September 17–21, 2023 | Prague | CR

UNIVERSITY OF PARDUBICE

FZU Institute of Physics of the Czech Academy of Sciences

Book of Abstracts
Programme
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19th European Conference on **Thermoelectrics**

Editors: Čestmír Drašar
Jiří Hejtmánek

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19th European Conference on **Thermoelectrics**

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Praha | Czech Republic

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Edited by: Čestmír Drašar and Jiří Hejtmánek

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PREFACE

Dear thermoelectricians,

It is a great pleasure for us to host the 18th European Conference on Thermoelectrics in Prague, Czech Republic. The conference is held under the auspices of the University of Pardubice in cooperation with the Institute of Physics of the Czech Academy of Sciences.

We are glad that so many people found time for their colleagues, for science. Some of us are more oriented towards technology and applications, some of us are stimulated by the ingenuity and beauty of nature and its subtlest laws. Let's come together and enjoy a moment of discovery and sharing of knowledge and experience.

Welcome to the mother of cities, Prague, the beautiful and vibrant capital of the Czech Republic. Prague is not only a modern city but also the historical center of Europe. The conference center is close to the historical center - Prague Castle. Therefore, you can enjoy not only science and research, but also deeply breathe the atmosphere of the present and the past.

Welcome to Prague!

Čestmír Drašar, *co-chair*
University of Pardubice,
Czech Republic

Jiří Hejtmánek, *co-chair*
Institute of Physics
of the Czech Academy of Sciences

on behalf of organizing committee

GENERAL INFORMATION

Conference venue

The conference will take place in OREA Hotel Pyramida.
OREA Hotel Pyramida - modern facilities near the places where history was made.
You can visit the nearby Strahov Monastery and it takes just a 15-minute walk to the Loreta, Prague Castle and St. Vitus Cathedral. From there you can continue down the Neruda Street to the Temple of St. Nicholas, over the Charles Bridge and Old Town Square to the Astronomical Clock and through the charming streets of Prague to Wenceslas Square, the centre of endless shoppings, cafés and restaurants.

Thanks to its strategic location, OREA Hotel Pyramida is the ideal venue for local and international events. Just a 15-minute drive from the airport, the hotel offers peaceful accommodation and a relaxation centre with a swimming pool, sauna, and fitness centre.

Address

Bělohorská 24, 169 01 Praha 6
GPS coordinates: 50.08558589758908, 14.379615640680806

Conference language

The conference language is English. Simultaneous translation will not be provided.

Conference office and on-site registration

The Conference office in the conference venue will be open for registration and information:

Sunday, September 17, 2023	15:00 – 20:00
Monday, September 18, 2023	8:00 – 12:00
Tuesday, September 19, 2023	8:30 – 12:00
Wednesday, September 20, 2023	8:30 – 12:00
Thursday, September 21, 2023	8:30 – 12:00

Conference Opening

The registration on site will open on Sunday, September 17, 2023, at 15:00.
All participants are cordially invited to a Welcome Drink, which will be served at 18:00.

The scientific programme of the conference will officially begin on Monday, September 18, 2023, at 9:00.

Student Award

All student poster contributions are automatically included in the Student Award contest. The best student's contributions will be awarded by valuable prices.

Students not wishing to participate are kindly asked to inform the Organising committee at the registration desk upon arrival.

Special issue of Solid State Sciences

Oral presentations and selected posters will be considered for publication in a special issue of Solid State Sciences (Elsevier, impact factor 3.5) after a standard peer review process. If you wish to publish your conference contribution, submit your manuscript at the submission website: https://www.editorialmanager.com/ssscie/ and select Article Type "VSI: Advances in thermoelectrics" at the beginning of the submission process. The deadline for submission is 30. 10. 2023.

Contacts

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PART I
PROGRAMME

SUNDAY, SEPTEMBER 17, 2023

15:00–20:00	**REGISTRATION**	
18:00–20:00	**Welcome Drink**	

MONDAY, SEPTEMBER 18, 2023

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09:15–10:00	**Half and Full-Heusler alloys: thermoelectricity beyond Bi_2Te_3** A. Riss, M. Parzer, F. Garmroudi, A. Grytsiv, G. Rogl, P. Rogl, T. Mori, E. Bauer	PT 01
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11:45–12:00	**Regulation of the intrinsic vacancies for high-performance GeTe thermoelectrics with ultrahigh carrier mobility** M. Zhang, Z. Gao, C. Hu, Q. Lou, Z. Han, C. Fu, T. Zhu	CT 04
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11:15–11:30	**Designing a high-precision instrument to characterize the thermoelectric material and device** H. R. Ren, C. P. Niu, Y. B. Zhao, Y. Q. Li, X. L. Chen, H. L. He	CT 07
11:30–11:45	**Understanding current-voltage curves of thermoelectric modules under low temperature difference operation** J. García-Cañadas, F. Vidan, B. Beltrán-Pitarch	CT 08

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11:45–12:00	**Enhancing thermoelectric generation with radiative cooling and phase change heat exchangers** M. Araiz, L. Catalán, P. Alegría, N. Pascual, D. Astrain	CT 14
12:00–12:15	**A design and verification of a non-icing and non-condensing waste-cold-recovery system** M. Ch. Lin, H. Y. Chen, F. T. Chung, M. J. Huang	CT 15

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14:15–14:30	**Transport properties of Co_2Hfsn Heusler alloy obtained by rapid solidification and sintering** A. Difalco, G. Barrera, P. Allia, M. Palumbo, S. Boldrini, A. Ferrario, P. M. Tiberto, M. Baricco, E. Alleno, A. Castellero	CT 16
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14:30–14:45	**An on-chip micro-thermoelectric temperature-controller** Q. Jin, N. Pérez, K. Nielsch, H. Reith	CT 25
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TUESDAY, SEPTEMBER 19, 2023

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11:30–11:45	**New architectures for heat sink less organic and inorganic thin film thermoelectric (TE) devices inspired by Kirigami** C. Zeng, E. Bilotti	CT 59
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14:15–14:30	**Interstitials in half-heusler compounds** W. Xie, R. Yan, A. Weidenkaff	CT 70
14:30–14:45	**Enhancing the thermoelectric performance of n-type $Mg_3(Sb,Bi)_2$ by high-temperature sintering and metallic inclusions** J. W. Li, H. L. Zhuang, J. F. Li	CT 71
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15:00–17:15	POSTER SESSION I

WEDNESDAY, SEPTEMBER 20, 2023

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11:15–11:30	**Rare Earth Chalcogenides: A Promising Group of Materials for Thermoelectric Applications** J. U. Rahman, K. Jang, Ch. Jung, S. Zhang, K. Nielsch, R. He	CT 75
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11:30–11:45	**Enhancing Low Temperature Thermoelectric Properties of n-type $Mg_{3.2-x}(Sb_{0.3}Bi_{0.7})_{1.996}Te_{0.004}$ through Nb Addition** M. Özen, A. B. Burçak, U. Aydemir	CT 81
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11:15–11:30	**Magneto-thermal switching using superconductors and importance of phonon-glass--electron-crystal states to the switching performance** M. Yoshida, M. R. Kasem, A. Yamashita, K. Uchida, Y. Mizuguchi	CT 85
11:30–11:45	**Soft optical phonons enabling ultralow and glass-like thermal transport in Argyrodite Cu_7PS_6** X. C. Shen, Y. Chen, E. Guilmeau	CT 86
11:45–12:00	**Temperature dependent Evolution of Optical Phonon Modes and Thermoelectric Properties in polycrystalline Bi_2Te_3** M. Tiadi, D. K. Satapathy, M. Battabyal	CT 87

12:00–13:30	Lunch

	SESSION I	
13:30–14:00	**Thermoelectricity and magnetism in selected oxides and chalcogenides** S. Hébert	IT 10
14:00–14:15	**Thermoelectric properties of defective half-Heusler $Nb_{0.80}CoSb$-TiCoSb solid solutions** Y. Huang, K. Y. Xia, Z. H. Gao, C. G. Fu, T. J. Zhu	CT 88
14:15–14:30	**Analysis of crystal structure and Thermoelectric properties of Sr-substituted $[Ca_2CoO_3]pCoO_2$** Y. Shimizu, K. Hayashi, Y. Miyazaki	CT 89
14:30–14:45	**Co-Cr-Fe-Mn-Ni oxide as a highly efficient thermoelectric high-entropy alloy** D. Pankratova, K. Yusupov, A. Vomiero1	CT 90
14:45–15:00	**Nanostructure Engineering and Thermoelectric Properties of $SrTiO_3$/TiN Nanocomposites Consolidated by Spark Plasma Sintering** M. Ohtaki, S. Umeno, S. Nagasaki, K. Suekuni	CT 91

	SESSION II	
13:30–14:00	**Electronic transport simulations in complex band materials beyond the constant relaxation time approximation** N. Neophytou, Z. Li, P. Graziosi	IT 11
14:00–14:15	**Thermoelectric figure of merit under constant Seebeck coefficients** J. Chung, B. Ryu, H. Seo	CT 92
14:15–14:30	**Efficient and accurate calculations of thermoelectric coefficients for materials with complex bands: The example of Mg_3Sb_2** Z. Li, P. Graziosi, N. Neophytou	CT 93
14:30–14:45	**Transport contribution to the Seebeck coefficient in the regime of transient delocalisation** J. Elsner, J. Blumberger	CT 94
14:45–15:00	**Unravelling the mystery: Does thermopower depend on specific heat or entropy?** M. Jazandari, J. Abouie, D. Vashaee	CT 95

	SESSION III	
13:30–14:00	**Unlocking high thermoelectric performance in metallic NiAu alloys via inter-orbital scattering** F. Garmroudi, M. Parzer, A. Riss, C. Bourgès, S. Khmelevskyi, T. Mori, E. Bauer, A. Pustogow	IT 12
14:00–14:15	**Playing with phonons: from the reduction of the thermal conductivity to the full control of the phonon flux** C. Capello, A. Masci, E. Dimaggio, G. Pennelli	CT 96
14:15–14:30	**Seebeck, Nernst and magnetotransport in dense $Co_3Sn_2S_2$ ceramic** A. Maignan, R. Daou, D. Pelloquin, S. Hébert	CT 97
14:30–14:45	**Sustainable metal phosphide thermoelectrics with promising performance** R. J. Quinn, J. W. G. Bos	CT 98
14:45–15:00	**Large atomic size mismatch induced novel meta-phase and high thermoelectric performance** K. Zhao, L. Chen, X. Shi	CT 99

15:00–17:15	POSTER SESSION II
19:00–22:00	CONFERENCE DINNER

THURSDAY, SEPTEMBER 21, 2023

09:00–09:45	**Development of enhanced thermoelectric materials and viable devices** T. Mori	PT 04
09:45–10:15	**The next generation RTG project – rebuilding the past and preparing for the future** J. P. Fleurial	IT 13
10:15–10:45	Coffee Break	

	SESSION I	
10:45–11:00	**Strong enhancement of the thermoelectric properties of nanostructured α-$SrSi_2$ by combining Melt-spinning and Spark Plasma Sintering** R. Ghannam, A. Moll, D. Bérardan, B. Villeroy, R. Viennois, M. Beaudhuin	CT 100
11:00–11:15	**Poly(3-hexylthiophene) layers modified by acids as promising p-type thermo-electric materials** S. Gogoc, P. Gnida, K. Wojciechowski, P. Data	CT 101
11:15–11:30	**Exploring the Potential of Nanostructured Ag_2Se in Hybrid Thermoelectric Films** B. Hamawandi, P. Genc, A. B. Ergül, M. S. Toprak	CT 102
11:30–11:45	**More than 3 times power factor improvement of PEDOT:PSS induced by electrolytes** M. Solis-de la Fuente, L. Márquez-García, S. Castro-Ruiz, E. Liautaud, L. Fournier, C. Chatard, A. Bouvet-Marchand, J. García-Cañadas	CT 103
11:45–12:00	**Thermoelectric properties of pedot: PSS thin films in different concentration** Ş. Özkan, G. Gürlek, M. Şener, Y. Seki, B. O. Gürses, L. Altay, M. Sarıkanat	CT 104
12:00–12:15	**Electrochemically grown bismuth telluride inside commercial polyester filters for flexible thermoelectric generators** O. Caballero-Calero, P. Cerviño Solana, M. Á. Tenaguillo, M. M. González	CT 105

	SESSION II	
10:45–11:00	**Ab-initio studies of electronic properties of tungsten carbide for thermoelectric applications** A. K. Vishwakarma, R. Saraswat, S. Bhattacharya, R. Verma	CT 106
11:00–11:15	**Does Zn form a resonant level in SnTe?** K. Pryga, B. Wiendlocha	CT 107
11:15–11:30	**In-gap states: mechanism of ZT improvement and their difference to resonant levels** B. Wiendlocha	CT 108
11:30–11:45	**Interplay Between Doping, Morphology and Lattice Thermal Conductivity in Organic Polymers** P. S. Floris, N. Zahabi, A. Cappai, I. Zozoulenko, C. Melis, R. Rurali	CT 109
11:45–12:00	**Criteria for erroneous substrate contribution to the thermoelectric properties of thin films** A. Riss, M. Stöger, M. Parzer, F. Garmroudi, T. Mori, E. Bauer	CT 110
12:00–12:15	**Lifetime prediction of a Bi_2Te_3 thermoelectric module** Y. Q. Zhang, C. P. Niu, H. L. He, Y. Wu, M. Rong	CT 111

	SESSION III	
10:45–11:00	**Advanced thermoelectric converter technologies for integration into a potential advanced radioisotope thermoelectric generator** T. Caillat, S. Pinkowski, I. Chi, J. Paik, K. Smith, R. Bennett, S. Keyser, A. Lane, K. Wefers	CT 112
11:00–11:15	**Feasibility of a Low-Power RTG Concept Utilizing a GPHS Heat Source** A. Ray, K. Sherick, P. Berneron, B. A. Tolson, C. Barklay, M. den Heijer	CT 113
11:15–11:30	**ISA-TEG: High temperature modules based on Half-Heusler compounds ready for commercialization** A. Fey, C. Klingelhöfer, S. Moos, B. Orth, B. Pfeiffer, N. Rink. J. Marien, D. Zuckermann	CT 114
11:30–11:45	**0.5 kW facility of geothermal thermoelectric generator from hot dry rocks on canary islands** D. Astrain, N. Pascual, P. Alegría, L. Catalán, M. Araiz, I. Erro	CT 115
11:45–12:00	**A new direct p-n junction based on Heusler compounds manufactured by co-sintering** G. Roy, M. Delcroix, N. Namazzade, V. Marchal-Marchant, C. van der Rest, P. J. Jacques	CT 116
12:00–12:15	**Development of thermoelectric modules based on magnesium and manganese silicide, derived from recycled Si-kerf** P. S. Ioannou, P. Mangelis, G. Mesaritis, A. Sousanis, I. Ioannou, A. K. Søiland, C. Kyriakou, K. Stylianou, S. Hadjipanteli, T. Kyratsi	CT 117

12:15–13:45	Lunch

	ROUND TABLE DISCUSSION	
13:45–14:30	**Identifying pathways for Successful Infusion of Recent Advances in Thermoelectric Materials into Power Generation Applications** J.-P. Fleurial1, C. Drasar	RTD

14:30–15:00	FAREWELL

15:00–17:15	**POSTER SESSION I** (Tuesday)

	Theory & Modelling
P 01	**First-principles study of structural disorder, site preference, chemical bonding and transport properties of Li-doped tetrahedrites** A. Kolezynski, K. Kapera
P 02	**Identification of dominant scattering mechanism and its influence on transport properties of half-Heusler compound** D. Bhattacharjee, P. R. Raghuvanshi, A. Bhattacharya, T. Dasgupta
P 03	**A multiband fitting technique for analyzing temperature dependent electronic band structure of thermoelectric materials** B. Agrawal, T. Tarachand, J. de Boor, T. Dasgupta
P 04	**Complex Fermi surface responsible for high zT** Ø. A. Grimenes, O. M. Løvvik, K. Berland
P 06	**High-throughput and accurate prediction of the thermal and electron transport properties of large chemical spaces accelerated by machine learning** J. J. Plata, A. M. Márquez, E. J. Blancas, V. Posligua, R. Grau-Crespo, J. Fdez Sanz
P 08	**Advancements and challenges in self-powering wearable technology: spotlight on energy collection via micro-power thermoelectric generators** D. Vashaee, P. Bhatnagar, B. Baraeinejad, A. R. Vazifeh
P 09	**Effect of PEDOT:PSS and bismuth tellure on electric potentials in the thermoelectric generator** G. Vardar, M. Şener, B. O. Gürses, G. Gürlek
P 10	**Thermoelectric algebraic representation: equations and inequalities for simple thermoelectric device design** B. Ryu, J. Chung, S. Park, S. D. Park
P 11	**The stability and role of defects in Bi_2O_2Se** K. Knížek, J. Navrátil, Č. Drašar
P 12	**Investigating the transport properties of CrN: Insights into phonon thermal conductivity and scattering** K. Ahn, J. Hejtmánek, K. Knížek
P 13	**First-principles calculations of thermal properties in the triangular lattice antiferromagnet $AgCrSe_2$** S.-J. Kim, H. Rosner
	Measurement & Characterization
P 15	**Establishing a protocol for the approval of thermoelectric materials used in biomedical applications** K. P. Walsh
P 16	**Novel methods of scattering parameter analysis for BiSbTe thermoelectric materials under constant temperature without Hall measurements** K. Hasezaki, J. Asai, M. Bumrungpon, T. Tsubochi, T. Kanaya, M. Tachii, T. Maeda, T. Iwamoto, C. Kanda, R. Yasuda, S. Uno, J. Kanaya
P 17	**Experimental estimation of electrical conductance of heterostructured Ge nanowires for thermoelectrical applications** T. Lahens, G. Hallais, L. Vincent, S. Dilhaire, S. Grauby
P 18	**Characterization and Seebeck coefficient of mesoporous silicon: effect of nanographene incorporation** S. Nar, A. Stolz, D. Machon, A. Boucherif, N. Semmar

P 19	**Lattice dynamics study of thermoelectric cubic $SrSi_2$ by Raman scattering experiments and *ab initio* calculations** R. Ghannam, J. Rouquette, M. Beaudhuin, R. Viennois
P 20	**In praise of the humble four point probe: Characterisation for scale up** R. S. Tuley, C. Koz, H. Hunter, E. Stefanaki, K. Simpson
P 21	**Thermal interface resistance analysis of thermoelectric devices by using thermoreflectance microscopy** H.-B. Kim, H. Jang
P 22	**A cross-plane Seebeck measurement system for sub-µm-thick films** H. Shin, S. Lee
P 23	**Test and simulation study for µ-TEGs based on screen-printed PbSe QDs** V. Sousa, R. Coelho, P. Alpuim, Y. V. Kolen'ko, F.P. Brito, A. P. Gonçalves, E. M. F. Vieira
P 24	**Hierarchically designed tetrahedrite with reduced thermal conductivity facilitated by all-scale phonon scattering** U. Rout, R. Ch. Mallik
P 25	**Mechanical properties characterization of thermoelectric materials** S. J. Jeon, S. Shin, D. H. Kim, S. Han
P 26	**Thermoelectric properties of doped SnSe alloys** F. Mihok, K. Saksl
P 27	**A Self-Independent Binary-Sublattice Construction in Cu2Se Thermoelectric Materials** H. Zhao, H. Hu, J.-W. Li, J.-F. Li, J. Zhu
	Thermoelectric Materials & Processing
P 28	**Development and evaluation of bismuth antimony telluride-PEDOT: PSS hybrid thermoelectric fiber using co-sputtering** D. H. Kim, S. Shin, S. J. Jeon, S. Han
P 29	**Experimental and DFT study of doped CrN thin films for thermoelectric applications** N. Singh, D. Gambino, A. Febvrier, B. Alling, P. Eklund
P 30	**Highly tailored gap-like structure for excellent thermoelectric performance** X. Xu, R. He, K. Nielsch, J. Q. Hex
P 31	**Anomalous thermal conductivity of alkaline-metals-substituted $EuTiO_3$ induced by resonant scattering** W. Xie, X. Xiao, A. Weidenkaff
P 32	**Manipulation with natural mineral chalcopyrite $CuFeS_2$ via mechanochemistry: properties and thermoelectric potential** P. Baláž, E. Dutková, M. Baláž, N. Daneu, L. Findoráková, J. Hejtmánek, P. Levinský, K. Knížek, M. Bali Hudáková, R. Džunda, R. Bureš, V. Puchý
P 33	**Enhance thermoelectric performance of Mg_3Sb_2-based materials via Ag doping strategy** J. Li, R. Chetty, T. Mori
P 34	**Chemical bonding origin of the excellent thermoelectric properties of Bi_2Te_3-based alloys** N. Lin, Y. Yu, M. Wuttig
P 35	**Synthesis, characterizabtion and thermoelectric properties of p-type $MnSi_{1.73}$ and Mg_2(Si, Sn) prepared using Si-kerf from PV cutting process** G. Mesaritis, I. Ioannou, A. K. Soiland, T. Kyratsi
P 36	**Growth and thermoelectric properties of ScN-based ternary alloys** S. Chowdhury, V. Hjort, N. Singh, F. A. F. Lahiji, M. Magnuson, A. L. Febvrier, P. Eklund
P 37	**Improving Thermoelectric Efficiency of InSb by Nano-Boron Doping** A. B. Burçak, R. Cardoso-Gil, U. Aydemir
P 38	**p-type copper iodide thin film for transparent and flexible thermoelectrics** P. Goel, W. Wojnicka, T. Koskinen, I. Tittonen

P 39	**Low purity elements based skutterudites for mid-temperature thermoelectric applications** R. Bhardwaj, E. Alleno
P 40	**Surface LASER processing effect on the thermoelectric properties of bismuth-antimony -tellurium alloy** G. Samourgkanidis, T. Kyratsi
P 41	**Effect of element substitution on thermoelectric properties and oxidation resistance of iron disilicide** H. Kohri
P 42	**Reduced contact resistance of Cu_2SnS_3 thermoelectric legs** S. Nakamura, H. Araki, Y. Akaki
P 43	**Thermoelectric materials grown by magnetron sputtering codeposition: a thin film approach** A. Conca, E. Ferreiro-Vila, J. M. Domínguez-Vázquez, C. V. Manzano, O. Caballero-Calero, A. Cebollada, M. Martin-Gonzalez
P 44	**Mechanochemical synthesis of tetrahedrite $Cu_{12}Sb_4S_{13}$ nanocomposites: challenge for thermoelectric performance** P. Baláž, A. Baran Burcak, U. Aydemir, A. Mikula, P. Nieroda, M. Baláž, L. Findoráková, R. Bureš, V. Puchý, M. Erdemoglu, M. Achimovičová, E. Guilmeau
P 45	**Design and properties of composites made of bismuth nanowires confined in mesoporous silica and alumina for Peltier applications** R. Viennois, M. Fabbiani, Y. Zhao, J. Haines, O. Cambon, J. Rouquette, M. Beaudhuin, V. Flaud, P. Toulemonde, M. Legendre, C. Goujon, J.-L. Bantignies, L. Alvarez, C. Levelut, L. Konczewicz, S. Contreras
P 46	**Thermoelectric properties of Cu_2Se obtained by the SPS and the "SPS melting" method** P. Nieroda, J. Leszczyński, M. J. Kruszewski, A. Koleżyński
P 47	**Thermoelectric properties of electrodeposited bismuth selenide thin films** R. Kaur, A. Tanwar, N. Padmanathan, K. M. Razeeb
P 48	**Comparison of different co-doping strategies in optimizing thermoelectric properties of tetrahedrites** J. Leszczyński, P. Nieroda, A. Koleżyński
P 49	**Organic/inorganic thermoelectric composites prepared via mechanical mixing** S. Hadjipanteli, Th. Krasia-Christoforou, Th. Kyratsi
P 50	**Thermoelectric properties of conventionally and mechanothermally prepared chalcogenide spinels $CuCr_2Se_4$** V. Kucek, M. Achimovičová, M. Baláž, V. Puchý
P 51	**Selective scatterings of phonons and electrons in defective Half-Heusler Nb1-dCoSb for the figure of merit zT > 1** Z. H. Gao, K. Y. Xia, P. F. Nan, L. Yin, B. H. Ge, Q. Zhang, C. G. Fu, T. J. Zhu
P 52	**Effect of sintering temperature on thermoelectric transport properties of n-type Mg_3Sb_2** J. H. Son, J. I. Jang, B. S. Kim, B. K. Min, S. J. Joo

15:00–17:15	**POSTER SESSION II** (Wednesday)

Thermoelectric Devices & Applications	
P 53	**Transient-Liquid-Phase bonding for Skutterudite-based thermoelectric modules** Ch. Stiewe, P. Ziolkowski, E. Müller
P 54	**Half-Heusler modules with high power density for nano-CHP application** N. Rink, C. Klingelhöfer, S. Moos, B. Orth, B. Pfeiffer, A. Fey, Dr. J. Marien, D. Zuckermann
P 55	**Fabrication of high power density telluride-based thermoelectric generator module for mid-temperature applications below 550 °C** J. Park, B. Ryu, S.D. Park
P 56	**Thermoelectric cooling system for the monolithic microwave integrated circuits chip** S. Shin, D. Kim, S. Jeon, S. Han
P 57	**Procedure of failure analysis on commercial available thermoelectric modules** K. H. Gresslehner, M. Krenn, J. Schaumberger, P. Kerepsi, E. Machado Charry, B. Sonderegger
P 58	**Thermoelectric generator for autarkic maritime heating systems** P. Ziolkowski, D. Zuckermann, P. Schmidt, E. Müller
P 59	**Development of thermoelectric generator for low-temperature waste heat recovery** R. Zybała, B. Bucholc, K. Kowiorski, G. Kuderski, A. Strojny-Nędza, M. Chmielewski, K. Krzyżak, A. Majcher, K. Kaszyca
P 60	**Optimization of a two-stage cascade type thermoelectric generator through finite element analysis** A. Miozzo, A. Ferrario, M. S. Natali, S. Boldrini
P 61	**Thermoelectric devices based on block copolymer nanostructured Si thin films** A. Rodríguez-Iglesias, I. Martín-Fernández, F. Pérez-Murano, J. Santander, F. Xavier Álvarez, A. F. Lopeandia, L. Fonseca, L. Abad, M. Salleras, M. Fernández-Regúlez
P 62	**Twist angle resolved thermal conductivity in bilayer $MoSe_2$** M. Mandal, N. Maity, P. K. Barman, A. K. Singh, P. K. Nayak, K. Sethupathi
P 63	**Reliability and electrical characterization of transient liquid phase sintering interconnects for thermoelectric devices** A. Ferrario, M. S. Natali, A. Castellero, C. Fanciulli, A. Miozzo, S. Barison, L. Armelao, S. Boldrini
P 64	**Difficulties in preparing a truly pure Bi_2O_2Se** A. Sojka, J. Zich, J. Navrátil, L. Beneš, T. Plecháček, Č. Drašar
P 65	**Inkjet printing flexible thermoelectric devices for sustainable power generation** Q. Zhang, A. Huang, L. Wang, W. Jiang, U. Lemmer
P 66	**Design optimization of printed thermoelectric generators tailored for plate heat exchangers in waste heat recovery applications** M. I. Khan, L. Franke, A. G. Rösch, U. Lemmer
Emerging Topics	
P 67	**A Cr complex solution able to produce a large power factor improvement in a nanostructured and porous oxide film** S. Castro-Ruiz, L. Márquez-García, M. Solis-de la Fuente, B. Beltrán-Pitarch, P. Íñigo-Rabinal, G. Guisado-Barrios, J. García-Cañadas
Others	
P 68	**Thermoelectric data analysis toward power generation evaluation and standardization** S. D. Park, J. Chung, J. Park, J. Jang, J. Lee, S. Park, B. Ryu

Thermoelectric Materials & Processing	
P 69	**Single-phase synthesis and thermoelectric properties of nowotony chimney-ladder FeGeγ** T. Kurosawa, K. Hayashi, Y. Miyazaki
P 70	**Textured $Ca_3Co_{4-x}O_{9-\delta}$ ceramics of electrospun nanoribbons with improved thermoelectric performance** K. Kruppa, I. I. Maor, F. Steinbach, M. Mann-Lahav, G. S. Grader, A. Feldhoff
P 71	**The comparison of properties of tellurides doped monocrystals** K. Kaszyca, G. Boczkal, B. Bucholc, K. Kowiorski, G. Kuderski, R. Zybała
P 72	**Properties of semiconductor-metal junctions obtained by the SPS/FAST process** K. Kowiorski, K. Kaszyca, B. Bucholc, M. Chmielewski, K. Krzyżak, G. Kuderski, R. Zybała
P 73	**The properties of tellurides fabricated by SHS technique** B. Bucholc, K. Mars, K. Kowiorski, G. Kuderski, A. Strojny-Nędza, K. Kaszyca, R. Zybała
P 74	**Role of the magnetism on the thermoelectric properties in $FeCr_2S_4$** S. El Haber, D. Pelloquin, O. Lebedev, R. Daou, A. Maignan, S. Hébert
P 75	**Impact of excess Cu on phase separation and thermoelectric properties of arc melted $Ti_{0.5}Zr_{0.5}NiCuySn$** B. F. Kennedy, J.W.G. Bos
P 76	**Band engineered and carrier modulated thermoelectric enhancement in half-Heusler** A. Kumar, P. Ghosh, S. Singh
P 77	**Engineering Thermoelectric Transport in Transparent Conducting Oxides** S. Biswas, S. Majumder, E Jagadeswarareddy, V. B. Kamble
P 78	**Modelling the lattice thermal conductivity of skutterudites: ab-initio calculations, machine learning and more** E. R. Remesal, A. M. Márquez, E. J. Blancas, V. Posligua, J. J. Plata, J. Fdez Sanz
P 79	**Preparation and thermoelectric properties of nonstoichiometric full-Heusler $Mn_{2+x}V_{1-x}Al$ alloys** G. Kanno, K. Hayashi, Z. Huang, H. Li, Y. Miyazaki
P 80	**Unraveling the origin of donor-like effect in bismuth-telluride-based thermoelectric materials** F. Liu, M. Zhang, P. F. Nan, X. Zheng, Y. Z. Li, K. Wu, Z. K. Han, B. H. Ge, X. B. Zhao, C. G. Fu, T. J. Zhu
P 81	**Enhanced thermoelectric properties by anion-engineering of 2-dimensional transition metal dichalcogenides** K. Ch. Kwon, H. Shin
P 82	**Enhancing thermoelectric and mechanical properties of p-type $(Bi, Sb)_2Te_3$ through Rickardite mineral ($Cu_{2.9}Te_2$) incorporation** K. Saglik, M. Yahyaoglu, C. Candolfi, U. Aydemir
P 83	**Effect of magnetic entropy in the thermoelectric properties of Fe-doped Fe_2VAl full-Heusler** T. Tarachand, N. Tsujii, T. Mori
P 84	**Carrier engineering-driven high thermoelectric performance in Ti doped $Yb_{0.4}Co_4Sb_{12}$** A. Dadhich, M. Saminathan, S. Perumal, M. S. Ramachandra Rao, K. Sethupathi
P 85	**Rapid synthesis and thermoelectric characterization of Ag_2S_{e1+x} compounds: Unveiling the secret of ultrafast formation and high performance** K. Gáborová, P. Levinský, J. Hejtmánek, K. Knížek, M. Achimovičová
P 86	**The enhancement of thermoelectric performance in MgAgSb via post-annealing process** S. Y. Back, W. Zhang, M. Yoshitaka, H. Cho, D. H. Nguyen, N. Kawamoto, D. Berthebaud, T. Mori
P 87	**Growth and TE properties of n-type Mg_3Bi_2-based thermoelectric thin film** S. Bano, P. Ying, A. Takashi, R. Chetty, T. Mori
P 88	**Porous Ag_2Se fabricated by a modified cold sintering process with the average ZT around unity near room temperature** D. Palaporn, S. Pinitsoontorn

P 89	**Enhanced thermoelectric performance of Al-doped ZnO nanocomposite obtained via chemical co-precipitation** I. Serhiienko, A. Novitskii, V. Khovaylo, T. Mori
P 90	**Energy harvesting from thermoelectric thin film by electromagnetic induction** M. Şener, G. Gürlek, B. O. Gürses, Ş. Özkan
P 91	**Thermoelectric properties of a novel $AgMnSbTe_3$ compound** P. Levinský, J. Hejtmánek, C. Candolfi, B. Lenoir
P 92	**Synthesizing double/triple Half-Heusler to explore larger compositional space** K. Imasato, P. Sauerschnig, T. Ishida, A. Yamamoto, M. Ohta
P 93	**Electronic/ thermal transport and thermoelectric phenomena in implanted diamond nanostructures** S. Salami, S. Pailhès, C. Adessi, V. Giordano, Z. Mthwesi, D. Régis, F. Rémy, B. Nicholas, A. Every, S. Naidoo
P 94	**Effects of annealing on thermoelectric properties of thin films and their application in micro-thermoelectric devices** H. Reith, M. Naumochkin, N. Pulumati, L. Wilkins, K. Nielsch
P 95	**Optimizing thermoelectric properties of electrodeposited chalcogenides by electrochemical reduction reaction of tellurium ion** J. Kim
P 96	**Improved thermoelectric performance of p-type tin monosulfide through tin precipitates** M. Y. Fakhri, T. T. Ho, W. J. Lai, S. M. Valiyaveettil, B. Jarwal, L. C. Chen, K. H. Chen
P 97	**High thermoelectric performance in Ag_2Se achieved through a sustainable solution synthesis** F. Milillo, T. Kleinhanns, M. Calcabrini, C. Fiedler, S. Horta, D. Balazs, M. Ibáñez
P 98	**Quantum and thermal fluctuations in spin configurations: deciphering their impact on magnetic order parameter and thermopower in MnSe across the critical temperature** M. Jazandari, J. Abouie, D. Vashaee
P 99	**High-performance n-type half-Heusler thermoelectrics exploiting interstitial Cu as dopants and phonon scattering centres** J.-W. Bos
P 100	**Study on Multi Scale Evaluation of Long-Term Reliability for Thermoelectric Devices and Legs** S. H. Park, E. A. Koo, S. W. Yoon, D. J. Wei, H. H. Lee, J. J. Choi

PART II
PLENARY TALK

PT01

Half and Full-Heusler alloys: thermoelectricity beyond Bi_2Te_3

A. Riss[1], M. Parzer[1], F. Garmroudi[1], A. Grytsiv[2], G. Rogl[2], P. Rogl[2], T. Mori[3], E. Bauer[1]*
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Keywords: Heusler compounds, electronic transport, thermal transport, DFT calculation, electronic structure, Boltzmann equation

Among the various families of thermoelectric materials, half-Heusler and full-Heusler systems are appreciated for their excellent mechanical properties and the outstanding thermal stability. While half-Heusler materials are also known for their superior thermoelectric performance as characterized by the so-called figure of merit, ZT, reaching ZT values above 1, the thermoelectric performance of full-Heusler systems is only moderate and ZT still keeps below 1. The latter follows from the unfavourable fact that the total thermal conductivity of such Heusler phases is pretty large, exceeding that of well behaving thermoelectric materials by more than one order of magnitude. Nevertheless, the optimal performance of the latter around 100 °C makes this family of compounds auspicious to replace, on the long run, Bi_2Te_3-based thermoelectric materials.

In order to arrive at better thermoelectric performances of these otherwise well behaving materials, we have developed a number of strategies to enhance to thermoelectric power factor and to reduce the thermal conductivity. Such strategies include modifications of the charge carrier effective mass, the width of the gap in the electronic density, charge carrier localisation, site-selective substitutions or off-stoichiometry in bulk and thin-film materials based on Fe_2VAl. Following such routes, power factors beyond 10 $mW/(m \times K^2)$ (3 times larger than pf's of Bi_2Te_3-based systems) are obtained around 100 °C. Our DFT-based calculations of the electron dispersion, as well as of electronic and thermal transport allow to perfectly guide experimental studies.

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Interface and grain boundary effects on thermoelectrics

PT02

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Keywords: thermal, electrical, boundary resistance, quality factor, electron filtering

Grain boundaries have a remarkable effect on the thermal and electrical transport properties of polycrystalline materials but are often ignored by prevailing physical theories. Grain boundaries and interfaces are often assumed to be beneficial to thermoelectrics but actually are detrimental in many materials. To devise strategies for improving the thermoelectric performance of materials, it is essential to understand the coupled charge and thermal transport mechanisms including interfacial electrical and thermal resistance (Kapitza resistance) and even an interfacial Seebeck effect. The inhomogeneous nature of materials, such as that caused by grain boundaries, must be taken into account to rethink engineering strategies based on Mathiessen's rule which interprets scattering homogeneously.

Electrical grain boundary resistance can be so high in some thermoelectric materials it is the dominant property that limits zT. While small grains are usually considered beneficial for thermoelectric performance due to reduced thermal conductivity, Mg_3Sb_2 based thermoelectric materials, so far at least, contradict that trend. The effect of grain boundary electrical resistance has been more striking and lead to the development of new electronic transport models in granular materials to explain and predict the electrical conductivity. Indeed, atomic segregation has been recently observed at the nanometer scale in grain boundaries in many materials suggesting interfacial or complexion phases should be specifically considered when understanding nearly all thermoelectric materials. These phases can even be engineered not only with thermodynamic quantities such as temperature and composition but also by adding 2D interfacial materials such as graphene.

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PT03

Enhanced atomic ordering leads to ultra-high thermoelectric performance

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Keywords: thermoelctrics, atomic ordering, nanoscale superstructures, weak localization, electron-electron interaction

With about 2/3 of all utilized energy is being lost as heat. Thermoelectric materials can convert waste heat to electrical energy, and it will have significant role in future energy management. High thermoelectric performance is generally achieved either by electronic structure modulations or through phonon scattering enhancements, which often counteract each other. A leap in performance requires innovative strategies that simultaneously optimize electronic and phonon transports. We demonstrate high thermoelectric performance with a near room-temperature figure of merit, zT ~1.5 and a maximum zT ~2.6 at 573 K by optimizing atomic disorder in Cd doped polycrystalline $AgSbTe_2$. [1,2] Cadmium doping in $AgSbTe_2$ enhances cationic ordering, which simultaneously improves electronic properties by tuning disorder-induced localization of electronic states and reduces lattice thermal conductivity via spontaneous formation of nanoscale (~2-4 nm) superstructures and coupling of soft vibrations localized within ~1 nm around Cd sites with local strain modulation. Furthermore, we have showcased the attainment of atomic ordering in $AgSbTe_2$ through a targeted elimination of Ag atoms from their disordered positions. This optimization of the stoichiometry has yielded remarkable results, with $Ag_{1-x}SbTe_2$ exhibiting a significantly high thermoelectric power density output of 267 $\mu W/cm^2$ at a temperature difference (ΔT) of 325 K with an estimated efficiency of ~7.5 %. [3] These achievements highlight the potential of our approach in enhancing the thermoelectric performance of the material by tuning its inherent atomic disorder which can be applicable to other thermoelectric materials.

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Development of enhanced thermoelectric materials and viable devices

PT04

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Keywords: enhancement principles, defect engineering, phonon engineering, TEG

Development of thermoelectric (TE) materials & devices is important, for energy saving via waste heat power generation [1], and as dynamic power sources for IoT sensors, etc. [2]. To enhance performance, ways to overcome the traditional tradeoffs between the key properties must be found. To enhance Seebeck coefficient *S*, and selectively lower thermal conductivity *k*, we are systematically developing principles and viable materials & devices [3], refs therein].

We have found that magnetism can be utilized to to enhance the Seebeck coefficent and overall power factor. Strong coupling of the electrical carriers with magnetic moments, can lead to effective magnon drag, e.g. like for $CuFeS_2$ chalcopyrite and the recently indicated origin of the huge power factor in metastable Fe_2VAl-based thin films, and furthermore paramagnon drag, where magnetic ion doping into nonmagnetic materials could enhance *S*. Spin fluctuation and spin entropy has also been demonstrated to enhance the Seebeck coefficient.

In addition to various nanostructurings, intrinsic low κ mechanisms have been demonstrated. Materials informatics approach led to identification of a material catalogue with low κ. Particular doping into SnTe was shown to lead to softening of the lattice and a dramatic reduction of thermal conductivity largely exceeding the contribution from phonon scattering. Finally, the heterogeneous bonding in mixed anion compounds was shown to result in exceptional low thermal conductivity [4].

Defect engineering has also been shown to be a powerful method, leading to high ZT in materials such as GeTe and Mg_3Sb_2. For the latter especially, high electrical mobilities similar to single crystals coupled to low thermal conductivity were achieved. Initial realistic 8 pair modules for temperatures up to ~320°C and also tuned for near RT, demonstrated efficiencies and power output rivalling the very best Bi_2Te_3 modules, with the performance of actually developed materials exhibiting much higher performance [5].

I will also present an overview on different thermoelectric power generation (TEG) devices which can be utilized for energy harvesting for possible applications. Bulk, microfabricated, hybrid, etc. Recent developments will be presented.

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PART III
INVITED TALK

IT01

Circular thermoelectrics and green innovations for sustainability

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The transformation of society to a future green circular economy will be based on green materials and innovations. The development of recyclable materials for thermoelectric generators requires sustainable large-scale production from secondary raw materials. The decision making for future resilient energy systems has to be based on environmental aspects as well as on performance criteria defined by a holistic life cycle assessment.

In this lecture an efficient circularity of thermoelectric converter materials with a programmable lifetime and regeneration will be introduced as a suitable approach. The design of circular high performance materials uses theoretical predictions and the criticality analysis of applied elements to improve the cycle life of future energy converters such as thermoelectric generators and refrigerators, batteries, electrolysers, fuel cells, plasmalysers, hydrides and solar watersplitting cells.

Multiscale phonon scattering in thermoelectric Fe_2VAl

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IT02

Keywords: Heusler alloys; Fe_2VAl; alloying; power factor optimization, first principles calculations; nanoprecipitates; mesostructuration

Upon doping, the Heusler alloy Fe_2VAl displays large values of power factor: PF = 4 mW m^{-1} K^{-2} in p-type $Fe_2V_{0.95}Al_{1.0}5$ [1] and 9.9 mW m^{-1} K^{-2} at 300 K in n-type $Fe_2V_{0.95}Ta_{0.05}Al_{0.9}Si_{0.1}$ [2] respectively. These values are close to or larger than in Bi_2Te_3 (PF = 5 mW m^{-1} K^{-2} at 300K) and this makes consider Fe_2VAl as a potential substitute to Bi_2Te_3. However, its thermoelectric performances are hampered by its large thermal conductivity, 29 W m^{-1} K^{-1} in pristine Fe_2VAl at 300 K. To tackle this problem, an approach where the heat carrying phonons are scattered at multiple length-scales has been implemented.

At the atomic scale, self-substitution as well as alloying with large atomic mass atoms (Ta, Sn) have been explored, leading to thermal conductivity smaller than 10 W m^{-1} K^{-1} at 300 K, in agreement with first principles calculations [3]. Self-substituted $Fe_2V_{1+x}Al_{1-x}$, ($-0.1 < x < 0.1$) compositions also allowed the optimization of the electronic transport properties, prior to nanostructuration [4]. A parabolic bands model yields values of the density of states (DOS) effective mass, $m_v^* = 3.7\ m_e$ and $m_c^* = 13.7\ m_e$ for the holes and electrons, respectively (m_e is the bare electron mass), in good agreement with first principles calculations [5]. Optimum thermoelectric power factor (PF) values are nearly reached experimentally in n-type $Fe_2V_{1.03}Al_{0.97}$ (PF = 6.6 mW m^{-1} K^{-2} for n = 1.4 × 1021 cm^3) whereas p-type $Fe_2V_{0.985}Al_{1.015}$ (PF = 3.3 mW m^{-1} K^{-2} for p = 6.7 × 1020 cm^{-3}) is not yet optimum. The easier optimization of the thermoelectric properties in n-type self-substituted Fe_2VAl can be traced back to the larger DOS effective mass of its electrons than of its holes.

At the nanometric scale, nanoprecipitates (~ 20 nm) of a secondary phase have been obtained in a Fe – V – Al matrix. But the Seebeck coefficient of this nanocomposite is too small to combine its thermal conductivity decrease with other reductions obtained for this last quantity at other length-scales.

At the mesoscopic scale, n-type Ta-substituted Fe2VAl samples, with an average grain size ~ 1 µm, were synthesized by powder metallurgy. Upon mesostructuration, the lattice thermal conductivity is reduced from 7.1 W m^{-1} K^{-1} to 4.2 W m^{-1} K^{-1} and the power factor reaches PF = 7.9 mW m^{-1} K^{-2} at 300 K. This leads to a figure of merit ZT = 0.3 at 300 K in meso-$Fe_2V_{0.96}Ta_{0.07}Al_{0.97}$, a value larger than in other Fe_2VAl alloys previously obtained by powder metallurgy [6].

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IT03

In operando X-ray scattering studies of degradation mechanisms in high-performance thermoelectric materials

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Keywords: *operando* studies, mixed ion electron conductor, X-ray scattering, degradation mechanism, material stability

Research on thermoelectric materials is primarily focused on maximizing the thermoelectric figure of merit, zT, since this value is eventually related to the conversion efficiency obtained in a working module. Immense progress has been achieved in improving zT, which has increased from unity two decades ago to current record values of around 3. [1] It is therefore somewhat peculiar that thermoelectric technology is still limited to niche applications. One of the major obstacles for actual implementation is that materials are unstable under the harsh conditions of an operating thermoelectric module, which is subjected to thermal and electrical gradients. Stability studies tend to be confined to the application side and often on macroscopic (module, property) level. [2] However, to understand, and eventually mitigate, degradation mechanism, it is desirable to have an atomistic understanding of the events. Furthermore, just as it is of fundamental academic interest to understand how materials form, it is also of fundamental academic interest to understand how they die.

We have developed the Aarhus Thermoelectric Operando Setup (ATOS) in order to simultaneously study the structure (PXRD, PDF) and transport properties (electrical resistivity, Seebeck coefficient) of materials under thermoelectric working conditions. [3,4] In this talk, I will present operando studies of important thermoelectric materials such as Zn_4Sb_3, Zn_4Sb_3 with nanoinclusion, segmented Zn_4Sb_3, PbTe, Mg_3Sb_2 and Cu_2Se. [5,6,7] The studies provide a particularly detailed insight into ion diffusion mechanisms in mixed ion electron conductors.

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Mg-based thermoelectric generators for near-room-temperature applications: device manufacturing and strategies for further improvement

IT04

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Keywords: magnesium silicide, TE modules, energy filtering, local characterization, transport analysis, MgAgSb

Alternative thermoelectric materials which can substitute the commercially dominant bismuth telluride technology are highly desirable for near-room-temperature heat conversion and thermal management applications. The combination of MgAgSb and n-type $Mg_2(Si,Sn)$ is highly promising due to the excellent thermoelectric properties of both materials and the higher availability of the constituting elements compared to BiTe. We have fabricated prototypes with conversion efficiencies > 6% (T_c = 25 °C, T_h = 300 °C) and power densities of ~1 W/cm^2, comparable in performance to commercial bismuth telluride modules. Analysis of the module measurement and comparative calculations using the constant property model indicates that a further performance gain of ~10% can be achieved by improved interface design.

Progress beyond that can only be achieved by improvement of the materials. $Mg_2Si_{1-x}Sn_x$, originally optimized for hot side temperatures of > 400 °C, can be improved by an (re)-optimizing of the Si:Sn ratio and the carrier concentration according to the targeted lower hot side temperature. Optimal compositions can be estimated using transport models considering the relevant conduction and valance band(s). Advanced strategies for material improvement include selective scattering of charge carriers on grain boundaries or nanostructures ("energy filtering"). This can be achieved by a locally varying electronic band structure, feasible in $Mg_2Si_{1-x}Sn_x$ by changing the band gap via the Sn content x and adjusting the energy levels of the electronic bands in grains of different compositions by selective doping. To test selective doping strategies a local charge carrier concentration measurement is highly useful. We'll show that transient microprobe measurements of the Seebeck coefficient can be used to that purpose with a local resolution down to ~5 µm. For carrier concentration determination with sub-µm resolution we employ a combination of the AFM-based Kelvin Probe Force Microscopy for work function measurements, SEM for determination of the composition, first-principles calculations for band offset predictions and modelling based on the Boltzmann transport equation. First results indicate an inhomogeneous distribution of the dopant Sb among several observed $Mg_2Si_{1-x}Sn_x$ phases, and confirm the feasibility to tune the local carrier concentration and influence the electronic band structure alignment.

IT05

Microscale imaging of thermal conductivity suppression at grain boundaries

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Keywords: grain boundaries, thermal conductivity, SnTe, frequency-domain thermoreflectance, Kapitza resistance

Grain boundaries have a central importance in materials science. In thermoelectrics, grain boundaries can be leveraged to suppress the thermal conductivity [1] this method of preparation holds out a possibility of improving the ‹figure of merit› of the thermocouple material and hence the conversion efficiency of the generator. Here the first measurements of the thermal diftusivity of fine grained bot pressed compacts of heavily doped n-type silicon germanium alloy are reported. The compacts investigated possessed grain sizes (L, but can also detrimentally suppress the carrier mobility [2]. Recent evidence suggests that some types of grain boundaries could be more beneficial than others for the thermoelectric performance [3,4] which is evaluated in terms of a dimensionless figure of merit (zT. Despite their importance, we lack a clear understanding of how grain boundaries modulate the microscale transport, owing to the scarcity of local investigations. Usually the role of grain boundaries is inferred from the grain-size dependance of the effective, bulk properties [2-4] which is evaluated in terms of a dimensionless figure of merit (zT. Nevertheless, understanding how grain boundaries impact micro- and nanoscale transport is crucial to enable grain-boundary engineering for the next generation of high-performance thermoelectrics.

Here, we demonstrate thermal imaging of individual grain boundaries in thermoelectric SnTe via spatially resolved frequency-domain thermoreflectance. Measurements with microscale resolution reveal a suppression in thermal conductivity at grain boundaries. In contrast to conventional thermal modeling, which assumes that all boundaries are perfect phonon scatters and lead to uniformly suppressed thermal conductivity, we observe a non-uniform thermal conductivity suppression localized within a few microns of a boundary. Furthermore, not all grain boundaries behave the same. Indeed, we find a correlation between the misorientation angle and the effective thermal boundary resistance at the grain boundaries.

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Structure-property relations in ternary copper sulphides for thermoelectric applications

IT06

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Keywords: copper sulphide, chalcopyrite, electrical properties, neutron diffraction, argyrodite

Binary copper chalcogenides have attracted considerable attention for their high thermoelectric performance, which may be traced to the onset of ionic mobility on heating. Effectively, this results in melting of the cation sub-lattice and entry into a liquid-like state, which significantly reduces the thermal conductivity. This has led to the description phonon-liquid electron-crystal (PLEC) being applied to such materials. However, the cation mobility that contributes to high performance is also responsible for materials degradation under operating conditions.

This instability of the binary phases has motivated us to investigate a range of more complex copper sulphides containing additional cations. The transport properties of ternary phases often exhibit unexpected behaviour, which can be associated with structural changes over a range of length scales. We have used both ex-situ and in-situ probes to examine the underlying structural features that gives rise to unexpected complexity in thermoelectric properties.

Here, recent work on ternary phases ($CuFeS_2$), adopting the chalcopyrite structure, will be described that reveals the impact that local structural distortions and the formation of micro-precipitates have on thermoelectric performance. We will also demonstrate that the identity of the product phase is sensitive to changes in stoichiometry with metal-rich phases adopting both talnakhite-and mooihoekite-type derivatives, depending on processing. A specially-constructed *in-situ* cell has been used to follow the temperature dependence of the electrical transport properties of these materials, while simultaneously probing structural changes through the collection of powder neutron diffraction data.

Extensions of work on chalcopyrite-related phases to copper sulphides which adopt the argyrodite structure will also be described. Analogous to the binary copper chalcogenides, these materials exhibit appreciable cation mobility, leading to superionic behaviour. However, the phase transition that precedes the onset of superionic behaviour introduces stresses into compressed pellets, resulting in cracking. Anion substitution has been used to suppress this phase transition, resulting in the production of mechanically-robust pellets, suitable for measurement of electrical and thermal transport properties.

