Transverse Effects in Thermoelectric Systems

819. WE-Heraeus-Seminar

13 – 16 October 2024

at the Physikzentrum Bad Honnef, Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 819. WE-Heraeus-Seminar:

This WE-Heraeus Seminar on Transverse Effects in Thermoelectric Systems will bring together practitioners of thermoelectric technologies in academia and industry for 3 days of talks, posters and discussions addressing the emergent area of transverse thermoelectrics. With uses in carbon-free energy generation, cooling, sensing and process monitoring, transverse thermoelectrics stands to play a role in several of society's most pressing technological challenges: generating green energy, cooling our infrastructure, maximizing the efficiency and safety of our chemical and power production, and exploring space.

Our invited and contributing speakers will represent the forefront of the field in theoretical and computational research, materials synthesis and characterization, device fabrication and integration, and end users of the technology, bringing broad representation in terms of geography, gender and seniority. The topics will include methodologies for high-throughput materials selection for efficient electrical-to-thermal energy conversion, innovations in the fabrication of anisotropic thermoelectric materials, novel crystal structures and compositions, characterization of structure and transport at interfaces, micro- and nanoscale thermoelectricity, advances in instrumentation and standardized measurement techniques, and small and large-scale deployment of thermoelectric devices.

The seminar will invigorate the field by facilitating scientific exchange, promoting new collaborations, and enhancing the visibility of transverse thermoelectric research in the various communities that will be represented in our meeting in Bonn.

Scientific Organizers:

Prof. Dr. Kornelius Nielsch, Leibniz Institute for Solid State and Materials Research Dresden / GER
E-mail: k.nielsch@ifw-dresden.de

Prof. Dr. Oded Rabin, University of Maryland / USA
E-mail: oded@umd.edu

Prof. Dr. Saskia Fischer, Humboldt University of Berlin / GER
E-mail: sfischer@physik.hu-berlin.de

Introduction

Administrative Organization:

Dr. Stefan Jorda
Mojca Peklaj

Wilhelm und Else Heraeus-Stiftung
Kurt-Blaum-Platz 1
63450 Hanau, Germany

Phone +49 6181 92325-11
Fax +49 6181 92325-15
E-mail peklaj@we-heraeus-stiftung.de
Internet: www.we-heraeus-stiftung.de

Venue:

Physikzentrum
Hauptstraße 5
53604 Bad Honnef, Germany

Conference Phone +49 2224 9010-120

Phone +49 2224 9010-113 or -114 or -117
Fax +49 2224 9010-130
E-mail gomer@pbh.de
Internet: www.pbh.de

Taxi Phone +49 2224 2222

Registration:

Mojca Peklaj (WE Heraeus Foundation)
at the Physikzentrum, Reception Office
Sunday (16:30 h - 21:00 h) and Monday morning

Program

Program

Sunday, 13 October 2024

16:30 – 21:00	Registration	
18:00	*BUFFET SUPPER and informal get together*	
19:30 – 19:45	Scientific organizers	**Welcome words**
19:45 – 20:45	Joshua Goldberger	**Paving Transverse Paths in Thermoelectrics**

Monday, 14 October 2024

08:00	*BREAKFAST*	
09:00 – 10:00	Yaxian Wang	**Goniopolar Thermoelectrics: A Theoretical Perspective**
10:00 – 11:00	Sunglae Cho	**Misfit Layered Composite Crystals: Growth and Thermoelectric Properties**
11:00 – 11:30	*COFFEE BREAK*	
11:30 – 12:20	Yosuke Goto	**Axis-dependent Conduction Polarity of Mg_3Sb_2 and Mg_3Bi_2 for Transverse Thermoelectric Devices**
12:20 – 12:40	Ryuji Okazaki	**Transverse Thermoelectric Effect in a Mixed-dimensional Material $LaPt_2B$**
12:40	*LUNCH*	

Program

Monday, 14 October 2024

14:00 – 15:00	Juri Grin (online)	**Transverse Seebeck Effect and Chemical Bonding in Complex Intermetallic Compound o-$Al_{13}Co_4$**
15:00 – 16:00	Silke Buehler-Paschen	**Topological Semimetals in Heavy Fermion Compounds**
16:00 – 16:40	**Poster Flashes**	
16:40 – 18:30	**Posters *+ coffee***	
18:30	*DINNER*	
19:30 – 20:30	Gabi Schierning	**Decoupling Transport Properties of Surface and Bulk Carriers in Topological Insulator Materials**

Program

Tuesday, 15 October 2024

08:00	*BREAKFAST*	
09:00 – 10:00	Ken-ichi Uchida	**Hybrid Transverse Magneto-thermoelectric Conversion in Artificially Tilted Multilayers and Thermoelectric Permanent Magnets**
10:00 – 11:00	Günter Reiss	**Seebeck, Spin Seebeck and Nernst Effects in Multilayered Thin Film Heterostructures**
11:00 – 11:30	*COFFEE BREAK*	
11:30 – 12:20	Sarah Watzman	**Topology and Anisotropy as Tuning Mechanisms for an Enhanced Nernst Effect**
12:20 – 12:40	Min Young Kim	**The Effect of Oxygen-vacancy Defects on Anomalous Nernst Thermopower**
12:40	*LUNCH*	

Program

Tuesday, 15 October 2024

14:00 – 15:00	Jörg Töpfer	**Transverse Multilayer Thermoelectric Generators with Thermoelectric Oxides**
15:00 – 16:00	Tim Roediger	**Fast Response Heat-flux Measurements Based on ALTP Sensors**
16:00 – 16:30	*COFFEE BREAK*	
16:30 – 16:50	Jan Spiece	**Peltier-Enhanced Anomalous Ettingshausen Effect in a Nano-Scale Magnetic Weyl Semimetal**
16:50 – 17:10	Matt Beekman	**An International Nernst Effect Measurement Round Robin**
17:10 – 17:30	Sang Jun Park	**Designing Flexible Hard Magnetic Materials for Zero-magnetic-field Operation of the Anomalous Nernst Effect**
17:30 – 18:30	Matthew Grayson	**Essential Role of Temperature-dependent Energy Gaps in (p x n)-type Transverse Thermoelectrics**
18:30	*HERAEUS DINNER* *(social event with cold & warm buffet with complimentary drinks)*	
after dinner	**Posters *+ coffee***	

Program

Wednesday, 16 October 2024

08:00	*BREAKFAST*	
09:00 – 10:00	Claudia Draxl	**Electronic and Thermodynamic Properties of Real Materials: Example of Thermoelectric Clathrates**
10:00 – 11:00	Christina Scheu	**New Insights Into Thermoelectric Materials Through Length-bridging Characterization**
11:00 – 11:20	*COFFEE BREAK*	
11:20 – 11:40	Alessandro Sola	**Transverse Thermopower of Polycrystalline MnBi with Tuned Microstructure and Magnetic Properties**
11:40 – 12:00	Lawrence Rhoads	**Method to Characterize Full Seebeck and Resistivity Tensors from a Single Sample of Transverse Thermoelectric**
12:00	*Conclusion and LUNCH*	

End of the seminar and departure

NO DINNER for participants leaving on Thursday; however, a self-service breakfast will be provided on Thursday morning

Posters

Poster Session, Monday, 14 October, 16:00 h (CEST)

Abdelkader Alleg	Theoretical Investigations of Electronic, Thermodynamic and Thermoelectric Properties of Filled Skutterudites ThFe 4 P 12 and CeFe 4 P 12 Using DFT Calculations
Sai Ram Goud Antharam	Thermoelectric Materials for Energy Generation and Infrared Sensors
Adriano Di Pietro	Dependence of Anomalous Nernst Coefficient on Electron Mean Free Path and Berry Curvature
Shuping Guo	Vacancy-mediated Anomalous Phononic and Electronic Transport in Defective Half-Heusler ZrNiBi
Xiaodong Guo	Onsager Reciprocal Relation between Anomalous Transverse Coefficients of an Anisotropic Antiferromagnet
Jangwoo Ha	Observation of Large Seebeck-driven Transverse Thermoelectric Generation in Bi/Sb Bulk Composites
Raymond Hartig	Thermoelectric Efficiency of Nanoscale Devices in the Nonlinear Regime
Fischer Harvel	Using Surface Interactions and Nanoconfinement to Prepare Heterostructures with Constituent Structures Not Found in Phase Diagrams: (PbSe)m(FeSe2)n, (MoSe2)m(FeSe2)n and (FeSe)m(MoSe2)n
Apoorva Joshi	Thermal Conductivity Reduction of Fe2VAl Thermoelectric Alloys Through Atomic Disorder Engineering
Abayomi Lawal	Enhanced Thermoelectric Cooling Through Improved Interfacial Bonding in 3D-Printed Materials

Poster Session, Monday, 14 October, 16:00 h (CEST)

Kwanyoung Lee	Coexistence of Kondo Effect and Weyl Semi-metallic States in Mn Doped VAl3 Compounds
Fu Li	High-throughput Design of Doped all-d-metal Heusler Compounds for Transverse Thermoelectric Applications
Romy Löhnert	TMLTEG based on substituted CaMnO(3-δ)
Kenneth McAfee	Robustness Through Simplicity: Leveraging the Transverse Seebeck Effect for Extreme Environment Heat Flux Sensing
Frantisek Mihok	Anisotropy Effect in Doped SnSe Materials Prepared by Spark Plasma Sintering
Francesco Milillo	High Thermoelectric Performance in Ag2Se Achieved Through a Sustainable Solution Synthesis
Shoya Ohsumi	Band-resolved Transport Properties and the Transverse Thermoelectric Conversion in a Semimetal WSi2
Junyoung Park	Optimizing Application-Specific Transverse Thermoelectric Properties of Binary Composites Using Topology Optimization
Nicolás Pérez Rodríguez	Interface-induced Transport Phenomena in Nanograined Thermoelectric Composites
Jose J. Plata Ramos	Modelling the Lattice Thermal Conductivity of Transverse Thermoelectric Materials: The Case of Re4Si7
Kacper Pryga	Electronic Band Structure and Thermoelectric Performance of SnBi2Te4

Poster Session, Monday, 14 October, 16:00 h (CEST)

Heiko Reith	Flexible Talbot Lithography for Fast-Response Heat Flux Sensors Using the Transverse Seebeck Effect
Jong-Soo Rhyee	Hierarchical Phonon Scattering in Nano-Ag/Micro-TiO2 Bismuth Telluride Bulk Composites and Cost-effective Module Structure
Katherine Schlaak	Characterization of the Anisotropic Nernst Effect in Antiferromagnetic YbMnSb2 and YbMnBi2
Shailja Sharma	Low-temperature Thermoelectric Properties of p-type Sb2SexTe3-x
Sanaz Shokri	Thermoelectric Transport in Atomically Thin van der Waals Cuprate Superconductors
Michael Staiger	Magnetotransport in (BixSb1-x)2Te3 Nanoparticles and the Challenges of Data Analysis
Tetiana Tavrina	Preparation and Characterization of 2D Molybdenum Dichalcogenides for Thermoelectric Applications
Tessera Alemneh Wubieneh	Engineering Tin Chalcogenides Thermo-electric Materials for Power Generation
Hyun Yu	Enhancing Transverse Thermoelectric Performance Using Topology Optimization Combined with Laser Powder Bed Fusion
Yi Zhou	Giant Pyroelectric Polarization Ripples in Transverse Thermoelectrics

Abstracts of Lectures

(in alphabetical order)

An international Nernst effect measurement round robin

M. Beekman[1] and S. J. Watzman[2]

[1] Department of Physics, California Polytechnic State University, San Luis Obispo, CA 93407 USA

[2] Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, OH 45221 USA

From the viewpoint of thermoelectricity, the Nernst effect has fundamental significance as an experimental probe of electronic structure and charge carrier transport in metals, semimetals, semiconductors, and superconductors [1, 2]. It also has practical significance as the governing effect underlying energy conversion and heat transport in Nernst-Ettingshausen generator and cooler applications, respectively [3]. While transverse thermoelectric and thermomagnetic measurements have historically received much less attention than the conventional Seebeck, Peltier, and other longitudinal thermoelectric transport effects, the former have gained considerably increased interest in recent years and are becoming more commonly studied in many research labs. However, currently there is very little literature reporting on the reproducibility of Nernst effect measurements. This presentation will describe a planned international round robin for Nernst effect measurements. In addition to reviewing common Nernst effect measurement protocols and recent related transport measurement round robins [4-6], we hope to solicit feedback from attendees on potential candidate materials, protocols, and measurement parameters, which will help guide the design of the planned round robin.