Phonons and thermal properties of complex crystals

IT07

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Keywords: crystal complexity; phonons; lattice thermal conductivity; heat capacity; clathrates

Exploiting the structural complexity of crystals at the scale of their unit cell is a well-established strategy in the search for efficient materials for energy conversion, which aims at disentangling and separately engineering heat and charge transport. Structural complexity, which can easily result in unit cells in the nanometer range that contain a large number of atoms of various types, is known to be an efficient way for designing thermal properties and the underlying phonon spectra. In the search for low lattice thermal conductivity, one of the main strategies is the use of complexity at multiple length scales, from structural complexity within the crystal unit cell, to disorder, short range order, and nanostructuring. This route has resulted in the discovery of clathrates with exceptionally low lattice thermal conductivity but essentially unaffected and tunable electronic properties. On the other hand, phonons measurements have revealed the existence of long-living acoustic phonons in the clathrates questioning the origin of their low lattice thermal conductivity [1]. In this talk, I will first review spectroscopic measurements by means of neutrons and/or X-rays of the phonon spectrum and transport properties and the comparison with perturbative ab initio DFT calculation [2,3]. We will see how the complexity acts on propagative phonons and is responsible for the anomalous behaviors in temperature of the lattice thermal conductivity. From this knowledge of the phonon, a simplified description of it and describe meaningful model which is enough to capture the dominant features for analyzing their thermal properties and extract microscopic properties from macroscopic measurements [4]. Another interesting case is that of High Entropy Alloys which exhibits a strong chemical disorder at the level of their unit cell leading also to a poor lattice thermal conduction. In a second part, I will introduce our recent measurements of phonons in High Entropy Alloys and show that these systems present a unique phonon dynamics at the frontier between fully disordered and ordered materials. [5]

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The concept of the composite thermoelectric materials with attuned electronic structure and mismatched phonon structure (AES-MPS)

IT08

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Keywords: inorganic composites, organic-inorganic composites, skutterudites, lead telluride, germanium telluride, effective media theory (EMT)

The energy conversion efficiency of thermoelectric elements depends directly on the so-called averaged thermoelectric figure of merit ZTaver. Achieving a high ZTaver in practice means producing a material that exhibits high ZT values over a wide temperature range. To this end, we have proposed a new strategy for the development of TE composites, which we call the Attuned Electronic Structure-Mismatched Phonon Structure (AES-MPS) concept The AES-MPS concept was developed based on the classical approach to heat and charge transport in inhomogeneous systems, in the framework of the Effective Medium Theory (EMT).

The experimental verification of AES-MPS concept has been carried out on various inorganic composites eg. $CoSb_3$ – PbTe [1], GeTe-WC [2], $La_{0.95}Sr_{0.05}Co_{0.95}Mn_{0.05}O_3$ – WC [3] $SrBi_4Ti_4O_{15}$-$La_{0.7}Sr_{0.3}MnO_3$, [4], In-In_4Se_3 [5] porous systems [6] as well as inorganic - polymer systems based on $Cu_{14}Sb_4SX$ tetrahedrites [7]. We have shown that in a composite consisting of Mn and Sb co-doped GeTe as a matrix and WC as a dispersed phase, the simultaneous effect of enhanced thermoelectric power factor and reduced phonon thermal conductivity results in an exceptionally high figure of merit ZTmax of 1.93 at 773K and great energy efficiency of 14%.

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IT09

Solution-processed inorganic thermoelectric materials: new avenues for material control

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Keywords: solution processing, Ag_2Se, defects, nanoparticles, polycrystalline, recycling

In recent years, solution processes have gained considerable attention as a cost-effective and scalable method for producing high-performance thermoelectric materials. In this strategy, powder material is prepared in a solution, then purified and processed thermally to render the desired dense polycrystalline material. Different from conventional methods, syntheses in solution can produce particles with unprecedented control over their size, shape, crystal structure, composition, and surface chemistry. Such control over the powder properties provides unique opportunities for the synthesis of thermoelectric materials with deterministic microstructural properties.

Herein, we propose the use of well-defined nanoparticles as precursors for the production of dense thermoelectric materials as a means to control the microstructure of the dense solid. We will show different examples in which the control over specific nanoparticle properties, such as surface or stoichiometry, translates into very particular properties of the dense material that allow for optimizing its performance. In particular, we will focus on the case of Ag_2Se, a highly relevant thermoelectric material for its use near room temperature.

Acknowledgments

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Thermoelectricity and magnetism in selected oxides and chalcogenides

IT10

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Keywords: Seebeck coefficient, magnetism, entropy, oxides, chalcogenides

The three different parameters ρ, S and κ defining the figure of merit ZT can be modified by the application of a magnetic field, depending on the magnetic properties of the materials. In particular, the magnetism can modify the band structure, and can induce extra entropic terms leading to a modification of the thermopower. These magnetic field dependences have been investigated in metals [1] but also in the case of localized carriers [2-6]. We will present here several examples of materials in which the magnetism can strongly modify the thermoelectric properties, with positive or negative magnetoresistance, associated to a positive or negative magnetothermopower. We will show that this effect can exist even at room temperature in the case of the double perovskite ferromagnetic $Sr_2Fe_{1+x}Re_{1-x}O_6$ [6].

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IT11

Electronic transport simulations in complex band materials beyond the constant relaxation time approximation

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Keywords: thermoelectrics, computation, bandstructure, electronic transport, anisotropy

The large variety of complex electronic structure materials and their alloys offer highly promising directions for improvements in ZT originating from the power factor (PF). The electronic structure of novel materials contains rich features such as many valleys (typically included in machine learning descriptors [1]), warped features, elongated features, anisotropic bands, resonant states, topological states, and more. The transport dynamics also involve complex scattering physics. Many theoretical studies provide very useful direction in identifying and optimizing these materials, most of them, however, based on the constant relaxation time approximation, which brings an arbitrary degree of error, both qualitatively and quantitatively.

Here we describe the advanced electronic Boltzmann transport simulator, *ElecTra* [2], that we have developed, and demonstrate its capabilities in a series of investigations: i) regarding the importance of including all relevant scattering mechanisms in electronic transport computation [3]; ii) regarding the possibility to obtain ultra-high PF in low bandgap materials with highly asymmetric transport properties between the conduction and valence bands [4,5]; iii) regarding the influence of the shape of the electronic structure with its elongated features and high band anisotropy on the PF, where we show that 2-3x PF variations are observed based on the band shape complexities alone; iv) regarding the possibility of reliably computing transport properties of complex band materials with low symmetry and large unit cells in realistic time scales entirely from first principles.

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Unlocking high thermoelectric performance in metallic NiAu alloys via inter-orbital scattering

IT12

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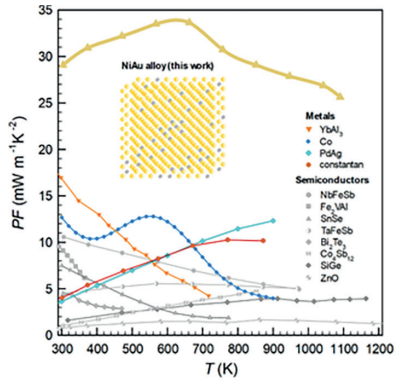
Keywords: giant power factors, high-*zT* metals, *s-d* scattering, metallic alloys, NiAu

Historically the thermoelectric effect was first discovered in metals, yet nowadays researchers focus on semiconductors with high figure of merit *zT*. While metallic alloys have superior functional properties, such as high ductility and mechanical strength, they have mostly been discarded from investigation in the past due to their small Seebeck effect. Here, we realize unprecedented thermoelectric performance in metals by tuning the energy-dependent electronic scattering [**arXiv:2303.03062**]. Based on our theoretical predictions, we identify binary NiAu alloys as promising candidate materials and experimentally discover colossal power factors up to 34 $mWm^{-1}K^{-2}$ (on average 30 $mWm^{-1}K^{-2}$ from 300 to 1100 K), which is more than two times larger than in any known bulk material above room temperature (see figure below). This system reaches a *zT* up to 0.5, setting a new world record value for metals. NiAu alloys are not only orders of magnitude more conductive than heavily doped semiconductors, but also have large Seebeck coefficients originating from an inherently different physical mechanism: within the Au *s* band conduction electrons are highly mobile while holes are scattered into more localized Ni *d* states, yielding a strongly energy-dependent carrier mobility. Our work challenges the common belief that good metals are bad thermoelectrics and presents a new paradigm for unlocking high thermoelectric performance in metallic alloys through engineering electron-hole selective scattering.



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IT13

The next generation RTG project – rebuilding the past and preparing for the future

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Keywords: radioisotope; heat; thermoelectric; converter; generator; power

NASA has long recognized the need to develop and provide reliable power sources for future deep space missions. The Next Generation Radioisotope Thermoelectric Generator (Next Gen RTG) Project's key objective is to assure the availability of high power, vacuum rated RTGs to missions later this decade. The Project team is developing that capability through a multi-phase effort that leverages the heritage General Purpose heat Source (GPHS)-RTG design, which is based on the SiGe unicouple-based converter technology initially developed in the mid-1970's as part of the Multi-Hundred Watt (MHW) RTG program [1]. The multi-phase Project plans for the following system variants ("Mods"): 1) Mod 0 seeks to refurbish an available GPHS-RTG Flight and verify its compliance with heritage requirements; 2) Mod 1 seeks to re-establish the capability to manufacture the heritage SiGe unicouple based thermoelectric converter and balance of plant hardware designs while accommodating the use of the current Step- 2 GPHS modules. This is the main focus of the Project at this time with the objective of delivering an unfueled Mod 1 flight unit before decade end; 3) Mod 2, which is not currently an active part of the Project, would explore development of thermoelectric technologies that could be an "in place" upgrade and significantly improve RTG efficiency. We report here on progress in "rebuilding the past" by re-establishing the SiGe unicouple production capability, which is the core of the critical path for the Mod 1 effort, with technical challenges being driven in many ways by the heritage techniques employed to produce the thermoelectric materials and assemble the devices. We discuss how the Project is also facilitating an effective partnership between industry and key government laboratories that have extensive experience with this technology, as well as ready-to-use facilities and equipment to be able to conduct pathfinder materials and couple development activities.

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PART IV
CONTRIBUTED TALK

CT01

Understanding thermal transport in GeTe thin films and impact of nanostructuration

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Keywords: chalcogenides, GeTe, thermal conductivity, thermoelectricity, nanostructuration

The study of the thermal properties of chalcogenide phase-change materials (PCMs) such as the prototypical GeTe compound will allow to improve and optimize future phase-change memories. The main challenge is to reduce programming currents, which need to reduce the thermal conductivity of the semiconducting PCM, without affecting its electrical properties [1]. The same need is met in thermoelectric applications of GeTe, which is indeed a promising thermoelectric material, [2] when it is doped to tailor both power factor and thermal conductivity. In this context, nanostructuration is a promising strategy, as it is expected to efficiently scatter phonons but not electrons. In this experimental work, we first investigate thermal transport in polycrystalline and amorphous GeTe thin films, providing, respectively, an upper and a lower limit for the thermal conductivity of nanostructured GeTe. Between these two limits, should fall the thermal conductivity of nanocomposites made of nanocrystalline GeTe grains embedded in amorphous carbon, where it should be possible to finely control the phonon mean free path (MFP) by tuning the GeTe grain size between approximatively 50 and 20 nm. The elastic contrast between the two materials is expected to strongly affect phonon propagation and thus mean free path [3].

To the purpose of our study, we have investigated the thermal conductivity of our samples combining a sensitive differential 3-omega method at low temperature and a pump-probe optical technique, the thermoreflectance, at high temperature. Our results for crystalline GeTe (k~3.7 $W.m^{-1}.K^{-1} \pm 0.9$ $W.m^{-1}.K^{-1}$ at RT) and amorphous GeTe (k~0.30 $W.m^{-1}.K^{-1} \pm 0.02$ $W.m^{-1}.K^{-1}$ at RT) are in nice agreement with recent literature results [4]. Their temperature dependence allows to identify the dominant phonon scattering mechanism. We show that GeTe-C nanocomposites with a grain size of about 20nm and 10 at % of C content exhibit a greatly reduced thermal conductivity (k~1.39 $W.m^{-1}.K^{-1} \pm 0.07$ $W.m^{-1}.K^{-1}$ at RT). Electrical conductivity and Seebeck coefficient have been also measured to investigate the effect on the power factor.

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Exploring the effect of resonant doping on thermoelectric properties of cubic Ge-Sb-Te thin films

CT02

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Keywords: thin films, cubic phase, resonant dopant, effective mass, carrier tuning

Germanium Antimony Telluride (GST), a pseudo-binary compound of GeTe known for its phase change applications has drawn enormous attention as a thermoelectric (TE) material owing to good electrical conductivity and low thermal conductivity [1]. However, the lower Seebeck coefficient remains a challenge. Also, studies on GeTe-based compounds suggest that it shows high thermoelectric performance at the high-temperature cubic phase [2]. Doping is a conventional but effective method in the TE community to obtain better TE properties. In this work, firstly a cubic phase of GST is stabilized at room temperature and then a simple and effective method was proposed to introduce Indium (In) inside the GST structure, and the insights into the effect of In were comprehensively studied. The results from advanced characterization techniques proved that with a two-step process (thermal evaporating and thermal annealing), In has been successfully and uniformly doped inside GST thin films. The gradual increase of doping amount (from 1.4 to 1.6, 1.9, 2.6 atomic %) indicated that the In content is controllable by adjusting the thickness of the evaporated-In layer. In doping enhanced the effective mass and increased the electron density inside the GST films reducing the overall p-type carrier concentration. As a result, it led to the essentially improved Seebeck coefficient. On the other hand, the existence of In also brings the suppression in thermal conductivity. Overall, a ZT for the GST-In1.9 sample increased to 1.9 at 575K compared with a ZT of 0.58 in GST film without In; and a higher average ZT of 1.2 was obtained in the temperature range of 300–575K useful for near room temperature applications.

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CT03

Origins of ultralow lattice thermal conductivity in $PbGa_{6-x}In_xTe_{10}$ filled-Mn-type phases

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Keywords: crystal structure, bonding inhomogeneity, polymorphic phase transition, lattice thermal conductivity, elastic properties

The understanding of the relationship between crystal structure arrangements, electronic and thermal transport properties of materials is among the main tasks in modern solid-state chemistry and material science. Here, we report the influence of cation substitution in tetrahedral voids on the structural and thermoelectric properties of $PbGa_{6-x}In_xTe_{10}$ filled **β**-manganese-type phases. The DSC analysis indicates that all investigated materials possess polymorphic phase transitions at ~580–700 K. The refined lattice parameters show that $PbGa_{6-x}In_xTe_{10}$ samples obey Zen's law which is reflected in a linear dependence of unit cell volume on *x*. The investigated materials show semiconducting behavior and the switch from *p*- to *n*-type conductivity can be explained by the change in the dominating mechanism of the defects formation. All investigated PbGa6-*x*In*x*Te10 materials possess extremely low lattice thermal conductivities due to the presence of lone-pair electrons on Te atoms which leads to significant anharmonicity of lattice vibrations reflected in high Grüneisen parameters. Bonding analysis also shows that in addition to strong Ga(In)-Te covalent interaction, Pb atoms have weak ionic interaction with the Te framework. As a result, the κ_L decreases with increasing *x* from 0.59 to 0.36 W m^{-1} K^{-1} at 298 K due to the weakening of Pb-Te interactions that probably facilitate the formation of the point defects. The fitting of the experimental κL with the results of Klemens-Callaway's calculations also suggests an increase in point defects. Moreover, the decrease in the lattice thermal conductivity is also in line with the reduction of the speed of sound and the bulk moduli of the investigated materials. This work evidences the filled β-Mn-type materials with transitional close-packed tetrahedra (TCP) structure and composition $PbGa_{6-x}In_xTe_{10}$, as a family of materials with extremely low lattice thermal conductivity.

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Regulation of the intrinsic vacancies for high-performance GeTe thermoelectrics with ultrahigh carrier mobility

CT04

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Keywords: GeTe, vacancy, mobility, thermoelectric, repeatability

GeTe is a promising thermoelectric material at medium temperature, but intrinsically forms in off-stoichiometric with Ge vacancies and Ge precipitates, leading to the carrier concentration beyond the optimal range for thermoelectric. It was formerly solved by counter doping. However, the existence of the high concentration of point defects not only deteriorates the carrier mobility but also harms the stability, which is a stubborn problem for GeTe-based materials. Herein, we discovered the distinct formation energy of Ge vacancies in the rhombohedral GeTe and the cubic GeTe. As a result, a significant decrease of Ge vacancies was realized in rhombohedral phase. By this way, the decline of carrier mobility by counter doping is avoided, and by virtue of the well lessened Ge vacancies the mobility achieved a high magnitude of 150 $cm^2 \cdot V^{-1} \cdot s^{-1}$ ($\leq$ 60 $cm^2V^{-1}s^{-1}$ for counter doped GeTe), realizing a decent electrical performance. Consequently, a high peak zT of 2.14 with a high level of reproducibility is obtained in the nominal composition $Ge_{0.93}Pb_{0.04}Bi_{0.03}Te$. This work provides a paradigm for tuning carrier concentration by point defect engineering entropy manipulation, but also demonstrated a route for improving the thermoelectric performance of GeTe.

CT05

Interplay of resonant level and band convergence in SnTe

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Keywords: chalcogenides, resonant level, band convergence, SnTe, electronic calculations

Over the last few decades, the dimensionless thermoelectric figure of merit, *ZT*, of various chalcogenide semiconductors was improved using band structure engineering tools that notably include resonant level (RL) and band convergence. Alloying with elements that give rise to a RL at the edge of either the valence or conduction bands provides a convenient way for optimizing the power factor of semiconductors by locally distorting the electronic band structure beyond the rigid-band model.[1-3] Furthermore, the convergence of several band extrema within a narrow energy window that leads to an increased number of degenerate valleys also yields enhanced power factor. In this presentation, we will discuss how the interplay between both mechanisms can result in a significant improvement in the thermoelectric performance of SnTe at high temperatures, providing guidelines to efficiently exploit both mechanisms in thermoelectric materials.

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Towards a complete characterization of thermoelectric figure of merit of individual nanowires

CT06

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Keywords: scanning thermal microscopy, nanowires, thermoelectric properties

Nanostructuration is a widely recognized and promising strategy for enhancing the efficiency of thermoelectric materials. This technique involves reducing the thermal conductivity of the material without compromising its electrical properties. Group IV semiconductor nanowires (NWs) are particularly well-suited for use in thermoelectric generators, especially when incorporated into vertical arrays. Additionally, introducing polytype heterostructures within the nanowires can further increase efficiency [1].

Recently, our team has conducted research on <111>-oriented 3C/2H heterostructured Ge and Si NWs. By utilizing a 3ω-SThM (Scanning Thermal Microscopy), we were able to evaluate the impact of several parameters on the thermal conductivity of the Si NWs [2].

In addition to our previous research, we have recently developed new instrumentation centered around the atomic force microscope presented in **Fig. 1**. This new equipment allows us to not only evaluate the thermal conductivity of heterostructured NWs, but also their electrical conductivity and Seebeck coefficient. By measuring these properties, we can estimate the thermoelectric figure of merit.

Our team has successfully validated the experimental set-up and obtained the first Seebeck and electrical conductivity maps of heterostructured NWs. Moving forward, our next step will involve calibrating these measurements to accurately assess the thermoelectric efficiency of nanostructured thermoelectric materials. By doing so, we hope to further advance the field of thermoelectric research and pave the way for the development of more efficient and sustainable energy conversion technologies.

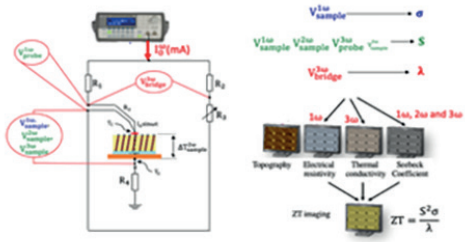

Figure 1: Set-up of complete thermoelectric imaging of individual nanowires.

Fig. 1:
Set-upof complete thermoeletric imaging of individual nanowires

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CT07

Designing a high-precision instrument to characterize the thermoelectric material and device

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Keywords: thermoelectric module, high-precision characterization instrument, electrical and thermal parameters, thermoelectric material.

Thermoelectric (TE) modules (TEMs) have been applied to many fields for its advantages of simple structure, quietness, and high reliability. Accurately characterizing the performance of TEM can contribute to its optimum design and guide its specific applications [1]. This study aims at accurately characterizing both the TE material and TEM by designing a high-precision instrument. This instrument mainly consists of five parts: vacuum system, heating system, pressurizing system, coolant system and measurement system. It can characterize the TEM with size of 3 × 7 mm^2 (single TE couple), 10 × 10 mm^2 (less TE couples), and 40 × 40 mm^2 (commercial TEM). For the vacuum system, a molecular pump is used to make the vacuum degree reach 10–3Pa level. The temperature of the heating system can be regulated up to 700 °C to meet the test requirement for different temperature-range TEMs. The pressurizing system is designed to satisfy the demand of clamping pressure imposed on the TEMs with different sizes, which can provide the pressure of 0–200 kg. A water-cooled machine is connected to the bottom plate in the coolant system to provide cooling effect. The measurement system is used to record two types physical parameters regarding the tested TEM. One is electrical parameter, including voltage, current and electrical power while the other is thermal parameter, mainly the heat flux rate. For the electrical parameters, a current source is used as external load to simulate various working conditions from open to short circuit especially allowing for the much small internal resistance of tiny TEM. For the thermal parameters, a series of high precision heat flux meter is designed, fabricated and calibrated to determine the heat flux of at TEM's cold side with a wide measurement range of 0.05W~400W. With the sampled electric power and heat flux at the TEM's cold side, its energy conversion efficiency can be directly derived. A lab-made TEM is characterized by the instrument and the error of its conversion efficiency is less than 4% compared with simulation. In addition, combined with the quasi steady-state method reported previously [2], the physical parameters(Seebeck coefficient, electrical conductivity and thermal conductivity) of TE material can be directly deduced using the instrument. The good precision and consistency of the results demonstrate that effectiveness and reliability of the instrument, which will assist to guide the design of TEMs and TE materials in the future.

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Understanding current-voltage curves of thermoelectric modules under low temperature difference operation

CT08

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Keywords: *I-V* curves, constant heat power, constant temperature difference, operating conditions, thermal contact resistance, spreading-constriction.

To determine the power output of a thermoelectirc module, an *I-V* curve is typically performed when the device is under a temperature gradient. These *I-V* curves generally follow a straight line, which can be defined by the open-ciruit voltage and its slope, which in the end is the total resistance of the system (R_{IV}). Here, we analyse the different contributions that R_{IV} can have when the system operates under a small temperature difference, which strongly depend on the operating conditions.

Two different modes of operation are analysed: (i) under constant heat power and (ii) under a constant temperature difference. In the first case, the total resistance of the system has two contributions, the ohmic resistance (R_Ω) and the thermoelectric resistance (R_{TE}, due to the variation of the temperature difference by the Peltier effect, governed by the thermal conductivity of the themoelectric materials). In the second case, apart from R_Ω and R_{TE}, three more resistances appear: R_C, R_{TC} and $R_{S/C}$. R_C is due to the variation of the temperature difference produced by the Peltier effect and governed by the thermal conductivity of the external ceramic layer. R_{TC} is related to the thermal contact resistance between the device and the heat exchangers. Finally, $R_{S/C}$ is due to the heat spreading-constriction, caused by the differences in the area between the legs an the ceramics (filling factor).

Apart from understanding the different processed mentioned affecting the *I-V* curves, it is also shown how the the thermal contact resistivity between the device and the heat exchangers can be determined [1], which resulted in a value of $3.57 \times 10^{-4}\,m^2KW^{-1}$ for a commercial Bi-Te module contacted using thermal grease as thermal contact interface material, which is in good agreement with reported values.

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Customized measuring station for Peltier modules

CT09

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Keywords: peltier module, measurement system, characterization, COP

Peltier modules control temperature in niche products such as wine coolers and camping fridges or are used to precisely temper processes such as the duplication of DNA sections. Accurate characterization of the modules is crucial in order to meet the high reliability requirements especially in critical applications such as in bio- and medical technology markets.

While most of the measurement stations are designed for thermoelectric generators, the measurement of Peltier modules is rarely described. In this contribution, we show a customized measuring station specifically for the characterization of Peltier modules and for the determination of temperature dependent properties such as I-max, Q-max, ΔT-max and the coefficient of performance (COP). Thus, it is possible to completely characterize a Peltier module with this setup. Furthermore, the software is able to create easily evaluable data sheets. An error analysis for the measured properties will be given as well.

In addition to the characterization of the modules, the long-term stability of the modules can be measured not only with static current and temperature but also at cyclical stimulation of temperature or current changes meaning that application-oriented long-term tests are possible as well.

Unlike most of the measurement stations described in literature [1,2,3], in this setup both the hot as well as the cold side consists of water driven heat exchangers with a range of -20 °C to 80 °C. The heat flow through the module is measured via two graphene heat flux meters at the hot and the cold side of the Peltier module.

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Mechanical and thermoelectric properties of AISI 4340 high-strength martensitic steel with ZnNi coating subjected to hydrogenation

CT10

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Keywords: 4340 martensitic steel, hydrogen embrittlement, Seebeck coefficient, mechanical properties, ZnNi coating

Hydrogen embrittlement and the interaction of hydrogen with steel have recently been of interest to many research groups. To our best knowledge, thermoelectric properties of high-strength steel have not been unequivocally correlated with the hydrogen content. AISI 4340 martensitic steel is very susceptible to hydrogen absorption and trapping due to its crystal structure. In our study, the surface Seebeck coefficient, Young modulus, breaking strength, and hydrogen content were measured after the electrochemical hydrogenation of steel. Measurements of mechanical and thermoelectric properties were also made for 4340 steel plated with galvanic zinc-nickel coating.

The results presented indicate a correlation between the hydrogen content in steel and the value of the Seebeck coefficient. With the increase of the hydrogen content (at electrochemical hydrogenation) to 1 ppm, the Seebeck coefficient decreases from 18.5 μV/K to about 11.5 μV/K. The change in mechanical properties can also be observed along with the increase in the hydrogen content in the steel samples.

Microstructural studies may ambiguously indicate the presence of the so-called hydrogen embrittlement. Thermal desorption studies (TDS) indicate the presence of two main hydrogens "traps". The first peak corresponds to the reversible traps identified as grain boundaries and dislocations. The second peak corresponds to irreversible traps, i.e. hydrogen bounded in the bcc structure. [1] Direct testing of the hydrogen content by the inert gas fusion method shows that even the hydrogen content below 1 ppm has a significant impact on the properties of 4340 steel.

Measurements of the surface Seebeck coefficient and the results obtained with direct tests of hydrogen content demonstrate strong correlation between the hydrogen content in 4340 steel and its thermoelectric properties. This study facilitated the development of new research methodology for hydrogen determination.

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CT11

Demonstration of the economic viability and energy savings potential of thermoelectric generators for pellet boilers

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Keywords: thermoelectric generator, pellet boiler, combined heat and power, renewable energy

Renewable energy utilization across all energy sectors is a crucial measure to mitigating climate change. For residential buildings, it is possible to meet a part their thermal and electrical energy demand with solar thermal energy and photovoltaic systems. As these technologies are limited to periods of high solar radiation, biomass-based heating systems, such as pellet boilers, are an effective complement. If the biomass is obtained from wood waste or sustainable agriculture, it represents a climate-neutral and permanently available fuel. However, most biomass-based heating systems supply only thermal energy, as current approaches to combined heat and power generation (CHP) are too complex and expensive for widespread application.

Thermoelectric generators (TEGs) can be integrated in heating systems and convert a part of the generated heat into electrical power. Their compact size, low maintenance and low noise make them an optimal technological solution. Additionally, their potentially competitive cost-benefit ratio is shown for some applications, such as waste heat recovery in vehicles [1] [2]. However, for biomass boilers, a sufficient cost-benefit ratio of TEGs for their commercial deployment is not proved [3].

To address this issue, this study uses a novel system-level development method for TEGs, elaborated together with partners in the project “PellTEG” [4]. It aims to optimize the system cost-efficiency and investigates whether commercial use is currently possible. The method is based on a numerical fluid dynamics simulation combined with an empirical model of professionally produced Half-Heusler thermoelectric modules under consideration of interactions with the heating system and manufacturing costs. The simulation results are used for a direct cost-benefit optimization of the system integrated in an 18 kW_{th} pellet boiler and are validated with a full-scale functional prototype on a hot gas test bench.

The first optimized TEG design produces 418 W_{el} at a pressure drop of 58 Pa and manufacturing costs of 1934 €. This cost-benefit ratio is competitive with existing CHP solutions. The next experiments involve long-term testing in the pellet boiler in laboratory and in application-related environment. Thereby, the first commercial development of this kind is possible, which can guide and support further research in the field.

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Utilising computational design tools to simulate novel thermoelectric systems for energy recovery in steel making processes

CT12

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Keywords: thermoelectric generators, waste energy recovery, numerical model simulation, TEG device testing, net-zero steel production

Steelmaking is an energy intensive process. Manufacturers are looking to transition to production methods with a net-zero impact on the global climate. Thermoelectric technologies can potentially be utilised to reduce the environmental cost of steel production. The EU-RFCS funded InTEGrated project seeks to investigate the use of thermoelectric generators (TEGs) to recover thermal energy from furnace cooling water and radiation from hot steel products.

Two experimental prototypes are under development and testing at operational steel plants, with additional design support provided with numerical modelling using COMSOL software. The thermal heat transfer involved in the movement of heat from radiative or hot water sources to the TEGs of the two prototypes has been simulated. This work shows how the experimental validation of key parts of the TEG system can be used to improve the accuracy of the simulation model and how numerical simulations can be used as a design tool for future prototype development. This allows for the implementation and optimisation of novel designs before experimental testing is undertaken.

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CT13

A TEG-based waste heat recovery system for atmospheric pressure plasma jets

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Keywords: green intelligent machines, atmospheric pressure plasma jet, waste heat recovery, thermoelectric power generators, compact thermal model

Many manufacturing machines use a lot of energy in the manufacturing process, most of which is lost to the atmosphere as heat. We propose a use of thermoelectric power generators (TEGs) to recover waste heat from such machines and utilize the generated electricity to monitor the operation of the machine, making the machines intelligent and green. Taking an atmospheric pressure plasma jet (APPJ) as a demonstration, TEGs are installed below the platform and heated when the glass on the top of the platform is being coated with a transparent conductive film. Experiments have confirmed the generated electricity is quite sufficient to simultaneously drive a fan for cooling TEGs and a multi-functional monitoring system which monitors the operating temperature of the APPJ and the air quality in the surroundings. A compact thermal model is also proposed to predict the power generation and obtain the detailed temperature distribution to ensure that the glass is maintained at proper temperature for coating.

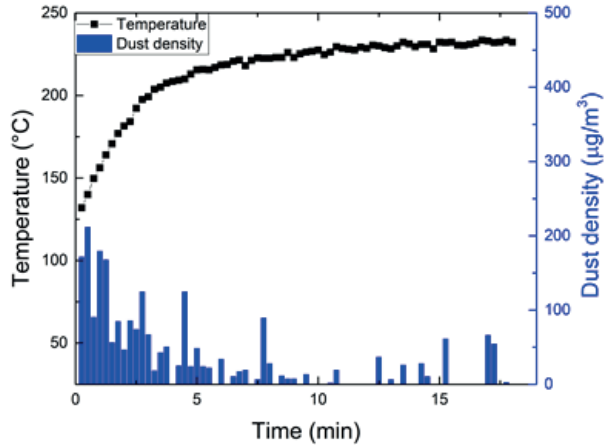

Fig. 1: A case study of the actual operation of the monitoring system powered by the TEG-based waste heat recovery system

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Enhancing thermoelectric generation with radiative cooling and phase change heat exchangers

CT14

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Keywords: thermoelectric generators, heat exchanger, radiative cooling, natural convection

Heat exchangers are critical for optimizing the efficiency of Thermoelectric Generators (TEGs) in energy conversion from waste heat to electrical power. Heat pipes without fans have emerged as an advantageous design for TEGs due to their robustness, low maintenance, and lack of moving parts [1]. However, the efficiency of these heat exchangers is reduced under natural convection conditions, leading to a decrease in heat transfer capacity and consequently, a decrease in thermoelectric power production.

In this work, we present a novel heat exchanger design that combines phase change and radiative cooling in a thermoelectric generator to improve its efficiency and increase the production of electrical energy, especially under natural convection. Two thermoelectric generators with heat pipes on their cold sides were tested: one with a radiative coating and the other without it. The thermal resistances of the heat exchangers were determined, and the electric power output was compared under different working conditions, including natural convection and forced convection indoors and outdoors.

Experimental tests demonstrated a clear reduction in the thermal resistance of the heat exchanger with the radiative coating, resulting in an increase in electric power production of 8.3% with outdoor wind velocities of 1 m/s, and up to 54.8% under free convection conditions. The application of the radiative surface treatment also resulted in a more stable electrical energy production, suppressing the drastic decrease in generated electric power that occurs in thermoelectric generators when they operate under free convection.

This study highlights the potential of combining phase change and radiative cooling in heat exchanger design to enhance the efficiency of thermoelectric generators, especially under natural convection conditions. The findings contribute to the development of more efficient and reliable thermoelectric power generation systems, with potential applications in waste heat recovery, renewable energy, and other industrial processes.

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CT15

A design and verification of a non-icing and non-condensing waste-cold-recovery system

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Keywords: waste cold recovery, non-icing, non-condensing, thermoelectric power generator, cryogenic

Cryogenic fluids are widely used in industries and research labs, frequently in the form of liquefied gases, which take a lot of energy to produce. These gases are usually still at very low temperatures when released into the atmosphere after use or must be warmed to room temperature before use. “Cold energy” is thus wasted. This work aims at recovering such cold energy by taking advantage of the thermoelectric chips. Icing and condensation are the toughest problems when dealing with cryogenic fluids. We present an ingeniously designed waste-cold-recovery device which is non-icing and non-condensing and demonstrate its success in extracting cold energy from the cryogenic nitrogen to generate electricity through experiments. Effects of both the layer number and the configuration of the TE chips are explored. Among all tests, the largest output power and the best efficiency obtained are 0.93W and 2.67%, respectively with a use of twelve TE chips and a nitrogen flow rate of 245 standard liter per minute (SLPM).

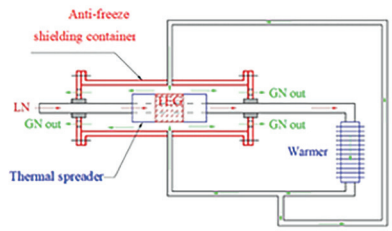

Fig. 1: A schematic diagram of the TEG waste-cold-recovery system.

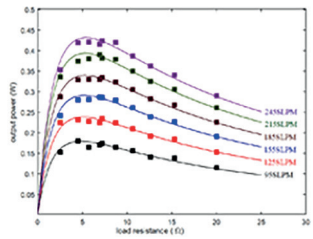

Fig. 2: The output power against the load resistance under various flow rate.

Transport properties of Co_2HfSn Heusler alloy obtained by rapid solidification and sintering

CT16

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Keywords: Heusler, half-metal, ferromagnetic, transport properties, *ab-initio*

Half-metallic ferromagnetic alloys are attracting considerable interest for their potential applications in spintronic devices. Since the development of spin-voltage generators is regarded as crucial in spintronics, thermoelectric properties are also of high interest for such technology, having been proved spin-Seebeck effect to be an effective way to generate and carry spin-polarized current over relatively long distances. Co-based Heusler alloys are considered to be among the most promising classes of half-metallic compounds as they combine suitable magnetic, electronic and transport properties with compositional versatility and high thermal stability. Also, several Co-based Heusler alloys were found to be suitable for spin-injection processes due to their semiconductive-like band gap located in one of the two electronic sub-bands. Thus, half-metallic alloys which show a constant, relatively large Seebeck coefficient (when compared with other thermoelectric materials) and a high Curie temperature (possibly above room temperature) are greatly looked after.

In this work, Co_2HfSn Heusler alloys was studied by combining experimental and ab-initio investigations in order to accurately estimate their electronic density of states in proximity of the Fermi level and to measure their transport properties over a wide range of temperatures. Samples were prepared by melt spinning followed by Spark Plasma Sintering (SPS). A comparison between the properties shown by the sintered samples, and arc-melted specimens is also proposed with the aim to understand how the synthesis route affect the thermoelectric behaviour of the alloy.

CT17

Enhancing the thermoelectric properties via modulation of defects in p-type MNiSn-based (M = Hf, Zr, Ti) half-Heusler materials

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Keywords: half-Heusler, thermoelectric, interstitial defect, p-type HfNiSn, mechanical alloying

The thermoelectric figure-of-merit (zT) of p-type MNiSn (M = Ti, Zr or Hf) half-Heusler compounds has long been reported much lower than their n-type counterparts. This can be ascribed to the presence of a donor in-gap state that is induced by the occupation of tetrahedral interstitials by Ni. Meanwhile, most p-type investigations focused on ZrNiSn and TiNiSn, yet the study of HfNiSn is absent. Herein, we report an improved thermoelectric property in p-type $HfNi_{1-x}Co_{x}$-Sn. Upon 5 at % Co doping at the Ni sites, the Seebeck coefficient are shifted to positive with the peak value exceeding 200 μV K^{-1} that breaks the record of previous reports. A maximum power factor of ~2.2 mW m^{-1} K^{-2} at 973 K is further obtained by optimizing the carrier concentration. The advanced p-type transport is ascribed to the reduced content of Ni defects, as evidenced by calculating the formation energies from first principles and refining the diffraction patterns. Concomitantly, Co doping leads to a synergistic effect of lattice softening and point-defect scattering for phonons, resulting in a minimum lattice thermal conductivity of ~1.8 W m^{-1} K^{-1}. A peak zT of 0.55 at 973 K is realized, which exceeds the state-of-the-art p-type MNiSn by 100%. Our strategy presents a new avenue to modulate the intrinsic atomic disorder degree of the half-Heusler system to facilitate further optimization of electronic and thermal properties of half-Heusler materials.

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Effect of isoelectronic substitution on the transport properties of $Co_2Zr_{1-x}Hf_xSn$ (x = 0, 0.25, 0.50, 0.75, 1) Heusler alloys

CT18

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Keywords: Heusler, thermoelectric, transport properties, phonon scattering, mass fluctuation

Heusler alloys represent a wide class of multifunctional materials with potential applications in the field of thermoelectricity, spintronics and magnetism [1].

In the case of Co_2ZrSn and Co_2HfSn, experimental investigations showed weak itinerant ferromagnetic behavior and ab-initio calculations, based on the plane-wave DFT approach, suggested a half-metallic behavior [2]. Measurement of the electrical conductivity showed a transition from metallic to semiconducting behavior in correspondence of the Curie temperature (T_C), while measurement of the Seebeck coefficient revealed n-type behavior and the presence of a plateau above T_C [3].

The aim of this work is to reduce the lattice thermal conductivity through mass fluctuation phonon scattering, by partial substitution of Zr with Hf in the aforementioned alloys. At this purpose, $Co_2Zr_{1-x}Hf_xSn$ (x = 0, 0.25, 0.50, 0.75, 1) alloys were synthesized by arc melting and annealed to ensure compositional homogeneity. The same alloys were prepared by rapid solidification and subsequently sintered by ultrafast high-temperature sintering.

The solubility of Hf in the Co_2ZrSn Heusler phase was explored for different Hf contents in samples prepared by different routes (i.e. arc melting, rapid solidification, sintering). The effect of the partial substitution of Zr with Hf on the thermoelectric properties (Seebeck coefficient, electrical conductivity and thermal conductivity) of $Co_2Zr_xHf_{1-x}Sn$ (x = 0.25, 0.50, 0.75) was investigated. The results of the partially substituted alloys were compared with those of the end-members (i.e. Co_2ZrSn and Co_2HfSn).

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CT19

Anisotropic magneto-thermal transport in Co_2MnGa thin films

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Keywords: anisotropic magnetoresistance, thermopower, Heusler alloys, magnetotransport, ferromagnets

The full Heusler compound Co_2MnGa belongs into the class of materials whose bandstructure features Weyl points [1]. Large anomalous Nernst effect has been observed in Co_2MnGa [2] and it was attributed to non-vanishing Berry curvature of the Weyl-points making the material also interesting for other transport phenomena. In this work, we systematically measure anisotropic magnetoresistance (AMR) and its thermoelectric counterpart anisotropic magnetothermopower (AMTP) in Co_2MnGa thin-films. The data is modeled using a Stoner-Wohlfarth formalism as well as a symmetry-based phenomelogical model. Our findings show the presence of both crystalline and non-crystalline components in both magneto-transport phenomena. While the AMR is small in relative terms, the AMTP is large, which is discussed in the context of the Mott rule [3].

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Machine learning enabled thermoelectric generator modelling and optimisation

CT20

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Keywords: thermoelectric generator, artificial neural network, genetic algorithm, optimisation, modelling

Modelling and design optimisation are essential tasks in developing thermoelectric generators (TEGs) with high performance. However, a compromise of the computational accuracy or computational speed is inevitable when using conventional modelling methods such as finite element method (e.g. COMSOL simulation) and mathematical modelling. The artificial neural network (ANN), a type of deep learning technique, can serve as a suitable forward modeller for TEGs that balances both accuracy and computational speed without any prior knowledge of the thermoelectric device.

This work demonstrates the application of the deep learning technique in forward modelling the power performance of different TEGs [1]. The ANN-based modeller considers a range of design parameters (e.g., leg height, width, and filling factor) with varying operating conditions (i.e., heat flux and electrical contact resistivity). After training using datasets from 3-D COMSOL simulations, the ANNs shows extremely high prediction accuracy of over 98%. Such high accuracy is accompanied by a significantly reduced prediction time of 1 ms, 60,000 times faster than the finite element method (FEM) approach. Furthermore, for the more complex segmented thermoelectric generators, we introduced a new iterative training approach that significantly improves the accuracy of ANN in predicting high-performing TEG designs [2]. Coupling with an optimisation algorithm, our trained ANN can perform geometrical and structural optimisation for TEG under different operating conditions. With almost identical optimised values obtained, our ANNs demonstrate superior optimisation efficiencies over 1000 times better than the COMSOL simulation coupled with genetic algorithm optimisation.

In addition to its application in TEG modelling and optimisation, we have also developed a novel ANN-based modelling architecture for the photovoltaic (PV)-TEG hybrid system. The novel architecture consists of a PV and a TEG ANN component, and is capable of predicting the power performance of the system under different operating conditions including xxx. The success of our work points towards using ANN for modelling complex TEG designs as well as other renewable energy technologies.

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CT21

Design theory of a tiny high-power-density thermoelectric harvester to power wireless sensor node

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Keywords: thermoelectric (TE) materials, figure-of-merit *zT*, tiny thermoelectric generators (TEGs), TEG's structural configuration, self-powered sensor node

Thermoelectric (TE) generators (TEGs) have recently attracted significant attention for harvesting ubiquitous heat energy to power industrial sensor nodes or wearable and implantable electronics. Such applications require that a small, fitted heat sink be incorporated into a tiny harvester to ensure conformal deployment and ease of use. Since the small heat sink will exhibit very poor heat rejection performance, the optimal structural design of the TEG device and the proper selection of its constituent TE materials are extremely important to ensure that sufficient electric power is provided to the connected post-stage circuits. Material scientists have long sought high-performance TE materials targeting higher figure-of-merit zT (or power factor PF). A fundamental and crucial issue is: what if zT (or PF) is not the right metric for determining the best TE material for a tiny harvester? Some have questioned the utility of these metrics, but a sophisticated theoretical explanation has not been reported thus far.

Here we establish a new set of theoretical formulas *via* a built 0–D analytical model for a tiny TE harvester. It creates a theoretical triangular bridge connecting the constituent TE material, the TEG design, and the harvester's performance, and fully reveals the interdependent relationships among them. Firstly, a practical concept of equivalent electrical resistivity of the TE material is proposed to enable the derivation of the 0-D model for a tiny TE harvester. Then the new metrics for gauging TE materials are constructed to meet the needs of the tiny TE harvester, the specific forms of which depend on the TEG structure and the external load. This breaks the long-standing consensus regarding zT and PF. Thirdly, the optimal configuration of the TEG is directly predicted without using any of the usual complicated and time-consuming optimization algorithms. A tiny TE harvester based on the optimized TEG is fabricated and is found to exhibit a power density nearly 100 times that of a harvester based on a commercial TEG. Finally, a low power circuit along with a Bluetooth wireless communication module are integrated. A self-powered temperature sensor node (25 mm × 25 mm × 16 mm) was developed. This work narrows the gap between advanced TE materials and their practical applications. All related methods and conclusions will foster a new understanding of microscale TE harvesters.

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Advanced simulations of hybrid porous-solid/electrolyte materials for enhanced power factors

CT22

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Keywords: self-consistent Monte-Carlo, nanostrctured thermoelectrics, electrolytes, efficient algorithm, hybrid thermoelectrics

Prior experimental work has demonstrated the possibility of large improvements in the thermoelectric (TE) power factor of porous media when intercalated with electrolytes filling their pores [1]. Surprisingly, in many cases both the electrical conductivity and Seebeck coefficient were increased, offering large improvements to the power factor (PF). These improvements were attributed to charge exchange between the solid medium and the electrolyte, with strong dependence on the type of solid and the type of electrolyte used.

In this work we examine theoretically this complex system and provide directions for optimization. For this, we have developed an advanced simulator and theoretical models to accurately describe the TE behavior of a hybrid porous-solid/electrolyte system in the presence of large degree of nanostructuring. We have developed a novel Monte Carlo algorithm specifically designed for large scale thermoelectric simulations in porous nanostructured media [2]. Our code includes many features beyond the state-of-the-art in Monte Carlo simulations, which allow for drastic computational savings of at least an order of magnitude, making large scale simulations feasible. We then developed a model for the addition of the electrolyte within the pores of the solid medium, whose interaction with the solid is computed in a self-consistent manner by solving the Poisson's equation. This provides the charge exchange and band variations that the solid thermoelectric material experiences. Once this is achieved, the Monte Carlo simulator provides the thermoelectric coefficients.

We find that under certain conditions, the electrolyte can cause favourable band bending in the solid material, resulting in increased carrier density and conductivity, creating conditions for largely improved power factors. The simulator we present, however, goes beyond this system, and can be generally used to enable the understanding of transport in highly disordered nanostructured TE materials in a very effective and efficient way.

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CT23

Influence of thermoelectric properties on the output power density of a new design of planar µ-TEG

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Keywords: thermoelectric, microgenerators, power density, numerical modelling, transport properties

Heat recovery systems based on thermoelectric microgenerators (µ-TEGs) can play an important role in the development of wireless, energy-autonomous electronics. However, to date, the power density that can be recovered with µ-TEGs at small temperature differences is limited to a few microwatts or less, which is not yet sufficient to power a wide range of wireless devices. To develop more efficient µ-TEGs, the material, device, and system requirements must be considered simultaneously. In this study, an innovative design of an in-plane µ-TEG integrating bismuth telluride and forming sinusoidal trenches is reported. Using 3D numerical simulation, the influence of boundary conditions, parasitic effects (electrical and thermal contact resistances), and transport properties of thermoelectric materials on the output power of these µ-TEGs are investigated in detail for a small temperature difference of 5 K between the hot and cold sources. Compared to wave-shaped trenches, this new shape enables an increase in output power. The results show that either the thermal conductivity or the Seebeck coefficient of the active n- and p-type semiconductors are the key parameter that should be minimized or maximized depending on the magnitude of the parasitic effects.

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Sustainable *n*-type $CuFeS_2$ thin-film thermoelectric generators

CT24

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Keywords: thermoelectric generator, thin-film, *n*-type semiconductor, thermal evaporation, sulfurization

$CuFeS_2$ chalcopyrite, with its *I-42d* structure, is a sustainable and earth-abundant *n*-type semiconductor that has been widely explored for various applications, particularly in the thermoelectricity (TE) field [1]. While it boasts high electric conductivity [2], its relatively high thermal conductivity of 6 W m^{-1} K^{-1} hinders its TE performance. Two alternatives have been proposed to overcome this limitation: (1) Microstructural engineering [3], which improves phonon scattering at the grain boundary without significantly decreasing the electronic conductivity, and (2) the production of the material in thin film form, for devices with 2D geometry, such that the sectional area through which the heat is transferred is reduced.

In this work, both strategies are employed together and tested in a proof-of-concept thin film TE generator (TEG). This was achieved by employing a new and innovative method of $CuFeS_2$ preparation: (1) ball milling of the metal precursors, (2) thermal evaporation onto soda lime glass substrates, and (3) sulfurization. Two legs were devised and connected by Ag thin film connections, each possessing a 3 mm × 25 mm active area (planar area covered by the legs). With a homemade setup, the complete TEG characterization was made possible, attaining the Voltage at Open Circuit (VOC) and Current vs Voltage (I–V) by a systematic change of the load resistance. The results showed a maximum power output of 270 nW cm^{-2} by actual area when maintaining a temperature gradient of 190 °C.

The performance of $CuFeS_2$ is comparable to other Cu-based materials produced by this research group [4,5]. Moreover, it is set as an adequate *n*-type junction with the already investigated *p*-type semiconductors.

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CT25

An on-chip micro-thermoelectric temperature-controller

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Keywords: temperature control, temperature-sensitive component, temperature controller, freestanding thermoelectric film, low-power electronic

To continue and extend Moore's Law in the development of modern microelectronics, multidimensional nanoelectronic integration and multifunctional component assembly have been greatly explored in recent years. However, these approaches will inevitably exacerbate the precise temperature control for temperature-sensitive electronic components [1-2] extremely challenging. Therefore, temperature control is critical in modern microelectronics as the temperature has multiple effects on the performance of almost all microelectronic devices.

Herein, we report an approach to integrating freestanding thermoelectric (TE) nano films [3] into micro on-chip TE temperature-controller for thermal management of macro electronics, its tunable effective thermal resistance can be controlled by electrical currents to achieve energy-efficient temperature control. A cooling temperature exceeding 44.5 K can be achieved using only 445 μW of power consumption, which is two orders of magnitude lower than that required in microheaters. We also observed an ultra-fast cooling rate exceeding 2,000 K/s and excellent reliability up to 1 million cycles. The proposed micro on-chip TE temperature-controller will play an important role in the development of modern electronics with numerous promising applications.

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Thermoelectric modules based on thin films for IoT applications

CT26

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Keywords: thin films; modules; PEDOT:PSS; skutterudites; oxides; power output

Compact, light thermoelectric modules based on thin film legs were prepared using different materials and techniques: (a) five ink-jet printed Ag electrode-legs alternated with five screen-printed *p*-type PEDOT:PSS legs on photo-paper scaffold [1]; (b) five *n*-type and five *p*-type skutterudite legs of the composition $Smy(Fe_xNi_{1-x})_4Sb_{12}$ (*n*-type: $x = 0.63$ and $y = 0.20$; *p*-type: $x = 0.70$ and $y = 0.40$) [2, 3] deposited on silica substrate by pulsed laser deposition (PLD); (c) 5 Al-doped ZnO (*n*-type) legs alternated with 5 $Ca_3Co_4O_9$ (*p*-type) legs deposited on $A_{l2}O_3$ and silica substrates by PLD [4].

The power output of the modules was measured with a custom-made apparatus. As displayed in **Fig. 1**, the maximum output power of the modules was measured as 60 nW (T = 75 °C) for the PEDOT:PSS/Ag module on photo-paper; 0.53 μW ($T = 300$ °C) for the skutterudite-based module; 3 nW ($T = 300$ °C) for the oxide-based module.

These encouraging results suggest the feasibility of miniaturized thermoelectric modules for powering out-of-the-grid IoT devices.

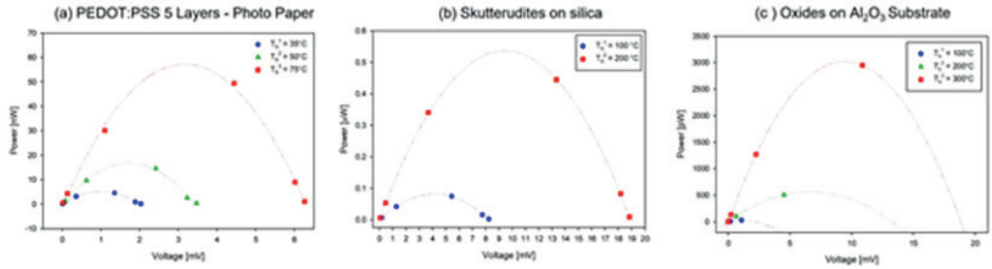

Fig. 1: Output power/voltage curves for: (a) PEDOT:PSS/Ag module; (b) skutterudites-based module and (c) oxides-based module

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CT27

High-sensitivity flexible thermocouple sensor arrays via printing and photonic curing

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Keywords: temperature sensor arrays, thermoelectrics, printed thermocouples, photonic curing

The research on thermoelectrics, so far, has been mainly for energy harvesting, waste heat recovery, and cooling applications. The thermoelectric (TE) technology is also widely employed for temperature sensor applications due to the following advantages: no resistance-related error, fast response, point temperature sensing, and wide temperature range operation. For a long time, metal-based thermocouples (TC) governed by the TE effect have been used as temperature sensors.