References

[1] T. C. Harman and J. M. Honig, *Thermoelectric and Thermomagnetic Effects and Applications* (McGraw-Hill, New York, 1967).
[2] K. Behnia and H. Aubin, Rep. Prog. Phys. **79**, 046502 (2016).
[3] K. Uchida and J. P. Heremans, Joule **6**, 2240 (2022).
[4] N. D. Lowhorn et al., Appl. Phys. A **94**, 231 (2009).
[5] H. Wang et al., J. Electron. Mater. **44**, 4482 (2015).
[6] A. Sola et al., IEEE Trans. Instrumen. Meas. **68**, 1765 (2019).

Topological semimetals in heavy fermion compounds

Silke Paschen

Institute of Solid State Physics, Vienna University of Technology (TU Wien),
Wiedner Hauptstr. 8-10, 1040 Vienna, Austria
e-mail: paschen@ifp.tuwien.ac.at

Gapless electronic topology driven by strong correlations is an emerging field of great interest, with heavy fermion compounds at its forefront. I will introduce the first such materials class, Weyl-Kondo semimetals [1-3], and report on the giant signatures of topology observed in $Ce_3Bi_4Pd_3$ [1,3] and the genuine topology control that can be achieved by magnetic field tuning [4]. I will also discuss design strategies for further correlation-driven topological phases [5], and highlight a new emergent topological phase that nucleates out of a strange metal state [6].

This work was supported by the Austrian Science Fund (FWF-I4047, I5868-FOR5249-QUAST, SFB F 86, Q-M&S), the European Union's Horizon 2020 Research and Innovation Programme (824109, EMP), and the European Research Council (ERC Advanced Grant 101055088, CorMeTop).

[1] S. Dzsaber et al., Phys. Rev. Lett. 118, 246601 (2017).
[2] H.-H. Lai et al., PNAS 115/1, 93 (2018).
[3] S. Dzsaber et al., PNAS 118, e2013386118 (2021).
[4] S. Dzsaber et al., Nat. Commun. 13, 5729 (2022).
[5] L. Chen et al., Nat. Phys. 18, 1341 (2022).
[6] D. M. Kirschbaum et al., arXiv2404.15924 (2024).

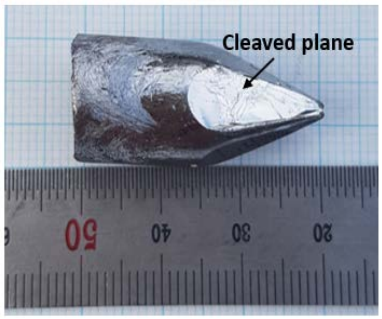
Misfit layered composite crystals: Growth and thermoelectric properties

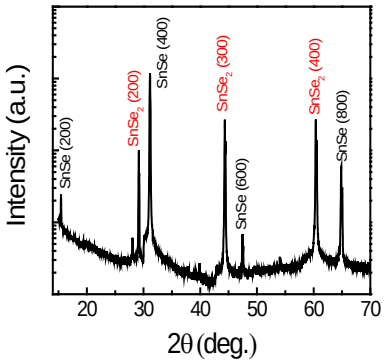
Van Quang Nguyen[1], Thi Huong Nguyen[2], and Sunglae Cho[1]

[1]Department of Physics, University of Ulsan, Ulsan 44610, South Korea
[2]Department of Physics, Natrang University, Vietnam

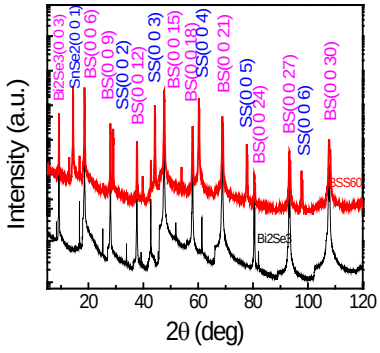
Researches have demonstrated the single crystal growth of van der Waals two-dimensional materials. $(BiSb)_2(TeSe)_3$ and SnSe are binary or ternary thermoelectric materials with va der Waals bonding. Regarding on the various and complex phases and several experimental clues, I have questioned the feasibility of single crystal growth in these systems. To address this issue, we have grown bulk crystals and thin films of Sn-Se, Fe-Te, Bi-Sn-Se, and Bi(Sb)-Se systems using the temperature gradient method and molecular beam epitaxy (MBE), respectively. In this talk, I will introduce "misfit layered composite crystals (MLCCs)," which feature a laminated structure comprising van der Waals layered materials, and discuss their related thermoelectric properties. We found that misfit layered composite crystals are very common in Van der Waals materials.

<$SnSe/SnSe_2$
bi-crystal & XRD>





<$Bi_2Se_3/SnSe_2$
bi-crystal & XRD>



Electronic and thermodynamic properties of real materials: example of thermoelectric clathrates

Claudia Draxl

Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany

Semiconducting behavior is a desired property for efficient thermoelectrics. This is often difficult to achieve due to the complex interplay of electronic structure, temperature, and disorder, as we find to be the case, for example, in thermoelectric clathrates [1]. In this talk, I will show how we can reliably describe the electronic structure of complex alloys as a function of composition and temperature, by combining state-of-the-art electronic structure theory, *ab initio* thermodynamics, cluster expansion [2], and machine learning [3]. With the example of $Ba_8Al_{16}Si_{30}$, I will first discuss, how a temperature-driven partial order-disorder transition leads to an effective closing of the band gap as a function of temperature. To model and predict nonlinear properties such as band gaps of materials with disorder and vacancies, I will introduce a novel method that looks at cluster expansion (CE) through the lens of machine learning, as demonstrated with the example of $Ba_8Al_xSi_{46-x}$. For the same material system, we show that this *nonlinear* CE can also be used for classification tasks, i.e. to distinguish metals from semiconductors.

References

[1] M. Troppenz, S. Rigamonti, J. O. Sofo, and C. Draxl, Phys. Rev. Lett. 130, 166402 (2023).

[2] S. Rigamonti, M. Troppenz, M. Kuban, A. Hübner, and C. Draxl, npj Comp. Mater. (in print).

[3] A. Stroth, C. Draxl, S. Rigamonti, preprint.

Paving Transverse Paths in Thermoelectrics

J. E. Goldberger[1]

[1]*The Ohio State University, Department of Chemistry and Biochemistry, 155 W. Woodruff Ave. Columbus, OH, USA*

Thermoelectrics have long been a promising technology for conversion between heat and electricity, allowing active cooling or power generation from waste heat. Conventional thermoelectric modules utilize hundreds of pairs of p-type and n-type semiconductors, with charge and heat flowing in the same ‘‘longitudinal’’ direction. Despite the decades of research that has led to 3-fold improvements in material efficiencies, little progress has been made in the practical use partly due to the inherent limitations of this device geometry; the main difficulty being the hundreds of contacts on the hot side that serve as sites for device failure as well as reducing overall efficiency. “Transverse” thermoelectrics, in which a thermal gradient induces a perpendicular voltage, promise to overcome these limitations by eliminating the need for hot side contacts and reducing the total number of contacts. Here we will provide a broad overview of the history and the state of the field of transverse thermoelectric technologies. We will review the variety of mechanisms for generating transverse thermoelectric effects in materials, especially highlighting recent advances over the past few years.[1] We will describe our recent progress in discovering materials that simultaneously exhibit majority p-type and n-type conduction along orthogonal directions,[2-4] and demonstrating their integration into transverse thermoelectric modules with efficiencies that rival state-of-the art commercial devices[5]. Finally, we will conclude by describing open questions in this emerging direction of thermoelectric research.

References

[1] K. Uchida, J. P. Heremans, Joule, 6, 2240-2245 (2022).

[2] B. He, Y. Wang, M.Q. Arguilla, N.D. Cultrara, M.R. Scudder, J.E. Goldberger, W. Windl, J. Heremans, Nature Materials. **18**, 568–572 (2019).

[3] Y. Wang, K. Koster, A. Ochs, M. R. Scudder, J. P. Heremans, W. Windl, J. E. Goldberger, Journal of the American Chemical Society **142**, 2812−2822 (2020).

[4] A. M. Ochs, G. H. Fecher, B. He, W. Schnelle, C. Felser, J. P. Heremans, J. E. Goldberger, Advanced Materials **366,** 2308151 (2024)

[5] M. R. Scudder, B. He, Y. Wang, A. Rai, D. G. Cahill, W. Windl, J. P. Heremans, J. E. Goldberger, Energy & Environmental Science **14,** 4009, (2021).

Axis-dependent conduction polarity of Mg_3Sb_2 and Mg_3Bi_2 for transverse thermoelectric devices

Y. Goto

National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, 305-8568, Japan

A thermoelectric device having a transverse configuration could mitigate long-standing challenges associated with such units, such as the long-term thermal stability of the device. One approach to the design of transverse thermoelectric devices is to use materials having axis-dependent conduction polarities, meaning simultaneous p-type and n-type conduction along different crystallographic directions. The present work demonstrates that layered Zintl phase Mg_3Sb_2 and Mg_3Bi_2 possess this property [1]. Single crystals of electron-doped Mg_3Sb_2 were found to show axis-dependent conduction polarity at low charge carrier concentrations (less than 10^{18} cm^{-3}) based on the contribution of holes to conduction in the cross-plane direction. Mg_3Bi_2 also exhibited this same characteristic but over a wider range of doping with carrier concentrations greater than 10^{19} cm^{-3}. This difference was attributed to the semi-metallic band structure of Mg_3Bi_2. First-principles calculations established that axis-dependent conduction polarity appeared in these compounds as a consequence of band anisotropy that arises from the isotropic conduction band minimum and anisotropic valence band maximum. Specifically, electron bands were primarily responsible for carrier conduction in the in-plane direction whereas hole bands were dominant in the cross-plane direction. On the basis of the present data, 122-type Zintl phases are proposed as a new family of materials having axis-dependent polarities, with the potential to allow band anisotropy engineering.

References

[1] Y. Goto, H. Usui, M. Murata, J. E. Goldberger, J. P. Heremans, and C.-H. Lee, Band Anisotropy Generates Axis-Dependent Conduction Polarity of Mg3Sb2 and Mg3Bi2, Chem. Mater. **36**, 2018 (2024).

Essential Role of Temperature-dependent Energy Gaps in ($p \times n$)-type Transverse Thermoelectrics

Q. Shao[1] J. Li[1] and M. Grayson[1]

[1]Northwestern University, Evanston, USA

In 2013, the concept of transverse thermoelectrics was reinvigorated [1] with the idea that single crystals of low-symmetry compounds could, on their own, exhibit a transverse thermoelectric effect if they hosted parallel *p*-type conduction along one axis and *n*-type conduction perpendicular. Such ($p \times n$)-type behavior, also subsequently referred to axis-dependent conduction polarity, allows a "single leg" of intrinsic semiconductor to achieve full thermoelectric device function, in contrast with standard thermoelectrics which require a "double leg" of one *p*- and one *n*-type extrinsic doped semiconductor. When this behavior arises from band conduction of two parallel, anisotropic electron and hole bands, the size of the semiconducting gap is critical in determining whether, and at what temperatures, the TTE can function. This talk will examine the transport modeling of these two-band TTEs and introduce novel TTE characterization methods for the energy gap.

The small energy gap in such TTEs, of order the thermal energy $k_B T$, can be comparable to the change in energy gap over the temperature range of interest, yet, thus far, transport simulations have assumed a temperature-independent energy gap, potentially misinterpreting the Fermi energy, mobility, and balance of electron-hole density. A *partial gap analysis* is introduced [2] which deduces the temperature-dependent energy gap directly from the experimental Seebeck and conductivity transport tensors and reveals this strong *T*-dependence. The partial gaps between the Fermi energy and the respective conduction/valence band edges are determined from a self-consistent analysis of the Peltier conductivity tensor in an effective mass, Boltzmann transport model. Analyzing the well-studied TTE Re_4Si_7, samples from two different research groups are shown to reproduce the same temperature dependent band gap decreasing by a factor of two over the measured temperature range, highlighting the necessity of considering T-dependent energy gaps.

References

[1] C. Zhou, Y. Tang, K. Heinselman, S. Birner, M. Grayson, *"Driving perpendicular heat flow: (p x n)-type transverse thermoelectrics for microscale and cryogenic Peltier cooling,"* Phys. Rev. Lett. **110**, 227701 (2013).

[2] Q. Shao, J. Li, X. Yan, C. Zhou, B. Cui, X. Li, J. Yang, C. J. Zeman IV, M. A. Mosquera, L. O. Jones, G. C. Schatz, M. Grayson, *"Temperature Dependence of Band Gaps in TTEs: Partial Gap Analysis of Re_4Si_7,"* (unpublished).

Transverse Seebeck effect and chemical bonding in complex intermetallic compound *o*-$Al_{13}Co_4$

Yu. Grin[1]*, P. Gille[2], M. Havrylyuk[3], M. Krnel[1], L. I. Anatychuk[3]

[1]*Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany*

[2]*Ludwig-Maximilia-Universität München, Germany*

[3]*Institute of Thermoelectrics NASU, Chernivtsi, Ukraine*

The intermetallic compound *o*-$Al_{13}Co_4$ is one of the aluminum-rich binary phases in the system Al-Co system. It shows special structural features. The recent refinements of the crystal structure using high-resolution X-ray diffraction data recently in a complex model of the crystal structure with a large number of split positions describing strong local violations of the translational symmetry, also confirmed by atomic-resolution TEM study [1]. The quantum chemical calculations by means of the positional space approach, yield two partial structures in *o*-$Al_{13}Co_4$ with different bonding patterns. The main three-dimensional structural matrix is formed by Al-Al and Al-Co interactions. Its cavities enclose three-atomic Co-Al-Co groups. The missed correlations between the configuration of the caping faces of the neighboring cages and the opposite caps of the same cage, combined with the stacking faults, are possible reasons for an extended crystallographic disorder [1].

The cm-sized single crystals grown by the Czochralski technique [2] were used for X-ray diffraction and thermoelectric experiments [3]. Electrical resistivity of *o*-$Al_{13}Co_4$ is relatively low in all crystallographic directions, but shows a significant anisotropy. Only the electronic component of thermal conductivity exhibits directional variations, while the phononic component demonstrates a more isotropic behavior, despite an anisotropic structure. In contrary to that, the Seebeck coefficient is strongly anisotropic. This feature was the starting point for exploring the transverse Seebeck effect, where the thermal and electrical flows are perpendicular to each other [4,5]. The study was performed conducted on the specially manufactured thermoelectric module within a setup designed for its thermoelectric characterization. The obtained results reveal the appearance of the transverse Seebeck effect in a material, which consists of two metals and shows metallic behavior in its transport properties.

References

[1] P. Simon et al. J. Alloy Compd. **820**, 153363 (2020).

[2] P. Gille, B. Bauer. Cryst. Res. Technol. **43**, 1161 (2008).

[3] J. Dolinsek et al. Phys. Rev. B **79**, 184201 (2009).

[4] L. I. Anatychuk et al. Phys. Thech. Poluporvodnikov, **9**, 1410 (1975).

[5] H. J. Goldsmid. J. Electr. Mater. **40**, 1254 (2020).

The effect of oxygen-vacancy defects on anomalous Nernst thermopower

Min Young Kim,[1,2] Dongkyu Lee,[2] June Ho Lee,[3] Donghwa Lee,[3] Gi-Yeop Kim,[4] Si-Young Choi,[4] Joseph P. Heremans,[1] and Hyungyu Jin[2]

[1]Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH, USA
[2]Department of Mechanical Engineering, Pohang University of Science and Technology (POSTECH), Pohang, South Korea
[3]Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Pohang, South Korea
[4]Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Pohang, South Korea

Recently, the anomalous Nernst effect (ANE) has been attracting much attention as a promising approach towards efficient thermoelectric generation. Accordingly, many of ANE materials have been found to deliver superior performance; in particular, intrinsically large Berry curvatures have been considered as an essential factor for a large ANE.[1,2] However, in addition to employing such intrinsically excellent materials, it is also imperative to develop design strategies for a high ANE performance from an engineering perspective. In that regard, we investigated how one of extrinsic factors, oxygen-vacancy defects, can play a key role in the enhancement of ANE thermopower. By choosing perovskite $Sr_3YCo_4O_{11-\delta}$ (δ = 0.02, 0.08 and 0.14, δ: oxygen deficiency) polycrystals, a promising thermoelectric ferromagnet,[3] as our experimental platform, we closely observed various ANE coefficients, S_{ANE}, depending on the amount of oxygen vacancies. For example, the maximum S_{ANE} of the vacancy-richest sample (δ = 0.14) is nearly twice that of pristine (δ = 0.02). We speculate that this immense increase of S_{ANE} results from the increase of diffusion thermopower between Co^{3+} and Co^{4+} ions, which strengthens total Seebeck currents following the linear response transport theory. Besides, the increase of anomalous Nernst angle with the oxygen vacancies also amplifies S_{ANE} due to improved hopping transport. The proposed facile approach can provide useful insight into artificially tunable ANE as well as help to expand the variety of ANE materials to other potential candidates such as a transition metal complex.

References

[1] S. N. Guin *et al.*, *Adv. Mater.* **31** 1806622 (2019).
[2] Y. Pan *et al.*, *Nat. Mater.* **21** 203-209 (2022).
[3] H. Takahashi *et al.*, *Phys. Rev. B* **98** 024405 (2018).

Transverse thermoelectric effect in a mixed-dimensional material $LaPt_2B$

R. Okazaki[1], Y. J. Sato[1], H. Manako[1], S. Ohsumi[1], and D. Aoki[2]

[1]Department of Physics and Astronomy, Tokyo Univ. of Science, Noda, Japan
[2]Institute for Materials Research, Tohoku Univ., Oarai, Ibaraki, Japan

Materials with axis-dependent conduction polarity (ADCP), known as p × n-type conductors [1] or goniopolar materials [2,3], are potential candidates toward the efficient transverse thermoelectric conversion. Such a function is realized even in zero magnetic field, in contrast to the transverse conversion using the Nernst effect, although the materials with ADCP are currently very limited. In this study, we have grown a single-crystalline boride $LaPt_2B$ and find a prominent ADCP in this boride; As shown in Fig. 1, the thermopower is negative along the crystalline *a*-axis direction while it is positive along the *c*-axis direction [4]. Using the first-principle calculations, we find that the mixed-dimensional Fermi surfaces, which consist of quasi-one-dimensional hole sheet with out-of-plane velocity and quasi-two-dimensional electron sheets with in-plane velocity, play a crucial role for the ADCP. We demonstrate the transverse thermoelectric conversion in $LaPt_2B$ and discuss such mixed-dimensional properties in other materials to explore the efficient transverse thermoelectrics.

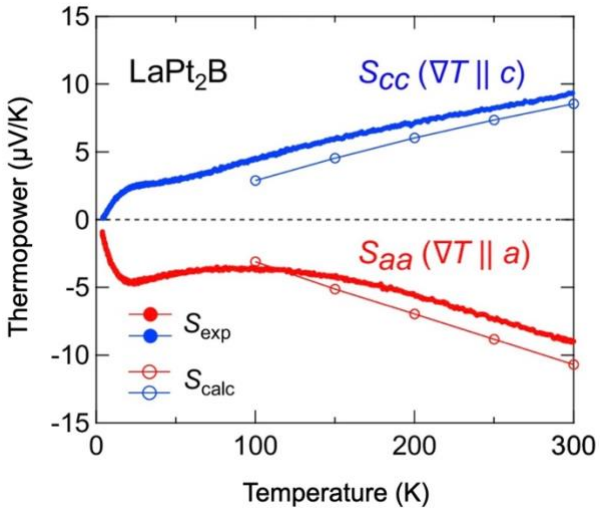


Fig. 1: Temperature dependence of the axis-dependent thermopower in $LaPt_2B$ single crystal.

References

[1] C. Zhou *et al.*, Phys. Rev. Lett. **110**, 227701 (2013).
[2] B. He *et al.*, Nat. Mater. **18**, 568 (2019).
[3] K. Uchida and J. Heremans, Joule **6**, 2240 (2022).
[4] H. Manako *et al.*, Nat. Commun. **15**, 3907 (2024).

Designing flexible hard magnetic materials for zero-magnetic-field operation of the anomalous Nernst effect

Sang J. Park[1,*], Rajkumar Modak[1], Ravi Gautam[1], Abdulkareem Alasli[2], Takamasa Hirai[1], Fuyuki Ando[1], Hosei Nagano[2], Hossein Sepehri-Amin[1] and Ken-ichi Uchida[1,3,*]

[1] National Institute for Materials Science, Tsukuba 305-0047, Japan
[2] Department of Mechanical Systems Engineering, Nagoya University, Nagoya 464-8601, Japan
[3] Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, Chiba 277-8561, Japan

* Correspondence to: PARK.SangJun@nims.go.jp (S.J.P.);
UCHIDA.Kenichi@nims.go.jp (K.U.);

The rising demand for energy has accelerated the shift towards a carbon-neutral society, driving research into efficient energy harvesting technologies from low-grade waste heat. Recently, transverse thermoelectrics based on the anomalous Nernst effect (ANE) has gained attention due to their simple device structure, scalability, and manufacturing-friendly nature [1,2]. While topological single crystals and epitaxial films have been focused for enhancing the ANE performance [3], further improvements in material design are necessary for practical applications. Here, we report an easy-to-implement strategy for designing mechanically flexible and magnetically hard transverse thermoelectric materials by creating amorphous-crystalline heterogeneous composites. We fabricated and optimized these heterogeneous composites through controlled heat treatment, achieving significant enhancements in the coercivity and anomalous Nernst coefficient, while maintaining flexibility. Additionally, using the developed material, we constructed a single-material-based coiled device and demonstrated the zero-field operation of the ANE-based energy harvesting from curved heat sources. These results validate the feasibility of using ANE-based flexible materials for energy harvesting applications.

Acknowledgements

This work was supported by ERATO "Magnetic Thermal Management Materials" (grant no. JPMJER2201) from JST, Japan.