Despite remarkable advances, high-performance TE materials-based TCs lack mechanical robustness and flexibility. Hence, conventional low Seebeck coefficient metals (Ni, Cu, Fe) wire-junction-based TCs have been used for temperature sensor applications. However, not only the sensitivity of the metal-based TC sensor is low, but also it is very difficult to fabricate a pixelated sensor using the conventional approach. In this work, we have employed high-performance $(SbBi)_2(TeSe)_3$-based printed flexible TE materials to fabricate two types of shape-conformable TC-based temperature sensor arrays with 25 pixels (TSA I and TSA II). $Bi_{0.5}Sb_{1.5}Te_3$-based p-type printed TE film and copper have been used to fabricate TSA I, and the p-type film together with the $Bi_2Te_{2.7}Se_{0.3}$-based n-type film has been used to fabricate TSA II. A high average sensitivity (S_{Exp}) value of ~124 µV °C^{-1} for TSA I and ~319 µV °C^{-1} for TSA II is attained with high linearity.

The high-performance n-type bismuth-telluride-based polycrystalline materials via constructing $MoSe_2$-2D heterojunction for power generation applications

CT28

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Keywords: n-type Bi_2Te_3, $MoSe_2$ 2D-heterojunction, thermal conductivity, mechanical performance, thermoelectric property

Bi_2T_3-based thermoelectric (TE) material is the only commercial application material for waste heat power generation. However, the poor TE and mechanical properties of commercial n-type Bi_2T_3-based material restrict its conversion efficiency and micro-scale applications. The energy conversion efficiency of TE materials depends on the dimensionless figure-of-merit $zT = S^2\sigma T/\kappa$, where S, σ, T, κ are the Seebeck coefficient, electric conductivity, absolute temperature, and thermal conductivity, respectively. The strong coupling relationship between the three parameters (S, σ, κ) is responsible for the non-ideal TE property. Thus, seeking a method to decouple this relationship is an urgent matter. In addition, simultaneously improving the zT values and mechanical performance has attracted many TE researchers' attention.

This work adopts traditional melting, ball-milling and hot deformation methods [1] for synthesizing outstanding TE property n-type Bi_2T_3-based polycrystalline materials. The specific mechanisms for improving its property are summarized as follows: 1) according to the reference reported by Li *et al* [2], we select the suitable Ag doping for n-Bi_2T_3-based materials to control the carrier concentration. 2) We construct in-suit $MoSe_2$ rigidity heterojunction in the matrix phase to reduce thermal conductivity and optimize mechanical performance. 3) We apply the hot deformation to ensure carrier mobility.

This strategy can effectively improve the TE properties, especially presenting a low thermal conductivity of 0.82 $W{\cdot}m^{-1}K^{-1}$ at 373 K. Meanwhile, a competitive electrical performance has been kept ($PF = S^2\sigma = 30$ $W{\cdot}m^{-1}K^{-2}$ at 300 K). Finally, a maximum zT value of 1.24 at 373 K can be obtained for the content of 2 wt% $MoSe_2$ (37% enhancement compared with the non-$MoSe_2$ and commercial n-type Bi_2T_3-based materials). Subsequently, the Vickers hardness can reach 1 GPa for the samples with $MoSe_2$ heterojunction structures (150% enhancement compared with commercial n-type Bi_2T_3-based materials). Finally, a TE harvester using this novel material is fabricated and tested, whose output power is nearly two times that of the harvester using commercial materials on the premise of identical structural configurations.

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CT29

The effect of the milling rotation speed of PbTe thermoelectric materials with nanostructure

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Keywords: chalcogenide; lead telluride; nanostructure; thermal conductivity; milling rotation speed

Lead telluride PbTe is a promising thermoelectric material for applications in the intermediate temperature range of 500–900 K. PbTe thermoelectric generators have been used in various ways, such as waste heat recovery systems for engine exhaust gases. The phonon thermal conductivity κ_{phonon} of PbTe is theoritical expected a decrease with a grain size below order [1]. J. Male *et al.* reported that doping PbTe with Na or Eu reduces κ_{phonon} due to lattice softening or increased defective phonon scattering [2]. However, the corrent mechanism has not been clarified.

In the previous study, thermal conductivity was investigated by changing the milling rotation speed of undoped PbTe prepared by PbTe ingot milling followed by hot-pressing method. It was reported reducing κ_{phonon} of undoped PbTe [3]. In the present study, the weighed Pb and Te were melted at 1223 K. The PbTe alloyed ingots were milled 140–220 rpm. The PbTe powder was sintered at 650 K and pressed under 196 MPa. The obtained PbTe were dense and *p*-type semiconductors. Thermal conductivity was measured using a static comparison method. The average grain size was measured by using focused ion beam (FIB)-scanning electron microscope (SEM) and transmission electron microscope (TEM).

The thermal conductivities were decreased from 2.0 $Vm^{-1}K^{-1}$ to 1.59 $Vm^{-1}K^{-1}$. The minimum κ_{phonon} was obtained at a milling rotation speed of 160 rpm. The average grain size of 620 nm was observed in the FIB-SEM observation. Furthermore, nanostructures with an average size of 87 nm were observed in their grains by TEM observation.

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Investigating both electronic structure and thermoelectric transport properties of $SnBi_2Te_4$

CT30

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Keywords: thermoelectric, tetradymite, $SnBi_2Te_4$, first-principles calculations, electronic structure, thermoelectric transport analysis

Homologous series of $(A^{IV}Te)_n(Bi_2Te_3)_m$ in which A^{IV} is Ge, Sn or Pb and *n* and *m* are integers, are theoretically investigated as potentially useful thermoelectric compounds due to their narrow bandgap and layered, complex crystal and electronic band structures stemming from their well-known parent compound Bi_2Te_3. Up to now, most of the results on this series have been obtained from cold-pressed samples with low density yielding moderate peak zT values of 0.25 at room temperature [1,2]. In addition, these values are likely overestimated due to the combination of in-plane and out-of-plane transport parameters. In this work, comprehensive first-principles calculations of the electronic structure of $SnBi_2Te_4$ will be discussed with the results of experimental thermoelectric transport properties. Additionally, optimization of the carrier concentration through doping will be further presented.

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CT31

High temperature crystal structure analysis, effect of substitution on phase transition and transport properties of $Cu_{2.9}Te_2$

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Keywords: Rickardite, phase changing material, modulated structure, $Cu_{2.9}Te_2$, thermoelectric

Phase diagram of Cu-Te systems has been experimentally studied by many authors, and one of the complex Cu-Te phases between Cu_2Te and CuTe in the phase diagram is $Cu_{3-x}Te_2$ known as rickardite mineral that displays an unconventional defective structure with a large amount of vacant metal positions. In our recent investigation on $Cu_{3-x}Te_2$, a specific set of weak reflections both on single-crystal and powder diffraction data was also observed suggesting that the crystal structure of $Cu_{3-x}Te_2$ has modulated type of ordering[1,2]. DSC analysis performed to study thermal transitions of both samples showed that $Cu_{2.9}Te_2$ undergoes two main phase transitions at around 458 and 647 K and the first phase transition coincide to a crystal structure change from orthorhombic to tetragonal. The second endothermic peak is sharp on the DSC thermogram, and it is attributed to the tetragonal to hexagonal phases.[3-5] HTXRD measurements confirm the reversible phase transitions following the sequence orthorhombic ↔ tetragonal ↔ hexagonal phases. The high temperature phase at 673 K was found to be a hexagonal unit cell with lattice parameters of a = 7.289 and c = 7.855 Å.[1] The effects of these transitions were observed on the electronic and thermal transport properties up to 733 K. While the first transition has little influence on the transport properties, the high-temperature transformation leads to a metallic-like to semiconducting-like properties at around 650 K. The substitution (Ag, Zn) in $Cu_{3-x}Te_2$ has influence on the phase transition temperature significantly thus the transport properties around same temperature. While the investigations on physical properties have recently been reported, the study on structural characteristics of this complex phase at high temperatures is still incomplete[1].

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Reducing the thermal conductivity of nanocrystalline CuNi alloys

CT32

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Keywords: thermal conductivity, nanocrystalline, alloys, electrodeposition, lithography

The application of inexpensive and scalable materials in the industry for thermoelectric applications has received great interest, such as CuNi alloys in the last ears. Nanocrystalline CuNi alloys with different compositions were grown by pulsed electrodeposition reducing the crystallite size of the CuNi down to 30–40 nm by the incorporation of saccharine in the electrolyte [1]. The thermoelectric properties, such as electrical conductivity, Seebeck coefficient, and thermal conductivity of these nanocrystalline alloys, were studied. The maximum figure of merit at room temperature obtained was $(6.4 \pm 1.5) \cdot 10^{-2}$ for nanocrystalline $Cu_{0.65}Ni_{0.35}$. The thermal conductivity of CuNi alloys was reduced by the nanostructuration to a value of 9.0 ± 0.9 W/m·K (**Fig. 1**), making these nanocrystalline CuNi alloys more competitive than other more classical thermoelectric materials [2]. These alloys were also nanostructured in order to improve the thermoelectric properties. This work opens a new field to be investigated, that can be described as the use of commercial alloys such as CuNi for thermoelectric applications, and shows the use of a new approach to enhance the thermoelectric properties of inexpensive and/or fewer pollutant materials.

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CT33

Precision interface engineering of CuNi alloys by powder ALD toward high thermoelectric performance

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Keywords: CuNi, thermoelectric, atomic layer deposition, surface modification, figure of merit

The main bottleneck in obtaining high-performance thermoelectric (TE) materials has been identified as how to decouple the strong interrelationship between electrical and thermal parameters. Herein, we present a precise interface modification approach based on the powder Atomic Layer Deposition (pALD) technology to enhance the performance of CuNi alloys. Single-layer ZnO and Al_2O_3 layers have been deposited on the surface of powders, typically in 10–100 cycles, and their effect on the TE performance of bulks has been thoroughly investigated.

A standard model is proposed and experimentally confirmed to build the relationship between the ALD oxide cycle numbers and Zn and Al content, which could be easily adapted to other pALD processes. The enhancement of the Seebeck coefficient, caused by the energy filtering effect, compensates for the electrical conductivity deterioration due to the low electrical conductivity of oxide layers. Furthermore, the oxide layers may significantly increase the phonon scattering. Therefore, to reduce the resistivity of coating layers, a multiple-layer structure is deposited on the surface of powders by inserting Al_2O_3 into ZnO is constructed on. The atom probe tomography shows that after pressing, the Al atoms diffused into ZnO and realized the doping effect. Al diffusion has the potential to increase the electrical conductivity and complexity of coating layers.

In comparison to pure CuNi, zT increased by 227.6% as a result of the decrease in resistivity and stronger phonon scattering in phase boundaries. The study demonstrates that ALD-based interface modification may be a versatile method for decoupling TE parameters and precisely modifying phase boundaries, which is practical for other thermoelectric materials.

Acknowledgments

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On the optimisation of the brazing process of Fe_2VAl Heusler compound-based thermoelectric modules

CT34

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Keywords: contact resistance, interface, brazing, Heusler, thermoelectric module

The Fe_2VAl Heusler compound is a promising thermoelectric material with a very special technical and economic profile. Indeed, it has a large power factor (> 5.10^{-3} [W/mK²]) higher than Bi_2Te_3, while being composed of cheap and abundant chemical elements. To become a serious competitor for thermoelectric applications, two challenges still need to be met: (i) the optimisation of thermal properties to improve the figure of merit (currently limited to 0.2–0.3) and (ii) the development of assembly methods allowing the realisation of efficient and reliable thermoelectric modules. This is the second point that is investigated in this study.

In a previous study [1], various solutions for joining Fe_2VAl with copper were investigated. It was found that the use of an Ag-Cu-Zn braze was a promising method for the production of modules. However, the electrical contact resistance between copper and Fe_2VAl still reaches a value of ~45 μΩ cm², whereas a value smaller than 10 μΩ cm² would be necessary for a negligible effect on the module performances. Therefore, this study aims at analysing and optimising the brazing process to meet this objective.

In a first part, the effect of the brazing parameters on the electrical properties and the microstructure of the interface have been studied. By combining these experimental results with a finite element model, the electrical properties of the interface at the microscale have been resolved. Based on this study, the brazing parameters allowing to reach an electrical contact resistance lower than 10 μΩ cm² have been determined. In a second part, the brazing process was adapted to produce thermoelectric modules comprising 18 p-n pairs with a contact resistance below 5 μΩ cm². Their performances in terms of power density and efficiency are in agreement with literature results and stable after 200 thermal cycles.

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CT35

$CoTe_2$- enhanced thermoelectric performance of nanocrystalline skutterudite thin films

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Keywords: composite, work function, band bending, interface scattering, carrier tuning

Metal-semiconductor (M-Sc) based nanocomposite offers an exciting opportunity to enhance the thermoelectric performance of parent materials by modulating both electronic and thermal transport properties. In this study, a co-sputtering method was used to synthesize nanocomposite thin films of metallic $CoTe_2$ embedded with Sb doped-ternary skutterudite. By comparing the transport properties of the pristine ternary phase and the nanocomposites, we demonstrated that the presence of metallic $CoTe_2$ decisively contributes to a strong increase in the charge carrier concentration of composite films due to the low work function of $CoTe_2$. This spillover of charge density translated into increased electrical conductivity and moderate Seebeck coefficient values. The balance between these two properties yields a two-fold enhancement in the power factor of the nanocomposite thin film. Furthermore, the presence of multiple phases results in a notable decrease in the lattice thermal conductivity to a minimum value of 0.48 $Wm^{-1}K^{-}1$ (at 513K) due to increased phonon scattering. As a result, a maximum figure of merit (zT) of 1.30 (at 655K) was achieved in 7 wt.% $CoTe_2$ nanophase embedded nanocomposites, which is twice as high as that of the pristine sample.

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Fabrication and evaluation of Co-based diffusion barriers for skutterudite thermoelectric materials obtained via pulse plasma sintering

CT36

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Keywords: skutterudites; diffusion barriers; contact resistivity; thermal stability; microstructure evolution; pulse plasma sintering

One of the key aspects determining the broad commercialization of thermoelectric modules is their durability. To guarantee long-term durability, stable and effective diffusion barriers must be used to separate the thermoelectric material from the solder or connectors. Among the numerous parameters that should be paid attention to is thermodynamic stability, which is related to the diffusion phenomenon, and matching the coefficients of linear thermal expansion (CTEs) of the module's component materials, thanks to which stresses arising as a result of temperature changes are minimized [1].

This work aims to design and fabricate stable and effective diffusion barriers to be used in thermoelectric modules based on skutterudites. Co-Ni-Cr, Co-Ni-W, Co-Cr, and Co-W systems were selected for the tests. The chemical composition of the barriers has been chosen to ensure maximum compatibility in terms of thermal expansion with the $CoSb_3$ material. At the work's initial stage, several consolidation tests via pulse plasma sintering (PPS) technique were performed to determine the optimal conditions for barrier fabrication. The density, microstructure, and CTE of the obtained materials were investigated. In the next stage of the work, joints between the tested barriers and $CoSb_3$ were manufactured. Two ways of producing joints were used: (1) a single-stage process of PPS consolidation of the diffusion barrier together with $CoSb_3$, and (2) a two-stage process in which the diffusion barriers were initially PPSed and then joined with $CoSb_3$ during its consolidation. The microstructure and phase composition of the joint area as well as the electrical contact resistance, were investigated in the as-fabricated state and after prolonged annealing. The results of this work were also discussed in the context of other works presented in the literature.

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CT37

Development of high-entropy-type thermoelectric materials

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Keywords: high-entropy-type compounds, high-entropy-alloy, metal chalcogenide, Zintl phase, skutterudite compound

High-entropy-alloys (HEAs) have attracted much attention in the fields of materials science and engineering because of their tunable properties as structural materials, such as excellent mechanical performance under extreme conditions [1]. HEAs are the alloys with 5 or more constituent elements and a 5–35% occupancy of each element, resulting a high configurational mixing entropy value (Δ*S*mix) above 1.5 [1]. Introduction of large disturbances and strains due to the multiple elements solid solution is the core of excellent mechanical performances. Even in thermoelectric materials, it is expected that the lattice thermal conductivity (kL) will be reduced by introducing such large disturbances. So far, we have developed a new high-entropy superconductors that extends the concept of HEA from an alloy to a compound. Among them, we successfully synthesized the new high-entropy-type (HE-type) metal chalcogenide superconductor by mixing the multi-site with multiple elements simultaneously, resulting the highest ΔSmix vaule of 2.00 [2]. We also applied this new concept for metal chalcogenide (PbSe-based) thermoelectric material [3]. At the same time, very high *ZT* value above 1.8 was reported in similar metal chalcogenide material [4]. Based on these results, we have been developing various new HE-type thermoelectric materials such as 122 Zintl phase, $CoSb_3$, and so on. We will talk details of the development of HE-type thermoelectric materials.

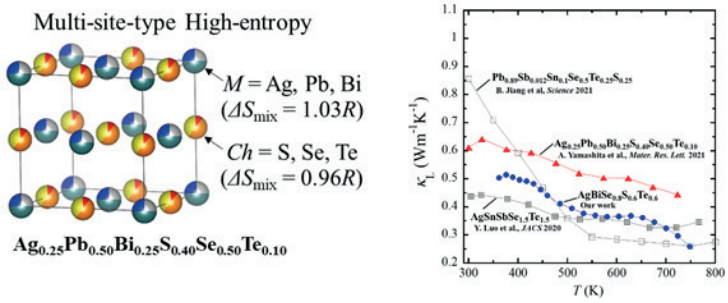

Fig1.: Crystal structure of high-entropy-type metal chalcogenide. Temperature dependence of midle- and high-entropy-type metal chalcogenide materials.

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Acknowledgments

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Electrochemical and thermoelectric characterization of mixed-conducting high-entropy oxides

CT38

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Keywords: mixed conductors; high-entropy oxides; protonic defects

The idea of entropy stabilization of inorganic materials triggered the intensive research activity. When various elements occupy one site in a crystal structure, the neighbourhood of each cation is different. This leads to a strong lattice strain that distorts the atom positions. The lattice distortions influence not only mechanical but also transport properties of HEO materials. In consequence, the transport properties, including both electrical and thermal properties, strongly depend on the structural properties [1-2]. Triple conducting oxides (TCOs) belong to mixed ion-electron conductors which may contain three mobile charge carriers - electrons, protons, and oxygen ions. We propose that the combination of the high configurational entropy and mixed oxygen ionic, protonic and electronic conductivity (HEOs-TCOs) of selected high-entropy perovskites may render them interesting thermoelectric and electrochemical materials [3].

This work is related to the systematic description and understanding of the thermoelectric and electrochemical properties of different (La, Sr, Ba)(Ce, Zr, Y, Ti, Sn, Fe, Co, Mn, Bi) O_3 oxides with compositions and structures based on the oxides being protonic, oxygen ionic and electronic conductors. The structure and microstructure of these materials will be analyzed with the use of X-ray Diffractometry (XRD) as well as Scanning Electron Microscopy (SEM). Electrochemical measurements will be performed both by DC four-wire technique and Electrochemical Impedance Spectroscopy (EIS) as a function of temperature and water vapour or oxygen partial pressures. The temperature dependence of the Seebeck coefficient and total thermal conductivity will be also measured and analysed.

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CT39

Thermoelectric properties of high-entropy type $AgBi(S, Se, Te)_2$

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Keywords: thermoelectric materials, high-entropy type compounds, entropy engineering, material design, order-disorder transition

High-entropy alloys (HEAs) have attracted much attention as a new approach to alloy design [1]. HEAs are typically defined as a solid solution with more than five elements and a 5 to 35% occupancy of each element, or a high configurational mixing entropy value () above 1.5*R* [1,2]. In recent years, this concept is adopted with thermoelectric compounds since it provides a good way to improve thermoelectric dimensionless figure of merit (*ZT*) by strengthening phonon scattering because of their disorder and distorted lattice, and the maximum *ZT* value was achieved 1.8 at 900 K [3].

So far, we synthesized $AgBi(S, Se, Te)_2$ as a high-entropy (HE) type $AgBiSe_2$ based compound. $AgBiSe_2$ based compounds show high *ZT* due to their low lattice thermal conductivity (κ_{lat} ~ 0.38 W/mK), however, crystal structure phase transitions of $AgBiSe_2$ (room temperature: hexagonal, middle temperature: rhombohedral, high temperature: cubic) should disturb utilizing as a practical module [4]. In the case of $AgBi(S, Se, Te)_2$, we succeeded in stabilizing the cubic phase at room temperature using HEAs concept, moreover, *ZT* ~ 0.9 was achieved at 747 K due to the ultra low lattice thermal conductivity of κ_{lat} ~ 0.24 W/mK. We will talk about details of this HE type thermoelectric compounds.

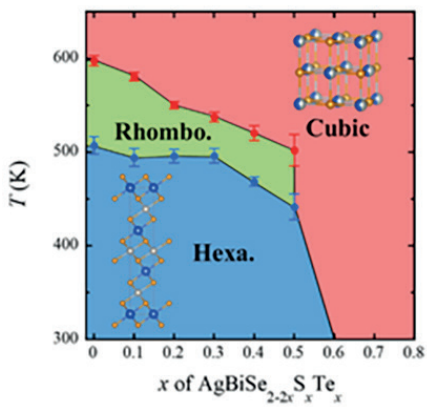

Fig. 1: *T* – *x* phase diagram

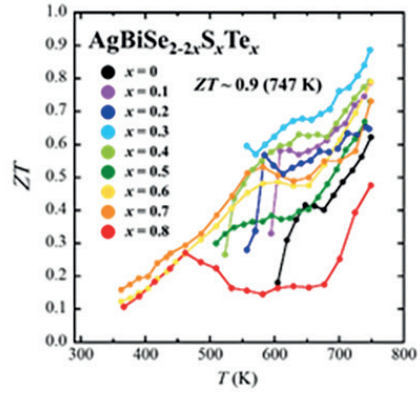

Fig. 2: Temperature dependent *ZT*

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Dynamic thermoelectric generators: increased efficiency at maximum power by modulation of heat fluxes

CT40

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Keywords: efficiency; autonomous heat engines; thermoelectric generators; thermodynamics; heat flux modulators

In the 1960s, Gray [1] analysed the dynamic operation of thermoelectric generators (TEGs) and coolers, but the mathematical complexity of the problem limited the assessment of this approach to the small-signal regime. In recent years, the issue has been reconsidered, still in the linear limit [2-6]. We present here the solution to the time-dependent nonlinear Domenicali's equation, discussing it both under Dirichlet and mixed boundary conditions. We show that the efficiency at maximum power (EMP) is always larger when input is time-modulated, but the enhancement largely depends on the characteristics of the electric load. With a fixed load, EMP increases by up to ≈ 50%, independently of the modulation frequency. Instead, coupling the TEG with a time-dependent synchronized resistance can improve EMP by up to 280% for currently available thermoelectric materials (tellurides). The importance of a proper matching load explains the controversial experimental results reported over the last years [7-10]. Along with the availability of more cost-effective materials, enhancing TEG EMP from 6–8% to around 20% could expand thermoelectric conversion from its current status of a niche technology to a more impactful method of recovering low-enthalpy heat from secondary power sources.

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CT41

In-situ electrode bonding process for improving the reliability and efficiency in nanostructured PbTe-based modules

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Keywords: PbTe, power generation, contact layer, contact resistance, thermal expansion

PbTe is among the best performing thermoelectric materials, both for p- and n-type, for intermediate temperature applications. However, the fabrication of PbTe-based modules for thermoelectric power generation still faces challenges related to the material mechanical stability and the bonding of electric contacts, particularly in the case of p-type PbTe. To address these challenges, in our previous work [1] we were able to successfully improve the high-temperature mechanical strength and stability in p-type $Pb_{0.993-x}Na_xGe_{0.007}Te$ by adjusting the Na dopant levels. At the same time, the excellent thermoelectric performance was maintained with peak $zT \sim 2.2$ at 813 K for $Pb_{0.973}Na_{0.02}Ge_{0.007}Te$. Subsequently, thermoelectric PbTe legs with Co-Fe alloy diffusion barriers were fabricated by co-sintering of the PbTe and Co-Fe powders. However, cracks in the PbTe were formed due to thermal stresses during the simultaneous densification and bonding of PbTe and Co-Fe powders, leading to increased module resistance and reduced output power. The thermal stresses are due to large differences in coefficients of linear thermal expansion (CTE) between PbTe and Co-Fe contact layers. In this work, we prevent crack formation by CTE mismatch through the modification of the contact bonding process. Legs of p-type $Pb_{0.973}Na_{0.02}Ge_{0.007}Te$ and n-type $Pb_{0.98}Ga_{0.02}Te$ are stacked with flexible Ag-foil interconnecting electrodes and Fe-foil contact layers on the hot side. Pressure is applied to the module to ensure intimate contact between all components. Consequently, maximum efficiency value ~7% was obtained for nanostructured PbTe modules for 773 K on the hot side and 293 K on the cold side, showing the viability of this approach.

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Height optimized micro-thermoelectric devices

CT42

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Keywords: geometry optimization, thermo-electrics, electrochemical deposition, micro-devices, solid state cooling

Micro thermoelectric devices are an excellent choice for hot spot cooling and energy-autonomous sensor applications in combination with fabrication methods that are fully compatible with on-chip integration.

To achieve maximum device performance, the geometry of the device must be optimized to match the electrical and thermal properties of the Thermoelectric materials. This is usually done by adjusting the cross-sectional areas which leads to a limitation of the maximum packing density. Here, we present a new design strategy for fabricating uTEDs in which we optimize the heights which allows higher packing densities, thus increasing cooling power density and output power, and also reduces the amount of thermoelectric materials needed, which are often toxic and expensive.

For the fabrication of the micro thermoelectric devices, we use a photolithography in combination with the electrochemical deposition of $Bi_2(Te_xSe_{1-x})_3$ and Te as n-type and p-type materials, respectively [1,2]. The optimized uTECs shows a maximum cooling of 10.5 K at room temperature and 21 K at an ambient temperature of 343 K. Simulations using the finite element method show that cooling power densities of hundreds of watts per square centimeter can be achieved. Which is 35%higher than unoptimized device and uses 75% less Te than cross-section optimized devices [2]. As a generator, the micro thermoelectric modules exhibit high open-circuit voltages and power densities in the range of a few milliwatts per square centimeter even at small temperature differences. Our results demonstrate the excellent suitability of micro thermoelectric modules for hot-spot cooling applications to increase integration density in circuits and energy-autonomous sensors for the Internet of Things.

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CT43

Long-term performance stability of all-Si based micro--thermoelectric generators with integrated heat sink

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Keywords: thermoelectric generator, silicon nanowires, internet of things

In Internet of Things (IoT) systems millions of interconnected devices demand for sustainable and long-term autonomous energy sources. Thermoelectricity offers an alternative to primary batteries for powering sensor nodes with energy harvesting in the 10–100 μW/cm^2 range.

Earlier, the group developed all-Si based μTEGs with planar architecture [1]. This approach benefits from silicon (Si) and microelectromechanical systems (MEMS) technologies for the downsizing and scalability, and from the fact that Si is abundant and environmentally sound. This work reports the studies on the performance stability with time of the power generation of the μTEGs in optimal working conditions (load and internal resistance matching). These studies have been carried out by exposing the μTEGs, with an integrated heat sink, to both a constant temperature and to cycles of different temperatures for a week.

The μTEG is based on arrays of p-doped Si nanowires (NWs) acting as the thermoelectric material, epitaxially grown connecting a Si bulk rim, in contact with the heat source, and a thermally isolated suspended platform, the cold end of the generator [2]. The thermal resistance from the suspended platform to the ambient, consequence of the small footprint of the platforms, limits the power generated by the μTEG. A heat sink enhances this heat exchange, increasing the temperature gradient across the NWs. Its integration on top of the fragile suspended platforms has only been possible by means of a μTEG-to-heat sink Si adapter that acts as an interface between the membranes and the heat sink. In order to carry out the heat sink integration a custom pick and place system has been developed to control the adapter placement on the μTEGs.

The μTEG with the heat sink generates output powers well within the range of IoT needs. When placing the μTEG on top of a heat source above 200 °C and in still air convection conditions it generates more than 10 μW/cm^2. The performance stability with time studies show that no degradation takes place on the μTEGs below 200 °C and that the power generation remains constant within 1 week. In the case of 250 °C, the power remains constant during the week but a degradation on the resistance of the Si NWs is observed. On the other hand, the V_{OC} is enhanced, compensating the increase in resistance and maintaining the power generation constant. These results demonstrate the validity of the μTEGs with heat sink as power supplies for IoT applications at the microscale.

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Development of Nano-CHP based on middle and low temperature thermoelectric modules arranged as a cascade

CT44

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Keywords: application, nano-CHP, heat transfer, middle temperature thermoelectric module, thermoelectric generator, heating unit

This paper presents results of an R&D project aimed at designing and optimizing a small-scale combined heat and power unit (Nano-CHP) based on middle and low-temperature thermoelectric modules arranged as a cascade.

The Nano-CHP mainly consists of a modified natural gas-fired condensing boiler equipped with a thermoelectric generator (TEG). The project's goal is to provide a low-cost Nano-CHP solution for single-family homes, with an electrical output of about 300 W at a firing heat output of about 5 kW. The focus of this paper is on heat transfer. The thermal flux from the combustion area and the hot gas to, through, and from the thermoelectric modules is discussed, with a particular emphasis on the aspects of bypass heat losses and heat transfer resistances.

The investigations were carried out by both experimental tests and CFD calculations. The experimental tests were performed on a full-scale Nano-CHP unit with a firing heat output ranging from 3 to 15 kW. The applied thermoelectric modules are based on Skutterudite material (middle temperature, up to about 500 °C) and BiTe (low temperature, up to about 200 °C), with the middle-temperature modules combined with low-temperature modules as a TEM-Cascade.

The results show that the concept works, with the amount of bypass heat losses and thermal resistances having a very strong influence on the thermoelectric performance. As a result, guidelines for an optimum design of a Nano-CHP are derived.

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CT45

300mm wafer level fabrication of CMOS-compatible thermoelectric energy-harvester and cooler devices

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Keywords: CMOS-compatible, 300-mm-wafer-level, thin film devices, FEM-simulations, Si-based thermoelectrics

The incessant downscaling of computer chip size and the ongoing increase in computing power require more and more energy-efficient devices to meet customer requirements. Thermoelectric-based cooling as well as energy harvesting could be useful methods for a reliable device performance and to achieve energy-efficient devices [1-3]. This approach requires optimized CMOS-compatible thin-films and device structures.

In this work, we demonstrate the realization of silicon-based thermoelectric thin film devices fabricated on 300 mm silicon wafers in a CMOS-compatible cleanroom. This required extensive preparatory work, which is represented by material development [4-5] and FEM-simulations. We use a lateral multistage approach with structure sizes from the micrometer to the nanometer range. Hotspots are simulated by integrated heating meanders and resistance thermometers serve as temperature sensors. Thin film properties such as elemental composition, crystallinity and microstructure are studied via XPS, XRD and SEM. All examined layers and structures are ready for industrial use and can be integrated into existing CMOS process flows. Thermoelectric approaches such as Peltier coolers or energy harvesters are discussed and represent a good option for thermal management of various electronic devices.

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Novel fabrication route for reproducible and high z_T in superionics Ag_2X (X = Se, Te)

CT46

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Keywords: superionic compounds, *n*-type, *p*-type, reproducibility, hierarchical nano-structuring, low thermal conductivity

The binary superionic compounds Ag_2Se and Ag_2Te have gained great attention from the thermoelectric (TE) community due to their favorable thermoelectric properties including very low thermal conductivity (~1 W m^{-1} K^{-1}) [1,2] and high carrier mobility (~ 3000 cm^2 V^{-1} s^{-1}) [3]. No wonder then that both Ag_2Se and Ag_2Te exhibit reasonably high zT. However, reproducibility and compositional inhomogeneity, both in part related to the migration of Ag ions during high temperature processing, remains an issue which limits their practical applicability [4,5]. In Ag_2Te in fact the problem is so severe that *n*-type and p-type behavior appears randomly for samples prepared with the same nominal composition Ag : Te = 2 : 1 [5].

In our study [6,7], we developed a novel synthesis method for producing nearly 100% dense nanostructured samples at room temperature without melting or sintering/annealing at high temperatures. This allows us to finely control the sample behavior and obtain reproducible transport properties for both the materials. We therefore obtained a high, reproducible and thermally stable, zT of 0.92 at 370 K in Ag_2Se. For Ag_2Te, fine-tuning of the Ag/Te molar ratio results in reproducible n- and p-type behaviors. A high and reproducible zT values of 1.2 and at 570 K for n-type and 0.64 at 570 K for p-type Ag_2Te samples are obtained. The average zT values of 0.81 and 0.99 have been achieved for n-type Ag_2Se and Ag_2Te samples, respectively, which are comparable to the state-of-the-art n-type Bi_2Te_3 material. Overall, the novel synthesis method that we developed allows us to control and improve the properties of Ag_2Se and Ag_2Te, making them potentially more suitable for thermoelectric applications.

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Metavalent bonding mediated high thermoelectric properties of SnSe-Ag_V_VI_2 alloys

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Keywords: SnSe, cubic structure, phase transition, thermoelectric, metavalent bonding

SnSe is a rising-star thermoelectric material due to its outstanding thermoelectric performance in conjunction with low toxicity and high abundance of constituent elements. However, SnSe only shows high ZT values above ~750 K when the structure transforms from the asymmetric Pnma phase to the higher symmetric Cmcm phase [1]. As a typical IV_VI compound bonded by p-state electrons, the Cmcm phase SnSe with an improved symmetry is expected to show the same chemical bonding with other rock-salt IV_VI compounds such as PbTe and SnTe, which could be responsible for its excellent thermoelectric performance [2,3]. Yet, it is very challenging to stabilize the Cmcm phase at room temperature to characterize the bonding indicators. Here, we alloyed SnSe with Ag_V_VI_2 (V = Sb and Bi; VI = Te and Se) compounds and obtained rock-salt SnSe bulk samples. All cubic SnSe alloys show a unique portfolio of properties including a high optical dielectric constant, a large Born effective charge, and abnormal bond-breaking behavior in laser-assisted atom probe tomography. All these characteristics are indicative of the metavalent bonding mechanism, which has not been found in the pristine SnSe. Our work demonstrates that metavalent bonding could be the origin of many special properties of the high-symmetric SnSe phase including excellent thermoelectric performance.

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In depth study on preparation of Bi_2O_2Se polycrystals

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Keywords: bismuth oxyselenide, Bi_2O_2Se, secondary phase doping, polycrystalline synthesis

Over the past decade, extensive research has been conducted on Bismuth oxyselenide (Bi_2O_2Se) as a promising TE material. It is known for its combination of advantageous transport properties, absence of toxic elements and reasonable price. However, its low electrical conductivity poses a significant challenge to its further utilization. [1]

Researchers have focused their efforts on enhancing thermoelectric properties through methods such as doping, grain boundary engineering, and the addition of secondary phases [2,3,4]. However, published results for the undoped material exhibit significant variation and are hardly reproducible, making it challenging to investigate the effect of doping accurately. To address this problem, we have prepared Bi_2O_2Se using various synthesis methods.

To ensure the phase purity of the prepared samples, we conducted an analysis using powder X-ray diffraction (PXRD), scanning electron microscopy/energy-dispersive X-ray spectroscopy (SEM/EDS), and Raman spectroscopy.

We have analyzed our experimental results and compared them with the existing literature data. This allowed us to identify multiple factors contributing to the variation of transport properties of undoped "pure" Bi_2O_2Se. Finally, we present a low-temperature reproducible synthesis process for pure Bi_2O_2Se, which is fundamental for further investigations into this material.

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CT49

Synthesis and thermoelectric properties of $Cr_{1-x}Me_xN$ (Me = Mo, V)

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Keywords: magnetron sputtering, epitaxial growth, thin films, alloying, CrN

Among emerging materials systems for thermoelectric applications, the early transition-metal nitrides based on ScN and CrN show unexpectedly promising properties in the form of high Seebeck coefficient, low thermal conductivity, and high electrical conductivity [1]. There is, however, still a need to improve their thermoelectric properties. One idea is to introduce dopants or alloying elements to alter the concentration, mobility, and/or type of charge carriers, such as $Cr_{1-x}V_xN$ [2]. Another is to focus on the different scattering mechanisms to manipulate the scattering of electrons or phonons. Electrical conductivity can be altered by grain boundary modifications, such as larger grains as well as metallic inclusions, for higher charge carrier concentrations and smoother interfaces. Such nanoinclusions could also potentially act as phonon scattering centra [3]. Phonon scattering can also occur due to mass contrast by site substitution of isoelectronic but heavier atoms, which could reduce the phonon mean free path while retaining the electrical conductivity.

This study investigates epitaxial thin films of CrN-based materials with Mo and V substitution, and their growth by DC-magnetron sputtering.

First, the growth condition of CrN films were optimized, with a varying substrate temperature and nitrogen flow ratio while the target power was fixed. The effect of in-situ annealing at the deposition temperature was also investigated. It was found that temperature, pressure, and ambient gas have a large effect on the decomposition of CrN to Cr_2N. Second, alloying with Mo and V was implemented. It was found that while Mo breaks the rock-salt structure, thin films of CrMoVN have higher solubility of Mo than what has previously been reported for bulk CrMoN [4].

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Influence of ion implantation on the thermoelectric properties of transition metal nitrides thin films

CT50

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Keywords: thin films, nitrides, implantation, defect engineering, nanostructuration, doping

Thin films transport properties have been extensively studied over the past decades for thermoelectric applications. On the one hand, the low dimensionality of these materials often allows them to exhibit unique electronic transport properties. On the other hand, phonon scattering through point defect engineering still remain a challenge to obtain high performance thermoelectric thin films. In this context, the ion-implantation technique, widely used for semiconductor doping, may present itself as a useful technique to generate various types of defects into the film and decrease the mean free path of phonons without disrupting the electronic transport properties. In addition, this technique offers access to a wide range of usable ions, which permits both generation of defects and doping of the material. In turn, this allows the control of the charge carrier concentration on top of the decreased thermal conductivity achieved in the process, leading to improved thermoelectric properties. This promising approach have been studied in the last few years for thermoelectric films and yielded encouraging results[1,2]. We propose in this work to study the influence of ion-implantation on the transport properties of transition metal nitrides thin films, in particular ScN and CrN, for possible thermoelectric applications (**Fig. 1**).

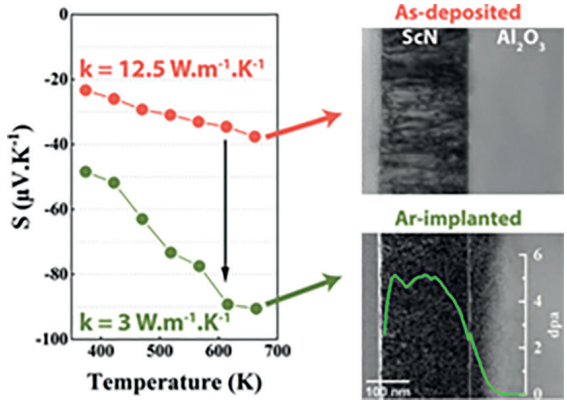

Figure 1: Effects of Ar-implantation on the structural and TE properties of ScN films [1]

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Understanding the mechanism of metal-assisted chemical etching to optimize thermoelectric devices based on Si nanopillars

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Keywords: silicon; nanowires; chemical etching; chemical mechanisms; thermoelectric generators

Quasi-1D nanostructures have shown the possibility of decoupling phonon and electron conductivities because of their different mean-free paths, therefore enabling major increases of thermoelectric figure of merits in several materials, including silicon. Among the many techniques, metal-assisted chemical etching (MACE) provides a simple yet very effective way to obtain nanopillars with lengths of some fractions of millimetres. The most significant limitations of MACE are related to its sensitivity to materials doping, nanopillar density and ordering. In a previous publication [1] we have investigated the mechanism of one-pot MACE, namely etching where Si is oxidized by the Ag^+/Ag couple where metallic Ag also acts as catalyst to localize Si etching. Aim of this communication is to clarify the role of Si surface preparation prior to MACE along with its relationship to nanopillar density and distribution. It will be shown the role played by hydrophobicity/hydrophilicity of Si surface, in good agreement with previous literature evidence [2]. We advance that it rules the eventual self-organization of gas (air) nanobubbles onto the surface. When hydrogenated Si surfaces are exposed to the etching solution, nanobubbles locally prevents Ag^+ ionosorption, leading to a sparser nucleation of metallic Ag nanoparticles. The opposite is true when Si surface is oxidized prior to its exposure to the etchant. Eventual presence of nanobubbles additionally rules the shape of the etched region – and therefore that of nanopillars, which may form either individual nanopillars or natively aggregated nanoridges.

Post-MACE treatments are also found to matter. Aggregation of nanopillars have been largely investigated in the past [3]. We confirm that drying conditions impact the final micromorphology, which is found to depend on solvent polarity, on the final hydrophobicity/hydrophilicity of the Si surface, and on its doping level as well.

Control of density, aggregation, and distribution of Si nanopillars impact their use for thermoelectric applications. While a high density is always required, the ideal nanopillared Si membrane should display little or no aggregation (to minimize contact resistances), which would be favoured by an ordered distribution of nanopillars. Conversely, MACE leading to the complete removal of any residual bulk Si requires nanopillar aggregation to grant mechanical stability. Ways to control all issues will be presented and discussed, along with prototypical devices based on Si nanopillars.

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Impact of the nanostructuring and Sr purity on the thermal and thermoelectric properties of -$SrSi_2$

CT52

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Keywords: nanostructured materials, thermoelectric materials, mechanical alloying, sintering, phonons

Alkaline earth – silicides alloys have been very useful in thermoelectricity due to the abundance of their precursors, their non toxicity and their performances comparable to conventional thermoelectric materials such as PbTe in the mid-temperature range. In the lower temperature range (200–500K) efforts must be performed to be competitive to Bi_2Te_3 alloys.

α-$SrSi_2$ could be a promising material for thermoelectric applications around room temperature if one can decrease the lattice contribution to its thermal conductivity. Its performances were limited by the phonon contribution to the thermal conductivity (about 5 $Wm^{-1}K^{-1}$ at RT) which led to maximum ZT about 0.15 at 300K. Thus, reducing the thermal conductivity should permit to improve the ZT.

In our work, we studied the effect of the nanostructuring and Sr purity on the thermal and thermoelectric properties of α-$SrSi_2$ using 2N and 3N Sr Combining ball milling and spark plasma sintering it was possible to decrease the lattice thermal conductivity by a factor 2 at 300K to 3 at 600K close to that expected to highly disordered or amorphous materials without impacting much the power factor. The results obtained in this study show that the figure of merit ZT was improved, after nanostructuring, from 0.08 to about 0.2 at 300K. A strong enhancement of the ZT is then expected for alloyed α-$SrSi_2$ samples which could permit to compete with Bi_2Te_3.

CT53

Thermal conductivity of GeSn alloys: a CMOS energy harvesting platform for green computing

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Keywords: GeSn, CMOS, IC, group IV alloy, Raman thermometry, 3ω-method

The development of suitable thermoelectric technologies for recycling of waste heat on chips could lead to a significant re-use of energy at operating temperatures of electronic circuits, which could make a significant contribution to reducing greenhouse gas emissions. Nowadays, thermoelectric elements are rarely used within integrated circuits with operation temperatures below <100 °C since there are no efficient thermoelectric semiconductors compatible with CMOS technology. Group IV elements (Si, Ge, Sn) have already been thoroughly studied as TE materials, but in combination with group VI elements such as Tellurium and and Selenium for thermal recovery applications above 400 °C. GeSn alloys with a few percent of Sn content show a lattice thermal conductivity 200 times lower than Si [1], while having a good electrical conductivity, which may lead to a ZT larger than the SiGe material system, especially at operating temperatures close to those normally measured on working electronic chips (80 °C). For the development of GeSn-based on-chip thermoelectric elements, a thorough characterization of their thermal properties is required. In this work, we measure one of the main thermoelectric parameters, the thermal conductivity of the lattice, for a large set of epitaxial GeSn/Ge/Si heterostructures with Sn content of up to 14 at.%. We leverage an electrical characterization technique, the 3ω-method, and compare the results with micro-Raman thermometry. The obtained values of thermal conductivity are in the range 5 to 20 W/m*K, parametrized as a function of Sn content, are then used to numerically predict the relevant thermoelectric figure of merit ZT. To this end, a multi-valley- bipolar Boltzmann transport model is developed, whose accuracy has been validated by reference measurement against magnetic transport measurements. The resulting values of ZT up to 0. 4, and power factor of up to 8 mW/m*K^2 for both p- and n-type GeSn in the temperature range of 0–200°C highlight the potential of GeSn as a CMOS-compatible thermal material for low-quality heat conversion, and body temperature energy harvesting for wearable electronics.

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Suppressing the thermal conductivity of type-I clathrates by mesostructuring

CT54

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Keywords: clathrates; thermal conductivity; size effects; mesowires; 3ω method

A popular route to achieving a high thermoelectric conversion efficiency is finding materials with low phonon thermal conductivities. Type-I clathrates are particularly interesting in this regard, due to their extremely low phonon thermal conductivities caused by a hybridization of the acoustic phonon modes with the low-energy rattling modes of the encapsulated guest atoms [1]. This hybridization effectively cuts off the high-frequency phonons and tilts the balance of phonons relevant for thermal transport to low-frequency, i.e., long-wavelength, ones, making type-I clathrates uniquely suited for mesostructuring approaches aimed at lowering the thermal conductivity even further. We demonstrate this with our study on $La_{1.2}Ba_{6.8}Au_{5.8}Si_{38.8}\square_{1.4}$, where we investigate single crystalline mesowires with diameters ranging from 630 to 1260 nm. We have implemented a self-heating 3ω method and measured the electrical resistivity and thermal conductivity at temperatures between 80 and 300 K. At high temperatures the influence of defects on the thermal transport is negligible, and the observed strong size effect supports the hypothesis of enhanced boundary scattering of the long-wavelength phonons [2]. Seeing that the thermal transport in type-I clathrates is defined by the Einstein temperature of the lowest-lying rattling mode, we furthermore plan to compare the material to other type-I clathrates with different Einstein temperatures and analyze their influence on the magnitude of the size effect.

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CT55

3High-performance *n*-type silicide thermoelectrics developed by recycled Si kerf

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Keywords: *n*-type silicides, circular economy, recyclable Si kerf, mechanical alloying, material characterization

In an effort to establish a circular economy and provide a cost-effective solution for the manufacturing of high-performance Thermoelectric Generators (TEGs), *n*-type silicides are currently developed by recycled Si-kerf from photovoltaic manufacturing and by using for the first time Mechanichal Alloying (MA) which is an energy-efficient and straightforward method making scaling up the material production from g- to kg-scale possible. Two types of Si kerf have been used for the synthesis of Mg_2Si-based materials. Electron doping has been applied through appropriate Bi substitution to enhance the electrical transport properties and improve their thermoelectric (TE) performance, since this strategy has shown quite promising results in the past. Therefore, in order to exploit the recyclable Si, Si-rich phases based on the formula Bi-doped $Mg_{2.2}Si_xSn_{1-x}$, ($0.6 \leq x \leq 1.0$) have been synthesized by MA, as a suitable method to avoid the oxidation of reactants and the volatilization of Mg, reducing consequently the possibility of impurities formation in the final products. Sintering by hot-pressing followed at appropriate temperatures in order to produce pellets with high density. The structural characterization was carried out using X-ray diffraction and the crystal structure of final phases was confirmed through the Rietveld method. Structural changes in lattice parameters and unit cell were determined as a function of Si content. SEM and EDS analysis were also carried out to investigate the possibility of secondary phases and to identify the elemental composition of the materials. TE measurements were carried out, providing promising TE properties in all cases of Si kerf. The use of Si-kerfs, instead of pure Si, for the production of high-performance silicide thermoelectrics is of great importance for the adoption of circularity in economy and materials re-usage for the development of sustainable energy technologies.

Acknowledgments

This work is part of ICARUS project funded by Horizon 2020 research and innovation programme under grant agreement No 958365. ICARUS project aims to process and refine secondary raw materials from silicon PV manufacturing.

A Heusler-based transverse thermoelectric generator processed by co-sintering

CT56

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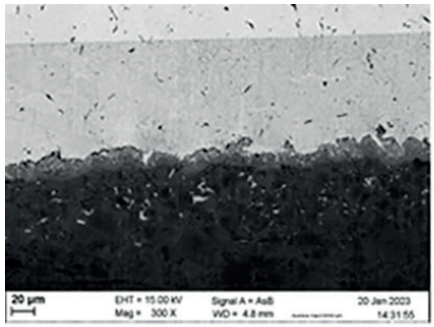
Keywords: Co-sintering, transverse TEG, Heusler, contact resistance, TEG assembly

Nowadays, the Heusler compound is well known as a promising thermoelectric material for near room temperature applications. Indeed, it presents some advantages such as the abundance of its constitutive elements, its low cost, and its good thermal stability. This material is therefore well-suited for large-scale applications. However, the process steps required to manufacture efficient integrated thermoelectric generators are numerous and it is economically intersting to reduce their number. In this context, metallization of Fe_2VAl obtained by co-sintering could ease the assembly process and bring opportunities to enlarge the scope of assembly geometries including ready-to-use transverse thermoelectric generators.

In this study, Cu and were co-sintered together by hot-pressing. The characterization of the interface between the materials revealed that Al tends to diffuse in Cu, creating a depletion in . This interface was electrically characterized with a home-made device and was found to have a contact resistivity significantly lower compared to the resistivity of .

A simple transverse thermoelectric generator was built. This type of module artificially generates an electric field perpendicular to the heat flux by tilting a stack of layers of one thermoelectric material and a good conductor. This module was fully characterized using a custom-build setup. Its performances were consistent with estimations made with finite element calculations of an ideal case. It demonstrates the effectiveness of co-sintering as an assembly technique for TEGs.

This study also enabled to show the trade-off behaviour between power factor and figure of merit in transverse TEG. Indeed, the power factor of the module was 50% higher than the one of the bulk thermoelectric materials while the ZT was 35% lower.



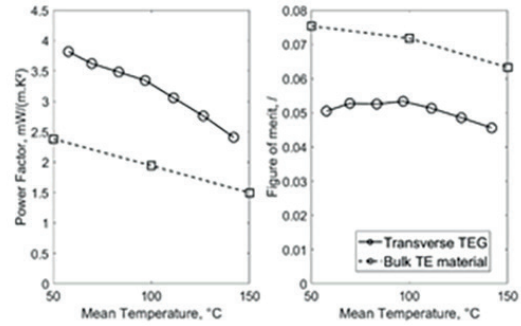


Figure 1: SEM image of the interface of a co-sintered part with Cu (on top) and Fe_2VAl (below)
Figure 2: Power factor and Figure of merit measurement of a 3-layers transverse TEG.

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CT57

Development and experimental validation of a computational model for geothermal thermoelectric generators

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Keywords: geothermal energy, thermoelectric generator, computational model, heat pipe, experimental

In the current climate and energy context, it is important to develop technologies that permit increase the use of renewable sources such as geothermal energy. Enhancing it is particularly important in some places, due to its availability and the enormous dependence on fossil fuels, as is the case of the Canary Islands. This work proposes the use of thermoelectric generators with heat exchangers working by phase change to harness the shallow geothermal anomalies on the island of Lanzarote, since the use of conventional geothermal power plants would not be possible because they would damage the protected environment. The proposed generators operate without moving parts, so they do not require maintenance nor auxiliary consumption, and produce a minimal environmental impact, are noiseless and the use of water as working fluid makes them completely harmless.

They were successfully installed in Timanfaya National Park with gases reaching 170 °C in the medium temperature zone and 465 °C in the high temperature one. Both generators have been working for more than 24 months in perfect conditions and each is generating more than 280 kWh per year [1,2]. Once demonstrated the viability of this technology, a computational model was developed with the aim to permit the design of a higher-scale installation. The model, based on the finite differences method, was successfully validated thanks to the experimental results, with relative errors of ±10% in terms of power and errors between 1.6% and 0.5% in the annual energy generation.

This research demonstrates not only the viability of this technology to generate clean energy in an area with geothermal anomalies, with very favourable results in terms of energy generation, but also the great potential for transforming the geothermal energy of Lanzarote into renewable electricity. Therefore, future installations would be adequately designed thanks to the developed computational model.

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High-efficiency printed radial thermoelectric generators utilizing photonic curing of p- and n-type inorganic chalcogenides-based inks

CT58

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Keywords: printed electronics, inorganic, photonic curing, screen-printing, shape-versatile, functional device

Printed thermoelectric generators (TEGs) are of particular interest due to their potential in terms of low cost and easy integration into standard heat exchanger systems. However, the most considerable drawback of printed TEGs is their low thermoelectric (TE) figure-of-merit (ZT), which is usually several orders of magnitude smaller than that of bulk TE materials. In the past, we reported an effective strategy to fabricate high-efficiency printed inorganic chalcogenide-based TE materials (p-type $ZT_{max} \approx 1.4$ and n-type $ZT_{max} \approx 0.7$) by utilizing highly conductive β-Cu_2Se as an interconnecting phase [1]. We, therefore, use photonic curing as an efficient and fast sintering process for the inorganic thermoelectric films [2]. Here, we present a functional, fully screen-printed, and photonically cured radial/disc TEG based on n- and p-type chalcogenide-based TE materials fabricated on a 25 µm polyimide (KAPTON) substrate for operation temperatures exceeding 200 °C. The disc device delivered 305.08 µW of power which relates to a power density of 107.9 W/m² at a hot side temperature of 220 °C when exposed to free convection of ambient air at 24 °C.

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CT59

New architectures for heat sink less organic and inorganic thin film thermoelectric (TE) devices inspired by Kirigami

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Keywords: thermoelectric device, heat sink, carbon nanotube veil, bismuth telluride, kirigami, honeycomb structure

Thermoelectric (TE) technology[1] presents a unique opportunity to convert waste heat directly into electricity, offering a promising solution to address energy harvesting and sustainability challenges. However, conventional TE devices with π-type structures always need a heat sink to thermally link to the air during operation which remains a significant limitation for their practical applications.

Herein, we report a new configuration of a TE device that has a built-in heat sink for the first time. Furthermore, the device modified with shape-memory polymer films can be self-folded into a hexagonal structure via heating above its glass transition temperature. We demonstrate the feasibility of our design through experimental characterization and modelling. The device with built-in fins exhibits superior thermoelectric performance with both organic (carbon nanotube veils) and inorganic (bismuth telluride, BiTe) TE materials. The maximum power output of the BiTe-based device can reach 180 μW, which is 4.4 times higher than that of the carbon-based device (41 μW) when the temperature difference is 43 K and airflow is 1.5 m s^{-1}. BiTe-based devices show better TE performance but less stability compared to carbon-based devices. Moreover, carbon-based devices can be self-folded via external temperature stimulus and keep resistance no change (95 Ω) while BiTe-based devices cannot.

This work provides a path to optimize the thermoelectric performance of TE devices by designing rational structures. This approach has the potential to reduce the cost, mass, and volume of TE devices, making them more attractive for a wide range of applications, such as waste heat recovery, energy harvesting, and thermal management.

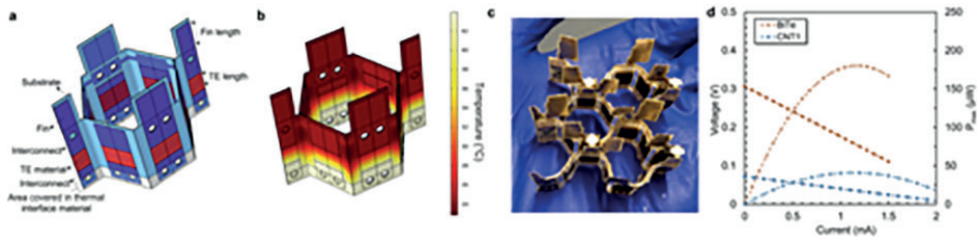

Figure 1: Design and performance of TE devices.

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Characterisation and optimisation of passive heat exchangers for enhancing the operation of thermoelectric generators under extreme environmental conditions

CT60

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Keywords: thermoelectric generator, efficiency, thermal resistance, phase change, heat pipe

Nowadays 10% of the world's population lives within 100 km radius of an active volcano. These geological formations are often remote, inaccessible, and off grid, making the installation of power supply and communication systems a major challenge. Consequently, only 30% of active volcanoes are equipped with the necessary instrumentation systems to measure their activity. These systems are usually powered by photovoltaic panels and batteries. Nevertheless, in regions with extreme meteorological conditions, such as Antarctica, it is not viable to use such equipment to monitor volcanic activity in real time.

The present work proposes the use of thermoelectric generators that harness the geothermal energy emanating from the fumaroles to generate electrical power to run the measuring equipment. The generator is mainly composed of thermoelectric modules and heat exchangers based on phase change. The energy conversion process is direct, and the heat exchangers operate by gravity, requiring no moving parts, which makes the system highly robust and reliable. The visual impact of the generator is minimal and stands out by its scalability. Furthermore, it is powered by a renewable and stable energy source, independent of meteorological conditions.

Despite its remarkable advantages, the major drawback of this technology is its low efficiency, which could be increased either by improving the efficiency of the thermoelectric modules through their materials or by increasing the temperature difference between the module faces by enhancing the heat exchangers' performance. In fact, a 10% reduction in thermal resistance leads to an 8% increase in electricity generation [1].

Consequently, this work focuses on the design and optimisation of cold side heat exchangers with the aim of improving the performance of the thermoelectric generator under extreme climatic conditions. It has been demonstrated that the most suitable heat exchangers are those based on phase change, as they are able to transfer large amounts of heat with minimal temperature drop [2]. Therefore, finned heat pipes have been chosen to dissipate the heat to the environment. These devices have been characterised by calculating their thermal resistance experimentally and computationally. Additionally, the entire thermoelectric generator has been modelled to predict its behaviour under different weather conditions, enabling the selection of the most suitable heat exchanger dimensions based on the prevailing circumstances.

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CT61

Enhanced electronic transport and low thermal conductivity in eco-friendly $Cu_2CoSnS_{4-x}Se_x$ diamond-like materials

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Keywords: crystal structure, carrier mobility, lattice thermal conductivity, thermoelectric figure of merit, ultrasonic properties

Lightweight diamond-like structure (DLS) materials are excellent candidates for thermoelectric (TE) applications due to their low costs, eco-friendly nature, and property stability. The main obstacles restricting the energy-conversion performance by the lightweight DLS materials are high lattice thermal conductivity and relatively low carrier mobility. Investigating the anion substitution effect on the structural, microstructural, electronic, and thermal properties of the $Cu_2CoSnS_{4-x}Se_x$, we show that the simultaneous enhancement of the crystal symmetry and bonding inhomogeneity engineering are the effective approaches to enhance the TE performance in lightweight DLS materials. Particularly, the increase of x in $Cu_2CoSnS_{4-x}Se_x$ makes favorable the DLS structure with the ideal tetrahedral bond angles of 109.5° leading to better crystal symmetry and higher carrier mobility in samples with higher selenium content. In turn, the phonon transport in the investigated DLS materials is strongly disturbed due to the bonding inhomogeneity between anions and three sorts of cations inducing large lattice anharmonicity. The increase of Se content in $Cu_2CoSnS_{4-x}Se_x$ only intensified this effect resulting in lower κ_L for Se-rich samples. As a result of the enhanced power factor $S^2\rho^{-1}$ and low thermal conductivity κ_L, the dimensionless thermoelectric figure of merit ZT achieves a high value of 0.75 for $Cu_2CoSnSe_4$ DLS material. This work demonstrates that crystal symmetry and bonding inhomogeneity play an important role in the transport properties of DLS materials and provides a path for the development of new perspective materials for TE energy conversion.

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Thermoelectric properties of $Cu_{12-x}Ni_xSb_4S_{13-y}Se_y$ tetrahedrite

CT62

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Keywords: thermoelectric materials; power factor; tetrahedrite; solid-state method; co-doping

The biggest obstacle to the wide application of thermoelectrics is the lack of cheap and sustainable materials with at least the same level of performance as commercial materials (e.g., Bi_2Te_3, PbTe), which achieve a zT close to or above unity.[1] Sulfide-based thermoelectric materials are being extensively studied for lower costs and toxicities. Among them, tetrahedrite ($Cu_{12}Sb_4S_{13}$) has been gaining popularity as a potential thermoelectric material, as it is a worldwide available mineral with low thermal conductivity due to its highly complex crystalline structure. Therefore, several studies were carried out to improve its thermoelectric performance, which has been achieved through the chemical replacement of small amounts of Cu, Sb and S by other elements. However, only few studies were made on the simultaneous doping of two or more elements. [2] Here, we present experimental and simulated results of the effect of doping with both Ni and Se on the thermoelectric properties of tetrahedrite. [3,4]

$Cu_{12-x}Ni_xSb_4S_{13-y}Se_y$ samples were successfully produced using the solid-state method, being almost monophasic after casting and after annealing, but copper/nickel sulfides and chalcostibite ($CuSbS_2$) are occasionally observed. SEM-EDS, powder X-ray and Raman spectroscopy revealed that both Ni and Se integrate the tetrahedrite matrix, which has a composition is close to the nominal one.

Computational (using Wien2K and BoltzTrap software's) and experimental results indicate the existence of an optimum composition for maximum performance, at around $Cu_{11.5}Ni_{0.5}Sb_4S_{12.5}Se_{0.5}$. Simulations placed the figure of merit as 0.30 at 300K, and experimental results yield a power factor of 1280 $\mu W/m.K^2$, which, after estimating thermal conductivity with the Wiedemann-Franz law, resulted in a figure of merit of ~0.32 at 300K, in good agreement with calculations. Pisarenko plots roughly point to the downward trend of Seebeck as Ni content decreases, but no clear change of Seebeck is observed for Se doping, as expected from previous results and DOS calculations. However, weighted mobility results show that, albeit changing several orders of magnitude, no constant trend with any doping exist. This behaviour most probably results from the negative impact of secondary phases and structural defects, indicating that there is still room for further optimization of the current materials thermoelectric properties.

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CT63

High-performance thermoelectric properties of Cu_2Se fabricated via cold sintering process

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Keywords: thermoelectric; Cu_2Se; cold sintering process; ZT; fabrication;

The phonon-liquid electron-crystal has become a fascinating concept for thermoelectric material in recent years. The Cu_2Se is a potential material for this concept. Although it exhibits excellent thermoelectric performance due to great electron transport properties, the thermal conductivity is still relatively large due to grain growth from high-temperature fabrication process. Herein, a cold sintering process (CSP) was employed to fabricate Cu_2Se bulk materials. By selecting a thiol-amine solution as a liquid sintering aid, 89% of bulk density can be achieved at a sintering temperature of only 473 K. The Cu_2Se + 3wt% of thiol-amine solution exhibits a high ZT value of 2.13 at 800 K, higher than that the counterpart sample prepared using a hot-pressing process (ZT = 0.65). The outstanding performance is ascribed to the remaining nonmetallic sulfer in the matrix from thermal decomposed thiol-amine solution leading to the high carrier concentration. Furthermore, the liquid phase and low-temperature sintering suppresses grain growth, which significantly enhances the phonon scattering resulting in ultralow lattice thermal conductivity. The advantage of CSP can serve not only in the fabrication of Cu_2Se but can be applied to other high-performance thermoelectric materials.

Acknowledgments

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Atomic and nanoscale order/disorder phenomena in thermoelectric copper-based sulfides

CT64

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Keywords: sulfides, sphalerite, thermoelectric, disorder, defects

Among the various possibilities offered by the periodic table, copper-rich sulfides represent a formidable source for the discovery of low cost and environmentally benign thermoelectric materials. Copper-rich sulfides form an important class where univalent copper is the dominant element, giving the possibility of creating hole carriers in the conductive "Cu–S" network for the generation of *p*-type thermoelectrics. During this presentation, recent advances in synthetic minerals and new sulphide compounds will be shown. Some peculiar structural features in connection with atomic and nanoscale order/disorder phenomena were carefully examined to establish rules and correlations between the crystal structures, nano-microstructures, electronic structures, vibrational and thermoelectric properties. [1-3]

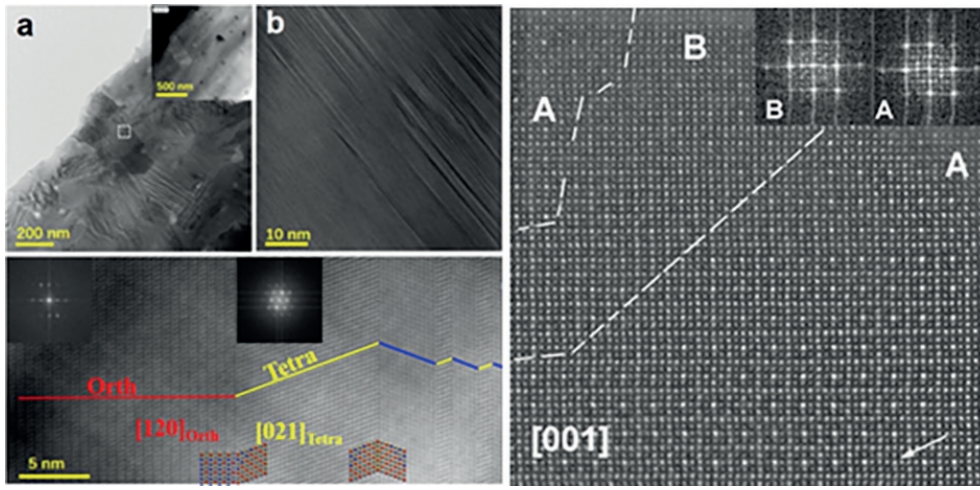

Figure 1: Left) interconnected stannite/enargite nanodomains in Cu_2MnGeS_4 [1] Right) Ordered/disordered clusters in colusite $Cu_{26}V_2Sn_6S_{32}$ [3]

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CT65

Predicting phonon transport in thermoelectric $Sr_2Si_{1-x}Ge_x$ alloys from a highly accurate machine learning interatomic potential

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Keywords: thermoelectric; phonon transport; $Sr_2Si_{1-x}Ge_x$ alloys; first-principles calculations; machine learning

The II2IV family of materials, such as Mg_2Si, Mg_2Sn, Sr_2Si, and Sr_2Ge, among others, are highly regarded as promising high-performance thermoelectric materials. In a previous study [1], the maximum figure of merit ZT of Sr_2Si and Sr_2Ge was calculated to be 1.15 and 1.44 at 900 K using first-principles calculations. To enhance thermoelectric properties, doping elements are commonly used to reduce the lattice thermal conductivity and improve Seebeck coefficient. However, finding an appropriate amount of doped elements using experimental or first-principles calculations can be challenged due to high costs. Classical molecular dynamics (MD) simulations can predict phonon transport in different compositions, but empirical interatomic potentials limit its accuracy in lattice thermal conductivity. Here, we introduce a highly accurate deep potential (DP) model of doped thermoelectric materials $Sr_2Si_{1-x}Ge_x$ alloys, created using a machine learning approach based on first-principles density functional theory (DFT) data. Our DP model achieves DFT-level accuracy, facilitating efficient MD simulations and accurate property predictions. Using the DP model, we investigate suitable compositions for $Sr_2Si_{1-x}Ge_x$ alloys, aiming to find high-performance thermoelectric materials while determining the contribution of phonon modes to phonon transport.

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Designing phonons for thermoelectric metamaterials with physics and machine learning optimization

CT66

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Keywords: thermoelectric energy conversion, phonon engineering, thermal conduction, machine learning, metamaterials

Minimizing phonon transmission across nanostructures is necessary for blocking parasitic heat conduction that limits the efficiency of heat management and energy conversion at the nanoscale. It can be achieved by designing the modulation profile of width-modulated nano-waveguides [1,2]. Aperiodic modulation profiles have been theoretically predicted to limit phonon transmission and heat conduction much more efficiently than periodic ones [3,4].

Optimizing the modulation profile is challenging due to the big number of possible configurations. We demonstrate efficient optimization using physics and machine learning. Bayesian optimization is shown to efficiently identify the optimal modulated nano-waveguide that minimizes phonon thermal transmission. The optimization has been validated by comparison with calculations. The identified optimal configuration is aperiodic, in agreement with physics predictions. The optimization has been tested for constraints, thermal broadening, material choice and modulation geometry.

Our work supports that machine learning is a valuable design tool of geometry-modulated nanostructures which are promising for efficient heat and energy applications.

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CT67

Comprehensive fitting tool to analyse temperature-dependent transport data: Introduction and examples of usage

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Keywords: thermoelectric transport, transport theory, transport modelling, temperature dependence, fitting model, open-source software, band gap opening, DFT calculations

Linking the fundamental physics of band structure and scattering theory with macroscopic features, such as measured temperature dependencies of thermoelectric transport, is indispensable for a thorough understanding of thermoelectric phenomena and ensures more targeted and efficient experimental research. Nonetheless, many experimental results in our field are only interpreted qualitatively, leaving us with a superficial understanding of the collected data. In this talk, we will present a comprehensive fitting tool to analyse temperature-dependent thermoelectric properties, particularly the Seebeck coefficient, to model the effective electronic structure. To make the fitting process widely accessible and effortless, we will introduce our easy-to-use, open-source software, which is freely available online, and explain it briefly. The interactive user window, showing the active fit as well effective band structure in real time allows for the user to predict doping-related changes by modifying the respective parameters, which returns the predicted transport properties. This will help to reach a better understanding of the interplay of band theory with the transport properties and has the potential to accelerate thermoelectric research.

To demonstrate the potency of the fitting tool, we will examine the effect of Ti substitution in $Fe_2V_{1.2-x}Ti_xAl_{0.8}$ for numerous samples by analysing the temperature-dependent properties and comparing the results with DFT calculations and supplemental measurement data. Lastly, we will present the case of highly off-stoichiometric full-Heusler systems [1], where the thorough analysis of temperature-dependent thermopower data using our fitting model has led to the discovery of an unexpected band gap opening, which now has been confirmed and understood by means of electron-bonding theory and DFT calculations.

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Best thermoelectric efficiency exploration by solving thermoelectric integral equation over material big data of Starrydata2

CT68

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Keywords: thermoelectric, best efficiency, integral equation, big data, Starrydata2

In this presentation, we report the best thermoelectric efficiency for thermoelectric power generation devices [1]. We develop a thermoelectric integral equation framework to calculate thermoelectric efficiency with temperature dependent properties within the long-leg approximation [2], which is fast and exact one-dimensional temperature-solving method. By combining the thermoelectric material database of Starrydata2 [3] and the integral framework, 100 million device efficiencies are calculated over approximately 13,000 published materials data (from roughly 3,000 publications) under various device geometries, interface qualities, thermal boundary conditions, and electrical currents. As a result, best thermoelectric efficiency is explored for a given hot side temperature range when cold side is 300 K.

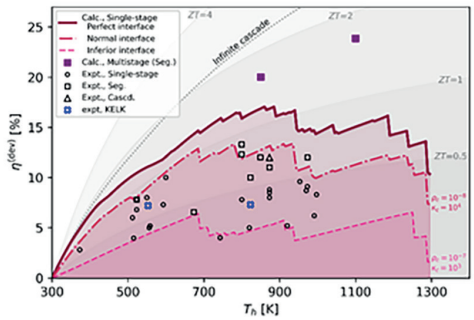

Fig. 1:
Best thermoelectric efficiency of ever-explored materials, adapted from ref [1]. Licensed under CC BY 4.0.

Our results show that the theoretical best efficiency is 17.1% for a single-stage P-N leg-pair device, surpassing 10% and 13.3% experimental records for single- and multiple-stage devices, respectively. It indicates that optimal material selection and advanced multistage structures with small interfacial/contact resistance may enhance thermoelectric efficiency significantly. From calculations we find that a very high efficiency more than 24% is achievable in a multistage device structure.

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Protective covers for $Cu_{10.5}Ni_{1.5}Sb_4S_{13}$ tetrahedrites

CT69

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Keywords: protective coatings, tetrahedrites, oxidation, degradation mechanisms, thermoelectric devices.

With the increase in global energy demand and the ambitious targets for greenhouse gas emissions cuts set by climate policy, searching for alternative and renewable energy sources is fundamental. In this context, thermoelectric (TE) materials play a vital role as alternative solutions with great potential for energy recovering, being capable of converting heat into electricity and vice-versa, using the Seebeck and Peltier effects, respectively. Due to their versatility and modularity, TE materials and devices can be excellent tools to increase the sustainability of energy-intense processes by maximizing energy usage (reducing waste) and reducing the carbon footprint of industries [1].

Despite the great potential for energy harvesting, most of the TE devices are based on toxic and rare elements such as Pb, Bi, and Te. This has made them expensive and only suitable for niche markets due to their weak chain of supply and reduced efficiencies (<12%). To overcome these challenges, new TE materials, such as tetrahedrites (a copper antimony sulfosalt), are being studied and developed. These materials are abundant, cheap, and therefore very suitable for large scale applications. They have a $Cu_{12-x}M_xSb_4S_{13}$ general formula (M = Mn, Ni, etc., and x = 0 – 2), and crystallize in a complex cubic cell ($\bar{I}43m$) [1]. Despite presenting low toxicity and good thermoelectric properties (zT ~1 at 600 K), tetrahedrites easily oxidize and degrade when exposed to air at medium temperatures, which consequently creates the need to protect or cover them to maintain their TE properties during operation.

In the present study, different coatings were deposited on Nickel-doped tetrahedrites. Then, the covered tetrahedrite legs were aged at 573 K for 300 h (~14 days) under air atmosphere. At the same time, coated and uncoated materials were submitted to identical aging conditions and compared to check for traces of oxidation and degradation. The effectiveness of these coatings was verified, with the materials being analysed by Xray Diffraction and Scanning Electron Microscopy. The identification of effective protective coatings and of the main degradation/oxidation mechanisms is expected to allow a future development of a novel generation of thermoelectric generators based on these materials. Such devices are anticipated to be low cost and able to work for long periods, allowing heat recovery applications to become more easily widespread.

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Interstitials in half-heusler compounds

CT70

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Keywords: at least five keywords required

The density functional theory (DFT) calculations and experiments have confirmed that in the *ABC*-type half-Heusler compounds, the 3*d* elements occupying the *B* position are natural over-stoichiometry. Such over-stoichiometry (interstitial defect) substantially impacts the crystal structure and the microstructure, providing a new starting point to understand and further manipulate the thermoelectric (TE) properties in HH compounds. Experimental results show the amount of interstitial defect, phase constitution, and microstructure can be modified by adjusting the starting composition. The interstitial defects can modify the position of the Fermi level inside the band gap and the value of the band gap, thus significantly influencing the electronic transport properties of HH compounds. Besides, interstitial defects enhance the phonon scattering, significantly suppressing thermal conductivity. This talk will take ZrNiSn as an example to show that interstitials formed in the arc-melted samples. The formation mechanism of the interstitial defects and the influence of interstitials on the transport properties of ZrNiSn will be discussed.

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CT71

Enhancing the thermoelectric performance of n-type $Mg_3(Sb,Bi)_2$ by high-temperature sintering and metallic inclusions

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Keywords: Mg_3Sb_2, thermoelectric, defect engineering, metallic inclusions, energy conversion

$Mg_3(Sb,Bi)_2$ is a promising near-room-temperature thermoelectric (TE) compound with earth-abundant elements, whilst further optimization of its TE properties relies on complex defect tuning and exceptional microstructural control. Herein, significant enhancement in both room-temperature and high-temperature zT of $Mg_3(Sb, Bi)_2$ was achieved through high-temperature sintering in combination with metallic inclusions addition. Although Mg is more volatile than Bi, the volatilization of Bi was found to be facilitated at higher sintering temperatures. Positron annihilation spectrometry and C_s-corrected scanning transmission electron microscopy analyses indicated that the V_{Mg} tended to coalesce and form vacancy clusters due to the formation of V_{Bi}. The defects generated by Bi deficiency effectively weakened the scattering effect of intrinsic V_{Mg} on electrons and enhanced the phonon scattering. Based on this optimized process, the nano-sized metallic inclusions were further introduced at the grain boundaries, which led to a strong energy filtering effect, thereby significantly enhancing the electrical conductivity with negligible changes to Seebeck coefficients. An exceptionally high room-temperature power factor >30 μW cm^{-1} K^{-2} was finally obtained. The increased zT values within the entire temperature range resulted in a high average zT and a conversion efficiency >10% under ΔT = 525 K for the fabricated TE device.

Acknowledgments

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Dilemma and opportunities: A review on industrial-scale applications of thermoelectric power generation

CT72

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Keywords: flexible thermoelectric generators (Flex-TEGs), thermal energy harvesting, industrial-scale applications, internet of things, return of investment, industry 4.0, green transition, life cycle assessment (LCA)

Thermoelectric power generation has great potentials in the transition towards industry 4.0 and Net Zero. However, there are lack of awareness on the market and profitable applications in large scales. The most successful use case is still the ones in the deep space (RTGs), which is known for decades but is not a scalable business. Other niche applications, such as the ones found in military and hobby markets, don't provide a strong enough demands to accelerate the commercialization of the R&D efforts.

In this talk, we are going to go through some of the key obstacles in implementing TEGs in industrial applications. By stressing the dilemma, we hope to draw more attention to the real working conditions in industry and the practical criteria for implementing TEGs in larger scale. And we want to make an appeal in putting more resources in exploiting suitable applications for the already available technologies, in parallel with developing new ones.

Acknowledgments

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CT73

Role of lone pair rotation in the ultralow thermal conductivity of aikinite

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Keywords: thermal conductivity, sulfides, minerals, phonons, inelastic neutron scattering, molecular dynamics

Minerals in the aikinite-bismuthinite series, $Cu_{1-x}\square_xPb_{1-x}Bi_{1+x}S_3$ ($0 \leq x \leq 1$, where $\square$ represents a vacancy), have been recently reported as promising *n*-type semiconductors with exceptionally low lattice thermal conductivities ($\kappa \approx 0.5$ W m^{-1} K^{-1} at room temperature) [1]. Here, we present a detailed investigation of the structure and vibrational properties of the aikinite end member, $CuPbBiS_3$ ($x = 0$), in order to establish the origin of its ultralow thermal conductivity. Rietveld refinements using neutron diffraction data collected on aikinite indicate that the Cu^+, Pb^{2+} and Bi^{3+} cations are fully ordered in the crystal structure, and that the atomic displacement parameters for the Cu^+ and Pb^{2+} cations, which are separated at distances of ~ 3.3 Å, are significantly larger than those for Bi^{3+}. Despite its highly crystalline nature, the lattice thermal conductivity of $CuPbBiS_3$ is close to the calculated minimum for amorphous and disordered solids. Sound velocity measurements reveal that the phonon mean-free-path is approximately 5 Å. Inelastic neutron scattering data unveil the presence of an anharmonic optical phonon mode at approximately 30 cm^{-1}, attributed mainly to the vibrations of the Pb^{2+} cations, and with an estimated lifetime of only 0.4 ps. Analysis of *ab-initio* molecular dynamics simulations shows that the Pb^{2+} lone pairs are rotating and that these rotations influence the Cu^+ dynamics. Our work reveals that the ultralow thermal conductivity of aikinite arises from the coupling of rotating Pb^{2+} lone pairs with the vibrational motion of the Cu^+ cations.

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Acknowledgments

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Innovative synthesis methods to reach quaternary thioantimonate $Ag_4MnSb_2S_6$

CT74

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Keywords: polyol, hydrothermal, solvothermal, samsonite, quaternary sulfide

Samsonite ($Ag_4MnSb_2S_6$) is a mineral that can be naturally found in hydrothermal veins. Its complex crystal structure – it crystallizes in the monoclinic crystal system (space group: $P2_1/n$ with a = 10.3861 Å, b = 8.1108 Å, c = 6.6637 Å, and β = 92.639°) – together with the electron lone pair of Sb^{3+} atoms and the lack of research about it (never synthesized so far through lab conditions), make this phase highly promising for thermoelectric applications.[1] Indeed, authors have shown through the tetrahedrite phase, that the electron lone pair of Sb^{3+} may explain the ultralow thermal conductivity of $Cu_{12}Sb_4S_{13}$.[2]

The objective is to synthesize $Ag_4MnSb_2S_6$ through unconventional synthesis ways (**hydrothermal** synthesis and **polyol** synthesis process) to mimic the high pressure and temperature found in natural conditions. Then, structural, magnetic, and thermoelectric properties would be assessed.

As such, this presentation will focus on these innovative synthesis methods and compare their respective efficiency while considering their advantages and drawbacks. On one hand, hydrothermal synthesis allows **highly crystalline** compounds with **simple precursors and solvents** involved but isn't easily scalable. On the other hand, the polyol synthesis is **fast** and can **easily scale up,** but the crystallinity of the compound formed is rather poor, necessitating a crystal growth processing as a follow-up.

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CT75

Rare earth chalcogenides: a promising material for thermoelectric applications

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Keywords: thermoelectric, energy harvesting, *n*-type materials, rare earth chalcogenides, defect engineering

Thermoelectric materials have attracted considerable attention in recent years due to their ability to directly convert heat into electricity, which has significant potential for energy harvesting and waste heat recovery applications. Rare earth chalcogenides (RECh) have attracted significant attention for their potential use in thermoelectric applications due to their unique electronic and thermal properties. In this study, we have optimized the thermoelectric performance of RECh by introducing defects in the RECh system to manipulate the carrier concentrations. This enhanced the electrical conductivity and improve the power factor. In addition to this, we have introduced a secondary phase that acts as a carrier filter and/or band engineering agent, which could further enhance the thermoelectric performance by improving the Seebeck coefficient and reducing the lattice thermal conductivity. Here, we have considered a new RECh material as an example and introduced point defects and secondary phases. It is interesting to see that the introduction of point defects and secondary phases in RECh has shown promising results for improving their thermoelectric performance. Further research is needed to fully understand the underlying mechanisms and optimize the materials for practical applications in thermoelectric devices.

Thermoelectric studies of synthetic mineral Kutinaite $Cu_{14}Ag_6As_7$

CT76

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Keywords: kutinaite, synthetic mineral, metal, thermoelectric, and hole carriers

Exploration of new materials that might have promising transport properties could be very much beneficial for the advancement of the thermoelectric field. In this context, natural minerals can act as a fountain of vast variety of novel compounds that might be potential candidates for thermoelectric applications. Recent studies showed that the natural minerals of tetrahedrites ($Cu_{12-x}M_xSb_4S_{13}$) and tennantite ($Cu_{12-x}M_xAs_4S_{13}$); (M = Mn, Fe, Ni, and Zn) exhibit promising thermoelectric performance due to their intrinsic low lattice thermal conductivity [1]. There are several mineral based compounds with complex crystal structures, which have not fully exploited from the thermoelectric perspective.

Here in, we have prepared a synthetic mineral, Kutinaite, $Cu_{14}Ag_6As_7$, whose transport properties have not been explored yet. $Cu_{14}Ag_6As_7$ crystallizes in a cubic structure, space group *Pm*, with a = 11.7808 Å [2]. In the present work, we investigated in detail the thermoelectric properties of solid solution of $Cu_{14}Ag_6As_{7-x}Se_x$ compositions in the temperature range of 2–700 K. Using a combination of synchrotron X-ray diffraction, first principles calculations and transport properties measurements, we discuss the structure–thermoelectric properties relationships and clarify the interesting crystal chemistry in this system. In agreement with band structure calculations, $Cu_{14}Ag_6As_7$ is a p-type metal with a resistivity of 8.5×10^{-5} Ω cm and carrier concentration of 2.0×10^{21} carriers/cm^3 at 300 K. Short metal-metal bonding interactions lead to the observation of interesting low temperature magnetic and transport properties, which will be shown in detail during the presentation.

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CT78

Optimization of magnesium-based materials for near room temperature applications

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Keywords: magnesium, room-temperature, SPB, experimental, n-type, p-type

Although it is a highly promising technology, with great potential to contribute to the mitigation of the global energy crisis, thermoelectrics still need to be optimized to increase their efficiency. Furthermore, the lack of viable sustainable substitutes for established thermoelectric (TE) materials, particularly for near room temperature applications (which are primarily based on Bi_2Te_3), also hampers a wider use. In this sense, investigations on Mg-based constituents have been made employing $Mg_2Si_{1-x}Sn_x$ (x = 0.6, 0.7) and MgAgSb, as n- and p-type materials, respectively.

Single Parabolic Band modelling (SPB) was first used to simulate the n-type material properties and better understand the influence of the different intrinsic parameters, hence predicting the carrier concentrations for the best TE properties. Thus, to maximize zT ($zT_{max} = 0.96$ at 600K) or improve the conversion efficiency ($\eta_{\%} = 8.9$, with $\Delta T = 300K$), the optimum carrier concentration is identified as $n = 1.2*10^{26}$ m^{-3} for $Mg_2Si_{0.3}Sn_{0.7}$, assuming $T_c = 285$ K and variable T_h.

Regarding the experimental part, two different production methods were used, a ball-milling and direct current sintering (DSP), and an original fast-production by high-frequency induction melting followed by hot-pressing. It should be noted that the latest was never used for MgAgSb.

Structural and microstructural characterizations were made employing XRD and SEM/EDS. The TE properties (thermal conductivity, electrical conductivity and Seebeck coefficient) were also measured for all the samples. In general, it was observed that method 2 produces more compacted samples and is less prone to form secondary phases.

Hitherto, preliminary TE data from undoped $Mg_{1.1}Ag_{0.97}Sb_{0.99}$ and $Mg_{2.1}Si_{0.3}Sn_{0.7}$ was obtained. P-type $Mg_{1.1}Ag_{0.97}Sb_{0.99}$ achieved a zT higher than 0.5 for both methods, being able to reach 0.9 with ball-mill route, whereas n-type $Mg_{2.1}Si_{0.3}Sn_{0.7}$ obtained lower values, below 0.7 for both. Further improvement of the n-type could be achieved by doping with Sb, yielding a zT of 1 at 640 K.

It is possible to conclude that the induction melting works quite well, achieving better results for the n-type, but method 2 looks more suitable for the p-type.

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On the stability of thermoelectric materials: investigating Mg diffusion in $Mg_2(Si,Sn)$ at room temperature

CT79

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Keywords: $Mg_2Si_{1-x}Sn_x$, TE properties, Mg diffusion, microstructure analysis, material stability

Due to their ability to convert (waste) heat into useful electrical energy through the Seebeck effect, thermoelectric generators (TEG) are highly attractive in fields like automotive or aerospace. Magnesium silicide-stannide $Mg_2(Si,Sn)$ solid solutions are part of a very interesting family of TE materials due to their low density, as well as cheap, abundant and nontoxic elements. While $Mg_2(Si, Sn)$ TE properties have been optimized and TEGs have been successfully fabricated, previous investigations have also shown limited stability against oxidation in air at high temperature and against Mg loss in inert atmosphere, identifying material stability as one of the major challenges to be overcome for large scale implementation. By integral measurement of the thermoelectric properties we furthermore found that under certain conditions the material also undergoes changes at room temperature (RT).

Our stability investigations focus on Mg-poor p-type $Mg_2Si_{0.3}Sn_{0.7}$ and Mg-rich n-type $Mg_{2+\delta}Si_{0.3}Sn_{0.7}$ due to their high TE performance and previous implementation in prototype devices. Samples were obtained by a melting route, resulting in the targeted main phase and a small amount (<3 % vol) of Si-rich $Mg_2Si_{1-x}Sn_x$ homogeneously distributed throughout the sample. While those Si-rich islands apparently don't affect the TE properties, they allow to investigate the relevance of the composition for the material stability on a single sample. Samples were stored in air at RT to investigate the impact of the storage condition over time.

By integral measurement of the TE properties, we show that Mg-rich n-type samples degrade over time (decrease of charge carrier concentration) while Mg-poor p-type samples remain stable, due to Mg-rich/poor content variation between both materials. Scanning electron microscopy (SEM) combined with energy dispersive X-ray spectroscopy (EDX) were used to analyse the microstructural changes at the surface of the samples and reveal the formation of magnesium oxide on the main phase of the sample only, while Si-rich regions remain unchanged. This provides evidence that the surface degradation is clearly selective to the Si:Sn ratio. Lastly, carrier concentration profiling by local scanning of the Seebeck coefficient also shows an increasing inhomogeneity of the samples with increasing age on a meso scale.

This work not only reports the effect of storing in air at RT on the TE properties and microstructure but also indicates that Mg in Mg-rich samples can be removed from the material by the following multi-step mechanism: (i) Mg sublimation ($Mg_{2+\delta}X \rightarrow Mg_2X + \delta$ Mg), (ii) Mg depletion at the surface from Mg-rich phases and (iii) Mg oxidation at the surface ($Mg + O_2 \rightarrow MgO$). Such degradation could be stopped by storing the samples in inert atmosphere.

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CT80

Tuning micro- and nanostructures by decomposition of $PbAgSbTe_3$ and the influence on thermoelectric properties

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Keywords: LAST; metastable phases; microstructure; decomposition; thermal conductivity

The system Pb/Ag/Sb/Te (LAST) is well known for thermoelectric materials with remarkable performance. For instance, $Pb_{18}AgSbTe_{20}$ reaches a record-high zT-value of 2.2 at 527 °C. This is due to very low lattice thermal conductivity, which has been attributed to significantly enhanced phonon scattering as a consequence of pronounced micro- or nanostructures. [1-3] The size and shape of precipitates embedded in a PbTe matrix can be adjusted by varying the synthesis conditions and enable a certain tuning of thermal conductivity.

While samples with the nominal composition $PbAgSbTe_3$ do not reach very high zT values, they are ideal model systems to study the influence of microstructure on properties. The 1:1 molar ratio of PbTe and $AgSbTe_2$ (with a small degree of mutual doping) in the thermodynamic equilibrium ensures microstructures that are not dominated by a main phase. Moreover, homogenous $PbAgSbTe_3$ is stable at high temperatures and can obtained as a metastable phase by quenching from 470 °C. Compact pellets obtained in a hotpress at 70 °C can be gradually decomposed by annealing e.g. at 250 °C for several minutes to a few hours. Both $PbAgSbTe_3$ and the products PbTe and $AgSbTe_2$ feature rocksalt-type structures (space group *Fmm*) that can be easily quantified from powder X-ray diffraction (PXRD) data due to their different lattice parameters. These decomposed samples exhibit laminar structures that sharpen and coarsen upon prolonged annealing. This has a significant impact on zT values. Tracking the decomposition by temperature-dependent PXRD with synchrotron radiation revealed the optimal conditions for controlled decomposition. The features and size regimes of the microstructures were analysed by SEM and Rietveld refinements with fundamental parameters that also included anisotropic size effects. It turned out that the electrical conductivity and the thermal conductivity can be varied and fine-tuned while the Seebeck coefficient remains nearly constant. This way we could the zT value at 50 °C could from 0.19 for macroscopic two-phase material to 0.28 for partially decomposed, nanostructured material.

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Enhancing low temperature thermoelectric properties of n-type $Mg_{3.2-x}(Sb_{0.3}Bi_{0.7})_{1.996}Te_{0.004}$ through Nb addition

CT81

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Keywords: thermoelectric, doping, low temperature, cooling, high zT

Thermoelectric materials became more attractive with the increasing demand on sustainable energy sources. While Seebeck effect is outstanding because of the conversion of waste heat to electricity, Peltier effect is also useful for cooling purposes because of their reliability, noise-free and emission-free characteristics. Mg_3Sb_2–Mg_3Bi_2 alloys display high thermoelectric efficiencies related to their layered crystal structure with inherently low thermal conductivity and tunable electronic transport properties. While near room temperature cooling applications dominated by Bi-Te alloys, researchers have showed that $Mg_{3.2-x}(Sb_{0.3}Bi_{0.7})_{1.996}Te_y$ (y = 0.001–0.004) is a significant candidate as an alternative to Bi-Te alloys for low temperature thermoelectric devices with high zT values. In this study, electrical and thermal transport properties of n-type $Mg_{3.2-x}Nb_x(Sb_{0.3}Bi_{0.7})_{1.996}Te_{0.004}$ was investigated through Nb addition with reference to the significant enhancement of thermoelectric properties of Cu-doped and Nb doped Mg_3Sb_2–Mg_3Bi_2 alloy based thermoelectric materials [1]. As a result, less hazardous and more efficient thermoelectric material applicable for both at low and middle temperatures was developed. The zT value of 1.1 was achieved for near room temperature in addition to the average zT value of 1.28 between 330 and 523 K.

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CT82

Low thermal conductivity in metal halide and chalcogenide

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Keywords: solid-state chemistry, metal halide perovskite, metal chalcogenide, thermal conductivity, soft crystal structure

Crystalline solids with low thermal conductivity are crucial for thermal barrier coating, thermoelectrics, and photovoltaics. The search for efficient materials with a fundamental understanding of lattice dynamics is of great research interest as well as practical application. Metal halide perovskites have experienced extraordinary rapid progress and attained momentous attention from worldwide scientific societies owing to their prospective multifunctional applications in the field of photovoltaic and optoelectronic devices. Recently, these halide perovskites have begun to receive fascination for future cost-effective thermoelectric applications beyond optoelectronic and photovoltaic devices. The promising research accomplishment of perovskite thermoelectrics was mainly recognized by the achievement of their ultra-low thermal conductivity. We demonstrate an ultralow (~0.20 W/m·K at room temperature) and glass-like temperature dependence (2–400 K) of κ_L in a single crystal of layered halide metal halide perovskite, $Cs_3Bi_2I_6Cl_3$. [1] Acoustic phonons with low cut-off frequency (20 cm^{-1}) are responsible for the low sound velocity in $Cs_3Bi_2I_6Cl_3$ and make the structure elastically soft. While a strong anharmonicity originates from the low energy and localized rattling-like vibration of Cs atoms, synchrotron X-ray pair-distribution function evidence a local structural distortion in the Bi-halide octahedra and Cl vacancy. Further we have also investigated the thermal transport properties of Pb-Sn-S system for efficient thermoelectric application and surprisingly we have observed very low lattice thermal conductivity due to the dual lone pair effect from Pb and Sn. The hierarchical chemical bonding and soft vibrations from selective sublattice leading to low κ_L is intriguing from lattice dynamical perspective as well as have potential applications.

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Large enhancement of the silicon power factor in on-chip multi-barrier nanodevices

CT83

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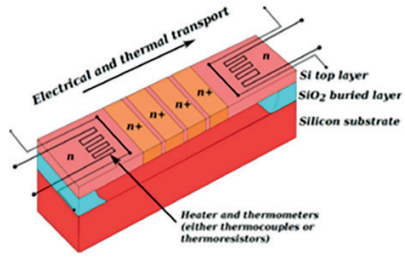
Keywords: silicon, multi-barrier, energy filtering, nanojunctions, nanolithography

Nanostructured silicon-based TEGs are very promising in the energy conversion field, and the research effort in this direction has the potential to lead to highly efficient and cost effective devices in the fields of battery-less devices for the internet of things, microelectronic cooling, and wearable electronics. Particularly for nanostructured Si, the electrical properties (electrical conductivity, Seebeck coefficient) can be well tailored as in bulk silicon, and the thermal conductivity is reduced to very low values due to the phonon scattering on the nanostructure walls: these elements can lead to highly efficient devices because the reduced thermal conductivity of silicon, combined with its very high Power Factor (PF) [1], results in a huge figure of merit. The Power Factor can be further increased by energy filtering, which allows to eliminate low-energy carriers through energy barriers, so that the Seebeck coefficient increases, at the expense of only a small reduction of the electrical conductivity. A power factor more than 5 times higher compared to bulk silicon has already been reported in disordered materials, such as heavily boron-doped silicon nanograins [2].



Our study focuses on developing top-down silicon nanodevice with a precisely controlled well/barrier design. To achieve this, we apply high resolution lithographic techniques and selective doping with phosphorus in order to define a succession of n++/i or n++/n- nanojunctions, and, hence, a 1D superlattice consisting of numerous well/barriers. Theoretical calculations showed that such designs can lead to even higher power factors, as the exclusion of doping in the barrier regions strongly mitigates the conductivity reduction [3]. These nanodevices have been thoroughly characterized, and preliminary results have already shown a significant enhancement in power factor of at least 10 mW/(m K^2). A detailed description of the results will be reported and discussed.

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CT84

Strong charge carrier scattering at grain boundaries of PbTe caused by the collapse of metavalent bonding

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Grain boundaries (GBs) play a significant role in controlling the transport of mass, heat and charge. To unravel the mechanisms underpinning the charge carrier scattering at GBs, correlative microscopy combined with local transport measurements is realized. For the PbTe material, the strength of carrier scattering at GBs depends on its misorientation angle. A concomitant change in the barrier height is observed, significantly increasing from low- to high-angle GBs. Atom probe tomography measurements reveal a disruption of metavalent bonding (MVB) at the dislocation cores of low-angle GBs, as evidenced by the abrupt change in bond-rupture behavior. In contrast, MVB is completely destroyed at high-angle GBs, presumably due to the increased Peierls distortion. The collapse of MVB is accompanied by a breakdown of the dielectric screening, which explains the enlarged GB barrier height. These findings correlate charge carrier scattering with bonding locally, promising new avenues for the design of advanced functional materials.

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Magneto-thermal switching using superconductors and importance of phonon-glass-electron-crystal states to the switching performance

CT85

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Keywords: thermal management, phonon-glass-electron-crystal, magneto-thermal switching, superconductor, thermal conductivity

Thermal management is one of the key technologies for developing nanoscale electronic devices. Thermal switching can control heat flow by the difference in thermal conductivity (κ) in the switching device. Furthermore, thermal switching by magnetic field is growing technology for thermal management [1,2]. In 2021, large thermal conductivity switching was observed in Co/CoFe spintronic multilayer film at room temperature [2].

In this study, we show a huge magneto-thermal-switching ratio (MTSR) in superconducting metals [3]. Generally, superconductors show low k because of the suppression of carrier contribution of κ (κ_{el}) below their superconducting transition temperature (T_c).

We measured κ of a Nb sheet (type-II superconductor with T_c = 9.2 K) by four-probe configuration using Thermal Transport Option (TTO) of Physical Property Measurement System (PPMS). We observed large MTSR, which is calculated by

MTSR = [κ (H) – κ (0 kOe)]/ κ (0 kOe), of 650% at T = 2.5 K and H = 4.0 kOe [3]. This huge MTSR in superconductors will be useful for the improvement of the performance of low-temperature electronic devices. In the presentation, we show the results for other superconductors and discuss the importance of phonon-glass-electron-crystal states to MTSR, which is a concept of thermoelectric.

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CT86

Soft optical phonons enabling ultralow and glass-like thermal transport in Argyrodite Cu_7PS_6

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Keywords: argyrodite Cu_7PS_6; crystal structure; Cu diffusion Lattice dynamics; glass-like thermal transport

Due to their ultralow and glass-like lattice thermal conductivity over a wide temperature range, Cu- and Ag-based Superionic Argyrodites with hierarchical crystal structures have gained widespread attention as promising thermoelectric materials [1]. However, despite their intriguing properties, quantifying their lattice thermal conductivities and fully understanding the microscopic dynamics that drive these extraordinary properties are still lacking. Here, we use an integrated experimental and theoretical approach to uncover the occurrence of enormous Cu-dominated soft optical phonons, which yield strong acoustic-optical phonon scattering and coherent thermal transport in a representative Argyrodite Cu_7PS_6. We employed the unified theory of thermal transport [2] to investigate the heat conduction of mutual coherence between degenerated phonon branches. Our results reproduce the experimental glass-like lattice thermal conductivities, ranging from ~0.40~0.60 W m^{-1} K^{-1}, in the 100 to 400 K temperature range. Moreover, we verify the superionic phase transition at ~509 K for Cu_7PS_6, identify the Cu diffusion pathways through synchrotron X-ray diffraction, and observe the footprint of Cu diffusion signals and over-damped phonon characters via simulated neutron scattering spectroscopy. Our study demonstrates that soft phonons enable ultralow and glass-like thermal transport and provides a comprehensive understanding of their underlying complex dynamics.

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Temperature dependent evolution of optical phonon modes and thermoelectric properties in polycrystalline Bi_2Te_3

CT87

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Keywords: doped Bi_2Te_3, Raman spectroscopy, optical phonon modes, crystal inversion symmetry, lattice thermal conductivity, thermoelectric properties

Due to its three-dimensional bulk-insulating nature and better room-temperature thermoelectric properties, Bi_2Te_3 is widely explored as potential thermoelectric material and topological insulator. The effect of smaller atoms (Ge, Se) doping on the evolution of the temperature-dependent optical phonon modes in polycrystalline single-phase Bi_2Te_3 are investigated. While undoped Bi_2Te_3 exhibits crystal inversion symmetry lowering in the investigated temperature range, the doped Bi_2Te_3 retains the inversion symmetry below 270 K. The increase in the full-width-half-maxima of Raman peaks and reduction in the phonon lifetime with an increase in temperature confirm the optical phonon decay in doped Bi_2Te_3, and hence lattice thermal conductivity is expected to decrease at higher temperatures. The lattice thermal conductivity estimated from the optical phonon modes is in line with the experimentally measured value, which affirms that optical phonon vibrations dominate the lattice thermal conductivity of Bi_2Te_3. At low temperature, the Ge-Se co-doped Bi_2Te_3 shows a four-fold enhancement of the Seebeck coefficient compared to that of undoped Bi_2Te_3. Our results give an insight into the optical phonon decay mechanism in the doped Bi_2Te_3 and corroborate that optical phonons play a vital role in the lattice thermal conductivity of polycrystalline Bi_2Te_3. The detailed optical phonon vibrations and thermoelectric properties of the light atom doped Bi_2Te_3 in the temperature range of 130 to 483 K will be presented.

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Thermoelectric properties of defective half-Heusler $Nb_{0.80}CoSb$-TiCoSb solid solutions

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Keywords: thermoelectric material, half-Heusler compound, NbCoSb, defective structure

Up until this decade, defective half-Heusler (HH) compounds with cation vacancies, such as $Nb_{1-d}CoSb$, have garnered increasing attention in the field of thermoelectric (TE) materials due to their degenerate semiconductor behaviour and competitive TE performance [1]. Unlike ideal HH compounds, the defective HH compounds exhibit significantly lower thermal conductivity due to strong point-defect scattering of phonons introduced by the cation vacancies, resulting in optimized TE performance with a peak zT of 0.9 at 1023 K [2]. However, these introduced vacancies can also have a negative effect on electrical properties. In the case of $Nb_{0.80}CoSb$ compounds, intrinsic cation vacancies inevitably lead to electron scattering, and low carrier mobility restricts the improvement of power factor. Moreover, $Nb_{0.80}CoSb$ compounds is limited by the optimal carrier concentration, which restricts the adjustment range of cation vacancies to a far lesser extent than the conventional HH compounds.

In this work, we examine the relationship between carrier concentration and cation vacancies concentration in $Nb_{0.80}CoSb$-based compounds by using TiCoSb isoelectronic solid solutions. We investigate the effects of Ti substitution on the TE properties of $Nb_{0.80}CoSb$-based compounds. To prepare $(Nb_{0.80-0.80x}Ti_x)CoSb$ samples, we use vacuum induction suspension melting, and then ball milling and subsequent spark plasma sintering. We explore the constitutive relationship between defect structure and TE properties in the solid solutions of the $Nb_{0.80}CoSb$-based compounds and reveal the regulatory mechanism of vacancies concentration in optimizing the TE properties of $Nb_{0.80}CoSb$-TiCoSb solid solutions. TiCoSb acts as a solid solvent and has the same outermost valence electron of 18 equilibrium state as $Nb_{0.80}CoSb$, maintaining the nominal valence electron number of the samples at 18 through composition design and optimization. Ti forms a continuous solid solution with $Nb_{0.80}CoSb$ in the form of TiCoSb, thereby decoupling the relationship between carrier concentration and the cation vacancies of the $Nb_{0.80}CoSb$-based compounds. Although reducing Nb vacancies helps to weaken carrier scattering in the $(Nb_{0.80-0.80x}Ti_x)$ CoSb samples, a large number of Ti generations also introduce strong alloy scattering.

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Analysis of crystal structure and thermoelectric properties of Sr-substituted $[Ca_2CoO_3]_pCoO_2$

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Keywords: Calcium Cobaltate, Ca349, Co-121, Misfit-layered, SPS

Misfit-layered cobaltate $[Ca_2CoO_3]_pCoO_2$ (Co-121, known as Ca349) has high Seebeck coefficient S but high electrical resistivity ρ in polycrystalline samples. It has a crystal structure that consists of an alternate stacking of a rock salt (RS)-type Ca_2CoO_3 block layer (BL) and a CdI_2-type CoO_2 conduction sheet parallel to the c-axis [1]. Owing to the size difference between the RS-type BL and the CoO_2 sheet, the compound has an incommensurate periodicity parallel to the b-axis, $p = b_{CoO2} / b_{RS} \sim 0.62$. Miyazaki *et al.* reported that the observed increase in S and ρ of the Bi-substituted phase can be explained in terms of the increase in p and decrease in career concentration n [2]. In this work, we perform a partial substitution for Ca atoms in RS-BL with Sr, which has the same valence state of Ca and a larger ionic radius.