References

[1] K. Uchida and J. P. Heremans, Joule **6**, 2240–2245 (2022).
[2] S. R. Boona, H. Jin and S. Watzman, J Appl Phys **130**, 171101 (2021).
[3] A. Sakai, S. Minami, T. Koretsune, T. Chen, T. Higo, Y. Wang, T. Nomoto, M. Hirayama, S. Miwa, D. Nishio-Hamane, F. Ishii, R. Arita and S. Nakatsuji, Nature **581**, 53–57 (2020).

Seebeck, Spin Seebeck and Nernst Effects in Multilayered Thin Film Heterostructures

G. Reiss[1], T. Kuschel[1], A. Boehnke[1], M. Münzenberg[2], H.-W. Schumacher[3], J. Schmalhorst[1]

[1] Bielefeld University, Physics Department, Bielefeld. Germany

[2] Greifswald University, Greifswald, Germany

[3] Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Transverse Thermoelectric effects such as the (anomalous) Nernst Effect, or the generation of voltages by the injection of spin currents will be discussed using the examples of normal-metal/ferromagnet bilayers with conducting and isolating ferromagnets as well as magnetic tunnel junctions. In such multilayered thin film systems, a thermally induced spin transport gives rise to a variety of effects, that often overlap each other. In particular, heavy normal metals such as Pt or Pd can exhibit proximity induced magnetic moments that additionally contribute to Nernst-voltages. Their identification and separation will be presented in the talk. Possible applications of such systems for sensing and/or power generation will be also discussed.

Method to Characterize Full Seebeck and Resistivity Tensors from a Single Sample of Transverse Thermoelectric

Juncen Li[1], Tyler Slade[2], Mercouri Kanatzidis[2], Lawrence A. Rhoads[3], Matthew Grayson[4]*

[1] *Material Science and Engineering, Northwestern University, Evanston, IL, 60208*
[2] *Chemistry department, Northwestern University, Evanston, IL, 60208*
[3] *Applied Physics, Northwestern University, Evanston, IL, 60208*
[4] *Electrical and Computer engineering, Northwestern University, Evanston, IL, 60208*
** Email: m-grayson@northwestern.edu*

(*p* × *n*)-Type transverse thermoelectrics were proposed for Peltier cooling at cryogenic temperature and integrated thermoelectric devices. In those materials, highly anisotropic ambipolar conduction can give rise to an off-diagonal Seebeck coefficient, generating a voltage drop perpendicular to an applied temperature gradient. However, typical thermoelectric characterization only measures the Seebeck coefficients along specific crystal axes, which is, in principle, insufficient to map the full Seebeck tensor of a low-symmetry crystal. Here, we report results for an all-in-one measurement set-up for measuring the full Seebeck tensor on a single sample with a custom-made reusable apparatus. In the case of a rectangular cut sample aligned with the principal axes, the Montgomery method can also be used to get the 3 principal resistivity components.

The sample of interest is sandwiched between anodized aluminum blocks. The aluminum is precision-machined and laser cut to make blind holes to house spring-loaded contact-pins and to make grooves for the thermocouples. Temperature gradients along 3 orthogonal directions are measured with these built-in thermocouples while voltages along different directions are measured by the contact pins, thus giving the full Seebeck tensor. The device was tested both on pre-characterized isotropic thermoelectric sintered polycrystalline PbTe and on anisotropic single-crystal bismuth as reference samples. The diagonal Seebeck coefficients agree with results from the standard measurement method within 10%, and the error introduced in the 6 off-diagonal terms are smaller than 5% of the diagonal values. In the case of deliberately miscut bismuth, we can both recover the correct anisotropic Seebeck tensor and respective orientation. Montgomery measurements of the resistivity tensors of bismuth show good agreement within 10% of the literature value. Preliminary results on TTE material $CsBi_4Te_6$ are also presented here.

Fast response heat-flux measurements based on ALTP sensors

Tim Rödiger

Chair of Fluid Mechanics, Heat Transfer, and Energy, UAS Landshut, Germany

In order to investigate heat transfer and fluid-wall interactions in thermodynamic applications, there is a strong demand for highly time-resolved heat flux measurements at the surface. ALTP sensors are based on transverse thermoelectric films and stand out by their unique temporal and spatial resolution. The development of sensor modules, static and dynamic calibration procedures as well as amplifier systems enable heat-transfer measurements with microsecond resolution in a broad range of flow speeds and heat loads.

As example, measurement results in combustion applications, high-speed flows and rotating detonation engines will be presented. In addition, a new methodology and circuit technology for a combined temperature and heat-flux measurement will be shown [2]. The procedure allows a direct, time-resolved determination of heat-transfer coefficients and local Nusselt numbers.

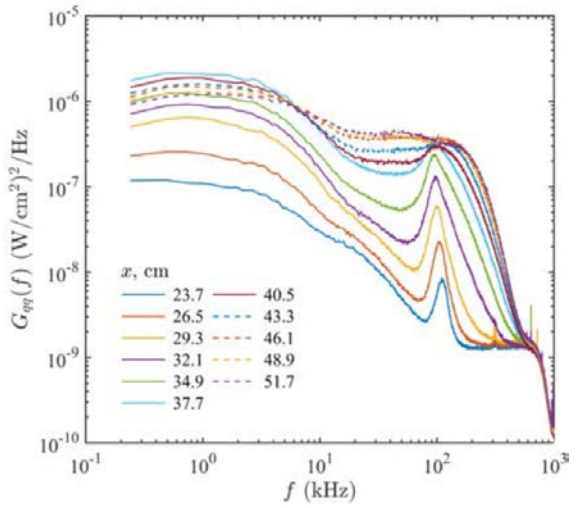


Figure 1a: NASA, Mach 6 Air Tunnel: Measured heat-flux auto-spectral densities by ALTP [3]

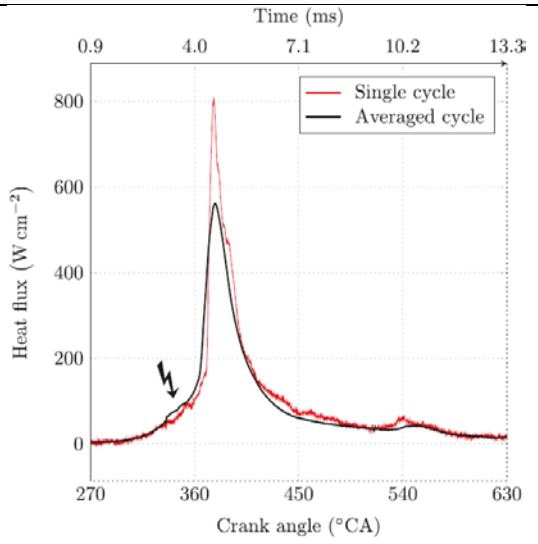


Figure 1b: Combustion cycle measurements in an internal engine [1]

[1] K. Huber, F. Gackstatter, T. Rödiger and M. Wensing, "Highly time-resolved heat flux measurement in a combustion engine," International Journal of Engine Research, p. 14680874221118970, 2022.

[2] K. Huber, F. Gackstatter and T. Rödiger, "A novel method for parallel measurement of temperature and heat flux with a single layer probe," Measurement, vol. 193, p. 110915, 2022.

[3] M. A. Kegerise and S. J. Rufer, "Unsteady heat-flux measurements of second-mode instability waves in a hypersonic flat-plate boundary layer," Experiments in fluids, vol. 57, p. 130, 2016.

New insights into thermoelectric materials through length-bridging characterization

S. Zhang, R. Bueno Villoro, L. Abdellaoui, D. Mattlat, C. Jung, B. Gault and C. Scheu

Max-Planck-Institute for Sustainable Materials, Düsseldorf, Germany

Thermoelectric materials can contribute to change the energy sector into an environmentally friendly one as they are able to convert waste heat into electricity. In order to obtain a high conversion efficiency the electrical conductivity should be high, while the thermal conductivity should be low. Several approaches exist to reduce the thermal conductivity, such as reducing grain size, insertion of point defects or precipitates and to add planar defects or dislocation. All of these defects can scatter phonons effectively. At the same time, they often reduce the electrical conductivity, which is unwanted. However, a few cases are reported, where defects can also show an enhanced electrical conductivity due to the formation of conductive pathways. In order to booster the efficiency further, it is of great importance to characterize the defects on different length scales – starting from the millimeter/micrometer level down to the atomic scale. The defect density has to be evaluated in a statistically relevant manner while at the same time the atomic arrangement and chemical composition need to be determined with high spatial resolution.

In order to fulfill this task, we developed a scale bridging methodology. Defects are characterized from the millimeter/micrometer level down to the atomic scale using a combined approach of various imaging and spectroscopic techniques. Electron channeling contrast imaging (ECCI) in conjunction with electron back-scatter diffraction (EBSD) experiments inside a scanning electron microscope (SEM) are used to determine the defect distribution and densities. (Scanning) transmission electron microscopy (STEM) imaging, energy-dispersive X-ray spectroscopy (EDX) and electron energy-loss spectroscopy (EELS) in STEM mode are often combined with atom probe tomography (APT) to unravel the atomic structure and composition of the defects. This novel methodology was applied to analyze defect types and their distribution within several different thermoelectric materials systems. Examples will be presented where grain boundary phases, dislocations or planar defects were analyzed in depth which strongly affect the thermoelectric properties [1,2].

[1] L. Abdellaoui, Z. Chen, Y. Yu, T. Luo, R. Hanus, T. Schwarz, R. Bueno Villoro, O. Cojocaru-Mirédin, G. J.Snyder, D. Raabe, Y. Pei, C. Scheu, S. Zhang, Adv. Funct. Mater. 2021, 31, 2101214

[2] R. Bueno Villoro, D. Zavanelli, C. Jung, D. A. Mattlat, R. Hatami Naderloo, N. Pérez, K. Nielsch, G. J. Snyder, C. Scheu, R. He, S. Zhang, Adv. Energy Mater. 2023, 13, 2204321

[4] The authors would like to acknowledge G. J. Snyder (Northwestern University, USA), Y. Pei (Tongji University, China), O. Cojocaru-Mirédin (Uni. Freiburg, Germany), K. Nielsch (IFW Dresden, Germany) and their teams for the fruitful collaboration.

Decoupling transport properties of surface and bulk carriers in topological insulator materials

N. Beryani Nezafat[1,2], M. Staiger[1,2], S. Izadi[1,2], C. van Halteren[3], S. Schulz[3,4], A. Bhattacharya[5], M. Mittendorff[5], and G. Schierning[1,2,4]

[1]Institute for Energy and Materials Processes, Applied Quantum Materials, University of Duisburg-Essen, Duisburg, Germany
[2]Research Center Future Energy Materials and Systems, Research Alliance Ruhr, Bochum, Germany
[3]Inorganic Chemistry, University of Duisburg-Essen, Essen, Germany
[4]Center for Nanointegration Duisburg-Essen (CENIDE), Duisburg, Germany
[5]Experimental Physics, University of Duisburg-Essen, Duisburg, Germany

Topological insulator materials (TI) are an interesting example of a material that contains different types of charge carriers and therefore largely decoupled transport channels. These TIs have two-dimensional (2D) charge carriers with special properties on their surfaces, and 3D charge carriers in the bulk. The topological protection of the 2D charge carriers prevents them from backscattering processes. As a result, their charge carrier mobility can be very high, in contrast to the mobility of the 3D charge carriers in the bulk. The bulk of TIs represents a highly doped semiconductor, usually with metallic transport properties (despite the misleading name: topological "insulators"). It is therefore difficult to show the special transport properties of the 2D charge carriers and different transport channels experimentally, since transport measurements contain the superposition of the proportions of both charge carriers – and normally the proportion of surface charge carriers is lost in the noise. However, by clever sample selection on the one hand and a combination of direct current (DC) measurements and frequency-dependent measurements on the other hand, the different types of charge carriers can be distinguished. All measurements shown here were carried out on samples that were nanogranular – either samples of compacted nanoparticles or sputtered thin films. In nanogranular samples there are sufficient free surfaces, interfaces and two-dimensional defects so that there are enough 2D charge carriers to be able to investigate their influence on transport. Investigated materials are Bi_2Te_3, $(Bi_{1-x}Sb_x)_2Te_3$ and SnTe – all materials that are known as excellent thermoelectric materials and often used in nanogranular form. These samples show a pronounced weak antilocalization in the low-temperature transport behaviour, indicating strong spin-orbit coupling and highly mobile charge carriers. The evaluation of the magnetotransport data using the Hikami-Larkin-Nagaoka (HLN) model yields 2D electron phase coherence lengths of up to 200 nm, which in some cases is almost two orders of magnitude larger than the average grain size in the analyzed samples. Terahertz spectroscopy is used to measure scattering rates of the 2D charge carriers. The 2D electron phase coherence lengths corresponds very well to the scattering rates. The average mobility of these 2D charge carriers is therefore in the order of 10^3 to 10^4 $cm^2V^{-1}s^{-1}$, even at room temperature. Hall data, on the other hand, address the 3D charge carriers. Consequently, the Hall-mobility is up to two orders of magnitude smaller.