The substituted samples are prepared using the standard solid-state reaction method of a stoichiometric mixture according to $[(Ca_{1-x}Sr_x)_2CoO_3]_{0.62}CoO_2$ (x = 0, 0.05, 0.10, 0.15, 0.20). The figure shows the result of the crystal structure analyzed using a Jana2006 [3]. It shows the change of lattice parameter p. According to the increased Sr-substitution, p decreases from 0.620 to 0.605. Assuming that the formal valence of the CoO_2 sheet is +3.5 to +3.6, all substituted samples are calculated n = 5.5 to 7.0 × 10^{20}/cm^3. The increase in ρ causes an increase in the formal valence of the CoO_2 sheet. Sr-substituted samples are expected to increase n, and decrease S and ρ. In the presentation, we will report the change in the other lattice parameters and TE properties. Additionally, we fabricate orientated bulk Co-121 samples using Spark plasma sintering to improve the TE properties.

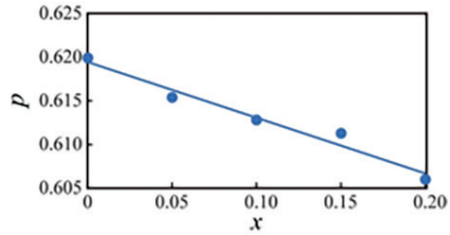

Fig.: Content of Sr-substituted dependence of lattice parameter.

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Co-Cr-Fe-Mn-Ni oxide as a highly efficient thermoelectric high-entropy alloy

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Keywords: high-entropy oxides, thermoelectricity, transport properties, spark plasma sintering, crystal structures, energy conversion

Ever-growing energy demand caused the rapid development of techniques for sustainable energy resources. Among the techniques, the most notorious one is a conversion of waste heat to electrical energy, i.e., the thermoelectric effect.

Recent studies show that multicomponent oxide systems with high configuration entropy can exhibit impressive electrical, thermal, catalytic, or magnetic properties. As a result, high entropy oxides (HEOs) are the alternative to conventional materials for different fields, such as microelectronics, catalytic converters, and energy storage. Such materials can be successfully obtained via various techniques, most of which require a very long processing time (from 15 to 50 hours). The main goal of the current study was to produce HEO composed of Co-Cr-Fe-Mn-Ni-O through the fast spark plasma sintering (SPS) and test their thermoelectric properties.

The samples were sintered in the temperature range between 1200–1300 °C with a pressure of 38 MPa under vacuum. Two main phases were formed: rock salt-structured Fm-3m and spinel-structured Fd-3m. The highest amount (81.4 wt.%) of the main structure (Fd-3m) was achieved by reaching the highest sintering temperature. The properties of this sample are comparable to the one obtained via a longer obtaining process: the highest value of the Seebeck coefficient reached -112.6 μV/K at room temperature (targeted value is -150 μV/K [1]); electrical conductivity is close to the single-phase material, i.e., $\sigma = 0.2148$ S/cm, $\sigma \approx 0.2009$ S/cm respectively.

These results indicate that SPS can be successfully applied to produce highly efficient TE high entropy alloys in a faster, 1.5 hours, and scalable process. Further optimization of the SPS parameters is needed for the production of a single-phase material [2].

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Nanostructure engineering and thermoelectric properties of $SrTiO_3$/TiN nanocomposites consolidated by spark plasma sintering

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Keywords: strontium titanate, oxide/nitride, hetero stricture, SPS, diffusion barrier

Nanostructure engineering is nowadays the most important and promising pathway to higher *ZT* values for any kind of thermoelectric (TE) materials. For instance, the TE performance of PbTe-based materials, which are one of the oldest and most well-developed TE materials, is still improving via nanostructure engineering. However, the complex nanostructures thus established are in principle thermodynamically non-equilibrial and hence thermally unstable, tending to transform toward energetically favourable coarser and simpler structures through thermal diffusion and grain growth. This natural tendency is crucial particularly for materials suitable for mid-to-high temperature TE applications such as oxides and other thermally durable compounds. In this paper, we have examined influences of metal nitrides as heat-resistant nano-inclusions dispersed in oxide matrix.

Strontium titanate $SrTiO_3$ (STO), known as one of the most promising oxide candidates for TE applications, was used as the oxide matrix with large thermopower due to its heavy electron effective mass as large as $m^* = 6–7\ m_0$. Titanium nitride TiN was employed as thermally durable conductive inclusions to be dispersed in the STO matrix. Samples were consolidated by using spark plasma sintering (SPS) in order to hinder grain growth during sintering at high temperatures required to densify the oxide/nitride composites. The sintered samples were examined by powder XRD and SEM. The TE properties of the samples, the electrical conductivity s, the Seebeck coefficient S, and the thermal conductivity k, were measured from room temperature to 800 °C for the sample pieces cut from the sintered bodies. The anisotropy of the TE properties were confirmed to be negligible.

The s values of the samples increased with increasing TiN content, reflecting the metallic characters of metal nitrides. Accordingly, the absolute values of the negative Seebeck coefficient, $|S|$, decreased with increasing TiN content. The k values of the samples were always higher for the samples containing TiN than that of STO, showing larger electron thermal conductivity for the samples with TiN as expected. However, most interestingly, the lattice thermal conductivity was lowest for the sample containing the largest proportion of TiN; this result can be attributed to enhanced phonon scattering at oxide/nitride hetero-interfaces at a large quantity in the sample. As a result, a highest *ZT* value among the samples was obtained for the sample containing 20 wt% (nominal) TiN as $ZT = 0.14$ at 800 °C, being 8 times higher than that of the sample without TiN.

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Thermoelectric figure of merit under constant Seebeck coefficients

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Keywords: thermoelectric power generation; thermoelectric figure of merit; energy conversion efficiency; integro-differential equation; mathematical analysis

When material properties are independent of temperature, the ideal energy conversion efficiency in thermoelectric power generation increases with the figure of merit introduced by A. F. Ioffe. However, when material properties depend on temperature, it appears that no single figure of merit can play the same role [1]. A recent result [2] shows that the efficiency can be represented by a set of three figures of merit.

If only some material properties are independent of temperature, is there a single figure of merit that is a generalization of Ioffe's figure of merit? Here we give an affirmative answer to this question.

In this talk, we show that Ioffe's figure of merit can be generalized when the Seebeck coefficient is temperature-independent but the electrical resistivity and the thermal conductivity are temperature-dependent. Our generalized figure of merit replaces the term in Ioffe's figure of merit with its temperature average. Assuming that the load resistance ratio is fixed, we can prove that the efficiency can be explicitly written in terms of the generalized figure of merit. We use the mathematical theory of ordinary differential equations for the proof. Details of the proof can be found in our publication [3].

Our figure of merit provides an accurate evaluation of materials when the Seebeck coefficient varies moderately with temperature.

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Efficient and accurate calculations of thermoelectric coefficients for materials with complex bands: The example of Mg_3Sb_2

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Keywords: thermoelectric, first-principle calculations, e-ph coupling, transport, Mg_3Sb_2

The computational prediction of thermoelectric transport properties in materials with complex band structures has gained significant attention in recent years. The most popular method involves combining first-principles electronic structure computations with the Boltzmann transport equation (BTE) within the constant relaxation time (CRT) approximation. However, the relaxation time is strongly dependent on factors such as material composition, carrier concentration, temperature, and electronic structure, whose omission can lead to significant uncertainties in the calculated transport properties [1,2]. Full ab initio calculations such as using EPW are computationally prohibitive.

In this study, we offer a feasible and highly accurate path beyond the CRT approximation. By combining density functional theory (DFT) and density functional perturbation theory (DFPT) calculations, we extract a limited number of electron-phonon matrix elements, from which we derive deformation potentials for all relevant acoustic, optical, and intervalley processes, to efficiently calculate scattering rates in materials with arbitrary band complexity. The transport properties are then calculated using our open-source Boltzmann transport code, *ElecTra*, which allows for detailed calculations of transport properties for each transport state, including polar optical phonon and ionized impurity scattering. The approach is validated using several materials, including the promising thermoelectric material Mg_3Sb_2 which is computationally one of the 'difficult' test cases due to its low symmetry, large unit cell, and conduction band minimum off high symmetry lines. Our results show good agreement with experiments and full ab initio computational methods, providing excellent accuracy while reducing computational costs by more than 90% in certain cases [3].

Overall, this study offers a valuable contribution to the field of computational materials science and provides a new, efficient method for accurately predicting thermoelectric transport properties in materials with complex band structures.

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Transport contribution to the Seebeck coefficient in the regime of transient delocalisation

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Keywords: organic semiconductors, Seebeck coefficient, nonadiabatic dynamics

Organic semiconductors (OS) are emerging as exciting materials for applications in flexible electronics. One relatively unexplored application is the use of OS as thermoelectrics, where high intrinsic Seebeck coefficients and low thermal conductivities indicate the possibility for high ZT figure of merit [1].

In the case of high mobility OS, charge transport operates in a regime where the charge carrier wavefunction undergoes transient delocalisation due to the opposing effects of large electronic couplings and strong electron-phonon coupling [2]. We capture this complicated dynamics with fully atomistic mixed quantum/classical dynamics simulations using the Fragment Orbital-Based Surface Hopping (FOBSH) method [3]. In this method, the quantum dynamics of an excess charge carrier is directly propagated under the influence of time-dependent classical nuclei according to Tully's fewest switches surface hopping method [4].

To study thermoelectric transport, we have applied the FOBSH method under an explicit temperature gradient. To the best of our knowledge, this is the first application of nonadiabatic dynamics under a temperature gradient. We show that there is a non-negligible contribution to the Seebeck coefficient (~ 100 μV/K) which arises from an asymmetry of nonadiabatic coupling elements towards the cold side compared to the hot side. This is a direct consequence of the increasing localisation of electronic states with temperature, due to increasing electronic disorder, leading to electronic states which are more delocalised at the cold side compared to the hot side. Our interpretation leads us to hypothesise that this contribution to the Seebeck coefficient should be larger in systems with a strong temperature dependence of wavefunction localisation and opens new avenues for materials design rules to maximise the Seebeck coefficient in this class of materials.

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Unravelling the mystery: Does thermopower depend on specific heat or entropy?

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Keywords: thermopower, specific heat, entropy, chemical potential, degenerate electron systems, thermodynamic equations

Thermopower, or the Seebeck coefficient, is a critical parameter in thermoelectric materials and devices, as it quantifies the voltage generated in response to a temperature difference, enabling efficient thermal to electrical energy conversion. The thermopower of particles depends on specific heat capacity, which indicates the heat storage capacity of a material, and entropy, which reflects the disorder or available energy states within a system.

Despite the significant impact of thermopower on the efficiency of thermoelectric devices, the dependence of thermopower on specific heat or entropy is still not fully understood. Various studies have used either specific heat or entropy to calculate thermopower, with some degree of success. In this work, we aim to examine the conditions under which thermopower can be accurately described by either specific heat or entropy. By employing fundamental thermodynamic equations, we will evaluate the accuracy and applicability of each approach in different scenarios.

We will demonstrate that, in a system with a temperature-dependent chemical potential, thermopower is directly proportional to entropy. This relationship can be expressed as the temperature integral of the specific heat divided by temperature. However, in systems with approximately constant chemical potential, such as metals, this relationship can be approximated, making the thermopower proportional to the specific heat. Consequently, it can be inferred that the proportionality to specific heat is a valid approximation only in metallic or degenerate systems, whereas the entropy-based description is the most general and accurate approach for understanding thermopower in a broader range of materials.

In conclusion, our work will provide a deeper understanding of the interplay between specific heat, entropy, and thermopower, shedding light on the conditions that favour each approach.

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Playing with phonons: from the reduction of the thermal conductivity to the full control of the phonon flux

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Keywords: phonon, thermal flux, rectification, diode

A large number of theoretical and experimental studies are currently focusing on phonon transport, particularly in nanostructures, where dimensions become comparable to the phonon mean free path [1]. One of the targets of these studies is to improve the conversion efficiency of thermoelectric devices based on nanostructured materials, such as silicon [2], which show a good power factor but a high thermal conductivity in its bulk form.

A new branch of these studies involves the investigation of methods for the control of the phonon flux, a process known as phonon engineering. The main target is to fabricate devices that work like conventional integrated circuit devices, but in which the principle of operation is based on heat propagation. The first step in this direction is the rectifying functionality (diode) applied to the heat conduction.

We will show the design and fabrication of a thermal rectifier device using NEMS techniques, and we will report its electrical and thermal characterizaton. The core component of the device is an asymmetrical holey silicon nanomembrane that allows heat flux to flow in one direction but is a thermal insulator in the other. The device design includes not only the membrane but also integrated heaters and temperature sensors for its characterization. All components, including the membrane, heaters and temperature sensors, are suspended to ensure precise control and measurement of the heat fluxes and to prevent any leakage through the substrate. The principles used to design the device will be outlined, and a comprehensive discussion of the measured thermal and electrical properties will be provided.

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Seebeck, Nernst and magnetotransport in dense $Co_3Sn_2S_2$ ceramic

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Keywords: ferromagnetic Weyl semi-metal, n-type sulfide, Nernst, Seebeck, magnetotransport

The search for magneto-Seebeck (S) effect is an active field in thermoelectricity. Interestingly, this quest meets also some aspects of the topological materials after the reports on magnetic topological thermoelectric materials, for which the topological band structures may affect S [1,2]. The $Co_3Sn_2S_2$ shandite attracts much attention: this ferromagnetic kagome lattice (T_C = 175K) is a Weyl-semimetal [1], with zT = 0.20 at 573K [3], it belongs to the TE n-type sulfides, a limited class as compared to p-type TE sulfides, and it exhibits a large Nernst effect in the absence of external magnetic field [2,4].

Using spark plasma synthesis (SPS) densification, we have produced a dense (>95%) $Co_3Sn_2S_2$ shandite which allowed (magneto) TE properties to be studied from low (T = 5K) to high (T = 675K) temperatures. The Nernst effect has also been evidenced for the first time in the ceramic form. A comparison between the ceramics and the crystals will be presented [5].

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Sustainable metal phosphide thermoelectrics with promising performance

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Keywords: metal phosphide, thermoelectric conversion, crystallography, thermal conductivity, electrical properties

There is a continued need for discovery of new thermoelectric materials. Metal phosphides are an emerging class of thermoelectrics with promising figures of merit, approaching $zT = 1$ in n-types and $zT = 0.5–0.8$ in p-types. [1]

Despite the low atomic mass of phosphorous, structural complexity leads to low thermal conductivities across a range of materials and the main challenge is to embed better electrical properties. [1] Phosphorous has a range of possible oxidation states, affording diverse chemical bonding and a wide range of available structures for exploration.

We have investigated a series of ternary metal phosphides and have discovered promising thermoelectric performance in MgCuP, CaCuP and CaAgP. [2,3] In all cases, metal deficiency leads to degenerate p-type conduction and the figures of merit fall between $zT = 0.4–0.5$ at 660–773 K. CaCuP in particular is promising as this composition has the best electronic properties amongst all reported metal phosphides. [2] Modelling shows CaCuP can reach $zT = 1$ in alloyed compositions if control of doping can be achieved. MgCuP has a lower symmetry structure and achieves a similar zT on account of a lower thermal conductivity. [2] CaAgP has been considered as a candidate topological nodal line semimetal. However, our work shows that CaAgP forms with high concentrations of Ag vacancies, and the stable phase $CaAg_{0.9}P$ behaves like a regular highly doped semiconductor. [3]

This contribution will summarise our recent metal phosphide work, including phase boundary mapping and alloying in the CaCuP system and discuss some of the general conclusions from our recent review.[1]

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Large atomic size mismatch induced novel meta-phase and high thermoelectric performance

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Keywords: atomic size mismatch, meta-phase, thermoelectric, Hume-Rothery rule, order-disorder

Discovery and regulation of new phases of matter drive science and technology forward. Here, we report unique meta-phase $Cu_2(S,Te)$, $Ag_2(S,Te)$ and $Mg_2(Si,Sn)$ over a wide composition range. In the formation of meta-phase, the large diffusion coefficient mismatch counterbalances the large atomic size and electronegativity mismatches, thereby escaping phase separation and creating stable single-phased exquisite atomic structures beyond the classic Hume-Rothery rule. Featured by the highly tunable, contrasting degree of order/disorder of the sublattice, the meta-phase showcases electron localization-delocalization in $Cu_2(S,Te)$, a rare co-existence of mechanical plasticity and amorphous characteristics in $Ag_2(S,Te)$, along with inherently low lattice thermal conductivity and high thermoelectric performance in all three compounds. We envisage that the concept of meta-phase will usher in more innovations in materials research and technical applications.

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CT100

Strong enhancement of the thermoelectric properties of nanostructured α-$SrSi_2$ by combining Melt-spinning and spark plasma sintering

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Keywords: alkaline-earth silicides, phonon scattering, melt spinning, spark plasma sintering, nanostructuring

Conventional thermoelectric materials such as Bi_2Te_3 have the best performances at room temperature and can reach a ZT about 1 [1]. However, the cost, the toxicity and the scarcity of Te limit the application of thermoelectric materials in the low temperature range (300–600K). The use of eco-friendly elements such as silicides alloys could overcome these concerns. Among them Mn-Si and $Mg_2(Si,Sn)$ reached a maximum figure of merit of 0.63 (723 K) and 0.8 (650 K) respectively [2,3] and α-$SrSi_2$ reaches a ZT about 0.15 at 300K which is the highest value for a silicide alloy at this temperature. The power factor of α-$SrSi_2$ is close to that of Bi_2Te_3 however its thermal conductivity (~5 W/m.K) limit its performances.

In this work, we investigate the effect of rapid solidification from liquid $SrSi_2$ on the microstructure of the α-$SrSi_2$ alloys. The use of melt-spinning technique unable to reach high cooling rates up to 105 K/s which permit to obtain high purity nanostructured ribbons which are then shaped into highly dense pellets by spark plasma sintering. Although the crystallite size obtained after these both processes reached 200 nm, one observed a strong decrease of the lattice thermal conductivity that permit to obtain a gain on the figure of merit up to 60% compared to our bulk reference.

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Poly(3-hexylthiophene) layers modified by acids as promising *p*-type thermoelectric materials

CT101

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Keywords: organic materials, acidic dopants, surfactants, conducting polymers, p-type materials, spin coating, atomic force microscopy

Nowadays, there is a trend to move into organic materials due to their versatility and the possibility to use them in flexible devices. Conducting polymers, such as poly(3,4-ethylene dioxythiophene) (PEDOT), have multiple applications – they can be used as photovoltaic devices, organic transistors, or light-emitting diodes. Polythiophene derivatives are well-known thermoelectric materials, modified by various dopants, such as F4TCNQ.[1,2]

In our work, we propose dodecylbenzenesulfonic acid (DBSA), as a cheaper alternative for F4TCNQ to dope poly(3-hexylthiophene) (P3HT). Aside from being a *p*-type dopant, DBSA serves also as a surfactant. Our research aimed to determine how the amount of dopant changes conductivity, Seebeck coefficient, and power factor. We used 3%, 2.25%, 1.5%, 0.75%, 0.1%, 0.01%, 0.001%, and 0.0001% of DBSA volume addition. Layers with 100 nm of thickness have been deposited with the spin coating method. As a result, we got the material with comparable thermoelectric parameters to P3HT doped with H_2SO_4 or F4TCNQ. Using atomic force microscopy (AFM) we observed the change in layer morphology. Higher addition of DBSA decreases layer roughness and improves materials' conductivity and decreases Seebeck coefficient. Comparing obtained *PF* of all materials, the most optimal P3HT:DBSA layer was the one with 2.25%v addition of acid which Seebeck coefficient, conductivity, and *PF* were 0.14 S/cm, 284 μV/K and 1.09 μW/(m·K2) respectively. Seebeck coefficient measured in the vacuum of our material differs between 177 μV/K for 3%v of DBSA addition and extraordinarily high 2120 μV/K for 0.1%v DBSA in P3HT which makes this material as promising *p*-type material for small appliances, like body sensors.

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CT102

Exploring the potential of nanostructured Ag_2Se in hybrid thermoelectric films

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Keywords: thermoelectric, organic–inorganic hybrids, power factor, interface engineering

To effectively harness thermal energy over large areas, thermoelectric (TE) materials need to maintain their performance over time. One promising approach to achieving large-area TE films is through hybrid materials, where a combination of TE materials and polymers can be applied as paint or coating. Ag_2Se is a promising n-type TE material with a high abundance of elements and low toxicity. In this study, we developed all solution-processed hybrid TE films, incorporating varying amounts of TE Ag_2Se nanomaterials within a polymer matrix and characterized their properties. The hybrid TE films were fabricated using (1-methoxy-2-propyl) acetate (MPA) as the solvent and poly (methyl methacrylate)-PMMA as the durable polymer, resulting in the n-type hybrid TE films.

Ag_2Se nanomaterials as the TE phase was synthesized using a high-throughput method via an energy-efficient microwave-assisted hydrothermal method. Scanning electron microscopy (SEM) characterized the as-made powder material, revealing the primary particles' size and morphology. The phase purity of the as-synthesized materials is high, as identified by the XRD analysis. In addition, the electronic transport properties of the hybrid TE films have been characterized by measuring the Seebeck coefficient and electrical resistance, and finally, the TE power factor was estimated.

Our findings show that the TE power factor of the hybrid films with a solid material fill factor of 60–90% reaches exceptional values, considering the system's absence of conducting polymers. Overall, this study presents a promising low-cost route for producing and implementing TE coatings on a large scale, which could be valuable for flexible, large-area energy harvesting technologies like the Internet of Things (IoT).

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More than 3 times power factor improvement of PEDOT: PSS induced by electrolytes

CT103

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Keywords: organic thermoelectrics, PEDOT:PSS, electrolytes, power factor, electrochemistry

In the search of more efficient thermoelectric (TE) materials, significant improvements in *ZT* have been achieved, mainly due to the reduction of the thermal conductivity. In contrast, enhancements in the power factor $PF = \sigma S^2$, being σ the electrical conductivity and S the Seebeck coefficient, have been minor. Recently, large *PF* improvements have been reported in a novel solid-liquid TE system, consisting of a porous nanostructured TE solid (Sb-doped SnO_2) in contact with an electrolyte (ions in a liquid media) [1].

Here, we try to implement this strategy in PEDOT:PSS films, which were prepared from a formulation from Specific Polymers with dymethyl sulfoxide and polyethylene glycol. Using this formulation, films were deposited by spin coating on glass substrates and contacted by Ag paint at their ends. Different electrolytes were added on top of certain area of the films using a homemade setup. The Seebeck coefficient of the system was found to increase more than double, accompanied by an increase of around two times in its electrical resistance. This led to a more than three times improvement in the power factor, which is a remarkable variation.

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CT104

Thermoelectric properties of pedot: PSS thin films in different concentration

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Keywords: pedot: PSS, thermoelectric, thermoelectric characterization thin film, seebeck coefficient

Today's needs include the maximum use of energy resources. The harvesting of waste energy is one of these needs. Thermoelectric systems give us an advantage in terms of energy efficiency. Thermoelectric materials produce energy according to the Seebeck principle. This occurs by taking advantage of the temperature difference between the two plates. To improve the thermoelectric properties of a material, a balance between the Seebeck coefficient, thermal and electrical conductivity are required [1] So, the choice of thermoelectric material is a significant subject.

Inorganic materials have good thermoelectric properties. These materials are advantageous to be worked in a wide temperature range. Unfortunately, it creates difficulties in terms of flexibility. Organic materials, on the other hand, provide the advantages of low thermal conductivity, lightness, and flexibility [1]. Conductive polymers are widely used in products such as solar cells, optoelectronics, and thermoelectric materials. PEDOT: PSS, an organic polymer in thermoelectric generators, has been widely used in recent years. In addition, it is unique about its commercially available aqueous solution, easy film formation, and thermal and mechanical properties [2].

For these reasons, PEDOT: PSS polymer was preferred in the study. PEDOT: PSS solutions were prepared in DMSO and water (15/85) solutions, proportioned as 1-3-5% and 7%. Prepared solutions were applied to the polypropylene substrate by Dr. Blade. It was turned into a thin film by the Dr. Blade method and was left to dry at room temperature. Then, the Seebeck coefficient measurement was carried out by using the Seebeck coefficient measurement setup prepared in the laboratory. In addition, electrical conductivity, thermal conductivity, and SEM characterization studies were performed and compared.

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Electrochemically grown bismuth telluride inside commercial polyester filters for flexible thermoelectric generators

CT105

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Keywords: electrochemical deposition, nanostructures, microgenerator, scalable fabrication, out-of-plane characterization.

We have fabricated via electrochemical deposition, thin films of nanostructured bismuth telluride (n-type) and tellurium (p-type) using commercial polyester filters as templates. Also via electrochemical deposition, metal electrodes have been deposited in both sides of the filter, and thus, a nanostructured thermal generator is obtained. The main application of such devices (with mm in area and only a few microns in thickness) is to harvest body wasted heat and, with the power obtained, feed wearable devices. Then, flexibility is mandatory to be able to adapt these generators to the human skin and the procedure is low cost and scalable fabrication.

The characterization of such structures, from the morphological point of view, show that an intricate network of nanowires is formed inside the template. The nanostructure is preferentially oriented along the [110] direction, with stoichiometric composition, and with a high filling ratio of the template, and thus, the material is optimal for out-of-plane applications [1], as is the objective of the work. These kinds of structures are somehow similar to that of the highly ordered and controlled 3D-nanowire networks that have been studied previously in our group, but with a lower order and lower number of connections between the wires.

Given that in the case of 3D-nanowire networks of bismuth telluride a high increase of the performance of the thermoelectric material due to both the nanostructure and the connections between the nanowires was found [2], a great effort is being made in obtaining reliable measurements of the transport properties in the out-of-plane direction to see if the filled polyester templates show also this enhancement. Nevertheless, the reduced thickness of the samples makes it challenging to maintain the temperature gradients necessary for Seebeck and efficiency measurements. Therefore, a new system is being developed (with the company Panco), which is being calibrated and, with the aid of COMSOL MULTIPHYSICS® simulations, allows the characterization of actual flexible polyester BiTe filled microgenerators.

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CT106

Ab-initio studies of electronic properties of tungsten carbide for thermoelectric applications

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Keywords: nanostructure, Seeebck coeficient, thermal conductivity, thermoelectric figure-of-merit, *ab-inito* approach

Nanostructuring (1D, 2D, thin-film, nanoparticles) of the materials exhibits an improved thermoelectric transport coefficient, due to the quantum confinement effects in low dimensional materials [1-3]. Also, nanostructuring leads to an increased phonon scattering due to the introduction of surface roughness, numerous interfaces, etc. in such materials, and thus results in reduction of the lattice thermal conductivity. This improves the overall thermoelectric figure-of-merit (zT). Experimental realization of nanostructures are really very challenging and costly affair. Ab-initio based theoretical studies allow the researchers to precisely and effectively calculate the transport properties of a material and fine tune them at a comparativley lower computational cost.

We study the electronic transport properties of 2D hexagonal tungsten carbide (h-WC) which exhibits a direct bandgap of ~ 2.71 eV. Being a wide bandgap and high temperature material, the h-WC can be explored for thermoelectric applications. With the help of ab-initio based computational appraoch, we calculate the electronic properties of the material. The Seebeck coefficient (S) comes out to be 0.26 mV/K, the electrical conductivity (σ) and the electronic thermal conductivity (κ_e) as 0.24 S/m and 0.27 W/mK respectivelt at 300 K. Using Electron-Phonon Wannier function, we calculate the electron-phonon interaction and thus the average scattering time in the reduced Brillouin zone as a function of temperature. The inclusion of temperautre dependent scattering time in the aforementioned quantitites provide more realistic estimation of the thermoelectric performnce of the material.

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Does Zn form a resonant level in SnTe?

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CT107

Keywords: SnTe, resonant level, electronic structure, band engineering, bloch spectral function, Korringa-Kohn-Rostoker method

Thermoelectric materials are often seen as a green alternative to conventional energy sources and yet, achieving competitive efficiency has been an elusive goal for many years. So far, various strategies were developed to push their performance further, and introducing resonant levels (RL) attracted increasing attention in the last 10 years due to ability to increase thermopower because of distorting local electronic structure of host material. Recently, p-type Zn doped SnTe was found to have an enhanced thermoelectric efficiency [1] with a peak ZT value of 1.49 at 840 K, compared to 0.5 at 900 K for pristine SnTe. Formation of resonant level on Zn atoms was proposed as an explanation of the thermopower and ZT enhancement. While SnTe itself is inferior to its sister compound PbTe, it has been revisited recently as a more eco-friendly, lead-free alternative. Despite this advancement, electronic structure of SnTe:Zn has not been studied in detail, leaving room for improvement.

Here we perform ab-initio calculations of SnTe doped with Zn to study the character of impurity and modifications of the electronic structure. Calculations are performed using two complementary methods based on Density Functional Theory, that is KKR-CPA (Korringa-Kohn-Rostoker with Coherent potential approximation) and pseudopotential method, where all calculations include spin-orbit coupling. Obtained densities of states and Bloch spectral functions (BSFs) suggest that Zn forms a RL but in the conduction band of the material, thus the experimentally observed enhancement in the thermopower and ZT of p-type SnTe:Zn cannot be directly explained using the RL idea. Those results are confirmed by using pseudopotential method with unfolded bandstructure of $3 \times 3 \times 3$ supercell.

So why SnTe:Zn has an improved thermoelectric efficiency? We found that besides formation of RL in the conduction band, Zn has a strong influence also on the valence band of SnTe. Analysis of BSFs shows that introducing high amounts of Zn not only decreases the offset between the last valence band maxima but also leads to band flattening, increasing carrier effective mass and as a result, increasing thermopower as seen in the experiment.

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CT108

In-gap states: mechanism of ZT improvement and their difference to resonant levels

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Keywords: in-gap states, resonant levels, impurities, electronic structure, doping, power factor

In-gap states and resonant levels are two special types of electronic states, which can be formed in a thermoelectric material upon doping. Both of them do not follow the rigid-band behavior, and strongly modify the electronic structure and electronic transport properties of the host material. As a consequence, they may improve the thermoelectric figure of merit beyond what is succeeded using the "conventional" doping, hence are among the strategies used to optimize the thermoelectric performance of the material. Because both, in-gap states and resonant levels, lead to a formation of local peaks in the electronic densities of states computed using density functional methods, in-gap states are quite often confused with resonant levels, leading to an inappropriate interpretation of the experimental results.

In my presentation, based on the electronic structure and transport calculations for real materials, I will explain the mechanism by which the in-gap state modifies the thermoelectric properties, which can result in improved power factor at high temperatures. Double, In and I-doped PbTe will be used as an example of successful implementation of this strategy, giving extraordinary peak and average ZT in n-type PbTe [1]. Then I will contrast it with the well-known resonant level cases of Tl-doped PbTe [2,3,4] and In-doped SnTe [5,6,7]. By showing the key differences between the two scenarios, from both the theoretical (calculated electronic structure) and experimental (measured thermopower, conductivity, and effective mass) point of view, I will advise how to avoid confusing one with the other.

Electronic structure in this work is calculated using the KKR-CPA method, electronic bands are studied using the Bloch spectral functions and electronic transport properties are computed using the Kubo-Greenwood formalism.

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Interplay between doping, morphology and lattice thermal conductivity in organic polymers

CT109

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Keywords: PEDOT:PSS, P3HT, organic polymers, thermal conductivity, doping, morphology

Organic thermoelectrics (TE) has attracted a fair amount of attention in recent years due to remarkable advances achieved in terms of the figure of merit, ZT. However, much of the efforts up until now have just been devoted towards the improvement of the power factor, whereas thermal properties have often been overlooked. In order to fill this gap, the thermal conductivity of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) and poly(3-hexylthiophene) (P3HT) is studied through the use of classical Molecular Dynamics (MD), both with and without taking into account doping, which is modeled at Density Functional Theory (DFT) level and then incorporated into a classical MD force field.

It is found that undoped amorphous PEDOT exhibits a positive correlation between average chain length and thermal conductivity, as is well known, while showing a weak negative correlation between sample density and average chain length. We find that doping is responsible for a general increase of the thermal conductivity and a reduction in the pi-stacking distance (from 4 to 3.6 Å). It also gives rise to a stronger negative correlation between sample density and average chain length. The mere presence of PSS as a counterion is another factor that contributes to the increase in thermal conductivity. [1]

The crystalline arrangement of doped PEDOT is also investigated, in the form of nanofibers. At odds with previously reported theoretical results [2], a surprisingly low thermal conductivity is observed along the backbone direction when the interchain transport is taken into account. Two types of interchain interactions along this direction are also observed and discussed.

Also, a new monoclinic unit cell is proposed for crystalline P3HT. The impact of chain length, doping and morphology are discussed as done similarly for PEDOT.

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CT110

Criteria for erroneous substrate contribution to the thermoelectric properties of thin films

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Keywords: multi-layer systems, thin films, substrate contribution, transport modeling, thermoelectric performance

Since the discovery of the Seebeck effect over 200 years ago, many different strategies to obtain high-performance thermoelectric materials have been invented and tested, including the synthesis of thin films and other multilayered structures. Although it has already been shown that the pure combination of the properties of each layer without interactions will yield worse performance compared to the best layer [1], a critical estimation of the size of the deviation to trace back individual properties is still missing.

In this talk, we present a comprehensive description of the total Seebeck coefficient, electrical and thermal conductivity, power factor, and zT value of a two-layer system from a simple model and elucidate the origin and size of the contribution of each layer to the total thermoelectric performance. We further show both mathematically as well as by comparison with experimental data from literature that the influence of the substrate can lead to large deviation between the measured and the film's properties, advising caution when analyzing such systems. Ultimately, our model allows to ensure that the contribution of the substrate is below a desired threshold by introducing material-related quantities.

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Lifetime prediction of a Bi_2Te_3 thermoelectric module

CT111

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Keywords: Bi_2Te_3 thermoelectric module, thermal cycles, lifetime prediction, solder layer fatigue, darveaux model

A thermoelectric module (TEMs) for power generation usually works once a temperature difference exerts on it, *i.e.*, with the lower temperature at its cold side and higher temperature at the hot side. The TEM's reliability is always high when the output power and temperature applied at the heat source end is continuous and uniform. However, in practical application scenarios, the temperature of its heat source is usually periodically changing between higher and lower temperature values, and the cyclic thermal stress generated by thermal cycling gives rise to a lower energy conversion efficiency and lifetime reduction of the TEM device. So far few studies have been reported on the actual service life assessment and failure mechanisms of TEMs under thermal cycling conditions, which limits the further industrialization and scale-up of thermoelectric power generation.

In this work, we combine the solder layer fatigue theory and finite element simulation to establish a life evaluation model for Bi_2Te_3 devices under thermal cycling conditions. The following assumptions are made: 1) the actual operating conditions of the device are simplified to equal-amplitude thermal cycling, which is equivalent to loading equal-amplitude thermal stress on the module; 2) according to the previous literature [1], the interface is usually where the stress is concentrated. And it is assumed that the fatigue cracking of the solder layer is the main reason for the increase in device resistance; 3) the Anand model is used to describe the viscoplastic properties of the solder layer. And the viscoplastic dissipation energy density accumulated in the solder layer during thermal cycling is used as the intrinsic driving force of the interface fatigue; 4) the Darveaux energy life model is used to describe the specific process of fatigue and establish the final life evaluation model.

According to the theoretical assumptions, the resistance of the TEM is expected to remain constant in the beginning and then grow at a constant rate. The experimental data we obtained agreed well with the aforementioned theoretical assumptions. The constants required to obtain an evaluation model that can predict the lifetime of Bi_2Te_3 devices under unknown operating conditions, were finally fitted by the resistance growth data under different operating conditions.

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Acknowledgments

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CT112

Advanced thermoelectric converter technologies for integration into a potential advanced radioisotope thermoelectric generator

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Keywords: skutterudite, RTG, space power

The flight-proven Multi-Mission Radioisotope Thermoelectric Generator (MMRTG) is currently powering NASA's Mars Curiosity and Perseverance rovers and selected for NASA's Dragonfly mission. The MMRTG design includes sixteen thermoelectric converter modules, each composed of 48 couples of PbTe/TAGS (Lead-Telluride/Tellurium-Antimony-Germanium-Silver) packaged in fibrous insulation and is operated under inert gas in a hermetically sealed environment. The skutterudite (SKD)-MMRTG design in development would be nearly identical except for upgraded 48-couple modules using skutterudite-based couples. While preserving the majority of the flight-qualified MMRTG design, fabrication tooling and flight support equipment, the new skutterudite-based couples would provide a substantial improvement in power output over time. A team composed of Aerojet Rocketdyne (AR), Teledyne Energy Systems, Inc. (TESI), and NASA's Jet Propulsion Laboratory (JPL) team has been maturing the SKD technology for integration into a potential SKD-MMRTG. From JPL-transferred skutterudite technology, TESI has developed manufacturing capabilities for skutterudite-based couples as well as 48-couple modules, a building block of the SKD-MMRTG. Life assessment testing of SKD couples is underway at JPL and TESI, with some couples achieving more than three years of continuous time-on-test. Testing of SKD couples and a 48-couple module has shown that their power output is in good agreement with the predicted values. Physics-based life performance prediction models developed at JPL, and a newly developed one at TESI, utilize the couple test data results and analysis to forecast the generator power output. The current best-estimate power predictions for the SKD-MMRTG meets specification requirements and offers up to about 37% more power at End-Of-Design-Life (EODL) than the MMRTG at equivalent operating conditions. The SKD-MMRTG would provide a substantial improvement in power output in the out years, making it ideal for many long-duration, deep-space missions.

Acknowledgments

This work was supported by NASA's Radioisotope Power Systems program.

Feasibility of a low-power RTG concept utilizing a GPHS heat source

CT113

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Keywords: GPHS, RTG, silicon, germanium, thermoelectric

Abstract - Over the past twenty-five years, the average cadence of National Aeronautics and Space Administration (NASA) missions that employ radioisotope power systems (RPS) is approximately one per decade. Currently, the only flight-qualified RPS in the NASA inventory is the Multi-Mission Radioisotope Thermoelectric Generator (MMRTG), which has a beginning-of-life (BOL) power output of approximately 120 We. In addition, NASA and the U.S. Department of Energy (DOE) also manage the Next Generation Radioisotope Thermoelectric Generator (NGRTG) development, with a projected BOL power ranging from 250–270 We. However, if a lower-power RPS unit were available, would there be sufficient mission pull to increase the cadence of RPS-powered missions? We believe the answer to this question is yes, which drove the evolution of a concept study that examines the feasibility of low-power RPS based on a single General Purpose Heat Source (GPHS). This paper discusses the results of a concept study of an RPS system that utilizes novel ruggedized silicon germanium thermoelectric modules, a projected BOL of 15 We. In addition, this paper addresses the next steps required to evolve the concept beyond its current status to conceptual design

CT114

ISA-TEG: High temperature modules based on Half-Heusler compounds ready for commercialization

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Keywords: thermoelectric module, halfheusler, application, commercialization, CHP

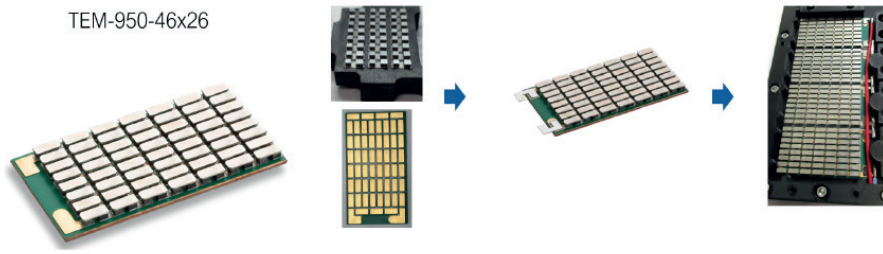
Commercialized high temperature TE-modules are not available up to day. This might the largest barrier for commercialization of TEGs. Now the company Isabellenhütte Heusler is able to provide a solution to solve this problem.

Dr. Fritz Heusler discovered the first Heusler alloy in 1901 at Isabellenhütte. Since 2009, Isabellenhütte has been actively engaged in Heusler alloy research. Our research efforts have been focused on thermoelectric Half-Heusler compounds since then. The goal of our research is to create a manufacturing process for these materials that can be scaled up for industrial production. In 2015, our research focus has shifted from the material to the development of modules using our Half-Heusler materials. Isabellenhütte established an industrial pilot production line in 2017, covering the entire process from raw elements to the creation of thermoelectric modules. Our ambition was to demonstrate the automated assembly process and industrial-scale material manufacturing of Half-Heusler modules, while maintaining a high level of quality. Starting in 2021, we initiated the development of tailored power electronics for our Half-Heusler modules, completing a full package solution.

Today, we are pleased to announce the introduction of our ISA-TEG product range. ISA-TEG is a two-step module concept that begins with the production of an unicouple. Our assembly process begins with the attachment of one P-type and one N-type thermoelectric leg, produced from the pilot line, onto a hot side contact by an automated assembly process. The next step involves the placement of multiple unicouples onto a flat, cold side substrate that can be customized in terms of size and shape.

In the first step, customers can select the most cost-effective heat transfer coefficient (HTC) that suits their specific application. We currently offer a choice of four unicouple designs, each with a different HTC. Customers have the flexibility to choose a module area in the second step. In the final step, we offer the option of a tailored power electronic design to meet customer specific application needs.

Over the past year, we have successfully demonstrated the ISA-TEG concept in a nano-CHP application. As a result, Isabellenhütte is now open to discussions regarding commercial TEG projects.



0.5 kW facility of geothermal thermoelectric generator from hot dry rocks on canary islands

CT115

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Keywords: geothermal energy, thermoelectric generator, thermosiphon, heat exchanger

Nowadays 81% of the world´s primary energy comes from the fossil fuel, causing a very serious climate crisis. In this context, it is important to develop technologies that permit increase the use of renewable sources such as wind and solar energy, but also geothermal energy, which is the only continuous renewable source that does not depend on the weather. There are areas where boosting the use of geothermal power is particularly important, due to its availability and the enormous dependence on fossil fuels as is the case of the Canary Islands. The Timanfaya National Park (TNP), in Lanzarote (Canary Islands, Spain), is one of the most important shallow hot dry rock fields in the world, but currently untapped. The geothermal anomalies are caused by the presence of a lava body at a depth of 1 km, corresponding to the last eruptions of 1730 and 1824. Thus, geothermal gases in this zone are heated by the magma and rises at a temperature between 170 °C and 470 °C [1]

The Thermal and Fluid Engineering Research Group (ITF) installed, for the first time in the world, a Geothermal Thermoelectric Generator (GTEG) prototype, placed on TNP in 2020. The generator developed in this work, composed by 16 thermoelectric modules with passive phase change heat exchangers, is capable of generating 36 W (2.6 W per module), with a temperature difference between the heat source and the environment of 160 °C, without any moving components [2]. In 2021 the second GTEG prototype was installed by ITF on TNP, where the temperature of the hot source is 465 °C. This prototype is capable of generating 36 W with 8 thermoelectric modules (4.5 W/TEM) [3].

Once the feasibility of thermoelectricity to generate electricity from high enthalpy geothermal anomalies in shallow hot dry rock fields has been experimentally demonstrated, this new work presents the development of a 0.5 kW GTEG in order to provide electric energy to the TNP. In addition, based on the experimentally validated computational model, the potential of total electric energy obtained increasing the number of the installed GTEG has been studied in TNP. The results show that it is possible to produce between 3.61 GWh and 11.35 GWh of electric energy per year, with an average Levelized Cost of Energy (LCOE) of 48 euros/MWh

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Acknowledgments

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CT116

A new direct p-n junction based on Heusler compounds manufactured by co-sintering

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Keywords: p-n junction, co-sintering, thermoelectric module, Heusler, interface

Thermoelectric modules have potential for widespread applications, but their cost needs to be reduced to make them economically feasible. When using low-cost thermoelectric materials, the cost drivers are material processing and assembly (including ceramic substrates). Innovative processing techniques and thermoelectric module geometries are necessary to mitigate these costs. In addition, the stability of hot side contacts is a significant concern when dealing with medium/high-temperature ranges. The p-n junction geometry (**Fig. 1**) could be a solution to these two challenges, simplifying the whole process and avoiding the need for a hot side metal contact.

In this work, we propose a low-cost Heusler p-n junction thermoelectric module. Finite element modelling (FEM) was used to perform a sensitivity analysis and determine the optimal geometry. A three-material co-sintering process was used to manufacture p-n junctions with the cold-side electrodes in a single step. Finally, experimental characterization was performed on the p-n junctions. The results show that the p-n junction is competitive with the π-type geometry but at a much lower production cost.

In conclusion, this work presents a low-cost Heusler p-n junction thermoelectric module with hot-side direct contact. The proposed manufacturing process and geometry could be used to reduce the cost of thermoelectric modules, making them a viable option for various applications at high temperature.

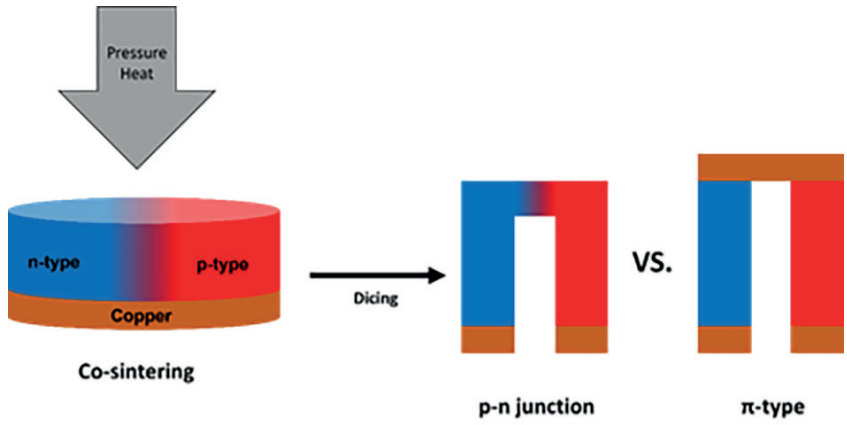

Figure 1: Sketch of the co-sintering process and the p-n junction geometry studied in this work

Development of thermoelectric modules based on magnesium and manganese silicide, derived from recycled Si-kerf

CT117

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Keywords: thermoelectric, module, silicon, kerf, recycle

Popularization of photovoltaic (PV) technology due to recent green-transition initiatives is generating increasing demand on Si-based PV cells, which hold the vast majority of the market share. Abrasive machining of Si ingots into wafers for the PV and electronics sectors results in significant material losses, in the form of Si-kerf. As purification of this waste material evolves as a viable technology, recycling of purified Si-kerf becomes a highly attractive route for supporting sustainability in the semiconductor industry. Fabrication of silicide-based thermoelectric (TE) compounds with competing figures of merit facilitates recycling of Si-kerf, while development of TE modules and generators from such materials and their integration in automotive-exhaust heat-recovery applications is also expected to conduce in CO_2 emission reductions.

This work describes the ongoing progress on the development of TE modules based on magnesium and manganese silicide (MSS and HMS respectively) synthesised from recycled Si-kerf. Both n-type MSS and p-type HMS pellets with nominal composition of $Mg_{2.2}Si_{x-0.03}Sn_{1-x}Bi_{0.03}$ (and $MnSi_{1.73}$ respectively, have been fabricated via mechanical alloying followed by hot press sintering. Mechanical polishing and precision grinding have been utilized for the parallelization and thickness regulation of the TE pellets, while metallization of the levelized pellets was conducted through sputtering of Ti/Ni bilayers. Metallized pellets are diced into TE-legs, ready to be assembled on Alumina plates patterned with direct bond copper (DBC) electrodes. Four TE legs have been silver-brazed in series (alternating p- and n-type) on the DBC Alumina, finalizing the fabrication of a two-couple TE module serving as a proof of concept for the utilization of recycled Si-kerf in TE applications

Materials were characterized using X-ray diffraction, electron microscopy, X-ray energy dispersion spectroscopy (EDS), laser flash analysis and direct-current four-probe measurements. TE legs where characterized with scanning-probe contact resistance measurements and EDS imaging, while devices where modelled in COMSOL Multiphysics® and characterized in a TE module testing apparatus.

Acknowledgments

This work is part of ICARUS project funded by Horizon 2020 research and innovation programme under grant agreement No 958365. ICARUS project aims to process and refine secondary raw materials from silicon PV manufacturing.

PART V
POSTERS

P01

First-principles study of structural disorder, site preference, chemical bonding and transport properties of Li-doped tetrahedrites

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Keywords: thermoelectric material, *ab initio* DFT calculations, tetrahedrites, electronic structure calculations, QTAiM topological analysis, WIEN2k

Tetrahedrite-based ($Cu_{12}Sb_4S_{13}$) materials [1] are candidates for good thermoelectric generators due to their intrinsic, very low thermal conductivity and high power factor [2]. One of the current limitations is virtual absence of tetrahedrites exhibiting n-type conductivity. In this work, first-principles calculations are carried out to study Li-doped tetrahedrite, $Li_xCu_{12}Sb_4S_{13}$ with possibility of predicting n-type material in mind.

Different concentrations and modifications of the structure are investigated for their formation energies, preferred site occupation and change in local environment around dopants. Li atoms, unlike Mg ones [3], more likely will occupy 24g than 6b site. Moreover, according to our theoretical results, Cu(12d) vacancy introduced into the structure should stabilize the whole structure. Introduction of dopant or excess copper into 6b/24g sites display different effect on nearby rattling Cu(2) atom. Topological analysis shows that tetrahedrite exhibits ionic, closed shell bonds with some degree of covalency. Majority of the bonds weakens with increasing content of Li; structure becomes increasingly less stable, which is also expressed by global instability and bond strain indexes. Achieving n-type conductivity was predicted by the calculations for structures with $x > 2.0$, however increasing enthalpy of formation and lack of stability might suggest the limit of solubility close to $x = 2$ and difficulties in obtaining those experimentally.

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Identification of dominant scattering mechanism and its influence on transport properties of half-Heusler compound

P02

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Keywords: half-Heusler, interstitial, anti-site disorder, scattering, annealing, SPB model

Ternary inter-metallic half-Heusler (HH) compounds (XYZ) with 18 valence electron count have revealed interesting thermoelectric (TE) properties pertaining to their narrow bandgap and flexibility in undergoing doping. Despite having good electronic transport properties, such materials oftentimes have inherent atomic disorders appearing in the HH structure arising during the synthesis processes. There is an ongoing controversy among the literature reports as to the most dominant disorders that is influencing the transport in such materials. Therefore, one needs to understand the underlying scattering mechanism in order to fine tune the material properties for its widespread application. The key focus of this work is to recognize these disorders and their influence on the transportation properties based on both theoretical (first-principles) and experimental perspectives. Additionally, this work examines how the annealing duration affects these disorders. Rietveld analysis on XRD data reveals that some of the disorder is still present even after 10 days of annealing. In order to decipher the types of scattering present in the compound single parabolic modelling of experimental transport parameters is employed. On exploration of mobility (μ) from theoretical calculations, a high dependence on scattering due to ionized impurity, and grain boundary is observed. With the incorporation of disorder (interstitial and anti-site), the ionized impurity becomes the most dominant scattering mechanism, limiting the total μ of the compound. This research upholds the main imperfections found in the widely studied ZrNiSn compound and calculates the reduction in such defects after annealing by analyzing the μ, scattering lifetime and comparing it with theoretical models.

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P03

A multiband fitting technique for analyzing temperature dependent electronic band structure of thermoelectric materials

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Keywords: electronic band structure, multi-band fitting technique (MBFT), thermoelectric, least square minimization, transport properties

The study and estimate of the Electronic Band Structure (EBS) parameters is vital for understanding the charge transport behaviour in thermoelectric (TE) materials. Experimental methods such as Cyclotron Resonance, ARPES, UV/IR Spectroscopy etc. can be used to calculate EBS properties of materials. However, the applicability of these techniques is limited due to difficulties associated with the sample preparation. Theoretical approaches based on *ab-initio* methods (such as Density Functional Theory (DFT) etc.) overcome this problem. However, theoretical predictions of temperature dependent EBS parameters have met limited success till date. Thus, the preferred approach for studying EBS details in TE materials is based on semi-classical models which utilize experimental charge transport measurements. In this work, we propose a modified refinement-based approach (Multi-Band Fitting Technique (MBFT)) which can handle higher number of variables compared to the existing solution-based techniques. In the MBFT method, electrical conductivity ($\sigma(T)$), Seebeck coefficient ($S(T)$) and Hall coefficient ($R_H(T)$) data are taken as input and the EBS variables are refined to minimize a residual function (*R-factor*) using the least square minimization technique. Trials were conducted on elemental Si and Mg_2Si samples. Excellent match with the reported band masses and temperature dependent band-gaps was obtained for Si. For Mg_2Si compositions, information about the upper conduction band, inter-band separation and the valence band were obtained from n-doped samples. The details of the MBFT technique along with the results obtained for Si and Mg_2Si will be presented.

Complex Fermi surface responsible for high zT

P04

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Keywords: transport distribution, fermi surface, electron transport, zT, modelling

Electron transport properties can be expressed in terms of the generalized transport coefficients:,

$$L^{(\alpha)}(\mu,T) = q^2 \int \sigma(\varepsilon,T)\,(\varepsilon-\mu)^{\alpha}\left(-\frac{\partial f^{(0)}(\varepsilon;\mu,T)}{}\right)d\varepsilon,$$

which in turn depend on the transport distribution:

$$\sigma(\varepsilon,T) = \int \Sigma_b\, v_{b,k}\, \Phi\, v_{b,k}\, \tau_{b,k}\, \delta(\varepsilon-\varepsilon_{b,k})\, dk/8\pi^3.$$

As a general rule of thumb, the transport distribution should increase rapidly and much close to the band gap for a high zT [1]. The transport distribution again depends on the density of states (DOS) and the electron group velocity of each state. A band with low effective mass will have high velocity but contribute less to the DOS and vice versa. To achieve both at the same time we need either many bands contributing states or high valley degeneracy [2].

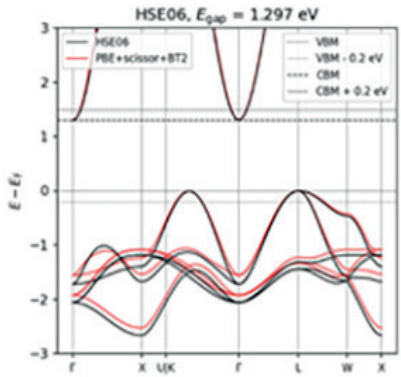

Fig. 1: HSE06 band structure of FCC material

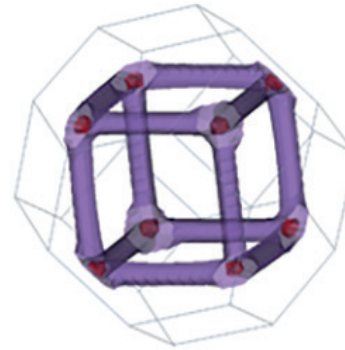

Fig. 2: Fermi surface of valence band at E = -0.1eV

While most materials have a few degenerate Fermi pockets in k-space, some have complex, extended Fermi surfaces close to the band gap, giving a large number of states. Inspection of the Fermi surface show that the valence band maximum exists in an extended volume of the Brillouin zone, see **Fig. 2**. This complex Fermi surface combined with a low lattice thermal conductivity result in a predicted zT of ~3.5 at 800K. The band structure and zT reported here is based on the band gap of a HSE06 calculation, see **Fig. 1**, as the material is semi-metallic at a PBE level.

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P06

High-throughput and accurate prediction of the thermal and electron transport properties of large chemical spaces accelerated by machine learning

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Keywords: thermal conductivity, high-throughput, modelling, optimization, *ab-initio*

The optimization of new and more efficient thermoelectric, TE, materials has been hindered by the interdependence of electronic and phonon transport properties and the multitude of variables that affect the thermoelectric figure of merit, *ZT*. Traditional approaches involving time-consuming and expensive synthesis and characterization processes are not practical for exploring sets of materials and optimizing properties that depend on numerous variables. This work employs a high-throughput framework that combines ab-initio calculations and machine learning to chart systematically and accurately the thermoelectric properties of large chemical spaces [1-2].

In addition to examining the already well-established temperature dependence of *ZT*, the study investigates the effect of carrier concentration and polycrystalline average grain size on *ZT*. By calculating the mean free paths of electrons and phonons, the study demonstrates the potential for automating and rationalizing the optimization of TE materials through nano-structuring.

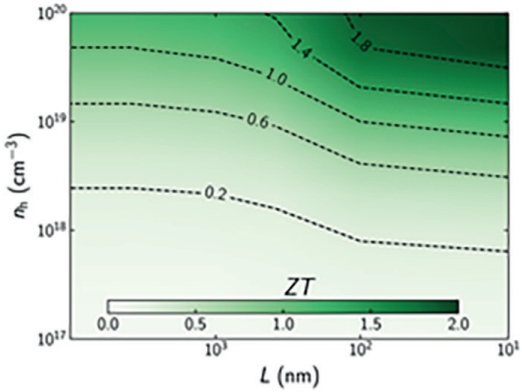

Fig. 1: Thermoelectric figure of merit, *ZT*, dependence on average grain size, *L*, and carrier concentration, *n*, at 700 K for a *p*-type chalcopyrite.

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Advancements and challenges in self-powering wearable technology: spotlight on energy collection via micro-power thermoelectric generators

P08

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Keywords: thermoelectric generators, wearables, IoT, microfabrication, flexible

The emergence of self-sustaining wearable sensor nodes and electronic devices has opened up countless opportunities for seamlessly incorporating health and wellness monitoring into people's everyday lives. Significant strides have been made in energy efficiency and harvesting, as well as in optimizing device form factors and expanding functionalities. A self-sustaining wearable system typically includes sensors, an energy harvesting mechanism, a power management unit, energy storage capability, a data transmission element, and a data processing platform. We will explore recent research and prominent challenges related to the components of a self-sustaining wearable system, with a special focus on thermal energy harvesting. A concise summary of fundamental concepts is complemented by an evaluation of several systems designed for wearable applications. Simultaneously, we will investigate current research and industrial efforts to develop a network of self-sustaining wearable devices that can continuously operate for extended periods by harvesting heat from accessible sources. Specifically, we will examine the use of micro-power thermoelectric generators, a burgeoning area with numerous innovative applications, such as self-sustaining wearable devices for consumers, ongoing health and performance monitoring devices for personal and clinical use, and sensors and communication equipment installed on pipelines and various industrial machines that necessitate constant, hassle-free monitoring.

Despite the strong push for self-sustaining wearable systems, the performance of micro-power thermoelectric generators (TEGs) produced thus far may not always meet the power demands of sensors and electronics that must operate continuously with high reliability. In some cases, TEGs can fulfil the power requirements of low-power sensors, while in others, they may fall short. Factors contributing to these devices' inefficiencies include incompatibility with cutting-edge thermoelectric materials, concessions made in device design due to the resolution and throughput of deposition techniques, and significant thermal parasitic resistances caused by supporting materials in their packaging. We present our findings that emphasize some challenging trade-offs encountered during the fabrication of rigid and flexible modular devices that can be integrated with a shirt and a smartwatch.

Acknowledgments

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P09

Effect of PEDOT:PSS and bismuth tellure on electric potentials in the thermoelectric generator

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Keywords: thermoelectric generator, seebeck effect, thermoelectric, thermoelectric generator system, comsol multiphysics, heat transfer

Nowadays, due to high population growth, diminishing energy resources, rising environmental pollution and the effects of global warming, living conditions are becoming more difficult. Therefore, scientists have focused on thermoelectric generators, which have the ability to collect energy that we can use the already existing energy [1-2]. In this context, the effects of different parameters on the electrical potential in a thermoelectric generator were investigated in this study. First of all, thermoelectric generator design (TEG) was carried out using the Comsol Multiphysics 6.0 design and analysis program. The designed generator consists of two pairs of thermoelectric couples with 4 legs. The legs are defined as P-type and N-type with the values entered into the program. In the study, the materials of the p and n type legs were chosen as the first variable. Insulating upper and lower blocks were determined as PDMS (Polydimethylcycloxane), and conductive lower and upper blocks were determined as Silver (Ag). The first material is Bismuth Tellurium as the P-Type and N-Type leg material, which is widely used in the market, and the other leg material is 5% Pedot:PSS, which is the material we have produced. Considering that the thermoelectric couples are placed on the skin, the contact surface temperature was accepted as 36 °C. The ambient temperature is determined as 10 °C, 20 °C, 30 °C, 40 °C. These temperature values were applied one by one for both leg materials.The aim of this study is to see the effect of different leg materials and the temperature difference applied while using these materials on the electrical potential. As a result of the study, the most optimum module was selected. In our previous Comsol analysis studies, it was observed that the leg length also increased the electrical potential value. For this reason, after the optimum module was selected, the leg lengths were also changed. The leg lengths were changed as 1.5mm, 1.25mm, 1mm, 0.75mm, 0.5mm and the electrical potential values were checked.

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Thermoelectric algebraic representation: equations and inequalities for simple thermoelectric device design

P10

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Keywords: thermoelectric, efficiency, integral equation, thermoelectric algebra, thermoelectric inequality

Thermoelectric devices enable direct energy conversion between heat and electricity via the Seebeck and Peltier effects. While the figure of merit ZT, based on a single parameter efficiency theory, has guided material discovery and evaluation, it is difficult to apply this theory for device design due to compatibility issues and temperature-dependent thermoelectric properties. In this presentation, we introduce a thermoelectric representation using algebraic equations and inequalities for material and device performance prediction, going beyond the constant-property model (CPM), ZT, and compatibility factor.

Starting from the thermoelectric differential equation for a one-dimensional thermoelectric power generator module, we derive the one-dimensional thermoelectric integral equations for temperature and temperature gradient [1,2]. Then, we generalize the CPM and extend it to the constant Seebeck coefficient model, generalizing the definition of average ZT [3]. It is also found that a proper temperature integral can be applied for segmented-leg device design.

Next, observing the transformation invariant property of temperature-dependent curves while maintaining average device parameters, we develop a multiple parameter theory for thermoelectric conversion, which we call the three thermoelectric degrees of freedom theory [2]. With numerical validation of the theory, we formulate an analytical approach describing thermoelectric performance at a device level, heat current at boundaries, power generation, and thereby thermoelectric efficiency. The theory is further extended for P-N leg pair devices with interfacial thermal and electrical resistances, so that it can be used for device performance even with non-Dirichlet boundary conditions.

We also derive several thermoelectric inequalities for device performance description. In the case of a single-leg device, where only one type of thermoelectric material is used for the device, it is found that the total performance of the single-leg device is approximately bounded by 1/4 of the single-leg ZT.

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The stability and role of defects in Bi_2O_2Se

P11

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Keywords: Bi_2O_2Se; defects; DFT calculation; transition metal substitution

Bi_2O_2Se is an emerging semiconducting, air-stable layered material in the next-generation high-speed and low-power electronics, optoelectronics, spintronics and thermoelectrics. One of the prominent features is the exceptionally high in-plane Hall mobility [1]. Electronic structure calculation revealed that most of the electron density close to Fermi level is spread in the Se-plane along xy-direction, see the **Fig. 1**. Therefore, it is anticipated that electronic transport is mediated mostly by Se layers while Bi_2O_2 layers are insulating.

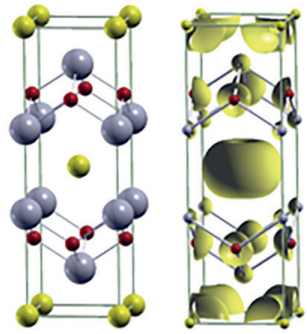

Fig. 1.:
Structure of Bi_2O_2Se (Bi: grey, O: red, Se: yellow) and electron density close to the Fermi level

It has been demonstrated that the role of defects for the properties of the real material may be essential [2,3,4]. Since Se vacancy has been identified as the most likely among the various possible defects, the transport properties of Bi_2O_2Se are expected to be sensitive to the presence of defects. The situation becomes more complicated for the substituted phases, where the interplay of substitutions and intrinsic defects inherent to the Bi_2O_2Se structure must be taken into account.

In our work we have studied the relative stability of defects by electronic structure calculations in substituted $Bi_2O_2Se$and their influence on the band structure near the Fermi level. We have focused on the substitution of 3d transition metals in the Bi_2O_2 layers. We have shown that the substituted metal alters the relative stability of individual defects, so that in some cases, the increased defect formation is comparably important to the resulting properties as the effect of the substitution itself in the ideal structure.

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Investigating the transport properties of CrN: Insights into phonon thermal conductivity and scattering

P12

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Keywords: CrN, antiferromagnetic semiconductor, magnon-phonon interaction, thermal conductivity, first-principles calculation

In this presentation, we focus on the transport properties of CrN, a semiconducting material with thermoelectric potential and widely employed in ceramic applications. The magnetic CrN exhibits a simultaneous magnetic and structural phase transition at the critical temperature T_N = 280 K [1]: below T_N, CrN adopts an antiferromagnetic phase with an orthorhombic crystal structure, while above T_N the paramagnetic phase is characterized by a cubic structure.

Of particular interest is the behaviour of the phonon-dominated thermal conductivity, κ(T), which displays dramatically different temperature dependencies on either side of the phase transition [1,2]. In this respect we note that standardly nonmagnetic materials exhibit a decline in phonon-dominated thermal conductivity by 1/T at higher temperatures due to temperature induced increasing phonon-phonon interactions.

However, CrN exhibits very low and nearly constant thermal conductivity κ(T) above T_N, setting it apart from its nonmagnetic counterparts. In addition, there is a remarkable and sudden drop in κ(T) from 6 $Wm^{-1}K^{-1}$ to 2 $Wm^{-1}K^{-1}$ at T_N, with a lack of clear explanation so far. We associate this unexpected behaviour of the thermal conductivity at T_N with the anomalous shortening of phonon lifetime in the paramagnetic phase, caused by the spin-lattice interaction above the magnetic ordering temperature [3].

In order to model the thermal conductivity, we have performed first-principles based calculations of the phonon thermal conductivity, accounting for various scattering mechanisms. Our analysis includes the effects of phonon-phonon (Umklapp), impurity and grain-boundary scattering. By adjusting the boundary-scattering characteristic mean free path, the grain-size of the ceramics showing T_N = 283 K was estimated as ~ 100 nm, which value is consistent with the recently reported data [4]. To reproduce the low temperature data, the influence of porosity of CrN ceramics was also considered.

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P13

First-principles calculations of thermal properties in the triangular lattice antiferromagnet $AgCrSe_2$

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Keywords: density functional theory, delafossites, antiferromagnet, lattice thermal conductivity, magnon-phonon interaction

In this study, we present pioneering first-principles calculations of the thermal properties in $AgCrSe_2$, employing density functional theory. $AgCrSe_2$ is a layered triangular lattice system characterized by the absence of inversion symmetry. Below the critical temperature $T_N = 32K$, a cycloidal coupling is observed within the $CrSe_2$ layer at a small angle, while adjacent layers exhibit antiferromagnetic coupling with a slight canting along the c-axis.[1] Building upon previous studies that reported the thermal conductivity measurements of $AgCrSe_2$ [2], our investigation aims to compare our phonon calculations with experimental results and further deepen our understanding of its thermal behaviour. Furthermore, we extend our analysis to predict the thermal properties of its sister compound. By elucidating the intricate interplay between crystal and magnetic structures in $AgCrSe_2$, our findings provide valuable insights for the design and optimization of advanced thermoelectric materials.

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Establishing a protocol for the approval of thermoelectric materials used in biomedical applications

P15

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Keywords: thermoelectric; eddy; biomedical; dental; amalgam

It is a commonly acknowledged principle in thermoelectric science that all materials display some degree of thermoelectric behaviour. It should therefore be considered incumbent upon those working in the field of biomedical science to be aware of the thermoelectric behaviour of any material, or any assembly of materials, intended for placement either within or at close proximity to the human body.

In particular, metals, mixtures of metals, and dissimilar metals in contact with each other may require careful attention in this respect in order to prevent the unintentional and possible harmful effects arising in bodily tissue as a result of thermoelectric activity.

However, it has been established that in certain areas of biomedical practice there is little or no appreciation of the thermoelectric effect.

This poster presentation highlights the requirement for the establishment of a scientifically rigorous protocol which can be implemented to ensure the thermoelectric compatibility of biomedical devices.

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P16

Novel methods of scattering parameter analysis for BiSbTe thermoelectric materials under constant temperature without Hall measurements

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Keywords: bismuth antimony telluride, mechanical alloying, Lorenz number, scattering parameter, reduced Fermi energy, phonon thermal conductivity

The transport properties of a conductor including thermoelectric materials depend not only on the concentration n of the charge carrier but also on the mean free path length between collisions. The Lorenz number L is given by the following expression on the basis of a one-electron approximation or single parabolic band model [1]:

$$L = (k_B e)^2 \left\{(1+\gamma)(3+\gamma)F_\gamma(\eta)F_{\gamma+2}(\eta) - (2+\gamma)^2 F_{\gamma+1}(\eta)^2\right\} / (1+\gamma)^2 F\gamma(\eta)^2 \quad (1)$$

where η is the reduced Fermi energy (= E_F/k_BT, E_F: Fermi energy, k_B: Boltzmann's constant), e is the electric charge, and $F\gamma(\eta)$ is the Fermi integral. The scattering parameter γ is representative of collision effects. The scattering parameter is an important parameter for understanding thermoelectric properties. The reduced Fermi energy η is usually found from the experimental values of the Seebeck coefficient a as follows:

$$\alpha = \pm k_B e \left((2+\gamma) F_{\gamma+1}(\eta) - \eta\right) / (1+\gamma) F_\gamma(\eta) \quad (2)$$

In the present study, the effects of the addition of lead as one of the multiple dopants in p-type $Bi_{0.3-x}Sb_{1.7}Te_{3.0+x}Pb_y$ (x = 0 – 0.01, y = 0 – 0.003) fabricated by mechanical alloying followed by hot pressing (MA-HP) were investigated [2]. If the phonon thermal conductivity is constant regardless of the doping amount, the L was evaluated to be 0.73–1.18 × 10−8 W $S^{-1}K^{-2}$. The γ and η were estimated by using eq. (1) and (2), measured a and the estimated L at room temperature. The γ was approximately from -1.06 to -0.60 and showed a mutual effect of acoustic and optical phonon scattering. The relationship between ZT and η was clarified, and the optimum η = -1.25 at ZT = 1.26 at room temperature.

From these results, it was found that the γ obtained by MA-HP is in the region where the γ cannot be analyzed by the Hall effect. This analysis method can also be widely applied to other thermoelectric materials to evaluate the transport properties of a conductor.

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Experimental estimation of the electrical conductance of heterostructured Ge nanowires for thermoelectrical applications

P17

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Keywords: electrical conductivity, heterostructuration, nanowires, scanning thermal microscopy

Nanostructuration is one of the various routes to improve the thermoelectric efficiency of materials at room temperature. It has been theoretically predicted and experimentally demonstrated that semiconductors such as Si, SiGe or Ge could enhance their figure of merit ZT through nanostructuration, in particular in the case of nanowires (NWs). Nevertheless, in addition to nanostructuration, it has been shown, using a 3ω-Scanning Thermal Microscopy (3ω-SThM) imaging set-up, that the creation of heterostructures along the NWs [1] could constitute another way to introduce new scattering mechanisms of phonons and then to reduce again their thermal conductivity [2].

However, it is then necessary to evaluate the heterostructured NW electrical properties to verify if the reduction in thermal conductivity is not accompanied by a reduction in electrical transport. The SThM set-up has then been upgraded to simultaneously image the thermal and electrical transport properties on individual NWs [3]. Among the different parameters that can be measured, the sample conductance enables to evaluate the electrical conductivity.

Different samples, either heterostructured or not, made of Ge NW arrays embedded in a matrix are being studied. A non heterostructured NW sample is used as a reference and its electrical conductance (**Fig.1**) is compared with the one of heterostructured NWs, which differ from each other by their diameter. Finally, we can then conclude on the influence of heterostructuration on the electrical conductivity of Ge NWs.

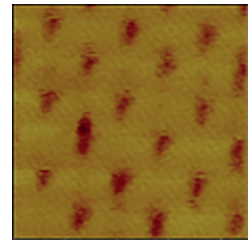

Fig. 1: electrical conductance image (9 µm × 9 µm) of a Ge NWs array sample

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P18

Characterization and Seebeck coefficient of mesoporous silicon: effect of nanographene incorporation

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Keywords: mesoporous silicon, electrochemical etching, Seebeck coefficient, homemade ZT-meter

As derived from silicon substrate, meso-porous Si could be a competitive candidate for many thermoelectric applications for micro-systems namely due to the huge decrease of its intrinsic thermal conductivity. As reported in the literature, this can offer a higher figure of merit as well as a more significant efficiency for energy harvesting at the microscale level at room temperature. In addition, to consider the electronic transport that is lowered by the fabrication process, a graphenisation step is investigated [2] both on the structural and thermoelectric behavior of the mesoporous complex Si matrix.

Porous silicon membrane is obtained by electrochemical etching process from an electrolytic solution of hydrofluoric acid and ethanol. Depending on numerous parameters (porosity, pore size distribution, porous thickness...) the Seebeck coefficient will be experimentally investigated accordingly to key process parameters and correlated to the membrane morphology and structural characteristics.

Using a new home-made thermoelectric device specifically designed for porous membranes will make possible to evaluate the Seebeck coefficient in the range of 30 to 70 °C [3]. Systematic investigation of graphenized and non-graphenized membranes is conducted to determine the contribution of the graphene in the thermoelectric properties, especially on Seebeck coefficient (S) and electrical conductivity (σ).

Thanks to these thermoelectrical properties, it will possible to evaluate the power factor (σS_s) for carbon coated and uncoated mesoporous matrix.

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Lattice dynamics study of thermoelectric cubic $SrSi_2$ by Raman scattering experiments and ab initio calculations

P19

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Keywords: silicides, lattice dynamics, Raman, ab initio calculations, pressure

Thermoelectric materials (TEM) attract high interest from many fields of science as a potential green energy resource. For a few decades the TEM community has been on the quest for more efficient and environment friendly compounds. At present, the drawback of the best-performing TEM compounds is their toxicity, rareness, and/or costs of the chemical elements they are synthesized from. For this reason, silicides have attracted high interest because they are made of abundant, cheap, and non-toxic elements.

Among silicides, cubic $SrSi_2$ has attracted the attention because of its good thermoelectric properties at the vicinity of the room temperature. A ZT of 0.15 was obtained for undoped $SrSi_2$ at 300 K [1] and ZT as large as 0.4 was reached for yttrium-doped $SrSi_2$ at 300 K [2] thanks to its moderate thermal conductivity (κ = 4–5 W/m.K) [1-2] compared to most of the silicides [3] and despite its simple cubic crystal structure containing 12 atoms. This suggests higher anharmonicity in $SrSi_2$ than in other silicides. Recent theoretical works suggested that cubic SrSi2 could be a topological Weyl semimetal [4] and the presence of quadratic double-Weyl phonons [5], making this material very attractive for topological science. However, despite the interest of this material, until now there is no experimental study of the lattice dynamics and the DFT study in ref. 5 was limited to the phonon dispersion curves of $SrSi_2$. We have therefore began to study the lattice dynamics of $SrSi_2$ both theoretically and experimentally.

In the present work, we present a combined pressure dependent Raman scattering study and ab initio study of the lattice dynamics of cubic $SrSi_2$. We find 5 of the 8 Raman-active modes predicted by the theory, but one of the missing mode is overlapping another observed mode. Good agreement is found for the frequencies and the calculated Grüneisen parameters follow qualitatively the experimental trend. We notably show that the phonons in the intermediate range 150–300 cm^{-1} have low Grüneisen parameters (less than 1) whereas moderate Grüneisen parameters (above 1) were found above 300 cm^{-1}. However, we found that the low energy optical mode predicted at 7.5 meV, which is optically silent, has large Grüneisen parameter (about 2.5) and its interaction with the acoustical phonons could explain the rather low lattice thermal conductivity of $SrSi_2$ compared to most of the silicides.

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P20

In praise of the humble four point probe: Characterisation for scale up

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Keywords: characterisation, measurement, electrical conductivity, scale up, industry

The thermoelectric field has seen strong academic research but has struggled to commercialise these results beyond the well-established bismuth telluride based devices. To enable larger scale adoption of new thermoelectric materials, it is necessary to be able to reproducibly make larger quantities of thermoelectric materials. This reproducibility requirement means that is it important to rapidly and non-destructively characterise these materials.

We find that the electrical conductivity often shows the largest and most easily measurable variation in material properties. We discuss how the humble 4 point probe is well suited to these types of measurement task, enabling rapid, non-destructive testing across a range of geometries. In addition it allows a range of potential further analysis including:

– coarse mapping of electrical properties
– improved understanding of anisotropy
– can be developed into a 6 probe method to enable puck level electrical contact testing

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Thermal interface resistance analysis of thermoelectric devices by using thermoreflectance microscopy

P21

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Keywords: interface, thermal resistance, thermoreflectance, microscopy, thermography

Thermoelectric devices have interfaces between the thermoelectric material, metallic electrodes, and barrier layers. [1] When the temperature gradient is applied for power generation, the thermal resistance of the interfaces lowers the actual temperature difference across the thermoelectric material, leading to a lower efficiency than expected. Therefore, it is important to characterize and reduce the thermal resistance for thermoelectric devices. While the contact-based thermometries, such as thermocouples, are widely used, they suffer from additional thermal resistance that arises at the contacts. [2] Also, it is difficult to map the temperature distribution near the interface simultaneously. These limitations challenge accurate measurement and understanding of the interfacial characteristics of devices under operating conditions. This study uses non-contact optical thermoreflectance microscopy (TRM) for temperature mapping of Bi-Te thermoelectric devices. The TRM has high spatial resolution of sub-micron and temperature resolution of 1 K. [3,4] We characterize the temperature distribution of the a Bi-Te thermoelectric material and adjacent metal electrode while applying electrical current. We believe that the quantitative information of temperature evolution and thermal loss of the thermoelectric device will help realize the high power efficiency of thermoelectric devices.

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P22

A cross-plane Seebeck measurement system for sub-µm-thick films

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Keywords: thin films, Seebeck coefficient, SThM, cross-plane measurement, 2D materials

Transport properties of a material is essential for its proper utilization and further expansion of application fields. In the case of highly anisotropic materials with 2D-layered structure, the transport properties can significantly differ for both in-plane and cross-plane direction. However, the measurement of transport properties in the cross-plane direction, particularly for sub-µm-thick films, is rarely adopted due to substrate effects and probe-tip damage. In this study, we present an AFM-based system to measure cross-plane Seebeck coefficient for sub-µm-thick films. A commercial AFM apparatus (TT-AFM, AFM Workshop) was equipped with a custom heater, scanning thermal microscopy (SThM) module, conductive metal probes and nanovoltmeters. A qualitative assessment of the system's temperature sensing capability was performed by spatial temperature mapping of exfoliated Bi-Te specimens containing well-defined sub-µm steps. The system was then calibrated by measuring temperature and Seebeck voltage of a certified reference material (SRM 3451, NIST).

Test and simulation study for μ-TEGs based on screen-printed PbSe QDs

P23

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Keywords: lead selenide; quantum dots; screen printing; μ-TEG; COMSOL software

The characterization of thin film micro-thermoelectric generators (μ-TEG) is still challenging, and simulation studies can enhance the understanding of the experimental results [1]. Here, we propose a screen-printing approach as an easy to scale-up and industry-relevant technology to fabricate thin film μ-TEGs. PbSe quantum dots (QDs) with spherical morphology and monodisperse size of 13 ± 1 nm were successfully synthesized by the colloidal heating-up method. Next, the PbSe QD ink was formulated, and used to manufacture the TE thin films through screen-printing followed by annealing. Notably, the phase composition, size, and morphology of the PbSe QDs were maintained after annealing at 600 °C (**Fig. 1a**) [2]. The characterization of the PbSe thin films was performed and a Seebeck coefficient and electrical conductivity of 58 μV K^{-1} and 50 S m^{-1} were obtained, respectively, under room temperature conditions. Several geometries were explored with 6 pairs of screen-printed *p*-type PbSe QDs and Ag commercial paste metal contacts. Device performance (**Fig. 1b**) was compared with simulation results through the COMSOL software.

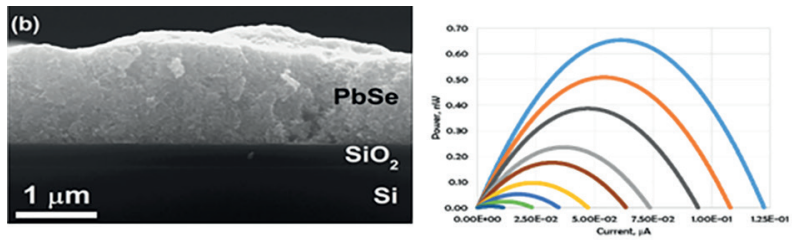

Figure 1: Cross-sectional (a) SEM images of the PbSe QD thin film, fabricated through screen printing followed by rapid heat treatmen. Power vs current (b) representation of 6 pair legs μ-TEG PbSe QD reaching P_{max} of 0.65 nW at ΔT = 44°C for 2.5 cm legs length.

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P24

Hierarchically designed tetrahedrite with reduced thermal conductivity facilitated by all-scale phonon scattering

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Keywords: seebeck coefficient, electrical resistivity, thermal conductivity, Raman spectroscopy, X-ray photoelectron spectroscopy

Tetrahedrite, $Cu_{12}Sb_4S_{13}$, an eco-friendly thermoelectric material with earth-abundant and low-cost constituents, has drawn worldwide attention. The thermoelectric performance of this material has been enhanced by various groups worldwide by focusing on the enhancement of the Seebeck coefficient via the substitution of higher valence substituents at the Cu/Sb site. Such substitutions reduce the carrier concentration and hence the electronic thermal conductivity. These samples also show reduced lattice thermal conductivity owing to the alloy scattering/mass difference scattering. However, in most cases, the reduction of total thermal conductivity and the average value of total thermal conductivity is minimal. The reason for the above observation is that the alloy scattering targets only the low-to-mid wavelength of phonons but a majority of mid-to-long wavelength phonons, which carry the majority of the heat, remain unaffected. Our findings show that via solid-state synthesis and sample processing through appropriate conditions of high-energy ball milling, the average value of total thermal conductivity of pristine tetrahedrite($Cu_{12}Sb_4S_{13}$) was reduced to ~ 0.83 W m^{-1} $K^{-1,}$ which is 43% lower as compared to the literature reported value 1.5 W m^{-1} K^{-1} [ACS Appl. Mater. Interfaces 2021, 13, 25092−25101]. This work demonstrates a simple procedure to enhance the average figure-of-merit(zT_{avg}) in tetrahedrite thermoelectrics by introducing all-scale hierarchical scattering centers.

Mechanical properties characterization of thermoelectric materials

P25

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Keywords: mechanical property, young's modulus, poisson's ratio, bending test, impulse excitation technique

Since thermoelectric devices are applied to thermoelectric power generation systems and are subjected to repeated thermal loads during use, it is very important to evaluate the reliability of thermoelectric devices. Since Bi_2Te_3-based alloys have a long history as direct energy conversion materials, their mechanical properties - tensile, compressive, hardness, fracture toughness, thermal shock and fatigue life - have been studied early on [1].

Among the above mechanical properties, Young's modulus, which represents the elastic properties of a material, is one of the most commonly known mechanical factors, describing the elastic response of a material to uniaxial loading (tension or compression) and evaluated as a linear ratio of the increase in stress with increasing displacement of the material.

In most studies, it has been evaluated by measuring the speed of sound to investigate the composition dependence of elastic properties [1]. The ASTM D 2845 method of measuring the propagation time of transverse and shear waves has been used to evaluate brittle materials, which are often difficult to produce standard specimens.

In this study, thermoelectric materials manufactured by zone melting, sintering, and extrusion processes were selected to produce specimens for mechanical property measurement, and mechanical properties were measured by bending test (ASTM C1161-13) and impulse excitation technique (ASTM E1876).

The mechanical property values derived from the test methods are elasticity, shear modulus, and Poisson's ratio. The elastic modulus of the n-type ranged from 28.78 to 47.99 GPa, the shear modulus from 14.84 to 19.65 GPa, and the Poisson's ratio from 0.18 to 0.29, while the p-type ranged from 34.96 to 53.33 GPa, 11.10 to 21.08 GPa, and 0.22 to 0.39, respectively.

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Thermoelectric properties of doped SnSe alloys

P26

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Keywords: polarity switch, direct synthesis, SnSe alloy, electrical conductivity, Seebeck's coefficient

Material selection for thermoelectric modules and generators always poses a significant challenge. Usually alloys with a high percentage of doping element must be used to achieve different semiconductor polarity. This introduces mechanical stresses to the system due to the varying thermal expansion rate of this material combination. It has been proven that semiconductor polarity of SnSe alloy can be changed with small amounts of Sb. However, to achieve the polarity change the material needs to be monocrystal [1].

This work describes modified synthesis process of SnSe alloys with Bi and Ag as dopants. This direct synthesis is scalable and more cost effective. Polarity switch in synthesized materials occurred in similar regions as when Sb was used. Electrical conductivity of Bi and Ag doped materials is comparable with monocrystal Sb doped materials while Seebeck's coefficient in N region is slightly lower. Doping elements had no noticeable effect on crystal lattice of material and only small shift in lattice parameters was observed. Significant preferred orientation was observed during crystallography analysis. This was attributed to the material tendency to form and align in layers which was observable even by naked eye and confirmed by an electron microscope.

We have in-house developed and thoroughly calibrated apparatus for determining Seebeck's coefficient and electrical conductivity of thermoelectric materials. This method is easily reproducible, reliable and capable of handling many shapes of solid samples. Method for determining electrical conductivity is based on the work of De Boor and is capable of obtaining real values of electrical conductivity for rod and disk shaped objects [2]. This method was also the base for determining Seebeck's coefficient. The instrument was modified with different modules to incorporate determination of some different physical material properties at different spots on the samples.

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A self-independent binary-sublattice construction in Cu_2Se thermoelectric materials

P27

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Keywords: cuprous selenide, ordered cooper fluctuation, binary-sublattice constructions, first-principle calculations, transmission electron microscopy

Among the state-of-the-art excellent thermoelectric materials, Cu_2Se has been widely studied due to its high performance and environmentally friendly nature compared to lead-based thermoelectric materials, in addition to its lower cost than tellurides. It is discovered that Cu_2Se shows extraordinary "liquid like" behavior of copper ions and reaches a zT of 1.5 at 1000 K, among the highest value for bulk material. The atomic-scale structure of cuprous selenide room temperature phase (α-Cu_2Se), which plays an important role in understanding the mechanism of its high thermoelectric performance, is still not fully determined.

Here, direct observation with atomic-scale resolution is realized to reveal the fine structure of α-Cu_2Se via spherical-aberration-corrected scanning transmission electron microscopy. It is observed to be an interesting self-independent binary-sublattice construction for Cu and Se in α-Cu_2Se, respectively, which shows a variety of ordered copper fluctuation structures are embedded in a rigid pseudo-cubic Se sublattice. Ordering of Cu uses a variety of configurations with little energy difference, forming considerable amounts of "boundaries," which may lead to ultrastrong phonon scattering and α-Cu_2Se exhibits an extremely low lattice thermal conductivity of around 0.42 W m^{-1} K^{-1} at 300 K. Furthermore, density functional theory calculations indicate that the electronic structures are mainly determined by the rigid Se face-centered cubic sublattice and not sensitive to the various copper fluctuations, which may guarantee the electron transfers with large carrier mobility. The self-independent binary-sublattice construction is speculated to enhance phonon scattering while still maintaining good electrical transport property. It is also illustrated that α-Cu_2Se is a semiconductor with an indirect bandgap of 1.21 eV, which is in good agreement with the optical experiments. This work provides new critical information for further understanding the possible correlation between the specific structure and thermoelectric performance of α-Cu_2Se, as well as designing new thermoelectric materials.

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Development and evaluation of bismuth antimony telluride-PEDOT: PSS hybrid thermoelectric fiber using co-sputtering

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Keywords: thermoelectric fiber, PEDOT:PSS, bismuth antimony telluride, wet-spinning, co-sputtering

Wearable thermoelectric generators that use the Seebeck effect to convert the temperature difference between the body and the environment into electrical energy show great promise for powering wearable devices. This technology efficiently converts thermal energy into electricity, with no noise or vibration, and is eco-friendly. The textile-based wearable thermoelectric generators, made with thermoelectric fibers, can be woven without bonding materials, which enhances their stability and comfort when worn. In addition, because the woven wearable thermoelectric generators have flexibility and elasticity, they enable smooth heat exchange with curved skin, enhance the thermoelectric performance.

PEDOT:PSS(poly(3,4-ethylenedioxythiophene):poly(styrene-sulfonate)) has low thermal conductivity, high electrical conductivity and is easily processed into fibers.[1] However, its Seebeck coefficient of 14 ~ 19 μV/K restricts its thermoelectric power generation performance. To address these limitations, we developed a p-type hybrid thermoelectric fiber by depositing a high-performance BST(bismuth antimony telluride) thin film using co-sputtering on a flexible PEDOT:PSS fiber. We fabricated the PEDOT:PSS fiber using the wet-spinning method, which is easy to mass-produce. We then deposited BST on the PEDOT:PSS fiber by magnetron sputtering at 200 K. We evaluated the thermoelectric performance of the hybrid thermoelectric fiber by measuring its Seebeck coefficient, electrical conductivity, and thermal conductivity with TDTR(-Time-domain thermoreflectance), calculating ZT value. Additionally, we improved the electrical conductivity of the PEDOT:PSS fiber by post-treatment. Our results demonstrate that our hybrid thermoelectric fiber combines the benefits of high-performance inorganic and flexible organic materials. This advancement provides exciting prospects for developing high-performance textile-based thermoelectric generators using these fibers.

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Experimental and DFT study of doped CrN thin films for thermoelectric applications

P29

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Keywords: thermoelectric, nitride thin films, phase formation, DFT, one more

Transition metal nitrides constitute an important class of functional materials which are mainly studied for their tribological applications but also possess promising thermoelectric properties. [1,2] Near room temperature, stoichiometric CrN shows high thermoelectric power factor (*PF*) of ~ 5 $\times 10^{-4}$ $Wm^{-1}K^{-2}$, however possess relatively higher thermal conductivity, $\kappa \sim 4$ $Wm^{-1}K^{-1}$. [3] Studying phase formation as a function of doping concentration supported by DFT calculations can provide crucial insights for the design of better thermoelectric materials for energy harvesting applications. We report on the phase formation of W and Nb doped CrN thin films grown by reactive magnetron sputtering on c-plane sapphire substrate. W doping lead to a change of phase formation during film growth from CrN to metallic Cr_2N along with segregation of W, whereas Nb showed relatively higher solid solubility inside CrN matrix. However, co-doping of W and Nb in CrN increased the electrical conductivity (σ) as compared to pristine CrN, giving a *PF* of ~ 3.4 $\times 10^{-4}$ $Wm^{-1}K^{-2}$ for $Cr_{0.87}Nb_{0.04}W_{0.09}N$ at room temperature. Doping induced enhancement of σ is supported by density functional theory calculations which revealed shifting of Fermi level in the conduction band along with formation of acceptor states near the Fermi level.

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P30

Highly tailored gap-like structure for excellent thermoelectric performance

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Keywords: gap-like structure, $Sb_2Te_3(GeTe)n$, thermoelectric properties, HAADF-STEM, thermoelectric module

The microstructure-dependent thermal transport property has drawn significant attention in the thermoelectric community for elevating thermoelectric performance. In this work, we characterized gap-like structures and improved their controllability in GeTe-rich $Sb_2Te_3(GeTe)_n$ samples. The statistics of the gap-like structures were studied through direct observation using a transmission electron microscope with atomic-resolved spherical aberration correction. We found a strong and unambiguous linear correlation of the nominal composition to the planar density and sizes of the gap-like structures. This microstructure tailoring further enabled a significant reduction in lattice thermal conductivity, an ultrahigh maximum ZT value of ~2.4 at 773 K, and an average ZT value of ~1.51 from 323 K to 773 K in p-type $Sb_2Te_3(Ge_{0.995}Yb_{0.005}Te)_{17}$. Together with n-type $Pb_{0.985}Sb_{0.015}Te$, we further fabricated a single-stage thermoelectric module that realized an exceptional output power density value of 1.25 W cm^{-2} and an efficiency of 7.5% under a temperature gradient of 480 K. Our pioneering strategy validated the beneficial effect of gap-like-structure tailoring for improving thermoelectric performance, laying the groundwork for similar studies on other thermoelectric materials.

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Anomalous thermal conductivity of alkaline-metals--substituted $EuTiO_3$ induced by resonant scattering

P31

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Keywords: $EuTiO_3$; thermal conductivity; disorder; soft lattice

Thermal conductivities (κ) of polycrystalline $Eu_{1-x}A_xTiO_3$ (A = Ca, Sr, Ba, $0 \leq x \leq 0.8$) bulk materials have been measured in the temperature range of ~ 2 K < T < 1173 K. An anomalous double peak feature of $\kappa(T)$ is only observed in the Ca-substituted samples with $x \geq 0.4$, which show orthorhombic crystal structure at room temperature (RT). All the other studied samples which display a cubic phase at RT exhibit glass-like $\kappa(T)$ behavior. After excluding the magnetic effects on κ and discussing the possible phonon scattering mechanisms in depth, the unusual low-temperature $\kappa(T)$ behavior is related to the delicate lattice structure. In the perovskite-type structure, Eu^{2+} acts as the root to cause complex disordered local structures and structural instability. The lattice structure of $Eu_{1-x}A_xTiO_3$ can be regarded as formed by part-soft part-rigid sublattice. The ultra-low κ of $Eu_{1-x}A_xTiO_3$ at low temperatures is attributed to resonant scattering, which significantly suppresses thermal transport. The anomalous double peak $\kappa(T)$ structure accounts for a competition between the normal phononic heat transport in the rigid sublattice and the strong damping of heat conduction by resonance scattering in the soft sublattice.

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P32

Manipulation with natural mineral chalcopyrite $CuFeS_2$ via mechanochemistry: properties and thermoelectric potential

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Keywords: chalcopyrite, mechanical activation, properties, thermoelectrics

The properties of natural mineral chalcopyrite $CuFeS_2$ after mechanical activation in a planetary mill have been studied. The intensity of mechanical activation was controlled by changing revolutions of the mill in the range 0–600 min^{-1}. Set of characterization techniques such as XRD, SEM, TEM, SA, TA (DTA, TG, DTG), particle size analysis and UV-Vis spectroscopy was applied. Reactivity studies were also performed. Several new effects were revealed for mechanically activated chalcopyrite, e.g. poly-modal distribution in micrometer scale of produced nanoparticles, agglomeration effects by prolonged milling, the possibility to modify the shape of particles, X-ray amorphization and the shift from the non-cubic (tetragonal) structure to pseudo-cubic structure. Thermoelectric response was evaluated on "softly" compacted powders via SPS method (very short time, low sintering temperature and moderate pressure) by measuring Seebeck coefficient, electrical and thermal conductivity above room temperature. Independently on the delivered energy supply the milling process led to samples with lower resistivity, compared to original nonactivated ceramics. The Seebeck data close to zero confirmed the "compensated" character of natural chalcopyrite reflecting its close to stoichiometric composition with low concentration of both n- and p-type charge carriers. On the other hand, the evident correlation between thermal conductivity and energy supply by milling is observed similarly with the possibility of bandgap manipulation associated with energy delivered by milling procedure.

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Enhancing thermoelectric performance of Mg_3Sb_2-based materials via Ag doping

P33

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Keywords: zintl compound, Mg_3Sb_2, Ag doping, phonon scattering, single-leg

Thermoelectric (TE) material can directly convert heat energy into electric energy using the Seebeck effect. The efficiency of TE materials can be evaluated by TE figure of merit $ZT = S^2\sigma T/\kappa$. Recently, Mg_3Sb_2-based compounds have become promising TE materials because they consist of low cost and environmentally friendly elements as well as high TE performance [1,2]. In this study, we explored possibility of Ag as a significant dopant in Mg_3Sb_2-based alloys.

The high purity elements were weighed in stoichiometry ratio and loaded into a stainless-steel vial, then subjected to ball milling for 5 hours. The resultant fine powder was transferred into a graphite die and sintered by spark plasma sintering (SPS). Phase identification of samples was confirmed by powder XRD. The microstructural analysis was performed by SEM. Hall coefficient R_H was measured using PPMS. Electrical properties and thermal conductivity were measured by ZEM-2 and LFA, respectively. The power generation characteristics of single TE leg were measured by the mini PEM.

The electrical conductivity increased for the Ag-doped samples, while maintaining moderate Seebeck coefficient, leading to an increase in the power factor (PF). Moreover, lattice thermal conductivity decreased to 0.50 W m^{-1} K^{-1}. As a result of high PF and low thermal conductivity, a maximum ZT of 1.72 is obtained at 673 K. Moreover, a conversion efficiency of ~11% for a single TE leg was obtained, which shows an exceptional potential in the practical application.

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P34

Chemical bonding origin of the excellent thermoelectric properties of Bi_2Te_3-based alloys

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Keywords: Bi_2Te_3, bonding mechanism, single crystal, transport properties, metavalent bonding

Bismuth-telluride-based alloys have been recognized as thermoelectric energy converters for decades due to their excellent thermoelectric performance. Recently, benefiting from a non-traditional bonding mechanism, coined metavalent bonding (MVB), a special combination of properties, such as large optical dielectric constant, small band gap and strong lattice anharmonicity, has been found in IV–VI and V_2-VI_3 compounds. The Bi_2Te_3 based alloy also utilizes MVB - which raises the question of whether the excellent thermoelectric performance originates from MVB.

In this work, single-crystal $Bi_xSb_{2-x}Te_3$ (x = 0.5, 0.6, and 0.7) single crystals were prepared by Bridgman oven, and then measured the transport properties by thermal transport option (TTO) in PPMS were measured. The optical properties and bond-breaking behaviour of these compounds were also investigated using Fourier transform infrared spectroscopy (FTIR) and atom probe tomography (APT), respectively, which proved the MVB mechanism in these compounds. Finally, the transport properties based on the unique bonding mechanism are analyzed from a "bond-to-band" perspective.

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Synthesis, characterization and thermoelectric properties of p-type $MnSi_{1.73}$ and $Mg_2(Si, Sn)$ prepared using Si-kerf from PV cutting process

P35

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Keywords: synthesis, Si kerf, Sintering, optimization and thermoelectrics

More than 50% of high purity material is disposing as waste kerf from the cutting process of photovoltaic technology. Recycling Si kerf is increasing interest focusing on various applications such as batteries, heat exchangers and thermoelectrics. In the field of thermoelectrics, sustainability and the development of using low cost, earth abundant and non-toxic materials are necessary to meet the environmental regulations.

Recently, a high figure of merit up to 1.3 were obtained for the n-type $Mg_2Si_{1-x-y}Sn_xGe_y$ based materials from waste Si kerf. In this work, our efforts to synthesize p-type silicides using Si kerf will be presented for the first time. Specifically, the preparation of Al-doped $MnSi_{1.73}$ and Li doped $Mg_2(Si,Sn)$ via mechanical alloying and the affect of alloying and sintering conditions will be discussed in terms of thermoelectric properties.

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P36

Growth and thermoelectric properties of ScN-based ternary alloys

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Keywords: ScN, thin films, epitaxial growth, alloying, synthetic mica, thermoelectrics

Conventional thermoelectric materials such as tellurides have shown promises to harvest thermoelectric power from waste energy [1,2]. Transition metal nitrides viz. ScN and CrN are seen as possible alternative materials to the benchmark thermoelectric materials. Despite the power factor (2.5–3.3 W m^{-1} K^{-2}) of ScN that is comparable to Bi_2Te_3 and PbTe, the thermal conductivity (10–12 W m^{-1} K^{-1}) of ScN requires further optimization [3]. Since natural 45Sc has no isotopes, defects induced by doping/alloying can reduce the thermal conductivity of ScN.

The present work aims to achieve enhanced thermoelectric properties with alloying of suitable dopants in ScN thin film matrix. Consequently, alloying of V (3d), Zr (4d) and W (5d) in ScN leads to different enthalpy of mixing and provides distinct structural stability to the ternary compounds. Variable carrier concentrations (n) of the dopants are intertwined to the Seebeck coefficient ($\propto 1/n^{2/3}$) and the electrical conductivity ($\propto n$) [3]. The variation in atomic masses of the dopants is expected to affect the scattering mechanism and in turn affects the thermal conductivities. The differences in the thermoelectric properties are also reflected in the electronic density of states of the ternary compounds at the Fermi level. The structural, electrical, and thermoelectric properties of the different alloyed films were investigated and the influence of each dopant on the carrier concentration, Seebeck and electrical conductivity was evaluated.

Furthermore, the work is an assessment to achieve epitaxial growth of ScN on thermally stable (1 100 °C) flexible inorganic synthetic mica substrates. The mica substrate can be exfoliated due to weak van der Waals forces which provides a window for flexible thermoelectric films.

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Improving thermoelectric efficiency of InSb by nano-boron doping

P37

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Keywords: InSb, nano-boron, single crystal, thermoelectric, mechanical properties

The intrinsically n-type narrow band gap semiconductor InSb features promising electrical conductivity and Seebeck coefficient values; however, due to the high thermal conductivity, its thermoelectric efficiency is limited [1]. In this study, single crystalline InSb samples were grown by Bridgman method and the crystal structure was characterized by single crystal X-ray diffraction method. Transport properties of single crystalline and polycrystalline InSb are evaluated both at low (2–300 K) and high temperatures (300–723K). By nano-boron doping thermoelectric and mechanical properties of the target materials were improved. A thermoelectric figure of merit (zT) value of 0.18 was achieved at 723 K for the $In_{0.975}SbB_{0.025}$ sample, which corresponds to an enhancement of approximately 50% compared to the pristine sample.

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P38

p-type copper iodide thin film for transparent and flexible thermoelectrics

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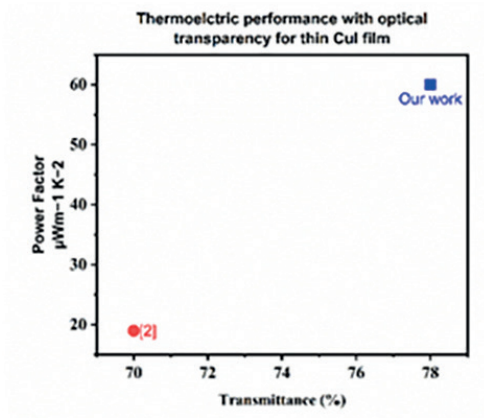
Keywords: electron beam evaporation, vapour iodization, power factor, transmittance, thermoelectrics

Transparent p-type copper iodide (CuI) is a promising material for thermoelectric p-n modules [1] which finds applications in wearable electronics, transparent electrodes, and solar cells.

We investigated the optical transparency and thermoelectric properties of nanostructured CuI films where Cu was deposited via electron beam evaporation at different glancing angles. Thereafter, Cu thin films were exposed to a rapid vapor iodination process, where instead of a long exposure in ambient temperature, the samples were treated at elevated temperature iodine vapor for a very short period of time, resulting in highly transparent CuI films. This method is relatively fast and also scalable leading to transparent films with a high conductivity of 1.3 × 103 Sm^{-1}, and a power factor of 60 $\mu Wm^{-1} K^{-2}$. The rapid, elevated temperature vapor iodination process yields comparable or better thermoelectric (TE) performance and transmittance when compared to previous results obtained by vapor iodization [2] and liquid iodization [3]. Our process results in > 75% average transmittance in the visible range, therefore enabling competition also with the solid iodination process.



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Low purity elements based skutterudites for mid-temperature thermoelectric applications

P39

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Keywords: skutterudites, cost-effective, low-purity, power generation

Thermoelectric Generators (TEGs) are one of the alternatives for clean power generation, and their performance is strongly influenced by the properties of the material used in the device fabrication. For the commercialization purpose of TEGs, the main objective is to enhance the figure of merit and reduce the processing cost of the materials used in device.

However, the cost and availability of high-purity elements have been identified as one of the hurdles to the widespread applications of thermoelectric (TE) materials. This has led to increased interest in the use of low-purity elements to synthesize efficient TE materials. Skutterudites (SKDs) based materials emerged out as potential candidates for mid-temperature TE applications owing to their high thermal and chemical stability, mechanical strength, possibility of synthesizing similar n- and p-type materials and cost-effectiveness [1].

The current work discusses the potential benefits of using low-purity elements and highlights the challenges associated with using low-purity elements. For this purpose, $In_xCo_4Sb_{12}$ samples were synthesized employing the conventional melting and annealing process and consolidated by spark plasma sintering (SPS). Further, the samples were characterized for structural and transport properties and the influence of impurities on the TE properties is studied in detail. Employing this strategy, the cost of the TE device is expected to reduce significantly (estimated to be ~50%) as the low purity elements are about 10 times less expensive than the high purity elements [2].