Transverse thermopower of polycrystalline MnBi with tuned microstructure and magnetic properties

A. Sola[1], V. Basso[1], E. Olivetti[1], L. Martino[1], G. Tesi[2] and R. Cabassi[2]

[1]Istituto Nazionale di Ricerca Metrologica INRIM, Torino, Italy
[2] Institute of Materials for Electronics and Magnetism (IMEM), Parma, Italy

In the field of thermoelectricity, there is growing attention on transverse thermoelectric effects, stimulated by the discovery of the spin Seebeck effect and the renewed interest in the anomalous Nernst effect (ANE) [1,2]. This last phenomenon refers to the thermoelectric generation within a magnetic material, where the thermal gradient, the magnetization and the generated voltage are all oriented perpendicularly to one another. Although the values of thermopower are relatively low, this configuration opens up new possibilities for designing devices such as thin or flexible sensors and heat-sensing coatings for surfaces with arbitrary shapes. Progress in developing easily shaped ferromagnetic materials, such as polycrystalline materials, is essential for these applications. Powder metallurgy is a highly adaptable technique for preparing samples, suitable for both fundamental research and practical applications, without significant technological or cost limitations. Our recent research has demonstrated that polycrystalline MnBi alloy produced through powder metallurgy [3] exhibits ANE in the μV/K range [4], comparable to that of single-crystal samples [5]. Differently from the latters, in our MnBi samples the contribution to the thermopower from the ordinary Nernst of elemental bismuth must be taken into account because of the presence of unreacted bismuth inside the polycrystalline framework.
Finally, polycrystalline materials offer the advantage of tunable magnetic properties, such as coercive field and remanent magnetization, and enable the production of composite materials, paving the way for optimized thermoelectric conversion.

References

[1] S. R. Boona, et al. Journal of Applied Physics **130.17** (2021)
[2] K. Uchida, Z. Weinan, and S. Yuya, Applied Physics Letters **118.14** (2021).
[3] C. Curcio, et al. Physics Procedia **75**, 1230-1237 (2015)
[4] A. Sola, et al. AIP Advances **13.3** (2023)
[5] B. He, et al. Joule **5.11**, 3057-3067 (2021)

Peltier-Enhanced Anomalous Ettingshausen Effect in a Nano-Scale Magnetic Weyl Semimetal

M. Razeghi[1], J. Spièce[1], V. Fonck[1], Y. Zhang[3,4], M. Rohde[1], R. Joris[2], P. S. Dobson[5], J. M. R. Weaver[5], L. da Costa Pereira[2], S. Granville[3,4], P. Gehring[1]

[1]IMCN/NAPS, Université Catholique de Louvain (UCLouvain), Louvain-la-Neuve, 1348, Belgium

[2]QSP, KU Leuven, Leuven, 1587, Belgium

[3]Robinson Research Institute, Victoria University of Wellington, Wellington, PO Box 600, New Zealand

[4]MacDiarmid for Advanced Materials and Nanotechnology, Wellington, PO Box 600, New Zealand

[5]James Watt School of Engineering, University of Glasgow, Glasgow, G12 8LT, United Kingdom

Solid-state cooling devices offer compact, quiet, reliable and environmentally friendly solutions that currently rely primarily on the thermoelectric (TE) effect. Despite more than two centuries of research, classical thermoelectric coolers suffer from low efficiency which hampers wider application. In this study, the less researched Anomalous Ettingshausen effect (AEE), a transverse thermoelectric phenomenon, is presented as a new approach for on-chip cooling. This effect can be boosted in materials with non-trivial band topologies as demonstrated in the Heusler alloy Co_2MnGa. Enabled by the high quality of our material, in situ scanning thermal microscopy experiments reveal a high anomalous Ettingshausen coefficient of -2.1 mV in µm-sized on-chip cooling devices at room temperature. A significant 37% of the effect is contributed by the intrinsic topological properties, particularly the Berry curvature of Co_2MnGa. Furthermore, by geometrically creating longitudinal thermoelectric junctions, we trigger a Peltier enhancement and amplify the cooling performance, making the Anomalous Ettingshausen Effect in magnetic Weyl semimetals a promising avenue for high-efficiency spot cooling in nanoscale devices.

Transverse Multilayer Thermoelectric Generators with Thermoelectric Oxides

J. Töpfer, A. Bochmann, R. Löhnert, A. Ibrahim,

Ernst-Abbe-Hochschule Jena, FB SciTec, C.-Zeiss-Promenade 2, 07745 Jena, Germany

Oxide thermoelectric generators (TEG) are typically fabricated using the standard dual-leg design including manufacturing, arranging and contacting many individual sintered p- and n-type ceramic blocks. Alternatively, the ceramic multilayer technology represents a promising option enabling fabrication of multilayer TEGs. A concept of transverse multilayer thermoelectric generators (TMLTEG) with charge transport perpendicular to the heat flow direction will be presented. Such generators consist of layers of tape-cast p- or n-type thermoelectric oxides in combination with metal layers printed at a certain angle with respect to the heat flow direction to create anisotropic thermoelectric properties [1-3].
The synthesis, sintering behavior and thermoelectric properties of the individual thermoelectric oxides, as well as the co-firing behavior of metal and oxides is presented. Based on analytical calculations, we have developed the concept of Babin-plots, describing the power output and conversion efficiency for a given material combination as function of the internal and external device geometry [4]. This approach is demonstrated in combination with device simulations for pellet-based and multilayer transverse generators. The fabrication of TMLTEGs using various thermoelectric oxides, e.g., $Ca_3Co_4O_9$, La_2CuO_4 and $CaMnO_3$ for low-power applications, is reported.

References

[1] S. Teichert, A. Bochmann, T. Reimann, T. Schulz, C. Dreßler, J. Töpfer, AIP Adv. 5, 077105 (2015)
[2] J. Töpfer, T. Reimann, T. Schulz, A. Bochmann, B. Capraro, S. Barth, A. Vogel, S. Teichert, Int. J. Appl. Ceram. Technol. 15, 716–722 (2018)
[3] A. Bochmann, T. Reimann, T. Schulz, S. Teichert, J. Töpfer, J. Europ. Ceram. Soc. 39, 2923–2929 (2019)
[4] R. Löhnert, A. Bochmann, A. Ibrahim, J. Töpfer, Phys. Stat. Sol. A 2400321 (2024)

Hybrid transverse magneto-thermoelectric conversion in artificially tilted multilayers and thermoelectric permanent magnets

Ken-ichi Uchida[1,2]

[1] *National Institute for Materials Science (NIMS), Tsukuba, Japan*
[2] *Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, Japan*

In artificially tilted multilayers comprising two different conductors that are alternately and obliquely stacked, transverse thermoelectric conversion occurs, in which charge and heat currents are interconverted in the orthogonal direction. Although transverse thermoelectric conversion also occurs in homogeneous materials as intrinsic transport phenomena owing to the effects of magnetic fields, magnetization, and spins on conduction carriers, such magneto-thermoelectric effects have been investigated independently of thermoelectrics for artificially tilted multilayers [1]. Here, we show that the synergy of these different principles improves the performance of transverse thermoelectric conversion [2,3]. Using lock-in thermography techniques, we visualize transverse thermoelectric conversion processes in artificially tilted multilayers and experimentally clarify how nonuniform charge currents are converted into orthogonal heat currents. Through the measurements of temperature change under magnetic fields, we quantify the contributions of the magneto-thermoelectric effects in the artificially tilted multilayers and demonstrate magnetically enhanced hybrid transverse thermoelectric conversion. By replacing one of the conductors in the multilayer with permanent magnets, the same functionality is obtained even in the absence of magnetic fields, paving the way for the creation of "thermoelectric permanent magnets" that exhibit efficient transverse thermoelectric conversion together with spontaneous magnetization [2,4]. This study provides a new material design guideline for transverse thermoelectrics.

References

[1] K. Uchida and J. P. Heremans, Joule **6**, 2240 (2022).
[2] K. Uchida, T. Hirai, F. Ando, and H. Sepehri-Amin, Adv. Energy Mater. **14**, 2302375 (2024).
[3] T. Hirai, F. Ando, and K. Uchida, arXiv:2406.05393
[4] F. Ando, T. Hirai, A. Alasli, H. Sepehri-Amin, Y. Iwasaki, H. Nagano, and K. Uchida, arXiv:2402.18019

Goniopolar thermoelectrics: a theoretical perspective

Yaxian Wang[1] and Wolfgang Windl[2]

[1]Institute of Physics, Chinese Academy of Sciences, Beijing, China
[2] Department of Materials Science and Engineering, The Ohio State University, OHIO, USA

At present, the vast majority of electronic devices rely on the integration of p-type (hole conduction) and n-type (electron conduction) materials to direct current flow and create functionality, including transistors, light-emitting diodes, photoelectrocatalysts, solar cells, and thermoelectrics. However, some metallic and semiconducting single crystals have been shown to exhibit opposite charge polarity along different crystallographic directions from their Seebeck coefficients, although a solid theory for this phenomenon has been lacking for the past few decades.

In this talk, I will present a theoretical perspective on axis-dependent conduction polarity, termed “goniopolar” or “goniopolarity,” where the same population of charge carriers can simultaneously conduct as n-type and p-type along orthogonal crystallographic axes, originating from the Fermi surface topology [1]. Furthermore, by bridging the chemist's molecular orbital theory with the physicist's band theory, we propose the chemical design principles for both goniopolar and pxn mechanisms and make predictions in a variety of semimetals and semiconductors [2]. This enables transverse thermoelectric devices with an unprecedentedly high figure of merit, serving as a promising route to improve energy conversion. Finally, perspectives on future research directions and other relevant applications will also be provided.

References

1. B. He et al. , *Nat. Mater.*, 18 (2019), 568
2. Y. Wang et al., *J. Am. Chem. Soc.,* 142 (2020), 2812

Topology and Anisotropy as Tuning Mechanisms for an Enhanced Nernst Effect

S. J. Watzman[1], E. F. Scott[1], and K. A. Schlaak[1]

[1]Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, OH, USA 45219

Previous work in the Type I, inversion symmetry-breaking Weyl semimetal NbP demonstrated the simultaneous presence of both a large Nernst and magneto-Seebeck effect, which is rarely seen in a singular material, and how doping strongly alters both thermopowers [1]. The theory underlying transport in NbP is now applied to the Dirac semimetal Cd_3As_2 to predict the carrier concentrations at which the combined Nernst and Seebeck thermopowers are maximized under various temperature and field conditions. Thin films of Te-doped Cd_3As_2 were grown via molecular-beam epitaxy at the predicted carrier density levels, and magneto-thermoelectric transport is characterized to determine the predictive power of the model for tuning the material to the specific operating conditions (i.e. temperature and magnetic field). This work is then extended to WTe_2, a Type II Weyl semimetal that breaks inversion symmetry. While Type I Weyl semimetals like NbP have symmetric Dirac bands, Type II Weyl semimetals have tilted Dirac bands. Through experimental transport results in conjunction with theoretical modeling and comparison to previous results in NbP [1], we determine that when Dirac bands are tilted, their signature contributions to transport are washed out by parabolic bands. Therefore, we offer this comparison between Type I and Type II Weyl semimetals as evidence supporting the use of Type I Weyl semimetals for future applications of topological materials in solid state energy conversion devices.

While non-magnetic topological materials do exhibit a large Nernst effect in externally applied magnetic fields, magnetic Weyl semimetals offer the potential to substantially decrease, or even eliminate, the need for the external field. $YbMnSb_2$, an antiferromagnetic Weyl semimetal that breaks time-reversal symmetry, has a highly anisotropic band structure. In this work, the relationship between the anisotropic band structure, the orientation of the Mn moments, and the geometry of the fluxes associated with the Nernst effect is explored. This will elucidate a crystallographic orientation in which the Nernst effect is maximized, offering insight for energy generation applications of topological materials.

This work is supported by the U.S. Department of Energy under Award No. DE-SC0020154 and the National Science Foundation Graduate Research Fellowship Program under Grant No. 2035701.

References

[1] E. F. Scott et al. *Phys. Rev. B* **107**, 115108 (2023).

Abstracts of Posters

(in alphabetical order)

Theoretical investigations of electronic, thermodynamic and thermoelectric properties of filled skutterudites ThFe 4 P 12 and CeFe 4 P 12 using DFT calculations

F. Alleg Abdelkader[1] and S. Moulay Noureddine[2]

[1]Laboratory Physico-Chemistry of Materials, Laghouat, Algeria
[2] Laboratory of Advanced Materials Physical Chemistry (LPCMA), Sidi-Bel-Abbes, Algeria

The structural, mechanical, electrical, thermodynamic, and thermoelectric properties of $CeFe_4P_{12}$ and $ThFe_4P_{12}$ have been explored using first-principles calculations combined with semi-classical Boltzmann transport equations. These materials are confirmed to be semiconductors based on their band gap characteristics. Both materials demonstrate mechanical and dynamic stability. The Seebeck coefficient for $ThFe_4P_{12}$ and $CeFe_4P_{12}$ at ambient temperature indicates their potential in thermoelectric applications. The theoretical results strongly suggest these materials warrant further experimental investigation..

References

[1] F. **Alleg Abdelkader**
[2] S. **Moulay Noureddine**

Dependence of Anomalous Nernst coefficient on electron mean free path and Berry curvature

V. Basso[1],A. Di Pietro[1], A. Sola[1]

[1],Istituto Nazionale di Ricerca Metrologica (INRIM), Turin, Italy

The spontaneous Nernst effect of metallic ferromagnets is currently an active topic of research because of the possibility to design passive heat sensing [1] and active cooling devices [2] based on it. Among the relevant materials we find MnBi [3], FeGa [4] and NiMnGa [5].

The spontaneous Nernst effect is caused by the spin orbit interaction felt by conduction electrons and shares its microscopic origin with the spontaneous Hall effect [6]. Recently, the introduction of the Berry phase formalism has permitted to compute the spontaneous Hall conductivity on magnetic metals by first principles methods as for example by spin DFT [7]. In the present paper we address the problem of deriving the Nernst coefficients of ferromagnets by using the Boltzmann transport approach. The ordinary Nernst coefficient is known to scale with the electron mean free path, implying that efficient Nernst materials are generally found as single crystal semimetals with reduced scattering. Introducing the thermal transverse effect in analogy to what is done for the spontaneous Hall effect, we show that the resulting spontaneous Nernst coefficient rescales with the inverse of the mean free path. We therefore predict that optimal spontaneous Nernst materials should have semimetallic properties, a strong spin orbit interaction and relatively strong scattering. In our work, together with the theory, we also show some exactly solvable models allowing to distinguish the relative importance of some basic physical parameters determining the magnitude of the Berry curvature and its effect on the Nernst coefficient.

References

[1] K. Uchida *Appl. Phys. Lett.* **118**, 140504 (2021).
[2] A. Miura *Appl. Phys. Lett.* **115**, 222403 (2019).
[3] B. He *Joule* **5**, 3057 (2021).
[4] A. Sakai *Nature* **581**, 53 (2020).
[5] A. De *Phys. Rev. B* **103**, L020404 (2021).
[6] N. Nagaosa *Rev. Mod. Phys.* **82**, 1539 (2010).
[7] J. Kubler *Phys. Rev. B* **85**, 012405 (2012).

Vacancy-mediated anomalous phononic and electronic transport in defective half-Heusler ZrNiBi

Wuyang Ren[1,2,†], Wenhua Xue[3,†], Shuping Guo[4,†], Ran He[4], Liangzi Deng[2], Shaowei Song[2], Andrei Sotnikov[4], Kornelius Nielsch[4], Jeroen van den Brink[4], Guanhui Gao[5], Shuo Chen[2], Yimo Han[5], Jiang Wu[1], Ching-Wu Chu[2], Zhiming Wang[1]*, Yumei Wang[3]* & Zhifeng Ren[2]*

[1]Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, Chengdu 610054, People's Republic of China.
[2]Department of Physics and Texas Center for Superconductivity at the University of Houston (TcSUH), Houston, TX 77204, USA.
[3]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Science, Beijing 100190, People's Republic of China.
[4]Leibniz Institute for Solid State and Materials Research, Dresden 01069, Germany.
[5]Department of Materials Science and Nano-Engineering, Rice University, Houston, TX 77005, USA.

Studies of vacancy-mediated anomalous transport properties have flourished in diverse fields since these properties endow solid materials with fascinating photoelectric, ferroelectric, and spin-electric behaviors. Although phononic and electronic transport underpin the physical origin of thermoelectrics, vacancy has only played a stereotyped role as a scattering center. Here we reveal the multifunctionality of vacancy in tailoring the transport properties of an emerging thermoelectric material, defective n-type ZrNiBi. The phonon kinetic process is mediated in both propagating velocity and relaxation time: vacancy-induced local soft bonds lower the phonon velocity while acoustic- optical phonon coupling, anisotropic vibrations, and point-defect scattering induced by vacancy shorten the relaxation time. Consequently, defective ZrNiBi exhibits the lowest lattice thermal conductivity among the half-Heusler family. In addition, a vacancy-induced flat band features prominently in its electronic band structure, which is not only desirable for electron-sufficient thermoelectric materials but also interesting for driving other novel physical phenomena. Finally, better thermoelectric performance is established in a ZrNiBi-based compound. Our findings not only demonstrate a promising thermoelectric material but also promote the fascinating vacancy-mediated anomalous transport properties for multidisciplinary explorations.

Onsager Reciprocal Relation between Anomalous Transverse Coefficients of an Anisotropic Antiferromagnet

X. Guo [1,2], X. Li [1], Z. Zhu [1], K. Behnia [1,2]

[1]Wuhan National High Magnetic Field Center and School of Physics, Huazhong University of Science and Technology, Wuhan 430074, China
[2]Laboratoire de Physique et d'Etude de Matériaux (CNRS) ESPCI Paris, PSL Research University, 75005 Paris, France

Whenever two irreversible processes occur simultaneously, time-reversal symmetry of microscopic dynamics gives rise, on a macroscopic level, to Onsager's reciprocal relations [1,2], which impose constraints on the number of independent components of any transport coefficient tensor [3,4]. Here, we show that in the anisotropic antiferromagnetic $YbMnBi_2$, which displays a strong temperature-dependent anisotropy, Onsager's reciprocal relations are strictly satisfied for anomalous electric (σ_{ij}^A) and anomalous thermoelectric (α_{ij}^A) conductivity tensors. In contradiction with what was recently reported by Pan et al. [3], we find that $\sigma_{ij}^A(H) = \sigma_{ij}^A(-H)$ and $\alpha_{ij}^A(H) = \alpha_{ji}^A(-H)$. This This equality holds in the whole temperature window irrespective of the relative weights of the intrinsic or extrinsic mechanisms. Furthermore, it should be note that the Nernst thermal power S_{ij} is not a true Onsager coefficient, which is apportioned by the mobility μ_{ii}, giving rise to an enhanced thermopower in one of the configurations for an anisotropic system. The $\alpha_{zy}^A/\sigma_{zy}^A$ ratio is close to k_B/e at room temperature but peaks to an unprecedented magnitude of 2.9 k_B/e at ~150 K, which may involve nondegenerate carriers of small Fermi surface pockets [6].

References

[1] L. Onsager, Phys. Rev. 37, 405 (1931).
[2] L. Onsager, Phys. Rev. 38, 2265 (1931).
[3] Y. Akgoz and G. Saunders, J. Phys. C 8, 1387 (1975).
[4] Y. Akgoz and G. Saunders, J. Phys. C 8, 2962 (1975).
[5] Y. Pan, C. Le, B. He, S. J. Watzman, M. Yao, J. Gooth, J. P. Heremans, Y. Sun, and C. Felser, Nat. Mater. 21, 203 (2022).
[6] Guo, X., Li, X., Zhu, Z., & Behnia, K. Phys. Rev. Lett. 131, 246302(2023).

Observation of large Seebeck-driven transverse thermoelectric generation in Bi/Sb bulk composites

Jangwoo Ha[1], Min Young Kim[2], Sang J. Park[1,3] and Hyungyu Jin[1]

[1]Department of Mechanical Engineering, Pohang University of Science and Technology (POSTECH), Pohang 37673, South Korea.
[2] Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH 43212, USA.
[3] Present address: National Institute for Materials Science, Tsukuba, 305-0046, Japan.

Transverse thermoelectric devices generate an electric field perpendicular to a temperature gradient, allowing for simple, sheet-like module designs that can circumvent the contact issues faced by conventional Seebeck-effect-based thermoelectric devices. Recently, significant transverse thermopower has been reported in bilayer structures composed of electrically connected Nernst and Seebeck materials [1], a phenomenon called Seebeck-driven transverse thermoelectric generation (STTG). However, most studies of STTG have focused on thin bilayers with in-plane heat flow, which restricts its scalability for large-area applications. Here, we extend the STTG concept to bulk composites composed of Nernst and Seebeck materials, which are isotropic and do not constrain the heat flux direction, making them scalable and suitable for large-area heat sources. Experimental validation on a Bi 51 vol% / Sb 49 vol% composite demonstrates a remarkable enhancement in transverse thermopower (5.55 $\mu V\ K^{-1}$ at 300 K and 0.3 T), a threefold increase compared to poly-Bi (1.97 $\mu V\ K^{-1}$). Under the same conditions, the transverse thermoelectric figure of merit increases sevenfold, suggesting that Nernst/Seebeck bulk composites are a promising pathway for efficient transverse thermoelectric generation.