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P40

Surface LASER processing effect on the thermoelectric properties of bismuth-antimony-tellurium alloy

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Keywords: bismuth-antimony-telluride; laser processing; thermoelectric materials; mechanical alloying; hot-press sintering

In this study, the effect of surface laser processing (LP) on the thermoelectric properties of bismuth-antimony-tellurium alloy pellets is investigated. The stoichiometric alloy used is $Bi_{0.4}Sb_{1.6}Te_{3.0}$ powder, which was prepared by mechanical alloying (MA) and hot pressed (HP) under optimal pressing and temperature conditions [1–2] to produce disk pellets for further processing. X-ray diffraction (XRD) and scanning electron microscopy (SEM) methods were used to characterize the alloy phase, composition, and morphology. The HP pellets were then exposed to different laser beam energies, keeping the laser beam power constant and varying the scanning speed, and the smoothness of the surface was evaluated to select the sample with the highest quality forming surface layer. Specifically, the beam scanning speed was varied from [500–1500] mm/s with a step size of 500 mm/s, and the power of the beam was kept at 25 W. The results showed smooth surface layers when the scanning speed of the laser beam is 1500 mm/s. Two different samples were prepared for thermoelectric characterization, one in the shape of a rod and one in the shape of a disk pellet. The electrical properties (Seebeck coefficient and electrical conductivity) were studied using the rod sample while the thermal properties (thermal conductivity) were studied using the disk pellet. The measurements were made before and after the LP, for comparison purposes. The results revealed an average increase of 20.1% in electrical conductivity and a decrease of 6.8% in the Seebeck coefficient, with the power factor remaining almost unchanged. No changes were observed in the thermal conductivity measurements, and the data were nearly identical before and after laser processing.

Based on these findings, the figure of merit ZT remained nearly constant. In general, laser surface processing only impacts the surface of the samples and changes the surface structure, transitioning from the sinter to the melted stage, which mainly alters the electrical properties. In this respect, this work is a proof-of-concept study aimed at evaluating the thermoelectric properties in conjunction with various LP parameters, such as laser beam power and scan speed, beam trajectory hatching, exposure patterns (single and double zig-zag cross) etc.

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Effect of element substitution on thermoelectric properties and oxidation resistance of iron disilicide

P41

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Keywords: iron disilicide, oxidation resistance, kitchen equipment, gas flame, auger electron spectroscopy

70% of primary energy in Japan is thrown away as waste heat. To aim for carbon neutrality, it is essential to improve the thermal efficiency of industrial combustion furnaces, garbage incinerator, kitchen equipment, and so on. If the flame with a large amount of heat can be directly used, a higher electric power can be expected. β-$FeSi_2$ has low performance but can be used in the flame [1]. In this study, the effects of substituting elements on thermoelectric properties and oxidation resistance of β-$FeSi_2$ were investigated.

The starting ingot of β-$Fe_{0.95}M_{0.05}Si_2$ (M is Ni, Nb, V, Cr) was synthesized by arc melting. Each sample was sintered by SPS (Spark Plasma Sintering) at 1173 K, 30 MPa, 15 min in a vacuum. These sintered samples were heat treated at 1203 K for 100 h in a vacuum. The crystal phases of the samples before and after heat treatment were identified by XRD. The high-temperature oxidation resistance was evaluated by heating the edge of the sample with a gas flame and measuring the change in thermoelectromotive force for 15 min, 30 min, or 1 h. After the measurement, the surface of the measured sample was analyzed using Auger electron spectroscopy.

From the results of XRD, each sample was a homogeneous β-$FeSi_2$ phase. From the results of the thermoelectromotive force of β-$Fe_{0.95}M_{0.05}Si_2$ (M is V, Nb, Cr, Ni), the thermoelectromotive force of the Nb-substituted sample did not decrease significantly. From the results of AES analysis, it was found that the oxide layer of the sample heat-treated for 1 h was thinner than that of the sample heat-treated for 30 min. This is considered that the oxidation of Si transitions from passive oxidation, in which SiO_2, which is a protective oxide film, is formed on the surface to active oxidation, which generates SiO gas and causes mass reduction [2]. In particular, the Nb-substituted sample had the thinnest oxide layer thickness when heated for 30 minutes, and the reduction of the oxide layer was less when heated for 1 h. These results suggest that Nb is a suitable substitution element for β-$FeSi_2$.

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Reduced contact resistance of Cu_2SnS_3 thermoelectric legs

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Keywords: Cu_2SnS_3, electrode, aluminium, mixed layer, contact resistance

Cu2SnS3 (CTS) is an attractive candidate for non-toxic and earth-abundant thermoelectric (TE) material because of its phonon-glass-electron-crystal features with ZT of 0.88 at 773 K [1]. To the best of our knowledge, there are no reports on the contact resistance (CR) for CTS TE legs and electrodes. Therefore, we have fabricated CTS TE legs with the electrodes and have attempts to reduce the CRs.

Detail of the fabrication and measurement methods of CTS TE legs has been described elsewhere [2]. Various metal electrodes were prepared with a monobloc sintering method, which CTS and metal powders were sintered simultaneously at 673 K and 40 MPa for 5 min. Then, to reduce the CRs a mixed layer of CTS and metal were inserted between the CTS and the electrodes. The CRs were obtained by subtracting the resistance of CTS alone from the total resistance including electrodes.

At first, we have searched for suitable metal materials as electrodes by monobloc sintering. Mo and W, which are used as the electrode for CTS solar cells, could not be sintered under the above condition. Cu and Sn, which are constituent elements of CTS, have completely been diffused to CTS during sintering under this sintering condition. Zn, which is sometimes used as a dopant for CTS TE, also have been diffused. Ag, which is the isoelectronic element of Cu, has partially be successful but sometimes peel off form CTS legs. Al, the most widely used wiring material for ICs, was found to have good adhesion to CTS.

Then we have measured the CRs and obtained a few Wcm^2, which is larger than the other TE materials, such as Mg_2Si, by a factor of 105 [3]. Therefore, to reduce CRs a mixed layer of CTS and metal were inserted between the CTS and the electrodes. Al and CTS powders were mixed with weight ratio of 1:1, 3:7 and 7:3, [Al/CTS] = 1, 0.42 and 2.33, respectively. Inserting the mixed layer reduces the CRs and the lowest CR in this experiment was 0.086 Wcm^2 with the sample of [Al/CTS] = 0.42.

Consequently, Al is found to be the most suitable electrode material for the CTS TE legs fabricated by the monobloc sintering among these elements. The mixed layer is found to be effective to reduce the contact resistance. However, further reduction is needed.

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Thermoelectric materials grown by magnetron sputtering codeposition: a thin film approach

P43

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Keywords: sputtering, thin film, codeposition, Si, SiGe, Heusler

Sputter deposition is a well-established, inexpensive, and very versatile technique for the fabrication of a wide variety of material systems. The chemical composition can be highly controlled by the simultaneous use of several magnetrons with the different elements (codeposition) to achieve the desired film content. DC and RF configurations allow depositing materials from conductive and insulating targets, with their relative powers controlling the composition in detail. In addition, the codeposition configuration also allows a fine tuning of the doping concentration in semiconductor materials, which is needed to optimize the thermoelectric properties [1].

In this contribution, we present results on three different materials systems under investigation by our group using this sputtering co-deposition technique. Boron doped Si, SiGe thin films and W-doped Fe_2VAl Heusler alloy. This last compound has recently attracted large interest due the extraordinary thermoelectric properties reported [2].

A complete characterization protocol will be followed, including morphological, structural, compositional, thermal and electronic transport measurements in the different materials studied.

With these results from different material systems, we prove the large potential of sputtering to produce, in a versatile way, thermoelectric materials with desired compositional variation and tuned doping concentrations.

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Mechanochemical synthesis of tetrahedrite $Cu_{12}Sb_4S_{13}$ nanocomposites: challenge for thermoelectric performance

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Keywords: tetrahedrite, mechanochemistry, composite, thermoelectrics

Tetrahedrite $Cu_{12}Sb_4S_{13}$ with its low thermal conductivity represents a flagship in sulphide thermoelectrics. However, to achieve a reasonable figure-of-merit ZT the adequate dopping is needed. In this work, a different approach (without dopping) is illustrated for two systems containing tetrahedrite. The using of mechanochemical treatment and/or the addition of foreign phase (applied in extrinsic and/or intrinsic mode) the tetrahedrite composites have been obtained:

1. Binary composite tetrahedrite $Cu_{12}Sb_4S_{13}$/muscovite $KAl_2(AlSi_3O_{10})(OH)_2$ was prepared by two-step *mechanical activation* where combined treatment by excentric vibratory and subsequent planetary milling was applied. Addition of muscovite did not give extraordinary results in comparison with pure tetrahedrite, where this two-step process (performed in extrinsic mode) has led to a value of ZT = 0.75@673 K which belongs to the highest in the tetrahedrite community.

2. Binary composite copper minerals tetrahedrite $Cu_{12}Sb_4S_{13}$/chalcopyrite $CuFeS_2$ was prepared by *mechanochemical leaching*. In this strategy frequently used in hydrometallurgy, the alkaline leaching medium (Na_2S + NaOH) was applied to partly extract antimony from tetrahedrite and thus changing and disordering of its structure. The obtained composite (gained in an intrinsic mode) gives low values of ZT = 0.0022@673 K in comparison with the non-treated tetrahedrite where ZT was 0.0090@673 K. The reason can be hidden behind the extremely low electric conductivity as a consequence of changes in tetrahedrite evoked by mechanochemical leaching.

Acknowledgments

This work was supported by the Slovak Research and Development Agency APVV (project APVV-18-0357) and the Slovak Grant Agency VEGA (projects 2/0112/22, 2/0036/23). The support by European ERA-MIN 3 Potassial 27 project is also acknowledged.

Design and properties of composites made of bismuth nanowires confined in mesoporous silica and alumina for Peltier applications

P45

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Keywords: bismuth, nanowires, composites, thermoelectric, Peltier

The creation of novel functional materials is a technological need and a scientific challenge for the production of innovative systems able to face the requirements of many application fields. Cooling technologies are useful in many fields related to daily life (domestic refrigeration, computer cooling, air conditioning ...) as well as high technology (cooling of optoelectronic devices, superconducting devices, thermal management of electronic devices ...) In this, all-solid technologies based on the thermoelectric effect such as Peltier cooling devices represent a real alternative, as they have no moving parts, are compact and reliable. Despite the technological advance of the system, large-scale applications of Peltier cooling devices have been limited so far, mainly due to their insufficient performance and their rather high cost. Because of better performance at the lowest temperature and of the absence of tellurium present in Bi_2Te_3, $Bi_{1-x}Sb_x$ alloys have a strong potential for cooling applications. Moreover, nano-structuring the TE phase from a bulk material to a nanometric sized mono-dimensional wire has the potential for obtaining original and improved properties. The specific aims are the decrease of thermal conductivity and the increase of the Seebeck coefficient by exploiting the quantum confinement of the metal phase.

Therefore, the insertion of the metallic Bi or Bi alloys inside of a porous structure, such as zeolite channels and silica pores, could improve the thermoelectrical properties with respect to the bulk materials. Among the many parameters, the channel arrangement and dimensionality are of crucial importance in obtaining metal nanowires affecting the outcome performances of the composite. Here, we introduced Bi metal under pressure from melt into ordered porous alumina and silica with 4–10 nm pores. Electron microscopy confirms the full filling of the pores and the negative variation of the thermal resistivity coefficient suggests a confinement effect on electrons in the case of mesoporous silica. Optical spectroscopy shows also significant changes in the composites compared to the bulk bismuth. In contrast, the absence of change in the Raman spectra indicate the absence of confinement effect on phonons. Thermoelectric properties will be also reported.

Acknowledgments

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P46

Thermoelectric properties of Cu_2Se obtained by the SPS and the "SPS melting" method

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Keywords: spark plasma sintering SPS, SPS melting, Copper(I) selenide, thermoelectric materials

The aim of the work was to develop a one-stage method for obtaining (synthesis and densification) of Cu_2Se sinters, using a modified SPS technique called here the "SPS melting method". The new approach consists of placing a special graphite container in a graphite die, which makes possible to pre-react the substrates at the temperature of $T = 475$ °C and then remelt at the temperature of $T = 1150$ °C in one process. In this way, high-density polycrystalline sinters with 99% theoretical density and homogeneous, in terms of phase and chemical composition, were obtained. In order to compare the properties of Cu_2Se samples obtained in one-stage SPS melting, a series of syntheses of Cu_2Se from pure elements were performed in quartz ampoules in rocking tube furnaces, and then densified using the classical SPS method, similarly to work [1]. The chemical composition was investigated via scanning electron microscopy (SEM) combined with the energy-dispersive spectroscopy (EDS) method, and the phase composition was established with *X*-ray diffraction (XRD). The uniformity of the thermoelectric properties of the materials was examined by scanning thermoelectric microprobe (STM). Measurements of thermoelectric transport properties, *i.e.*, electrical conductivity, the Seebeck coefficient and thermal conductivity in the temperature range from 300 to 965 K were carried out. Based on these results, the temperature dependence of the thermoelectric figure of merit ZT as a function of temperature for Cu_2Se samples densified by SPS and "SPS melting" method was determined. The proposed new approach of one-stage preparation of Cu_2Se sinters seems to be suitable also for many other congruently melting materials.

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Thermoelectric properties of electrodeposited bismuth selenide thin films

P47

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Keywords: thermoelectric material, electrodeposition, thin films, Seebeck coefficient, power factor

Due to their ability to convert waste heat into electricity, thermoelectric materials are becoming very popular in energy harvesting. Telluride-based compounds are well-known thermoelectric materials as they exhibit high figure-of-merit *ZT* near room temperature. However, there is a lot of research being done to replace tellurides with selenides due to their toxicity and scarcity. Bismuth selenide is one of the V–VI binary chalcogenide compounds with a similar structure to bismuth telluride and has great potential to be used for thermoelectric applications [1,2]. In this work, bismuth selenide thin films are electrodeposited at five different reduction potentials (between -40 mV to -120 mV) from a binary Bi–Se electrolyte solution. Later on, the films are annealed at 150 °C for 1 hour under a nitrogen atmosphere. Morphological, compositional and structural analysis of both as-deposited and annealed films are conducted along with the thermoelectric measurements at room temperature. The crystallinity of the films is improved after annealing without showing a significant change in the elemental composition of Bi and Se. As-deposited bismuth selenide films show positive Seebeck coefficient, which is decreased upon annealing. Among them, the annealed film deposited at -40 mV shows a maximum Seebeck coefficient of 54.72 µV/K and a power factor of 0.8 mW/mK^2. This study concludes that annealing does change the crystal structure of bismuth selenide, which leads to an improved power factor.

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P48

Comparison of different co-doping strategies in optimizing thermoelectric properties of tetrahedrites

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Keywords: tetrahedrites, thermoelectric properties, co-doping

Tetrahedrites continue to be an interesting group of thermoelectric materials due to their low cost, low toxicity and complex structure that can be modified in various ways. The use of multiple dopants for a number of thermoelectrics has resulted in a significant improvement in transport properties and an increase in thermoelectric figure-of-merit ZT. The introduction of several dopants into one atomic position or into several atomic positions of tetrahedrite should, through a significant modification of the structure and introduction of additional disorder, improve the transport properties of the charge carriers while increasing the scattering of phonons and, as a result, increase the thermoelectric figure-of-merit ZT of the obtained materials.

The aim of this study was to develop new tetrahedrite materials with improved thermoelectric properties by using different co-doping approaches. Tetrahedrites co-doped with two dopants in the copper sublattice $Cu_{11.5}(T1,T2)_{0.5}Sb_4S_{13}$ (T_x – transition metal) in the antimony sublattice $Cu_{12}Sb_{4-x}(Bi,Te)_xS_{13}$ and simultaneously doped in the copper and antimony sublattice $Cu_{12-x}Tx_xSb_{4-y}M_yS_{13}$ were obtained by means of a high-temperature reaction of high-purity elements and subsequent sintering using the SPS (Spark Plasma Sintering) method. The obtained pellets were characterised by structural (XRD) and microstructural (SEM-EDX) methods to confirm their chemical and phase composition and homogeneity. Electrical conductivity, Seebeck coefficient and thermal conductivity were studied from room temperature to 720 K and used to calculate thermoelectric figure-of-merit ZT. Experimental studies were supported by FP-LAPW DFT electronic band structure calculations. Benefits of various co-doping strategies were discussed using both experimental and theoretical results.

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Organic/inorganic thermoelectric composites prepared via mechanical mixing

P49

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Keywords: polymers, thermoelectric, additives, mechanical press, physical mixing

Thermoelectrics are widely researched for energy conversion from thermal to electrical, with inorganic thermoelectric materials being the main focus in the past years. However, in recent years it became known that organic-based thermoelectric materials can be more appropriate for low temperature waste heat. In comparison to the classic inorganic thermoelectric materials, organic thermoelectric materials such as conductive polymers and their composites can be easily synthesized and processed, they exhibit flexibility, low toxicity and cost-effectiveness. A wide range of methodologies are currently available for the development of organic thermoelectric devices. Among others, in-situ polymerization can be employed in the preparation of composite thermoelectric powders whereas simply physical mixing can be also used *via* printing methods, mechanical pressing, electrospinning, spin coating etc.

In this work, physical mixing of poly(aniline) (PANI) powder introduced as the polymer matrix and an inorganic bismuth/antimony telluride additive followed by mechanical pressing was attempted. Furthermore, various experimental parameters such as the additive content, processing time, temperature and applied pressure were investigated in terms of thermoelectric properties.

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P50

Thermoelectric properties of conventionally and mechanothermally prepared chalcogenide spinels $CuCr_2Se_4$

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Keywords: chalcogenide, solid-state reaction, milling, transport properties

Nowadays, research on thermoelectric materials as alternative power resources that can effectively convert heat into electricity and vice versa is very active. $CuCr_2Se_4$ belongs to the group of chalcogenide spinels with ferromagnetic arrangement which can strongly affect its thermoelectric properties [1-2]. Two polycrystalline samples of the composition $CuCr_2Se_4$ have been prepared by two-step solid-state reaction at 1123 K over 10 days and at 1073 K over 14 days and by high-energy milling for 16 hours and one-minute heating to 473 K from elemental powder precursors. The products were identified by X-ray diffraction. The samples for physical measurements were hot-pressed (823 and 953 K, 70 MPa, 1 h) and spark plasma sintered (873 K, 50 MPa, 10 min). The electrical conductivity σ, Seebeck coefficient S and total thermal conductivity κtotal as a function of the temperature of variously synthesized $CuCr_2Se_4$ were measured and compared. The positive sign of the Seebeck coefficient suggested the p-type conductivity. There was a great match of transport properties between the sample hot-pressed at 823 K prepared by conventional solid-state reaction and the sample hot-pressed at 913 K prepared by fast mechanothermal route. Lattice thermal conductivity was $\approx 2 Wm^{-1}K^{-1}$ at room temperature and decreased with increasing temperature, so the $CuCr_2Se_4$ is from this point of view a good candidate for TE applications. The resulting value of Power Factor σS_2 was an order of magnitude lower than that of commonly used thermoelectric materials. The value of the ZT parameter was around 0.012 at 575 K. To achieve higher thermoelectric efficiency doping with a monovalent element at the copper position or forming a solid solution with a suitable ternary compound e.g. $ZnCr_2Se_4$ is necessary.

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Selective scatterings of phonons and electrons in defective Half-Heusler $Nb_{1-\delta}CoSb$ for the figure of merit $zT > 1$

P51

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Keywords: thermoelectric materials, half-Heusler, NbCoSb, isoelectronic alloying, lanthanide contraction

The recently developed defective 19-electron half-Heusler (HH) compounds, represented by Nb1-δCoSb, possess massive intrinsic vacancies at the cation site and thus intrinsically low lattice thermal conductivity that is desirable for thermoelectric (TE) applications. Yet the TE performance of defective HHs with a maximum zT less than 1.0 is still inferior to that of the conventional 18-electron ones. Here, a peak zT exceeding unity is obtained at 1123 K for both $Nb_{0.7}Ta_{0.13}CoSb$ and $Nb_{0.6}Ta_{0.23}CoSb$, a benchmark value for defective 19-electron HHs. The improved zT results from the achievement of selective scatterings of phonons and electrons in defective $Nb_{0.83}CoSb$, using lanthanide contraction as a design factor to select alloying elements that can strongly impede the phonon propagation but weakly disturb the periodic potential. Despite the massive vacancies induced strong point defect scattering of phonons in $Nb_{0.83}CoSb$, Ta alloying is still found effective in suppressing lattice thermal conductivity while maintaining the carrier mobility almost unchanged. In comparison, V alloying significantly deteriorates the carrier transport and thus the TE performance. These results enlarge the category of high-performance HH TE materials beyond the conventional 18-electron ones and highlight the effectiveness of selective scatterings of phonons and electrons in developing TE materials even with massive vacancies.

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P52

Effect of sintering temperature on thermoelectric transport properties of n-type Mg_3Sb_2

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Keywords: thermoelectric, Mg_3Sb_2, ball milling, SPS, sintering temperature

Mg_3Sb_2 based compounds have shown the best thermoelectric performance around room and mid temperature. Mg_3Sb_2 based materials have the advantage of being inexpensive and eco-friendly, but it is difficult to synthesize stable n-type materials due to the high vapor pressure of Mg. Many efforts to stably synthesize n-type Mg_3Sb_2-based compounds with high thermoelectric properties were fulfilled, it has various synthesis methods, including ball milling and melting method [1,2]. Recently, Zihang Liu were reported that adjusting the sintering temperature significantly improves the thermoelectric properties of n-type Mg_3Sb_2 based materials [3]. In this work, we have investigated the effects of sintering temperature (923K–1073K) on the thermoelectric properties of the $Mg^{3+}\alpha SbBi_{0.99}Te_{0.01}$ with excess Mg. These Mg_3Sb_2 materials were synthesized with ball milling and Spark Plasma Sintering. The highest value of ZT = 1.2 was achieved at 623K for the samples with sintered at 1073K. This value was 70% higher than that sintered sample at 923K. The variation of the thermoelectric properties was supported and discussed with carrier concentration and mobility and so on.

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Transient-Liquid-Phase bonding for Skutterudite-based thermoelectric modules

P53

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Keywords: thermoelectric; Skutterudite; module simulation; contact resistances

Thermoelectric (TE) generators are an option for waste heat recovery in a large diversity of applications, such as automotive, aerospace or high temperature industrial processes with high energy throughput. Skutterudite materials are among the most interesting candidates for high efficiency modules in the high-temperature range up to 500 °C. However, Skutterudite-based TE modules still lack published results on reliable solutions for electrical and thermal contacts between the semiconducting TE pellets and metallic bridges and their stability under thermal treatment, leaving room for suggestions on durable joining and assembly technology.

Here we present contacting schemes for TE modules using different diffusion barriers and a transient liquid phase (TLP) joining process. The modules have been characterized using a high-precision, in-house built TEG measurement apparatus (TEGMA) to characterize electrical power output, efficiency and heat flux under given temperature conditions. Furthermore, the stability under thermal cycling and high temperature treatment has been tested. Experimental data of the module properties will be compared to 1D simulation based on measured temperature-dependent TE properties of p- and n-type materials used in the modules.

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Half-Heusler modules with high power density for nano-CHP application

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Keywords: thermoelectric module, halfheusler, power density, CHP, application

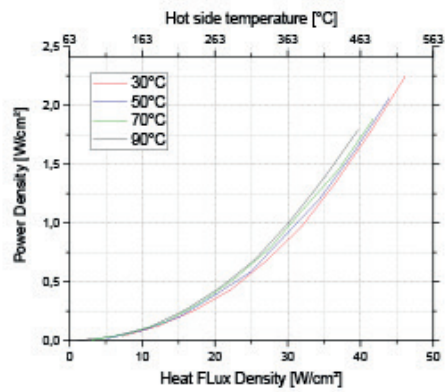
The primary barrier to the widespread adoption of TEGs is the insufficient cost-benefit ratio for commercialization. TEGs have high module and system costs relative to the amount of electrical energy generated. The company Isabellenhütte Heusler has the potential to contribute to solving this issue.

Dr. Fritz Heusler discovered the first Heusler alloy in 1901 at Isabellenhütte. Since 2009, Isabellenhütte has been actively engaged in Heusler alloy research. Our research efforts have been focused on thermoelectric Half-Heusler compounds since then. The goal of our research is to create a manufacturing process for these materials that can be scaled up for industrial production. In 2015, our research focus has shifted from the material to the development of modules using our Half-Heusler materials. Isabellenhütte established an industrial pilot production line in 2017, covering the entire process from raw elements to the creation of thermoelectric modules. Our ambition was to demonstrate the automated assembly process and industrial-scale material manufacturing of Half-Heusler modules, while maintaining a high level of quality. Starting in 2021, we initiated the development of tailored power electronics for our Half-Heusler modules, completing a full package solution.

The power density of a TEG is a critical part in the development of small, lightweight, and cost-effective systems. A key factor in achieving high power density is the use of suitable materials and module designs. Compared to other materials, Half-Heusler material combine high thermal conductivity and excellent conversion efficiency. Isabellenhütte has designed an ISA-TEG Half-Heusler module with a high power density of 950W/m²K to demonstrate its feasibility.

Today we able to present module performance measurement results in comparison with an ideal simulation. Furthermore, successful measurements have been taken for an entire TEG system utilized in a nano-CHP setting.

Electrical power density and heat flux density measurement of Isabellenhütte module TEM-950-46x26:



Fabrication of high power density telluride-based thermoelectric generator module for mid-temperature applications below 550 °C

P55

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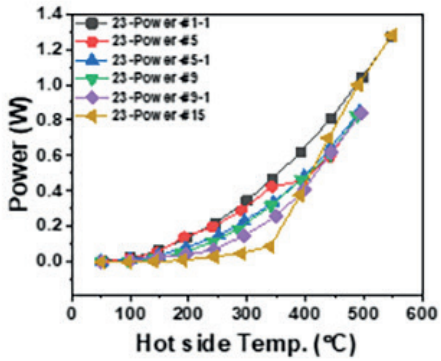
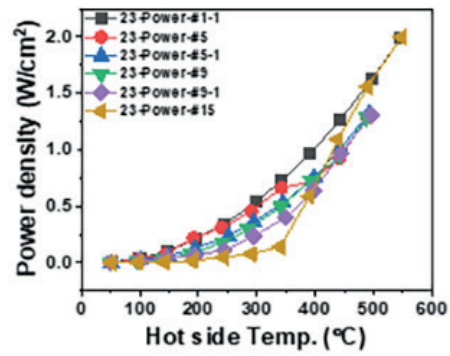
Keywords: thermoelectric, lead telluride, germanium telluride, diffusion barrier, power module

A high-power thermoelectric module is a critical component for thermoelectric power conversion [1,2]. In this study, we focus on the fabrication of a telluride-based thermoelectric power generator module for high power density in mid-temperature applications below 550 °C. We use N-type PbTe and P-type GeTe-based alloys, which have peak *ZT* values of 0.88 and 1.43 at 350 °C and 450 °C, respectively. To achieve high-electric power generation, we design a short-leg geometry and synthesize 3 × 3 × 2.5 mm^3 legs by a one-step hot-press sintering process with 0.5 mm Co diffusion barriers at the ends of each leg. Then, we fabricate 2 P-N leg-pair power modules with Al_2O_3 electrically insulating substrates by soldering or brazing joining technique. The performance characteristics of our module are measured using a mini-PEM system [3]. Our high power module shows an output power of 1.28 W at a hot-side temperature is 547 °C and a temperature difference of 512 °C, corresponding to a very high *leg-power density* of up to 2.0 W/cm^2. With device scaling technology of 8 P-N leg-pair AlN substrate or 50 P-N leg-pair Al_2O_3, a very high *device-power density* of 2.0 W/cm^2 can be achieved when a leg spacing is 1 mm.





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Thermoelectric cooling system for the monolithic microwave integrated circuits chip

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Keywords: monolithic microwave integrated circuits, thermoelectric device, cooling system, performance evaluation, finite element analysis

MMIC (Monolithic Microwave Integrated Circuits) is a core technology of microwave systems that are widely used as RF (Radio Frequency) components for satellite communication and mobile communication as well as radar. The miniaturization trend by MMIC is oriented to high integration level, versatile multi-function and high power density. It is necessary to provide a high level integration solution with sufficient cooling capability for the high power density to maintain the chip operating reliable and effective. The maximum temperature within the chip is required to be limited, otherwise the reliability and electrical performance will decline exponentially.

In this study thermoelectric devices were employed to cool MMIC chip for the purpose of controlling the heat flux of the chip. A thermoelectric cooling system is composed of carrier, housing, heat sink, measuring parts and a heater to simulate the MMIC chip. The performance of the cooling system was evaluated using the temperature of the MMIC chip. And the maximum cooling performance according to the applied current supplied to the thermoelectric element was evaluated. The performance of thermoelectric cooling system was compared with a cooling system without thermoelectric devices, and A governing equation that can predict the temperature of the chip according to the current supplied to the thermoelectric element was derived. FEA (Finite Element Analysis) was performed to investigate the effect of heat transfer coefficient which is related with forced convection on the performance of thermoelectric cooling systems. As a result of the analysis, it was found that as the convective heat transfer coefficient increases, the performance difference between the thermoelectric cooling system and the existing cooling system increases.

Based on the results of this study, a method for evaluating and predicting the performance of a thermoelectric cooling system has been proposed, and the proposed method will be widely used for chip cooling that needs to cool a small area.

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Procedure of failure analysis on commercial available thermoelectric modules

P57

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Keywords: thermoelectric, failure analysis, IR-thermography, scanning acoustic microscopy, X-Ray computed tomography

In this work, the procedure of a failure analysis on commercial available thermoelectric modules (TE-M) is presented. Due to the research activities in recent years, TE-materials become excellent candidates for power generation devices (TEG) which can be used in the mid- and high-temperature range up to 500 °C on the hot side of the TE-M. Now, in order to bring TE-M from laboratory status to industrial applications, it is very important that the intrinsic positive properties of a TEG, such as no moving parts, easy scalability, etc. can be fully exploited through a high long-term stability / reliability.

To quantify reliability, appropriate stress tests / reliability tests must be performed and defective modules must be analyzed for their failure mode and failure cause / failure location using non destructive (NDE) and destructive evaluation (DE) techniques. Failure analysis is a complex process of collecting and analyzing data to determine the failure mode / failure mechanism and location of the failure in a TE-M (root cause failure analysis). The results of failure analysis now allow the weaknesses of the component to be identified and help to understand the mechanisms and causes of failures, making it possible to undertake corrective measures to optimize the product and guarantee its quality and reliability. In this context, a rough distinction between so-called ‘soft’ and ‘hard’ failures is helpful. A soft failure means that the TE-M is working, but is out of specification, generally resulting in an increased internal resistance due to degeneration. A hard failure means that the TE-M is completely inoperable, i. e. no current can flow due to delamination or a gap (e. g. defective soldering or broken leg).

In this work we present the applicability of the NDE methods measuring the internal resistance (for soft and hard failures), IR-thermography (for soft failures), scanning acoustic microscopy (for hard failures) and X-ray computed tomography (mainly for hard failures). After NDE, DE methods of embedding the TE-M, cutting, grinding and polishing the surface where applied, followed by the NDE analysis methods using optical microscopy, SEM and EDS to determine the location of the defect.

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Thermoelectric generator for autarkic maritime heating systems

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Keywords: heating system, maritime, ship, thermoelectric generator, half Heusler

Heating systems for ships can be operated with gaseous or liquid fossil or regenerative fuels. Their operation requires electric energy, which has to be supplied either from on-board batteries or generators or from shore power during stays at the port. The limited capacity of batteries and the occasional lack of shore power or associated costs force ship owners to run auxiliary engines continuously in order to drive on-board generators for electric power generation. Fully autarkic heating systems could reduce corresponding costs and the emission of pollutants, which makes them very interesting for the maritime sector, particularly for passenger vessels with an increased demand for warm water.

Thermoelectric generators (TEG) convert heat into electric energy. In combination with small batteries for the system start-up, TEG can enable a fully autarkic operation of heating systems by supplying enough power to drive oil, fuel and circulating pumps, ignition transformers, blowers, sensors and valves. We describe first results of the development of a maritime heating system with an integrated TEG. A commercially available heating system from the manufacturer Scheer builds the starting point of the work. This very compact system, which can be can be operated with different types of fuels, is rated with an electric power consumption of 200 W_{el} and offers a heating power of 10 kW_{th}. The aim of the project is to generate more than 200 W_{el} by the TEG in order to charge the start-up battery and to supply energy additionally to other electric consumers on board. Half-heusler based TEG modules from the manufacturer Isabellenhütte are the centerpiece of the energy conversion and will be integrated into the heating system in order to fulfill the targeted power output. In this work we start with a simulation-based survey on the heat flow and temperature distribution of the original heating system and corresponding assessments on the extractable heat and potential power generation. We suggest a basic integration concept of the TEG including a preliminary design for highly compact heat exchangers to absorb combustion heat with flame temperatures up to 1,450 °C and to reject heat to the water circulation with a temperature between 70–90 °C. According to our results a power output of 200 W_{el} can be achieved at a TEG efficiency between 3%–4% if the heat exchangers offer an integral heat transfer coefficient in the range between 170 W/m² K–220 W/m² K, which is a realistic level in view of the given temperatures and installation space.

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Development of thermoelectric generator for low-temperature waste heat recovery

P59

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Keywords: thermoelectric generator; energy harvesting; waste heat recovery; TEG; thermoelectric module characterization

Thermoelectric Generators (TEGs) are devices that convert heat energy directly into electricity due to the thermoelectric effect. TEGs can be used in large-scale applications, e.g. industrial installations that produce a significant amount of so-called waste heat. Even partial recovery of this energy by converting it into electricity may remarkably increase the overall efficiency of such facilities and reduce its negative impact on the natural environment. Nowadays, several major development paths in thermoelectric materials and their applications can be distinguished. One group of research subjects contains the development of industrial parametrised, easy-to-deploy, and application-optimised systems, which have a huge potential for large-scale applications.

This work presents the results to date of the COTEG project, which aims to produce a series of thermoelectric generators for the recovery of low-temperature waste heat in industrial process installations. The project involves the development of a complete technological process, including the synthesis of materials with satisfactory thermoelectric performance, optimisation of the soldering technique as well as module assembly. Voltage-current and power-current characteristics of the fabricated thermogenerators were performed. The work employed cutting-edge approaches unprecedented in the literature.

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Optimization of a two-stage cascade type thermoelectric generator through finite element analysis

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Keywords: cascade-type thermoelectric modules, thermoelectric generation, conversion efficiency, optimization, finite element method

The cascade arrangement of thermoelectric modules is a suitable way to increase the conversion efficiency in energy production. The evaluation of optimized overall conversion efficiency has been made firstly by Harman [1] in 1958, and was further discussed, including recent works (as Fujisaka et al. [2] for a three-stage thermoelectric generators and Tian et al. [3] for a two-stage assembly). Meanwhile, optimized configurations have been investigated for thermoelectric coolers (see, e.g., [4]), cooling being an application of wider use of cascade-type thermoelectric modules.

In general, all evaluations should not avoid numerical analysis, also to take into account the contribution of passive elements and all contributions to heat flux. Furthermore, numerical analysis can evaluate chosen configurations in non-stationary operations. In particular, Multi-physics simulation, provided by Finite Element and Finite Volume Methods, allows the study of considered assembly in various operating conditions. So, whereas the evaluation of Harman was based on analytical calculations with constant properties of materials, more recent works are also based on numerical analysis (e. g., the evaluations of Fujisaka are based on both analytical and numerical analyses, using as numerical technique the Finite Volume Method).

In this work, Finite Element Analysis is used to identify the configuration of a two-stage cascade arrangement of thermoelectric modules giving the maximum conversion efficiency, taking into account all passive elements and the actual temperature distribution in the modules, which can affect the overall stability of the assembly. Unexpected high temperature on the modules, in particular on hot side of the cold stage, can lead to dangerous thermal stress on the element and eventually cause the failure of one or both stages. Therefore, the control of the thermal behaviour of the cascade appears to be as important as the evaluation of the electrical one, and both aspects have to be considered in efficiency calculations. The optimized configuration of the two-stage cascade is thus sought by means of the Finite Element Method, which yields the solution of the coupled system of differential equations governing the thermoelectric effect in both temperature and voltage. Through Finite Element Analysis, also side-effects of the cascade can be considered, as mentioned unsuitable high thermal stress and/or geometry mismatch of cascade stages.

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Thermoelectric devices based on block copolymer nanostructured Si thin films

P61

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Keywords: thermoelectric generator, nanostructuration, silicon thin films, block copolymers

In Internet of Things (IoT) systems millions of interconnected devices for sustainable and long-term autonomous energy sources. Thermoelectricity offers an alternative to primary batteries for powering sensor nodes with energy harvesting in sub-Watt applications.

In this contribution, we present the study of suspended silicon ultra-thin films as thermoelectric material. Although the enhancement in thermoelectric performance of thin films could be modest when compared to one-dimensional structures [1], this is compensated by introducing surface nanostructuration with the aim to reach power densities competitive with batteries for IoT nodes. Here, we present a cost-effective and scalable approach for the fabrication of the membranes by block copolymer (BCP) nanopatterning. BCP based technologies emerge as an appealing option, as it is a technology easy to scale for high-volume manufacturing, very cost-effective and capable of achieving sub-10 nm resolution [2].

Nanostructurated Si membranes are fabricated on the device layer of a Silicon on Insulator (SOI) wafer with ultrathin device layer (30–50 nm). A thin film BCP is self-assembled perpendicularly oriented to the Si surface. The BCP used for surface nanostructuration is polystyrene-block-polymethylmethacrylate (PS-b-PMMA) with cylindrical or lamellar morphology and a period between 28 and 80 nm. After self-assembly, the PMMA block is selectively removed, and PS features are transferred into the Si underneath by reactive ion etching (RIE). As a result, we obtain a surface nanostructurated with a hexagonal distribution of holes when a BCP with cylindrical morphology is used (**Fig. 1**). The period of such structures is controlled by properly blending BCPs of different molecular weights and depth and shape of the walls are tuned by RIE conditions. Final structures will be doped by spin on dopant to achieve optimal doping concentration, 10^{19}–10^{20} cm^{-3} for thermoelectric applications.

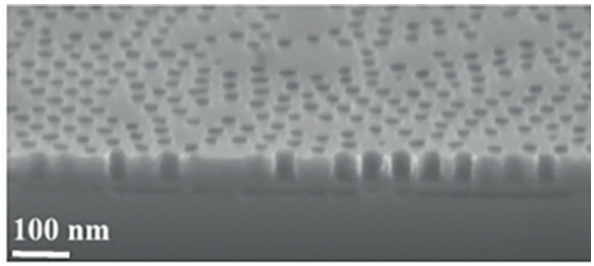

Fig. 1: SEM image of a 50 nm holley silicon thin film above the buried oxide layer (BOX). The holes array period is 57 nm. The film is suspended by eliminating the bulk silicon below the BOX with a KOH wet etching.

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Twist angle resolved thermal conductivity in bilayer $MoSe_2$

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Keywords: twisted bilayer $MoSe_2$, thermal conductivity, optothermal Raman, moiré superlattice, phonon lifetime

Twisted bilayer (t-BL) transition metal dichalcogenides (TMDCs) have attracted significant attention in recent times due to their unique electronic properties arises because of moiré superlattices that leads to the emergence of flat bands and correlated electron phenomena. Also, these materials can exhibit interesting thermal properties, including a reduction in thermal conductivity. In the present work, we report the manipulation of thermal conductivity in BL $MoSe_2$ based on some specific twist angles around two symmetric stacking AB (0°) and AB′ (60°) and intermediate angle (31°) using the optothermal Raman technique [1]. The observed thermal conductivity values are found to be ~ 13 ± 1 W/m. K, ~23 ± 3 W/m. K and, ~30 ± 4 W/m. K for twist angle [θ] = 58°, 31°and, 3° respectively, which is well supported by our first-principles calculation results. The reduction in thermal conductivity in t-BL $MoSe_2$ compared to monolayer can be attributed to the presence of phonon scattering due to the formation of moiré superlattice. Besides the change of the Brillouin zone [2] due to in-plane rotation and the appearance of multiple folded phonon branches are also responsible for the reduction in thermal conductivity seen in t-BL $MoSe_2$. The theoretical phonon lifetime study and electron localization function (ELF) analysis further reveals the origin of angle dependent thermal conductivity in t-BL $MoSe_2$. This work paves the way towards tuning the angle dependent thermal conductivity for any bilayer TMDCs system.

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Reliability and electrical characterization of transient liquid phase sintering interconnects for thermoelectric devices

P63

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Keywords: thermoelectric devices, TE module, transient liquid phase sintering, electrical contact resistance, cascade thermoelectric

The design process of a full scale thermoelectric (TE) device for medium to high temperature requires the feasibility and reliability of electronic contacts assembly. This point is particularly tricky in the case of multistage device fabrication.

Taking advantage of power devices technology [1], here we investigate transient liquid phase sintering (TLPS) technique for practical joining procedure of metal electrodes with thermoelectric materials below 300 °C. Different sintering pastes are tested to provide a low temperature process and a re-melting operational temperature above 500 °C. Accurate combination of elements (Ni, Cu, Sn) and particle size drives the temperature boundaries.

Compositional and morphological characterization of the interfaces between TE pellets and metal electrodes are obtained by Field Emission Scanning Electron microscopy (FE-SEM) coupled with Energy Dispersive Spectroscopy.

Electrical properties of the metal-semiconductor joints are investigated in term of their Ohmic or Schottky behaviours. Schottky barrier height was extrapolated from current-voltage (I-V) characteristics while contact resistance and diffusion layers are obtained with a custom-built scanning apparatus [2]. Electrical characterizations are combined with x-ray photoelectron spectroscopy (XPS) to deeper analyse the interface composition and interdiffusion or oxidation effects.

Mechanical bonding strength of contacts was investigated with a tensile testing apparatus.

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Difficulties in preparing a truly pure Bi_2O_2Se

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Keywords: Bi_2O_2Se, thermoelectric properties, stoichiometry, doping, foreign phases

Bi_2O_2Se is a 2D layered material with potential applications in thermoelectrics. In this work, a series of polycrystalline Bi_2O_2Se samples with altered stoichiometry were prepared. They were characterized by X-ray diffraction, electrical conductivity, Seebeck coefficient and thermal conductivity. Thermoelectric (TE) data were measured as a function of temperature in the range of 300 K to 773 K. We came across a specific issue where significant variations in TE properties compared to the recently published data on undoped Bi_2O_2Se are apparent. Furthermore, even the published data from various sources are inconsistent. We also compared TE properties of published data on doped samples with our samples with altered stoichiometry and found similarities. Based on a thorough investigation, we have reached several conclusions that are relevant to this problem. We argue that the solubility of the doped elements is very limited. Instead, the doping process mainly induces changes in the stoichiometry of the parent Bi_2O_2Se. This is associated with formation of native point defects and foreign phases. It is worth noting that both native defects and foreign phases are mostly not observable by X-ray methods.

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Inkjet printing flexible thermoelectric devices for sustainable power generation

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Keywords: flexible thermoelectric devices, inkjet printing, silver selenide, normalized power density, sustainable power sources

Flexible thermoelectric devices show great promise as sustainable power units for the explosively increasing self-powered wearable electronics and ultra-widely distributed wireless sensor networks. While exciting proof-of-concept demonstrations have been reported, their large-scale implementation is impeded by unsatisfactory device performance and costly device fabrication techniques. Here, we develop thermoelectric films and flexible devices via inkjet printing. Taking Ag_2Se-based inks as an example, large-area patterned arrays with microscale resolution are obtained in a dimensionally controlled manner by manipulating ink formulations and tuning printing parameters. Printed Ag_2Se-based films exhibit (00*l*)-textured feature and an exceptional power factor (1097 $\mu Wm^{-1}K^{-2}$ at 377 K) is obtained by engineering the film composition and microstructure. Benefiting from the outstanding behavior of printed films and high-resolution device integration, fully inkjet-printed Ag_2Se-based flexible devices achieve an outstanding normalized power density (2 $\mu WK^{-2}cm^{-2}$) and excellent flexibility (surviving 3,000 bending tests at bending radii of 3~4 mm). Furthermore, to enable inkjet printing of more thermoelectric materials, we employ a general templated-directed chemical transformation process to synthesize several types of 1D metal chalcogenide nanowires, such as Ag_2Te, Cu_7Te_4, and $Bi_2Te_{2.7}Se_{0.3}$, which can be made into inks suitable for inkjet printing by dispersing them in ethanol without any additives. Our work demonstrates the great potential of inkjet printing for scalable manufacturing of next-generation, high-performance flexible thermoelectric devices.

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Design optimization of printed thermoelectric generators tailored for plate heat exchangers in waste heat recovery applications

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Keywords: design and fabrication, printed thermoelectric generators, plate heat exchangers, waste heat recovery

A substantial proportion of the global primary energy production is lost to the environment as waste heat through exhaust systems. Effective exploitation and conversion of this lost thermal energy into useful energy would not only improve the thermal performance of the systems, but will also be a step towards mitigation of carbon emissions. Thermoelectric generators (TEGs) are a viable solution for waste heat recovery in a wide range of energy recovery applications. To achieve economical feasibility, TEGs can be printed in large area by screen printing.

In this study, an optimum planarly printed TEG tailored for plate heat exchanger (PHE) has been designed to transform some portion of low-grade thermal energy to high grade electrical energy. As a preliminary step, the temperature and heat flow boundary conditions for a PHE in energy recovery applications were explicitly stated. Then, a dedicated software environment implemented in Python was used to determine optimum thickness of the planar TEG against fill factor at previously defined PHE boundary conditions [1]. The optimum thickness of 100 µm [2] which is also the maximum limit given by printing process, was achieved at 0.62 fill factor. Furthermore, simulations indicated that a TEG integrated PHE should be about 115% of larger size than a simple one for the same heat transfer value. In trade-off, an optimized printed TEG tarnsformed about 1.34% of the total heat available (8575 watts) at hot side to electrical power (115 watts) and remaining heat (8460 watts) transmitted to the cold side.

In a nutshell, focus of this research is on the conversion of waste heat into electricity by using an optimized, cost-effective and tailored printed TEG for PHE with certain geometrical constraints and boundary conditions. Future investigations should delve into incorporating different printed TEGs into other potential energy recovery applications, like combined heat and power (CHP) systems, solar thermal systems, geothermal energy systems, and seasonal thermal storages.

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A Cr complex solution able to produce a large power factor improvement in a nanostructured and porous oxide film

P67

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Keywords: power factor, electrolyte, chromium complex, redox molecule, porous film

In the search of more efficient thermoelectric (TE) materials, significant improvements in *ZT* have been achieved, mainly due to the reduction of the thermal conductivity. In contrast, enhancements in the power factor $PF = \sigma S^2$, being σ the electrical conductivity and *S* the Seebeck coefficient, have been minor. Recently, large *PF* improvements have been shown in a novel solid-liquid TE system, consisting of a porous nanostructured TE solid (Sb-doped SnO_2) in contact with different electrolytes (salts in a liquid media) [1].

Here, we have investigated a new electrolyte for this system, a Cr (III) complex [chromium (III) acetylacetonate], which is dissolved in 3-methoxypropionitrile (3-MPN) in 0.1M concentration. Using this electrolyte in contact with the Sb-doped SnO_2 film, an average 3.4 times *PF* enhancement was achieved. This was due to an average decrease of 23% and 83% in the absolute value of the Seebeck coefficient and the electrical resistivity, respectively.

In order to understand these results, we tested possible changes in either the morphology or the film composition by scanning electron microscopy (SEM) and energy-dispersive X-ray (EDX) spectroscopy analysis, which were not present. In addition, ^{1}H NMR results showed no presence of H_2O, which can act as a donor of electrons [2]. On the other hand, impedance spectroscopy experiments determined that the electrical current only flows through the oxide film (ohmic behaviour). All these results led to the conclusion that electron injection from the electrolyte takes place, which increases the charge carrier density in the film and decreases the Seebeck coefficient. Our results demonstrate that electroactive molecules, such as inorganic complexes, can produce significant *PF* improvements when in contact with porous TE solids, which opens a new way of significantly improving the *PF*.

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Acknowledgments

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P68

Thermoelectric data analysis toward power generation evaluation and standardization

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Keywords: thermoelectric, data

Since the discovery of the Seebeck effect more than two hundred years ago, thermoelectricity has been continuously studied to apply the thermoelectric effects to the energy transformation from thermal energy into electrical energy. Thermoelectric technology has been utilized in special environments such as space, starting with the lunar exploration in the 20th century, and has recently been used/considered as an active heat management technology. Recently, thermoelectric power generation technology has been reconsidered to improve system efficiency such as waste heat recovery, but the lack of a performance evaluation system at the device level adds difficulties to industrialization.

In this presentation, we will present the results of a thermoelectric data study for the development of a thermoelectric power generation performance evaluation system. From a variety of data, including published papers and internet company brochures, we analyse the average material compositions and properties observed in thermoelectrics, as well as the average geometry of the legs and the performance scale of the devices. Based on these data, the characteristics of the most technologically advanced BiTe-based thermoelectric generator modules are derived. Furthermore, we will discuss the direction of thermoelectric device standardization and efficiency-oriented research for the application and industrialization of thermoelectric technology, moving away from the material and ZT-based evaluation system.

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Single-phase synthesis and thermoelectric properties of nowotony chimney-ladder FeGe

P69

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Keywords: FeGe, chimney-ladder phase, thermoelectric material, crystal structure, thermoelectric property

The chimney-ladder compound $FeGe_\gamma$ is expected to be an n-type thermoelectric (TE) material that can be paired with a promising p-type TE material $MnSi_\gamma$, as their thermal expansion coefficients at 700 K are nearly equal, which is desirable for module fabrication [1]. Sato et al. reported the synthesis and TE properties for $FeGe_\gamma$. However, their samples contain secondary phases, in which their contribution to TE properties cannot be negligible [2]. Therefore, this study aimed to synthesize single-phase $FeGe_\gamma$ samples and measure their TE properties.

The nominal composition x in $FeGe_x$ was varied for x = 1.52, 1.53, 1.54, and 1.55, and the samples were weighed accordingly. The starting materials, Fe and Ge grains, were arc-melted and subsequently ball-milled. The obtained powder was annealed to promote the reaction, and the annealing process was repeated several times. The resulting samples were densified using spark plasma sintering (SPS). Powder X-ray diffraction and TE property measurements were performed on the SPS-treated samples. The value of γ was determined using the Le Bail analysis of Jana2020 package [3].

For the sample with a stoichiometric composition of x = 1.54, a nearly single-phase sample was obtained. The refined γ values in all stoichiometric compositions were approximately 1.51700(5), indicating that the phase is almost a line compound. After the SPS process, the γ-value was slightly changed. The TE properties of the x = 1.54 sample were zT = 0.6(1) and TE power factor, PF = 2.1(3) × 10^{-3} W/m^{2}K at 623 K. The effect of partial substitution on the crystal structure and TE properties will be presented in the poster presentation.

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Textured $Ca_3Co_{4-x}O_{9-\delta}$ ceramics of electrospun nanoribbons with improved thermoelectric performance

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Keywords: calcium cobaltite, electrospinning, thermoelectric material, nanoribbons, texturing, nanostructuring

Calcium cobaltite $Ca_3Co_{4-x}O_{9+\delta}$ is a promising p-type thermoelectric oxide material with superior functional properties for high-temperature applications in air. Since the material has strong anisotropic properties, texturing and nanostructuring should be targeted to improve the thermoelectric performance. Electrospinning is particularly suitable for this purpose, which is a low-cost method and meets the requirements for texturing and nanostructuring of a material. In this study, flat-shaped $Ca_3Co_{4-x}O_{9+\delta}$ nanofibers, referred to as nanoribbons, were electrospun and the resulting nanoribbon mats were further processed into a textured $Ca_3Co_{4-x}O_{9+\delta}$ ceramic. In earlier work, we have demonstrated that mixtured mats of nanoribbons and cylindrical nanofibers feature strong thermoelectric properties [1]. Still, it is anticipated that the thermoelectric properties of the compacted specimen can be further enhanced by mats consisting only of flat nanoribbons. Nanoribbons are hypothesized to provide more efficient packing due to their flatness relative to cylindrical nanofibers, allowing for higher densification in the green body and ceramic, and contribute to sample texturing, since the primary particles in the nanoribbons are assumed to be aligned in the nanoribbons plane. Accordingly, we investigated the influence of the electrospinning conditions and the composition of the precursor material on the microstructure of the electrospun material to achieve pure nanoribbon mats. We noted a strong correlation of nanoribbon formation with the polymer concentration in the electrospun precursor and summarized the possible formation mechanisms. We also highlight an important step in the nanoribbon calcination process to obtain texturing of the primary particles. Lastly, we have fabricated ceramics from nanoribbon mats and analyzed their texturing by X-ray diffraction with measurement of the pole figures of the (0002) lattice planes associated with the 4-dimensonal superspace group of the C face-centered monoclinic aperiodic crystal structure. Additionally, we evaluated the Seebeck coefficient and electrical conductivity of the nanoribbon-based samples to assess their thermoelectric capabilities.