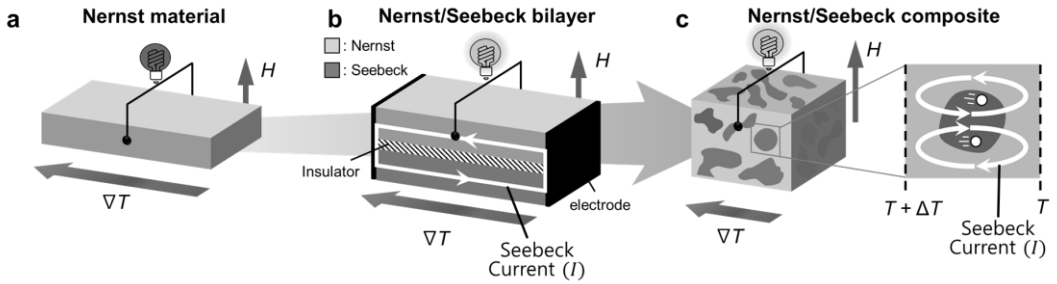


Figure 1. Schematic representation of Seebeck-driven transverse thermoelectric generation (STTG). (a) Nernst effect, where an electric field occurs perpendicular to both the temperature gradient ∇T and the magnetic field H. (b) STTG in bilayer structures, where the Nernst and Seebeck materials are electrically connected in series and thermally connected in parallel. (c) STTG in bulk composites.

References

[1] W. Zhou, et al., *Nature Materials* **20**, 463-467 (2021).

Title: Thermoelectric efficiency of nanoscale devices in the nonlinear regime

Raymond Hartig

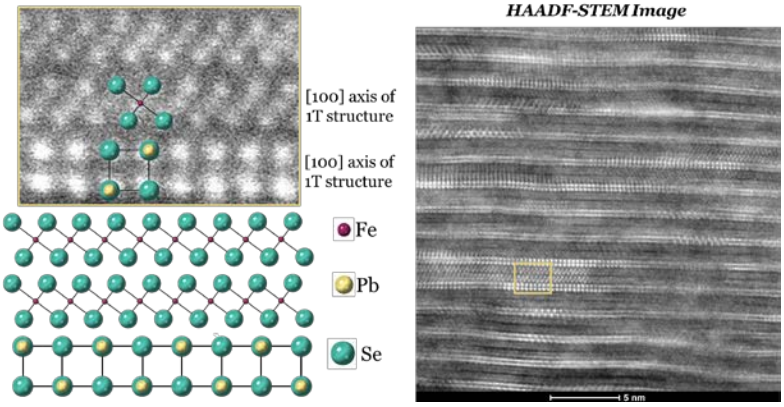
Abstract: We considered the quantum thermoelectric transport through a two-terminal nanoscale device whose two terminals are subject to a temperature and voltage difference. We present general expressions for the charge and heat currents and the efficiency of energy transfer in the nonlinear regime. For the particular cases of Lorentzian resonances and antiresonance transmission functions and Fano transmission functions the electric and heat currents expressions are *analytical* and can be expressed in terms of Riemann zeta functions and Bernoulli numbers. These results allowed us to optimize the efficiency of the thermoelectric transport in the nonlinear regime.

Using surface interactions and nanoconfinement to prepare heterostructures with constituent structures not found in phase diagrams: $(PbSe)_m(FeSe_2)_n$, $(MoSe_2)_m(FeSe_2)_n$ and $(FeSe)_m(MoSe_2)_n$

Fischer Harvel and David Johnson

University of Oregon, US, Eugene, OR.

β-FeSe and related Fe_xSe_y compounds have attracted significant attention for diverse applications including superconductors, thermoelectrics, photocatalysts, and batteries. The equilibrium phase diagram is relatively complex and consists of six phases between $FeSe_{1 \le y \le 2}$ composition, in addition to other kinetic compounds reported in literature. Therefore, understanding the reactions between Fe and Se in the 2D regime is crucial for optimizing growth conditions and subsequent device manufacturing. We used surface interactions with stable compounds PbSe, $MoSe_2$, and $NbSe_2$ to control structure of nanoconfined volumes of Fe-Se (~6 Å - ~18Å). We show that the favored Fe_xSe_y phase is influenced by local composition, annealing temperature, volume of the confined space and the identity of the adjacent layer. For example, PbSe stabilizes the nucleation and growth of metastable 1T-$FeSe_2$, forming $(PbSe)_{1.07}(FeSe_2)_n$ compounds (see figure).[1] Additionally, confining Fe and Se between thick layers of $MoSe_2$ (18 Å laterally) results in initial formation of 1T-$FeSe_2$, which converts to β-FeSe upon selenium vaporization during low-temperature annealing. We also formed a new alloy structure of $Pb_{1-x}Fe_xSe$ that is stabilized by adjacent $NbSe_2$ layers in the heterostructure $[(Pb_{1-x}Fe_xSe)_{1+\delta}]_3(NbSe_2)$. These results provide insights into controlling phase formation in confined volumes, where surface energies stabilize structures not found in binary phase diagrams.



References

[1] F. Harvel[II]; M. Lemon[II]; R. Gannon; S. Rudin; P. Lu; H. Blackwood; D. C. Johnson. 1T-$FeSe_2$ Layers in $(PbSe)_{1+\delta}(FeSe_2)_n$ - An Interlayer-Stabilized 2D Structure. *Chem Mater.* **2023**, 35, 18, 7521 – 7528.

Thermal conductivity reduction of Fe2VAl thermoelectric alloys through atomic disorder engineering

Apoorva Joshi[1] , James Russel Taylor[1] , Tao Fang[1] , Cory Cline[1] , Weiling Dong[1] , Jifeng Liu[1] , Ian Baker[1] , Geoffroy Hautier[1] ,

[1]Thayer School of Engineering, Dartmouth College, Hanover, United States of America

We report temperature-dependent thermal conductivity to reveal the microscopic phonon scattering mechanisms of Fe2VAl, an emerging and promising thermoelectric material due to its low cost and non-toxicity. As a pseudo-gap semiconductor, Fe2VAl has a good power factor, but its figure of merit is limited by high thermal conductivity. We found that the thermal conductivity can be greatly reduced by Ge doping and atomic site disorder engineering via water quenching from 1120ºC, which is above the order-disorder transition temperature between the fully ordered L21 and partially disordered B2 phase. While the base alloy without doping reports a high thermal conductivity of 28 W/K-m at 300 K, consistent with previous reports in the literature, it is greatly reduced by ~7x to 4W/K-m for Fe2VAl0.9Ge0.1 alloy water-quenched from 1120ºC. Temperature-dependent thermal conductivity measurement from 4K to 400K reveals that a nearly phonon-glass state is achieved with behavior comparable to that of silica glass, leading to a significant reduction in thermal conductivity because of increased disorder from quenching. The thermal conductivity at a low temperature <100K also shows a linear temperature dependence, suggesting strong electron-phonon scattering. We fit our data to the Debye-Callaway model including boundary scattering, point-defect scattering, phonon-phonon scattering, and electron-phonon scattering terms, which provided new insights into the optimization of thermal conductivity. Our investigation into the fundamental mechanisms revealed that a strong enhancement in point defect scattering and electron-phonon scattering plays the most significant roles in reducing thermal conductivity, particularly obvious at low temperatures but also extends to at least 400 K. We further examined the effects of different heat treatments i.e slow cooling versus water quenching on the material's properties, finding that the electron-phonon scattering parameter increases nearly 3x for water-quenched samples, consistent with our computational findings that the water quenching induces metastable L21* phase with a notable increased the effective mass of electrons as well as the experimental measurement of a larger electronic heat capacity. These findings offer valuable strategies for tailoring the thermal properties of Fe2VAl.

Enhanced Thermoelectric Cooling Through Improved Interfacial Bonding in 3D-Printed Materials

Shengduo Xu *, Sharona Horta, Abayomi Lawal, Magali Lorion, Maria Ibáñez *

Institute of Science and Technology Austria (ISTA), Am Campus 1, Klosterneuburg 3400, Austria

To date, Thermoelectric (TE) materials are used in niche applications, such as powering space missions and precise temperature controller. [1] However, their broader use in everyday devices is limited by low efficiency and high production costs. Hence, the dire need for performance enhancements and more cost-effective and scalable techniques. Despite considerable efforts made in improving the conversion efficiency of TE materials, there is still a huge gap to bridge when it comes to making practical devices form these materials. Conventional TE devices with cubic geometries are unable to effectively ensure thermal contact with non-flat heat sources. Non-cuboid geometries are challenging to mass-produce due to lack of shape control associated with traditional densification techniques for bulk materials. [2]

Additive Manufacturing (AM), also known as 3D printing, is a viable substitute for traditional fabrication that allows for the quick prototyping of intricate shapes. Compared to conventional methods, AM offers simplicity, flexibility, and speed by depositing material layer by layer. It also produces less waste, and is more adaptable to different materials. [3]

Even with the numerous advantages of 3D printing, performance of printed materials is low compared to their bulk counterpart owing minimal connection between the grains leading to porosity of the printed material which negatively impacts charge transport. Herein, we address this challenge by designing an ink formulation that ensure effective particle bonding during sintering. This leads to significant improvement in charge mobility of the printed material, thereby improving the printed material's performance. Through our approach we printed p-type and n-type TE legs with outstanding performance from which we assemble a TE cooler with COP comparable to that of dense materials.

Through this work we have demonstrated the potential of 3D printed materials for cost-effective and scalable production of high-performance TECs, avoiding the energy-consuming and lest cost effective steps such commonly used

References

[1] Yang. L, Advanced Energy Materials, 8(6), 1701797 (2018).
[2] Park. S, Nature communications, 7(1), 13403 (2016).
[3] Oztan. C, Energies, 15(9), 3121 (2022).

Coexistence of Kondo effect and Weyl semi-metallic states in Mn doped VAl3 compounds

Kwan-Young Lee[1,2] and Jong Soo Rhyee[*]

[1,]Kyung Hee Univ., Seoul, Korea*
[2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany
E-mail : k.y.lee@ifw-dresden.de

In condensed matter physics, the strong correlation effect in Weyl semimetal is of fundamental interest, and critical changes in electronic structure are relevant for many fields of current applied Physics like electronics, thermoelectricity, or quantum computing, to name a few. Although it hasn't yet been observed experimentally, diluted Mn-doping in type-II Dirac semimetal VAl3 is expected to bring about the Weyl semimetal phase transition, raising the chemical potential to a point where the Dirac point is near the Fermi energy, thus lifting band degeneracy. Our experimental work shows a resistivity minimum at Tk = 40 K, logarithmic increase in electrical resistivity, magnetic susceptibility, and specific heat divided by temperature, with a significant Sommerfeld coefficient at low temperatures, supporting the existence of Kondo effect. Because of the chiral anomaly in Mn-doped MnxVAl3, the angle-dependent magnetoresistance has shown the negative longitudinal magnetoresistance below Kondo temperature. Time-reversal symmetry is broken by the exchange interaction by RKKY interaction in MnxVAl3 even in Kondo screening at low temperature below Kondo temperature ($T \leq Tk$), leading to the topological phase transition from Dirac to Weyl semimetal. This study demonstrates the coexistence of the temperature-induced topological phase transition and the Kondo effect with the Weyl semi-metallic state.