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The comparison of properties of tellurides doped monocrystals

P71

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Keywords: Bi_2Te_3, Sb_2Te_3, monocrystal, thermoelectric properties, properties optimization

Bismuth and Antimony tellurides are well known as a non-toxic and relatively inexpensive thermoelectric material. One of the most popular parameters generally describing thermoelectric properties of any material is Figure of Merit (ZT). There is possible to enhance operational parameters of semiconductor material by doping its chemical composition with other elements, resulting with modification of career concentration as well as intensification of phonon scattering. Optimization of these parameters leads to enhancement of ZT not only by decreasing lattice part of thermal conductivity, but also by ensuring a proper balance between Seebeck coefficient, electrical conductivity and electron part of thermal conductivity. The research presented in this work is focused on comparison of doped Bi_2Te_3 and Sb_2Te_3 monocrystals and the powder metallurgy fabricated bulk materials.

Material fabrication procedure, sintering parameters, phase and chemical composition, microstructure, physical and thermoelectric properties are presented. Experiments results showed that monocrystals achieved better thermoelectric parameters, but their application is limited due to the higher costs of fabrication and further processing.

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Properties of semiconductor-metal junctions obtained by the SPS/FAST process

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Keywords: thermoelectric material, bismuth telluride, connectors, spark plasma sintering, SPS

One of the most important topic while thermoelectric modules fabrication is combining semiconductor materials with metallic electrodes. The efficiency of devices using thermoelectric phenomena essentially depends not only on the physicochemical properties of thermoelectric materials but also on other factors. According to research that has been carried out for many years, not much less important influence on the efficiency of the modules is the quality of the electrical contacts. During the design of devices based on thermoelectric materials, it is also important to pay attention to the selection of appropriate protective barriers that inhibit diffusion processes at the interface boundary, as well as test methods to determine the quality of metal/semiconductor junctions. It is necessary to study the properties of the resulting junctions to confirm the quality of adhesion, mechanical strength, electrical and thermal properties and, due to the operating conditions, excellent chemical and temperature stability during the device life cycle.

This paper presents the results of tests on joining bismuth telluride and copper using lead-free solder and discusses the properties of the joints produced. The properties of the samples (electrical conductivity and Seebeck coefficient) were characterized and presented. Microstructure studies (SEM) and elemental distribution analysis were also carried out to investigate the progress of corrosion/diffusion.

The detailed characterization of the obtained joints presented here facilitates quality control, enabling confirmation of the relevant joint parameters by simple electrical measurements.

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The properties of tellurides fabricated by SHS technique

P73

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Keywords: SHS, SPS, tellurides, materials fabrication, thermoelectric properties

The development of innovative applications must be supported not only by scientific analysis and basic research of novel materials but also by finding new methods to synthesise well-known semiconductor materials in a simpler and more economically attractive way. Nowadays a few main directions within thermoelectric society can be identified. One group of research subjects focuses on adopting new methods of synthesis to fabricate thermoelectric material. While the classical approach involves many stages of synthesis in vacuum quartz ampules, milling, vacuum quartz annealing, another milling, followed by a sintering, new ways should aim to reduce the number of steps or simplify them. Simplification of tellurides' fabrication process has a huge potential for thermoelectric applications, where lack of good-quality and economically viable material availability limits the implementation potential. This work shows the way of fabrication of doped bismuth and antimony tellurides using the self-propagating high-temperature synthesis (SHS) method inside the spark plasma sintering (SPS) apparatus, presents material properties and compares them to material fabricated in vacuum-sealed quartz ampules. Experimental results proved that properly conducted SHS process can be a promising alternative for the most popular direct synthesis method in quartz tubes, providing material with similar operational parameters in a simpler and faster way.

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Role of the magnetism on the thermoelectric properties in $FeCr_2S_4$

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Keywords: thiospinel, chalcogenides, magnetism, thermopower, magnetoresistance

Among sulfides, spinels have attracted significant research interest due to their interesting magnetic and electronic properties, which can exhibit metallic, insulating, or superconducting behavior [1]. The thermoelectric properties of spinels can be modified by doping, but magnetism can also play a significant role in shaping them.

The impact of magnetism has already been observed in transition metal oxides such as misfits [2] or Na_xCoO_2 [3], in pyrites [4] or in $CuGaTe_2$ chalcopyrites [5]. Its impact can induce entropic terms, beneficial for the thermopower S as for example in oxides with paramagnetic Co^{3+} and Co^{4+} [2,3], or it can induce a modification of the band structure as in pyrites [4] and thereby modify S. More recently, a clear impact of magnetism has been observed in the thiospinel $CuCr_{1-x}Ti_{1+x}S_4$ where, depending on x, a negative or positive magnetothermopower effect has been observed [6].

In that respect, as a significant impact of magnetism was previously observed for the $FeCr_2S_4$ thiospinel, with a very large and negative magnetoresistance (MR) effect [7], and considering that $FeCr_2S_4$ crystallizes also in the monoclinic NiAs structure (Cr_3S_4) [8], we present here the magnetic field dependence of thermoelectric properties for both $FeCr_2S_4$ polymorphs.

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Impact of excess Cu on phase separation and thermoelectric properties of arc melted $Ti_{0.5}Zr_{0.5}NiCu_ySn$

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Keywords: thermoelectrics, half-Heusler alloy, phase separation, excess Cu, processing, stability

Half Heusler (HH) alloys are characterised by high power factors $S^2\sigma$, abundant low-toxicity precursors, good stability and engineering properties.[1] The perfomance of the HH alloys is limited by an inherently high κ_{lat}. XNiSn (X = Ti, Zr, Hf) has been the prominent n-type HH thermoelectric material for the last decade, with alloying on the X site proven to significantly reduce κ_{lat}. [1] However, Ti and Zr/Hf mix poorly during materials synthesis, resulting in the presence of multiple HH phases. [2,3]

In this poster, the impact of excess Cu on the HH phase distribution of $Ti_{0.5}Zr_{0.5}NiCu_ySn$ (y = 0.025, 0.1) is presented. Thorough characterisation using XRD and SEM of samples treated at varying temperatures shows minimal impact by 2.5 at% Cu; whilst increased Cu content of 10 at% affords dramatically improved homogenity, as seen in **Fig. 1**. This nearly homogeneous sample has the lowest $\kappa_{lat,}$ confirming the effectivenes of alloying. Peak zT = 0.7 is found for $Ti_{0.5}Zr_{0.5}NiCu_{0.025}Sn$ with a lower zT = 0.5 for $Ti_{0.5}Zr_{0.5}NiCu_{0.1}Sn$ due to over-doping. Our results suggest that the poor mixing of Ti and Zr/Hf in XNiSn alloys is a kinetic effect and not driven by phase seperation.

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Band engineered and carrier modulated thermoelectric enhancement in half-Heusler

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Keywords: thermoelectric, Half-Heusler, band engineering, charge modulation, DFT

Inspired by the recent advancements in band engineering [1] to improve the thermoelectric properties, we have succeeded in enhancing the power factor and hence the figure of merit (zT) of half Heusler (hH) alloys based on TiCoSb. From the first-principle electronic structure calculations we show conduction band convergence at the X-point in the Brillouin zone upon 10% lattice expansion. To achieve degeneracy, we tried doping at the Ti site with Hf, Zr and Nb. We found that Nb doping is most conducive to obtaining the desired results. However, experimental attempts to dope Nb at the Ti site resulted in phase separation into phases $Ti_{1-y}Nb_yCoSb$ and $Nb_{0.80}CoSb$. The composition of Nb in $Ti_{1-y}Nb_yCoSb$ is found to scale with the starting composition TiCoSb : NbCoSb, the higher the Nb composition the larger the concentration of Nb in $Ti_{1-y}Nb_yCoSb$ whereas the second phase $Nb_{0.80+\delta}CoSb$ always appeared without change. Equipped with these findings, we made a series of alloys with compositions $(TiCoSb)_{1-x}(Nb_{0.8}CoSb)_x$, $(0 \leq x \leq 0.5)$. As x increases, y takes larger and larger values in $Ti_{1-y}Nb_yCoSb$. The carrier concentration of $Ti_{1-y}Nb_yCoSb$ phase accordingly increases and for a certain x exceeds the carrier concentration in $Nb_{0.80+\delta}CoSb$. This allows for carrier modulation [2] doping with electron migration from one electron-rich phase to another. A maximum power factor of 28 $\mu Wcm^{-1} K^{-2}$ is recorded for x = 0.3 composition for which the Nb doping in $Ti_{1-y}Nb_yCoSb$ is optimal to benefit from the band alignment. The Hall carrier concentration for this sample is also same as the concentration one can estimate theoretically from the valence electron count therefore Fermii level alignment resulting in maximum mobility. Reduction of the lattice thermal conductivity due to alloying and phase segregation is also observed in these alloys. A maximum zT of 0.81 at 973 K was obtained for x = 0.4 composite. We have therefore shown that band engineering along with modulation doping can be a very effective method to improve thermoelectric properties.

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Engineering thermoelectric transport in transparent conducting oxides

P77

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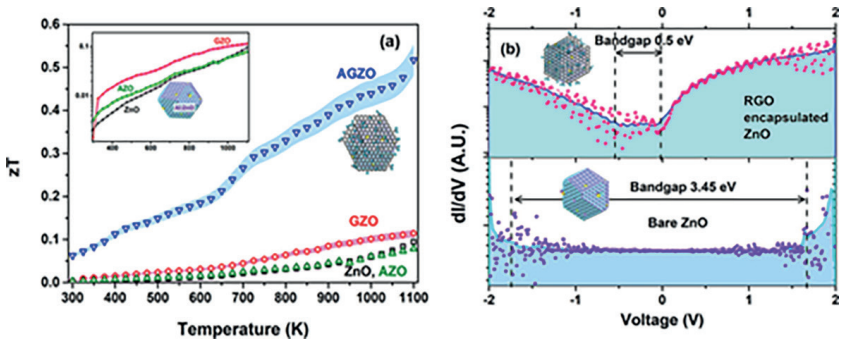
Keywords: oxides, thermoelectric transport, microstructure, defects, energy filtering



A number of oxides, including ZnO, ITO, $SrTiO_3$ and cobalt oxides are promising candidate as environment friendly thermoelectric (TE) materials [1-3]. However, high thermal conductivity is the primary factor which hinders their application and leads to poor TE figure of merit (zT). Here we demonstrate that microstructure engineering through Al doping and reduced graphene oxide /graphite additives leads to selective enhancement in phonon scattering in ZnO thereby increasing its TE efficiency [4]. The incorporation of trace Al doping with 1.5 wt% RGO into ZnO (AGZO) has been found to show significant improvement in zT (= 0.52 at 1100 K) which is an order of magnitude larger compared to that of bare undoped ZnO. Tunneling spectroscopy performed on bare as well as composite particles reveals that the band gap of ~ 3.4 eV for bare ZnO reduces effectively to ~ 0.5 eV upon RGO encapsulation, facilitating charge transport. The Al doping, defect engineering and RGO encapsulation synergistically brings about drastic reduction of thermal conductivity, through enhanced interfacial and point defect-phonon scatterings. These opposing effects on electrical and thermal conductivities leads to enhancement in the power factors as well as the zT value [5]. Our subsequent efforts with highly ITO oxides will be presented in the later half.

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Modelling the lattice thermal conductivity of skutterudites: *ab-initio* calculations, machine learning and more

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Keywords: thermal conductivity, high-throughput, modelling, optimization, *ab-initio*

Skutterudites have been reported as very good thermoelectric materials and very recently have been demonstrated to present one of the richest chemical spaces [1]. These materials combine high electron mobility with low thermal conductivity. However accurately predicting the transport properties that determines the thermoelectric figure of merit of such a large set of materials is a challenging task.

In this work, a high-throughput framework that combines ab-initio calculations, Machine Learning and the solution of the Boltzmann transport equation has been developed to explore the lattice thermal conductivity of skutterudites [2-3]. We systematically explore the effects of physical variables such as temperature, pressure, or crystallinity but also chemical variables such as composition, the presence of rattlers, and alloying. This strategy gives the opportunity to unravel the chemical and physical phenomena that govern lattice thermal conductivity in skutterudites, opening the door to the optimization of the thermoelectric efficiency of this family of materials.

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Preparation and thermoelectric properties of nonstoichiometric full- Heusler $Mn_{2+x}V_{1-x}Al$ alloys

P79

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Keywords: nonstoichiometry, full Heusler, half-metal, power factor, electronic structure

Half-metallic full-Heusler alloys have attracted attention as thermoelectric materials [1-5]. Li et al. [2,3,5] have shown that power factor, PF, of Mn_2VAl can be improved by controlling the amount of antisite defects and by partial substitution in Mn_2VAl. The maximum PF was reported to be 4.46×10^{-4} W/mK^2 for $Mn_2VAl_{0.96}Si_{0.04}$ [5]. In this study, we aimed to further improve the PF of Mn_2VAl by shifting the ratio of Mn to V from 2:1 to a nonstoichiometric composition, $Mn_{2+x}V_{1-x}Al$. The preparation method was based on previous research using ball milling and spark plasma sintering [3]. The prepared samples with x = -0.2, -0.1, 0, +0.1, and +0.2 were found to be almost single-phase. The Seebeck coefficient, S, was the highest for the $x = 0$ sample. This is contrary to the case of Fe_2VAl where nonstoichiometry increased S [6]. The temperature where S reached a maximum value decreased as x increased and decreased. This result may correspond to the change in magnetic transition temperature. Although the electrical conductivity, σ, increased with increasing x, the maximum PF was recorded for the $x = 0$ sample, reflecting the sample dependence of S. At the conference, we will also present calculation results of electronic structures of $Mn_{2+x}V_{1-x}Al$ to comprehend the change in measured S and σ.

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P80

Unraveling the origin of donor-like effect in bismuth-telluride-based thermoelectric materials

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Keywords: Bismuth-tellurides, donor-like effect, point defects, thermoelectric properties

The donor-like effect, depicting the uncontrollable increase of electron density that can significantly alter the thermoelectric performance of both p-type and n-type polycrystalline Bi_2Te_3-based materials, has long been an intriguing phenomenon while its origin is still elusive. Here, we found that, different from the common argument, the donor-like effect in Bi_2Te_3-based polycrystals is a result of the oxygen adsorption-induced evolution of the point defects. The dominant point defect in stoichiometric zone-melted Bi_2Te_3 ingot is the acceptor-like Bi'_{Te}, making it weak p-type. When subjected to the mechanical and thermal deformation processes to achieve high-strength polycrystals, the exposure of the ball milled powders to the air leads to their absorption of oxygen and the formation of secondary phase Bi_2TeO_5 in the following pressing process. This brings about the change of local chemical equilibrium and promotes the evolution of the intrinsic point defect from acceptor-like Bi'_{Te} to donor-like $Te^{\bullet}_{Bi}$. Notably, if the fabrication process is strictly controlled to minimize oxygen absorption, the evolution of the point defects will be avoided, whereby the donor-like effect disappears. As a result, a reproducible high zT value of 1.0 at 325 K can be achieved in $Bi_2Te_{2.7}Se_{0.3}$-based polycrystals. These results highlight the importance for understanding the evolution of point defects that is crucial for developing high-performance Bi_2Te_3-based polycrystals and corresponding fabrication processes.

Acknowledgments

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Enhanced thermoelectric properties by anion-engineering of 2-dimensional transition metal dichalcogenides

P81

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Keywords: 2-dimensional materials, molybdenum disulphide, thermoelectrics, nanomaterials

2D transition metal dichalcogenides (2D TMDs) have attracted considerable attention recently owing to their superior physical and chemical properties. These 2D materials have shown great potential for thermoelectric (TE) energy generation due to their unique electrical and thermal transport properties originated from their unique atomic structures. The calculated and predicted thermoelectric performance should exhibit outstanding TE performance, however, it still lacks of experimental confirmation. Furthermore, a reliable and a robust preparation and characterization methodologies for proving the 2D TMDs-based TE materials are underdeveloped. The measured and reported TE performance of 2D TMDs is still much lower than that of conventional bulk TE materials such as BST, because of higher thermal conductivity and lower seebeck coefficient.

Here, we demonstrate that the enhanced TE performance of 2D TMDs by a facile anion-engineering. Phosphorus doped 2D TMDs show the highly enhanced seebeck coefficient and electrical conductivity, which can lead high power factor. Furthermore, the low thermal conductivity can be achieved by defects and doped phosphorous atoms in 2D TMDs atomic structure. This work can pave a way to achieve high TE performance of 2D TMDs-based TE materials.

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P82

Enhancing thermoelectric and mechanical properties of p-type $(Bi, Sb)_2Te_3$ through Rickardite mineral ($Cu_{2.9}Te_2$) incorporation

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Keywords: $Bi_{0.5}Sb_{1.5}Te_3$, $Bi_{0.3}Sb_{1.7}Te_3$, Rickardite, thermoelectric, microhardness

Bi_2Te_3-based alloys are widely utilized in Peltier coolers owing to their highest thermoelectric performance at near-room-temperatures [1,2]. However, their peak dimensionless thermoelectric figure of merit, zT, is limited to a narrow temperature window due to minority carrier excitation emerging upon heating at around 400 K. Here, we show how this issue can be overcome by incorporating synthetic rickardite mineral, $Cu_{3-x}Te_2$, in p-type $(Bi, Sb)_2Te_3$. The significant enhancement of the electronic and thermal properties could be achieved due to small Cu incorporation into the crystal structure of $(Bi, Sb)_2Te_3$ and homogenous precipitation of $Cu_{3-x}Te_2$ at the grain boundaries. This leads to high average zT value (zT_{ave}) of 1.22 between 350 and 500 K for two compositions, $Bi_{0.5}Sb_{1.5}Te_3$ (BST-5) and $Bi_{0.3}Sb_{1.7}Te_3$ (BST-3), with peak zT values of 1.32 at 467 K and 1.30 at 400 K, respectively. These high zT values result in a considerably high maximum device ZT of ca. 1.15 and a theoretical efficiency of up to 7 % between 325 K and 525 K. Additionally, room-temperature micro-hardness is substantially improved, which is desirable for constructing reliable and durable thermoelectric modules.

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Effect of magnetic entropy in the thermoelectric properties of Fe-doped Fe_2VAl full-Heusler

P83

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Keywords: thermoelectric, Fe_2VAl, full-Heusler, spin fluctuation, point defects

Spin entropy is involved in the transport of heat/charge carriers in magnetic materials, and can provide new opportunities to improve the conversion efficiency of thermoelectric materials over that of the conventional case [1-3]. Here, we have explored the effect of magnetic entropy on thermoelectric properties of well-characterized Fe-doped full-Heusler, $Fe_{2+x}VAl_{1-x}$ with x = 0 – 0.1. These samples are prepared by arc melting, followed by spark plasma sintering and annealing, producing high-density crystalline products. The low-temperature magneto-thermoelectric measurement shows exotic results, including a significantly high power factor near 300 K.

The itinerant weak ferromagnetic behavior of studied samples is confirmed from the magnetization. A systematic increase in magnetic transition temperature (T_c; 40 K to 223 K) and saturation magnetization (M_s; 0.13 to 0.41μ_B/Fe) with increasing Fe doping (x = 0 to 0.1) is observed. Applying a magnetic field causes a clear suppression in the magnitude of thermopower (S) and electrical resistivity (i.e. negative magnetoresistance) near the T_c for all the samples, demonstrating a clear effect of spin fluctuation [2]. This difference further increases with increasing magnetic entropy by Fe-doping, with the highest of $|S_{0T}–S_{7T}|/S_{7T}$ of 13% for x = 0.1. The temperature-dependent behavior of S ruled out the contribution of magnon drag. Interestingly, we can shift the T_c towards room temperature to get the advantage of the spin fluctuation in enhancing the S, but Fe doping also increases the overall carrier density, leading to lower S. Callaway model fitting of thermal conductivity reveals Fe doping increases the number of point defects causing a significant reduction in lattice thermal conductivity. This study demonstrates a strategy for further enhancing the thermopower/ thermoelectric performance of Fe_2VAl by magnetic doping.

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P84

Carrier engineering-driven high thermoelectric performance in Ti doped $Yb_{0.4}Co_4Sb_{12}$

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Keywords: coupling, filling fraction, rattling, skutterudites, voids

$CoSb_3$ based skutterudite systems are one of the promising candidate for the intermediate temperature range thermeoelctric application beacause of their cage-type crystal structure and non-toxic constituting elements. The rattling behaviour of multiple-filler atoms in the voids have shown wide range of phonon scattering phenomenon. Also, the electrical conductivity and Seebeck coefficient are not influenced unpreferably which turns these systems suitable to induce decoupling effects between electrical and thermal transport under phonon glass electron crystal (PGEC) approach. $Yb_{0.4}Co_4Sb_{12}$ compound being a well studied system showed higher electronic performance due to the enhancement in carrier concentration. The rattling Yb atoms provided lowering effects in thermal conductivity. However, further strategies are needed to be adopted for enhancement in thermoelectric efficiency. Herein, the effect of Ti at Co site in $Yb_zCo_{4-x}Ti_xSb_{12}$ (z = 0, and 0.4; x = 0, 0.04, and 0.08) has been studied. The presence of Ti^{+4} at Co^{3+} site provided extra electron charge carriers and enhanced the electrical conductivity from 797 S/cm for x = 0 to 1043 S/cm for x = 0.04 at 577K. The scattering originating via point defects, rattling and umklapp mechnaisms provided additional reduction in thermal conductivity upto 3.5 W/mK at 300 K for $Yb_{0.4}Co_{3.96}Ti_{0.04}Sb_{12}$. Overall the power factor enhaced upto 44 W/cm. K^2, which leads to maximum zT value of 0.85 for the compsostions $Yb_{0.4}Co_{3.96}Ti_{0.04}Sb_{12}$ at 623 K. This improvement shows the suitablity of these compounds for thermoelectric applications.

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Rapid synthesis and thermoelectric characterization of Ag_2Se_{1+x} compounds: Unveiling the secret of ultrafast formation and high performance

P85

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Keywords: thermoelectrics; silver selenide; ball milling; mechanochemical synthesis

The challenge to create high performance thermoelectric materials lies in achieving simultaneously large Seebeck coefficient, high electrical conductivity and low thermal conductivity [1]. Notably, the high zT values near unity of Ag_2Se [2,3] make it a potential candidate for room-temperature thermoelectric application.

In this study, the thermoelectric properties of Ag_2Se_{1+x} compounds, where x is a variable that ranges from 0 to 0.04, through a comprehensive experimental and theoretical analysis were investigated. We synthesized Ag_2Se_{1+x} compounds using high-energy ball milling in only 10 minutes and characterized their electrical resistivity, Seebeck coefficient, thermal conductivity and figure of merit zT.

The results showed that despite the short time required for synthesis, the Ag_2Se_{1+x} compounds exhibited thermoelectric performance comparable to samples obtained by other synthesis routes. With increasing x, carrier concentration is reduced, resulting in increased electrical resistivity and magnitude of Seebeck coefficient. The maximum dimensionless figure of merit zT of the Ag_2Se_{1+x} compounds is achieved at $x = 0.01$, for which is the value is around 0.6 at 300 K and increased to 0.9 at 380 K, indicating their promising thermoelectric performance.

In conclusion, the study provided a comprehensive understanding of the thermoelectric properties of Ag_2Se_{1+x} compounds prepared by ultrafast high-energy ball milling. These findings contributed to the development of high-performance thermoelectric materials and open up new possibilities for optimizing the thermoelectric properties of Ag_2Se-based compounds.

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The enhancement of thermoelectric performance in MgAgSb via annealing process

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Keywords: MgAgSb, synthesis, defect, secondary phase, carrier mobility

The formation of defects in a material can generally modify the electronic transport properties of its mother compound. The controlling of defects in thermoelectric materials is advantageous to optimize the charge carrier concentration to achieve high thermoelectric performance. The α-MgAgSb has attracted attention as a promising thermoelectric material due to its intrinsically low lattice thermal conductivity, which leads to the high thermoelectric performance. It has been reported that the thermoelectric properties of α-MgAgSb are highly sensitive to the synthesis procedure[1-5]. The synthesis conditions for α-MgAgSb compounds not only influence the formation of secondary phases but also contribute the electronic transport properties.

In this work, we investigate the effect of annealing on thermoelectric properties and crystal structure of α-MgAgSb compounds at elevated temperatures. It is found that the heat-treatment plays an important role in determining the concentration and type of secondary phases, which impacts the electronic transport properties. For annealed sample, the α-MgAgSb phase become more stable with less secondary phases for wide temperature ranges than that of sample before annealed. The carrier mobility is significantly increased due to the annealing process and further improved by Fe-doping, leading to the enhancement of thermoelectric performance.

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Growth and TE properties of n-type Mg_3Bi_2-based thermoelectric thin film

P87

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Keywords: thin films, co-sputtering, defects, XRD, SEM, and thermoelectric properties

Mg_3Bi_2-based materials have become a topic of interest for possible room-temperature thermoelectric applications. These materials are highly explored in bulk, ensuring their n-type high-performance behaviour [1-3]. In contrast, there are very few reports on these thin films, mostly showing p-type behaviour. In this study, we reported the n-type Mg_3Bi_2-based thin films through a co-sputtering method for the first time. Here in present work several numbers of attempts have been made by varying the deposition power and pre-annealing temperature. The structural and thermoelectric properties of all these deposited thin films of Mg_3Bi_2-based are examined. We adjusted the Mg ratio by co-sputtering of Mg and $Mg_3Bi_{0.5}Sb_{1.5}$ targets simultaneously and achieved a maximum power factor of approximately 110 μW/m K^2 at 423 K along with n-type behaviour. This article reports the first n-type co-sputtered $Mg_3Bi_{0.5}Sb_{1.5}$ thin film and explains role of Mg concentration in adjusting the conduction of Mg_3Bi_2-based thin films from p-type to n-type.

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Porous Ag_2Se fabricated by a modified cold sintering process with the average ZT around unity near room temperature

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Keywords: thermoelectric, cold sintering process, chalcogenide, Ag_2Se, porous structure

Ag_2Se thermoelectric material was calculated to enhance ZT close to 1.0 by the decrease in carrier concentration to approximately 1×10^{18} cm^{-3}. [1] In this work, we present the strategy to reduce carrier concentration by performing porosity by the addition of dissolvable liquid during the sintering process. It is called the modified cold sintering process (CSP). The mixed solution between thiol-1, ethylenediamine (amine) and 1,2-ethanedithiol (thiol) in the ratio of 10:1 wt% was added with Ag_2Se powders before hot-pressing by a homemade instrument. In this work, the quantity of thiol–amine and holding time of sintering was optimized while the sintering temperature and pressure were controlled at 423 K and 600 MPa, respectively, under a room environment. Scanning electron microscopy (SEM) exhibits the existence of porosity with the addition of thiol-amine contributing to a decrease in carrier concentration from 1.4×10^{19} to 5.0×10^{18} cm^{-3}. Although the electrical conductivity decreased via this addition, the Seebeck coefficient increased contributing to an increase in power factor (PF) to 2200 $\mu W/mK^2$ for the best condition. Moreover, the decrease in carrier concentration not only affects electrical conductivity but also decreases thermal conductivity to lower than 1.0 W/mK throughout the measured temperature due to the reduction in electronic thermal conductivity. Finally, the average ZT from room temperature to 400 K of 0.9 was recorded and was comparable to the works of literature.

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Enhanced thermoelectric performance of Al-doped ZnO nanocomposite obtained via chemical co-precipitation

P89

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Keywords: ZnO; thermoelectric materials; oxides; wet chemistry; chemical co-precipitation

Recently, ZnO-based thermoelectric materials have attracted significant attention due to their low price and high thermal stability. ZnO is an *n*-type semiconductor with a wide direct bandgap of ~3.4 eV, and a Wurtzite crystal structure. For a long time, ZnO-based materials are considered as promising high-temperature thermoelectric due to its moderate power factor, low price, and high thermal stability. However, the high thermal conductivity of ZnO, originated from its simple crystal structure and light constituents, hinders its thermoelectric performance and thus widespread use. Prior studies have reported that doping ZnO with elements such as Ni, Al, In, Ti or Sb leads to a significant enhancement in its thermoelectric performance[1].

This research presents a study on the fabrication of nanostructured ZnO doped with aluminum (x = 0.02; 0.04; 0.06) via spark plasma sintering. $Zn_{1-x}Al_xO$ powder was produced directly by co-precipitation of $Zn(NO_3)_2$ and $Al(NO_3)_2$ as precursors. The resulting bulks exhibited high relative density of 95%. X-ray phase analysis revealed that a $ZnAl_2O_4$ spinel was formed for with $x > 0.04$ obtained by precipitation technique. Additionally, a peak shift for XRD patterns of samples indicated a successful formation of $Zn_{1-x}Al_xO$ solid solution.

This research presents a study on the fabrication of nanostructured $Zn_{1-x}Al_xO$ (x = 0; 0.02; 0.04; 0.06) via chemical co-precipitation followed by spark plasma sintering. Overall the solid solution was formed and only for $x > 0.04$ a $ZnAl_2O_4$ spinel phase was formed indicating that the Al solubility limit is reached in the ZnO in Wurtzite crystal structure. For the obtained samples, we observed quite an unusual behavior when the Seebeck coefficient and electrical conductivity increased simultaneously with temperature due to nanostructuring. The high σ values were attributed to the increase of electron concentration induced by Al doping, while high S values were due to Fermi energy tuning and heavier effective masses initiated by Al. Besides increasing the power factor, the double-phase structure played a vital role in reducing the lattice thermal conductivity due to phonon scattering by the Umklapp and point defect mechanisms. This approach yielded an increase of the figure of merit for $Zn_{0.96}Al_{0.04}O$ up to zT = 0.5 at 1100 K, which is one of the highest-ever reported results for single-doped ZnO.

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P90

Energy harvesting from thermoelectric thin film by electromagnetic induction

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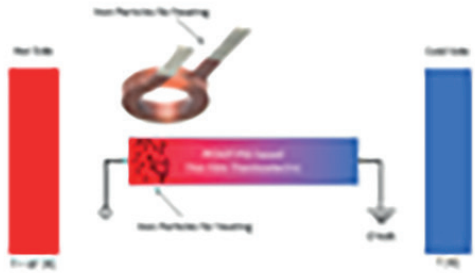
Keywords: pedot, PSS, energy harvesting, thermoelectric, thin film, electromagnetic induction

Researchers have focused on wearable technology in recent years. Wearable electronic devices need power supply. The capacity of the power supply affects the operating time and performance of the device. The use of wearable devices has been postponed due to problems such as low battery. In this case, devices need an efficient energy harvest [1]. Energy harvesting of thermoelectric modules can provide the energy needed by wearable technology [2]. Organic thermoelectric modules stand out in terms of being light and flexible [3]. Therefore, the use of organic materials is becoming widespread. Known as organic polymer, Pedot: PSS is one of the most common polymers used in flexible modules. The reason this; easy workability, high electrical and low thermal conductivity [4].

During the study, Pedot: PSS and Iron Oxide powder were used together. Iron oxide powder was added to one side of the thin films prepared with different Pedot:PSS ratios. The part where iron powders are located; exposed to the high frequency magnetic field produced by the designed induction coils. Here, an increase in temperature is observed. The part without iron powder is exposed to room temperature. Energy is obtained from the temperature difference obtained here. During this study, the magnetic modelling of the induction coil was made in COMSOL Multiphysics.



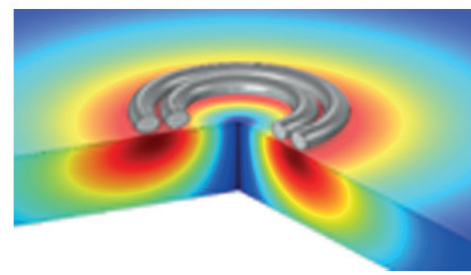


Figure 1: Finite element model mesh structure of auricular excitation coil
Figure 2: Heat dissipation of induction heating

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Thermoelectric properties of a novel $AgMnSbTe_3$ compound

P91

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Keywords: $AgMnSbTe_3$; narrow gap semiconductor; material synthesis; thermoelectric properties; thermoelectric measurements

A novel compound with the chemical formula $AgMnSbTe_3$ and the figure of merit ZT reaching 1.4 has recently been identified [1]. This narrow band gap, cubic semiconductor is obtained by alloying cubic $AgSbTe_2$ with hexagonal MnTe. We report a detailed investigation of a series of $AgMnSbTe_3$ samples with various doping and describe its synthesis, structural and thermoelectric properties.

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This work was supported by the Operational Program Research, Development and Education financed by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports (Project No. SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760).

P92

Synthesizing double/triple Half-Heusler to explore larger compositional space

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Keywords: half Heusler, thermal conductivity, alloying, p-n transition, module

Extensive research has been conducted on Half-Heusler materials due to their potential applications in thermoelectric materials, spintronics, and magnetic fields. Recently, the idea of higher order half-Heusler materials was proposed to enhance thermoelectric performance by reducing lattice thermal conductivity. In this presentation, we will explain the concept of double/triple half-Heusler (DHH/THH) materials, and their thermoelectric properties will be presented. The synthesized compositions using an unconventional valence balance strategy showed a low lattice thermal conductivity (κL) of less than 2.5W/m K. This value is significantly lower than the standards for half-Heusler (κL>10W/m K). [1] The high thermal conductivity of HH-based thermoelectric materials has always been a challenge, but the successful synthesis of DHH/THH materials with very low κL may open new possibilities for high-performance HH thermoelectric. In addition, achieving both n and p-type materials enable us to fabricate thermoelectric module with very similar composition and generate electricity with various temperature differences. These findings promote the benefit of exploring the huge compositional space of higher order half-Heuslers for further development of thermoelectric materials and devices.

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Electronic/ thermal transport and thermoelectric phenomena in implanted diamond nanostructures

P93

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Keywords: electron-phonon interaction, seebeck, implanted diamond, phonons, confinemet

The interaction between phonons and electrons is known to be at the origin of large values of the Seebeck coefficient at low temperatures, a phenomenon known as “phonon drag” in the Seebeck perspective in which a fraction of the phonon momentum, induced by an applied thermal gradient, is transferred to the electron gas. While phonon drag produces high Seebeck values, the thermoelectric community has long ignored it, since it is associated with phonons of long mean free paths and therefore high lattice thermal conductivity. This was the case until 2008 when Boukai et *al*. [1] confirmed in a study with Silicon nanowires, that it is possible to have a large phonon drag at high temperatures even if the system has low thermal conductivity. In 2015, the group of ZX Chen, at MIT published a paper where they rationalize it with *ab-initio* simulations by considering the coupling between the two Boltzmann equations (electron and phonon transport) through the electron-phonon interaction [2]. In this project, we investigate the thermal and electronic transport properties of conductive channels embedded in crystalline diamond. We aim to separate the phonon gas and the electron gas into two different media and try to have them interact to produce the phonon drag effect. This poster demonstrates how to create a conductive buried region of low thermal conductivity in a matrix of the highest known thermally conductive material in nature and the sample preparation for transport studies with some initial results.

P94

Effects of annealing on thermoelectric properties of thin films and their application in micro-thermoelectric devices

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Keywords: thin films, PVD, micro thermoelectric devices, thermoelectric characterization, *in-situ*, annealing

Demand for micro-thermoelectric harvesting or Peltier cooling devices for use in autonomous sensor systems needed for the Internet of Things is expected to increase dramatically in the coming years. Such microdevices are usually fabricated by electrochemical deposition or physical vapor deposition (PVD) in combination with photolithography. [1] In order to obtain good thermoelectric properties, PVD materials in particular are deposited at higher substrate temperatures. However, when using a template-based approach to fabricate micro-thermoelectric devices, the temperature during deposition is limited by the photoresist used. Therefore, the use of post-deposition heat treatment to optimize the thermoelectric figure of merit zT, which determines the performance of the device, is inevitable.

In this study, we discuss the influence of the post heat treatment process for n-type Bi_2Te_3 and p-type Sb_2Te_3 films in dependency of annealing temperature, time and film thickness. [2] By optimizing the annealing conditions, an increase in the zT value of up to 400% can be achieved. A thin film analyzer was used to determine the Seebeck coefficient, Hall coefficient, electrical conductivity and thermal conductivity in-situ during heat treatment. The influence of temperature effects on transport properties, including in-situ annealing experiments and the relationship to structure, grain size, and chemical composition will be discussed. In addition, we substantiate these results with finite element method simulations and discuss possible device designs and applications.

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This work was supported by the DFG (Deutsche Forschungsgemeinschaft) within grant no. RE3973/1–1 and SCHI 1010/11-1.

Optimizing thermoelectric properties of electrodeposited chalcogenides by electrochemical reduction reaction of tellurium ion

P95

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Keywords: electrodeposition, electrochemical kinetics, solubility of TeO_2, underpotential deposition, control of morphology

In order to apply metal chalcogenides for a thermoelectric application, morphology, crystal structure, and size must be precisely controlled to exhibit excellent thermoelectric properties. Thus, it is critical to understand the relationship between operating conditions of electrodeposition – such as electrolyte concentration, pH, temperature, and agitaion rate – and resulting physical proeprties of electrodeposits. In addition, because the satisfactory quality of tellurium-based chacogenides hinges on a critial control of a technique with a detailed understanding of deposition mechanism, it has been emphasized to investigate the reduction mechanisms in a wide range of electrodeposition conditions.

In this work, a systematic electrochemcial study was conducted on a varity of pH to control the solubiltiy of TeO_2, which is a key parameter for an underpotential deposition mechanism of chalcogenides, during the electrodeposition process. The morphology, composition, crystallinity, and crystal structure was varied to optimize their thermoelectric properties showning the relationship between the physical properties and the electrical proeprties of them.

Accordingly, a key target material property is able to be demonstrated by simply selecting the rate-limiting step in the specific deposition conditions, which leading to achieve the substances with meaningful thermoelectric properties. This finding also addresses the major challenge associated with the electrodeposition by the successful deposition of complex chalcogenides on an insulating substrate that expands its applications in fields for advanced electronics.

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P96

Improved thermoelectric performance of p-type tin monosulfide through tin precipitates

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Keywords: tin monosulfide, polycrystalline, precipitates

Tin monosulfide (SnS) has emerged as a promising thermoelectric material due to its abundance, low toxicity, and potential for high performance. As an analog of tin selenide, SnS exhibits anharmonicity that softens chemical bonds, resulting in ultralow thermal conductivity at moderate temperatures. However, despite its similarities to its analog, the polycrystalline form of SnS still lacks in terms of thermoelectric performance. The primary challenge lies in the significant decrease in electrical conductivity observed in polycrystalline SnS compared to its single crystal counterpart. In this study, we successfully synthesized polycrystalline Na-doped SnS through a precipitate design approach under tin-rich conditions. Tin precipitates were formed using a low-temperature solid-state reaction process at 973 K, followed by hot pressing at 923 K. These processing steps resulted in small grain sizes for the tin monosulfide, effectively reducing thermal conductivity. Although having the large grain size alone did not significantly enhance the electrical conductivity, the tin precipitates decorating the grain boundaries exhibited a remarkable improvement in electrical conductivity. As a result, we achieved a high power factor of approximately 2 μW/cmK at 473 K for the polycrystalline SnS. This corresponds to a relatively high thermoelectric figure of merit (zT) of nearly 0.2 at 473 K, which is relatively high for low-temperature applications involving this class of materials. Therefore, the precipitate strategy presented in this work is promissing for enabling high-performance polycrystalline tin monosulfide.

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Acknowledgments

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High thermoelectric performance in Ag_2Se achieved through a sustainable solution synthesis

P97

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Keywords: solution processing, Ag_2Se, defects, nanoparticles, polycrystalline, sustainability

Silver selenide, Ag_2Se, has been explored as one of the most promising candidates for room-temperature thermoelectric applications.

However, proper evaluation of its performance is hampered by the large discrepancy in the reported thermoelectric properties.

Herein, we propose a new synthetic approach based on the solution synthesis of Ag_2Se nanoparticles in a solvent mixture of amines and thiols. The resulting powder is then consolidated using spark plasma sintering at different temperatures. The sintering temperature allows us to control the material's microstructure and optimize it to reach a reproducible average figure of merit of ca. 1, from room temperature to 120 °C.

While this synthetic approach is scalable and robust, the use of the thiol/amine mixture can be problematic due to the cost of these solvents and how to dispose of them properly. A sustainable synthetic approach should account for minimizing waste. With this aim, we developed a strategy to reuse the byproducts (mainly solvents) after the reaction is finished. The protocol developed is based on the thermodynamics of the reaction that allows for using the supernatant directly to dissolve the new reactants with just a minor addition of thiols. Despite the repeated reuse of the supernatant, the performance of the resulting material remains the same. This synthetic method represents a breakthrough in solution-processed thermoelectric materials as it has overcome one of the biggest issues of solution processing, the large quantities of wasted solvents, yet without compromising on the final material performance.

Acknowledgments

ISTA and the Werner Siemens Foundation financially supported this work.

P98

Quantum and thermal fluctuations in spin configurations: deciphering their impact on magnetic order parameter and thermopower in MnSe across the critical temperature

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Keywords: quantum fluctuations, thermal fluctuations, thermopower, MnSe, magnetic order

MnSe is a semiconductor with notable thermoelectric properties due to its NaCl structure and two exchange interactions, J_1 and J_2. This structure is susceptible to frustration, leading to diverse initial spin states. Stabilizing the spin structure and achieving a specific antiferromagnetic order is possible when $J_2/J_1 > 0.5$. In this study, we explore undoped MnSe's properties, focusing on spin-driven effects. We utilize self-consistent spin-wave theory (SSWT) near and above the Néel temperature (TN), applying the Heisenberg model with nearest and next-nearest neighbor interactions. The Baryakhtar-Krivoruchko-Jablonsky representation allows examination of MnSe's magnetic order above the critical temperature by defining short-range order (SRO) parameters.

Our findings show strong quantum fluctuations at zero temperatures for anti-parallel nearest and next-nearest neighbors, with negligible fluctuations for parallel nearest neighbors. As temperature increases, thermal fluctuations intensify, reducing both long-range order and SRO. The influence of thermal fluctuations on anti-parallel and next-nearest spin SRO surpasses that on parallel spin SRO, indicating that temperature-dependent properties are mainly governed by anti-parallel nearest and next-nearest neighbors.

A comparison with MnTe demonstrates that MnSe's unique fluctuations arise from its lattice structure and frustration. Non-zero SRO parameter values above T_N suggest a non-zero entropy transfer and paramagnon drag thermopower similar to MnTe.[1–3] Consequently, MnSe presents potential as a spin-driven thermoelectric material. Additionally, the ternary alloy $MnSe_{1-x}Tex$ offers a versatile magnetic material system for developing efficient spin-driven thermoelectrics, with structures ranging from NaCl to NaAs hexagonal depending on the x value.

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Acknowledgments

This study was supported partially by NSF grant CBET-2110603.

High-performance n-type half-Heusler thermoelectrics exploiting interstitial Cu as dopants and phonon scattering centres

P99

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Keywords: half-Heusler alloys, thermoelectric conversion, TiNiSn, processing, empirical modelling

Half-Heusler alloys are leading contenders for application in commercial thermoelectric generators. They combine strong performance with good engineering properties and thermal stability. [1] There has been great progress in p-type half-Heusler alloys in the past decade, with $zT = 1.5$ achieved in NbFeSb and ZrCoBi. There have been fewer developments in n-type Heusler alloys with the best performance in compositions based on ZrNiSn, with peak $zT = 1.2–1.3$.

We have investigated the use of interstitial Cu in the XNiSn half-Heusler alloys. This cheap base metal is an alternative to the usual n-type dopant Sb. In addition to being an efficient n-type donor, its use leads to a suppression of thermal conductivity and a more homogeneous microstructure.[2-4] Our latest work reveals an enhanced density of states effective mass, $m_{DoS}^* \sim 4.1\ m_e$, for Cu-doped XNiSn half-Heusler samples rich in X = Ti. This enhancement over typical values of 3 m_e occurs without substantial drop in electron mobility. This enables improved power factors and peak $zT = 1$ at 773 K in TiNiSn-based samples with interstitial Cu used as a mineraliser, dopant and to suppress thermal transport.[5] Bandstructure calculations show the emergence of a second band at the conduction band minimum. This brings the performance of TiNiSn-based compositions close to the leading n-types based on Sb-doped ZrNiSn and is a significant development.

This contribution will summarise our current understanding of the impact of interstitial Cu in the XNiSn Heuslers, which goes beyond carrier doping and affects underlying electronic properties and microstructure of these materials.

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Study on multi scale evaluation of long-term reliability for thermoelectric devices and legs

P100

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Keywords: long-term reliability, leg-scale, device-scale, contact resistance, leg sample

In general, the long-term reliability of thermoelectric devices was evaluated by analyzing their overall device resistance and output power variation during accelerated thermal cycles. This overall device-scale evaluation could provide a rough understanding of device degradation over several or tens of years. However, a more specific understanding of the causes of device power generation degradation could not be investigated in detail after this overall device-scale cycling test. Considering recent thermoelectric power generation systems that increase the hot side temperature to around 200°C or even up to 250°C, detailed individual leg-scale and interface-scale evaluations are essential to gain a full understanding of thermoelectric device degradation. After the thermal cycling of the thermoelectric devices, the devices could not be fully disassembled to the individual leg size scale for detailed electrical and microstructural evaluations.

This study will evaluate both leg-scale and device-scale accelerated thermal cycling tests simultaneously and conduct a detailed analysis of thermoelectric device long-term power generation degradation. A typical single thermoelectric leg sample with all the layer structures, including the metallization layer, solder, and Cu electrode layer, will be fabricated except for the alumina substrate layer. This specially designed individual thermoelectric leg sample will enable an in-depth analysis of electrical and micro-structural degradation after the accelerated thermal cycling test, which could not be fully evaluated by the overall device-scale evaluation. In this specific leg-scale test, electrical contact resistances at each interface and the microstructural degradation will be evaluated after the accelerated thermal cycling test. A correlated analysis of these two different scale degradation tests will be reported, and the resultant long-term reliability calculation of thermoelectric devices will be discussed.

Acknowledgments

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PART VI
ROUND TABLE DISCUSSION

RTD

ROUND TABLE DISCUSSION: Identifying pathways for Successful Infusion of Recent Advances in Thermoelectric Materials into Power Generation Applications

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Keywords: thermoelectric; converter; generator; power

The field of solid-state thermoelectric technology serves a limited set of applications, with most of the current commercial market aimed at thermal management for operation in a narrow range of temperatures. This market is based on Bi_2Te_3-based materials discovered in the 1950's and offered in the form of standardized stand-alone modules, also known as "Peltier" coolers, that can be integrated with the end user subsystem.

For thermoelectric power generation, the need to achieve impactful performance often means being able to take advantage of a wide range of low-, mid- and high-grade heat sources. Current niche applications are based on PbTe/TAGS (medium temperatures) and SiGe (high temperatures) using technologies developed in the 1960's and 1970's as specialized fossil fuel- and radioisotope-powered generators in support of operations in extreme terrestrial and space environments.

Extensive work by the thermoelectric community at large has been successful in the last 25 years in identifying and characterizing new materials for power generation applications that clearly outperform older state-of-practice materials in their thermal and electrical properties. "Paradoxically", they are not used and it appears that more recent strategies for furthering the performance of high ZT materials may be largely at odds with addressing the key drivers for effective infusion into device-level and generator-level applications.

The thermoelectric material is only the starting point and high ZT values alone do not reflect the usability of thermoelectric materials. Many of the recent efforts have focused on achieving impressive "peak" ZT values, but one should keep in mind that these results can often be redeemed by difficulties in developing technology for its actual use in a thermoelectric generator. This is illustrated in the diagram below, which contrasts key high ZT approaches (upper box) with possible consequences relative to some important material requirements in terms of thermoelectric generator applications (lower box). It should be noted that these challenges are much less acute for Peltier cooling-type applications near room temperature.

Instead of "peak" ZT values, we postulate that an application "factor of merit" such as $ZT_{[average]} \times \Delta T_{[practical]}$ is a better initial measure of the efficiency and practical application "potential" of that material. It is then critical to recognize that practical thermoelectric generator designs are really "electrical power-generating heat exchanger" designs and consist of multiple subsystems that must be thermally, mechanically and electrically integrated and/or interconnected, which must demonstrate its long-term thermal, chemical and mechanical resilience in the targeted operating environment. In addition, understanding cost drivers and being able to satisfactorily address them is paramount.

Leaving aside the most technical aspects, we discuss some insights and pathways to help answering the challenging journey of higher performance modern thermoelectric materials from their discovery to their infusion into potential applications.

Acknowledgments

We gratefully acknowledge the support from the Czech Science Foundation (project no. 22-05919S).

RTD

A. Approaching anharmonic structure/near phase transition ($\kappa \downarrow$)

B. Nanostructuring/inclusions ($\kappa \downarrow$)

C. Multi-element composition/high number of atoms in the unit cell/alloying ($\kappa \downarrow$, ...)

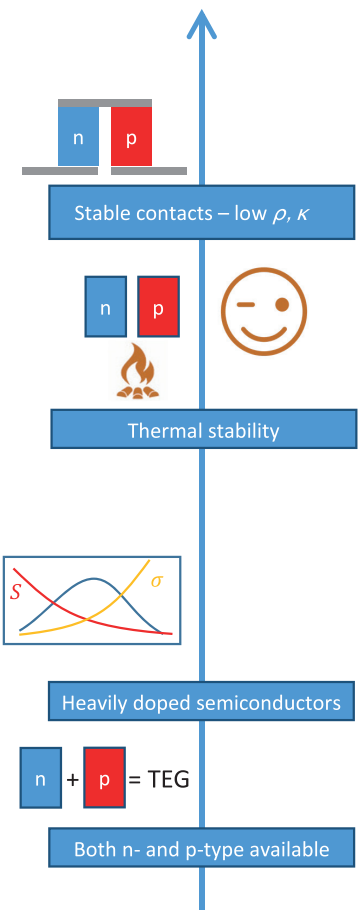
D. High DOS + high $\frac{\mathrm{d}\,(\ln \sigma)}{\mathrm{d}E}$ ($\sigma S^2 \uparrow$, $S_{dif} \uparrow$)

E. High mobility carriers ($\sigma S^2 \uparrow$) due to modulation doping, remote doping or δ-doping

F. Low dimensional/high symmetry structures ($m_{DOS} \uparrow \rightarrow S \uparrow$) ($m_{eff\ in\ particular\ direction} \downarrow \rightarrow \rho \downarrow$)

LEGEND:
κ...thermal conductivity, ρ...electrical resistivity
*S...Seebeck coefficient, *...solution to a problem*
↑...high or increasing, ↓...low or decreasing
→...implies or cause

Application tree
„what we need for applications "



Impact of A-F material parameters on device design

+) positive
0) neutral
-) negative

+)
0) D, E
-) A - thermodynamically unstable - reactive
B - nanoinclusions may increase reactivity
C - many elements increase number of possible reactions
F – superstoichiometry of one element increases reactivity

+)
0) D, E
-) A - materials at the limit of stability - decomposition, increased reactivity
B - nanostructuring increases reactivity)
C - large number elements increase the number of possible phases = reactions along T-gradient)
F - low-dimensional systems tend to be rich in one component, which increases reactivity

e.g. SnSe2+contact M → SnSe + MSe

+) C, D (DOS + high $\frac{\mathrm{d}\,(\ln \sigma)}{\mathrm{d}E}$ tends to increase with energy distance from the band edge
0) A, B, E, F
-)

+)
0) A, B, F,
-) C (native defects – either *n* or *p*, but not both)
D, E (unlikely to occur for both *e* and *h*)

* It is better to have 2 or 3 sister compounds (e.g. from n-Bi2Se3 to p-Sb2Te3

PART VII
LIST OF PARTICIPANTS

A

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		Zhang M.	Binninger R.	Araiz M.	Bouteiller H.	Mangelis P.	Pascual N.	Malik Z.	Acharyya P.	Battabyal M.	Özkan S.	Riss A.	Roy G.	
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		Lunch									Lunch			
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