References

[1] G.Sharma et al., Phys. Rev. B. 96, 045112 (2017)
[2] K.-W.Chen et al., Phys. Rev. Lett. 120, 206401 (2018)
[3] R. Singha et al., Phys. Rev. B. 98, 081103® (2018)

High-throughput design of doped all-d-metal Heusler compounds for transverse thermoelectric applications

Fu Li, Shen Chen, Hao Wang, Ruiwen Xie, Hongbin Zhang

Institute of Materials Science, Technical University of Darmstadt, 64287 Darmstadt, Germany
E-mail: fu.li@tu-darmstadt.de

Weyl semimetals have been attracting significant attention due to it topological features, Furthermore, a prominent class of Weyl semimetals is Weyl magnetic materials such as the ferromagnetic Heusler alloy. Many Heusler compounds have been theoretically predicted to be topological semimetals [1]. Chemical doping is an efficient method to optimize the physical properties of Heusler compounds [2], particularly their anomalous transport properties, including anomalous Hall conductivity (AHC) and anomalous Nernst conductivity (ANC). The correlations between these transport properties and the electronic structure will be thoroughly investigated, providing practical guidance for tailoring AHC and ANC through chemical doping for transverse thermoelectric applications.

References

[1] M. F. Tanzim, et al., Adv. Funct. Mater. **33**, 2214967 (2023)
[2] G. Xing, et al., Acta Mater. **270**, 119856 (2024)

TMLTEG based on substituted $CaMnO_{3-\delta}$

R. Löhnert[1] and J. Töpfer[1]

[1]Ernst-Abbe-Hochschule Jena, University of Applied Sciences, Jena, Germany

An artificial anisotropic material (AAM) is created by embedding parallel metal strips in a block of an oxide ceramic with thermoelectric properties. By tilting the metal strips with respect to an applied temperature gradient, an electrical voltage is generated across the AAM due to the transverse thermoelectric effect [1]. This ceramic-metal composite material can be fabricated as transverse multilayer thermoelectric generator (TMLTEG) using the established ceramic multilayer technology [2].

Among the thermoelectric oxides, the semiconducting compound $CaMnO_{3-\delta}$ displays attractive characteristics. Its thermoelectric properties were optimized by the substitution of Ca^{2+} or Mn^{4+} with ions of different charge (heterovalent substitution), which increased the number of mobile charge carriers. The electrical conductivity therefore rose as the degree of substitution increased, while the absolute value of the Seebeck coefficient declined. In addition, the smaller the ionic radius of the substituent, the greater the electrical conductivity for the same degree of substitution. However, the Seebeck coefficient was not dependent on the substituent introduced. The substitution of Ca^{2+} by ions of the same charge (homovalent substitution) enabled further improvement. These “lattice defects” increased the phonon scattering and thus reduced the thermal conductivity [3]. With regard to material optimization, the processing of ceramic powder is also of interest. Soft chemistry synthesis methods enabled the production of fine-grained, homogeneously substituted calcium-manganese ceramics with improved thermoelectric properties [4].

The suitability of different metals in combination with substituted $CaMnO_{3-\delta}$ in a TMLTEG was evaluated using micro-Babin plots [1]. For the use of an AgPd alloy (6:1), it was necessary to reduce the sintering temperature of $CaMnO_{3-\delta}$ from 1200 °C to below 1060 °C. This was achieved by using the sintering additive CuO. Compatibility tests of AgPd screen printing paste and Ca-Mn oxide ceramic showed diffusion of a metallic phase at sintering temperatures above 1000 °C. Finally, a TMLTEG based on substituted $CaMnO_{3-\delta}$ was sintered at 980 °C in combination with AgPd 6:1 metal strips. The produced module generated an electrical power of 1 mW at ΔT of 75 K and 25 °C at the cold side. Current research topics are the optimization of sintering temperature and component geometry with regard to the material properties.

References

[1] R. Löhnert *et al.*, Phys. Status Solidi A, 2400321 (2024)

[2] J. Töpfer *et al.*, Int. J. Appl. Ceram. Technol. **15**, 716–722 (2018)

[3] R. Löhnert *et al.*, J. Solid State Chem. **315**, 123437 (2022)

[4] R. Löhnert *et al.*, Mater. Sci. Eng. B **223**, 185–193 (2017)

Robustness Through Simplicity: Leveraging the Transverse Seebeck Effect for Extreme Environment Heat Flux Sensing

K. McAfee[1], P. B. Sunderland[1], and O. Rabin[1,2]

[1]University of Maryland, College Park, MD, USA
[2]Institute for Research in Electronics and Applied Physics, College Park, MD, USA

Direct heat flux sensors compatible with harsh, high-temperature environments are critical for applications such as space exploration, combustion, and hypersonic flight. In this work, we report on the development of a heat flux sensor tailored for operation in extreme environments using the Transverse Seebeck Effect (TSE). In contrast with sensors that rely on conventional thermoelectric effects, TSE-based heat flux sensors exhibit more simple and robust constructions and may be better suited for harsh environments. A TSE-based heat flux sensor is fabricated using anisotropic rhenium single crystals and high-temperature ceramic packaging. Through careful arrangement of the single crystal transducers within the package, the TSE is isolated as the sole transduction mechanism. Using an in-house calibration facility that can independently modulate the sensor temperature and incident heat flux, the responsivity of the heat flux sensor is characterized over a wide range of temperatures spanning from room temperature to 500°C. The TSE-based sensor exhibits a responsivity of -1.7 μV/(W/cm^2) at room temperature and a responsivity of 2.6 μV/(W/cm^2) at 500°C. A theoretical prediction of the temperature-dependence of the responsivity of the sensor is developed using literature-based thermoelectric transport properties and is shown to be in good agreement with experimental data. This work is supported by the US DOE Award DE-FE0031902.

Anisotropy effect in doped SnSe materials prepared by spark plasma sintering

F. Mihok[1]

[1] Institute of materials research, Slovak Academy of Sciences, Watsonova 47, 04001 Košice

Thermoelectric generators represent one of the most reliable ways to generate electricity even in challenging conditions. Hence their widespread use for space missions. Their reliability can be greatly reduced when materials are periodically exposed to mechanical stresses due to different rates of thermal expansion in a thermoelectric couple. SnSe is a promising material for a creation of homojuction pairs for thermoelectric generators which reduce internal stresses and improve reliability of the modules further. This can be achieved because of observed polarity switching in Sb and Bi doped SnSe [1], [2], [3]. This submission focuses on anisotropic behavior of polycrystalline SnSe doped with either Bi, Ag, Ni, Mg and In prepared by powder metallurgy and spark plasma sintering.

Prepared materials are arranged in layers with a tendency for preferred orientation that is observable even before sintering. This results in an anisotropic behavior that is further emphasized by the sintering process. Due to the nature of sintering anisotropy is observed in 2 dimensions only. The effect of different dopants on the bulk material anisotropy was determined. Furthermore, in the bulk form Bi-doped materials exhibit polarity switch from P to N region with certain dopant concentrations having the strongest effect.

Doping element not only changed the polarity of SnSe but its potent thermoelectric properties were not significantly affected. Additionally, mechanical properties of the material show improvements with a rising amount of dopant. Lastly, the polarity did not revert even with further excessive doping concentrations as opposed to doping with Sb. Therefore, this material lends itself well for creation of homojunction pairs for thermoelectric generators with enhanced longevity, better resistance to external mechanical stresses, without compromise on output, with a very forgiving synthesis pathway and long-term material stability.

References

[1] C. Yamamoto, *Adv. Funct. Mater.* **31**, 2008092 (2021)
[2] A. T. Duong, *Nat Commun* **7**, 13713 (2016)
[3] V. Q. Nguyen, *Nanoscale Res Lett* **13**, 200 (2018)

High thermoelectric performance in Ag_2Se achieved through a sustainable solution synthesis

F. Milillo[1], T. Kleinhanns[1], M. Calcabrini[1], C. Fiedler[1], S. Horta[1], D. Balazs[1], M. Ibáñez[1]

[1]Institute of Science and Technology Austria (ISTA), Klosterneuburg, Austria

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.

References

[1] T. Kleinhanns, Advanced Energy Materials, volume 14, issue 22, June 12, 2024, 2400408.

Band-resolved transport properties and the transverse thermoelectric conversion in a semimetal WSi_2

S. Ohsumi[1], Y. J. Sato[2], and R. Okazaki[1]

[1]Tokyo University of Science, Noda 278-8510, Japan
[2] Saitama University, Saitama 338-8570, Japan

WSi_2 single crystal exhibits axis-dependent conduction polarity (ADCP) of thermopower [1], which is expected to induce transverse thermoelectric voltage in zero magnetic field [2].

Figure 1(a) shows the temperature dependence of thermopower of two single crystals along the *a*- and *c*-axis directions. The ADCP of thermopower was confirmed at low temperatures and we revealed that the ADCP originates from the mixed-dimensional Fermi surfaces, which distinguished by the coexistence of quasi-one-dimensional electron-like and quasi-two-dimensional hole-like sheets [Fig. 1(b)].

In addition, we found strong sample dependence in thermopower along *c*-axis direction as shown in Fig. 1(a). Based on the computational study, we elucidated that the sample-dependent thermopower can be explained by band-dependent relaxation time.

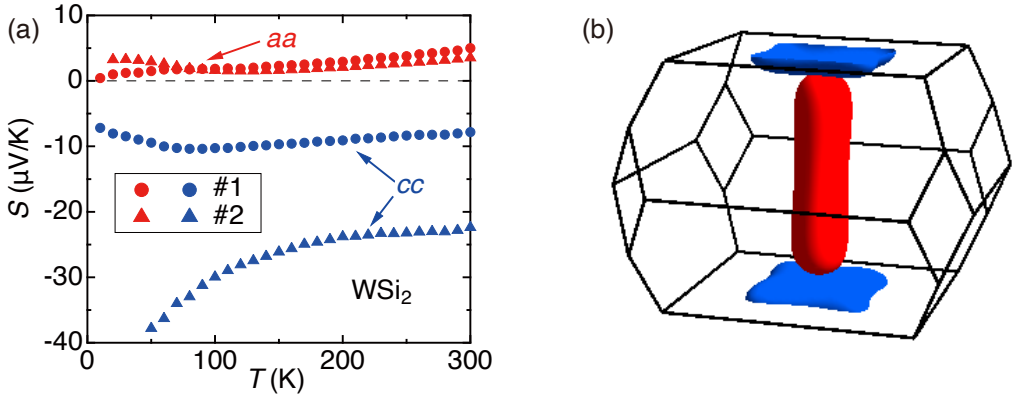


Fig. 1. (a) Temperature dependence of thermopower along the *a*- and *c*-axis directions. (b) Mixed-dimensional Fermi surfaces obtained by first-principles calculations

References

[1] Karl G. Koster *et al.*, Chem. Mater. **35**, 11 (2023).
[2] K. Uchida and J. P. Heremans, Joule **6**, 10 (2022).

Optimizing Application-Specific Transverse Thermoelectric Properties of Binary Composites Using Topology Optimization

Junyoung Park[1], Hyun Yu[1], Hyungyu Jin[1]

[1] Department of Mechanical Engineering, Pohang University of Science and Technology (POSTECH), Pohang 37673, South Korea.

Transverse thermoelectric (TTE) devices have demonstrated significant potential as generators, coolers, and heat flux sensors owing to their innovative architecture. To enhance their performance, TTE research have been focused on increasing the figure of merit, zT, which is directly related to the conversion efficiency in generators and the coefficient of performance in coolers. However, recent studies indicate that zT is not the sole determinant of thermoelectric (TE) performance. Depending on the application, indicators such as power factor, cooling rate, and heat flux sensitivity could better represent TE performance than zT. Consequently, simply utilizing TTE materials with high zTs may lead to suboptimal performance in certain applications. Thus, an emergent challenge in the field of TTE is to find a novel way to optimize TTE devices for each specific application.

To address such a challenge, we attempted to employ topology optimization (TO), a robust shape optimization method, for designing TTE devices with optimized performance for targeted specific applications. The TO was performed on TE legs constituted with a binary composite; $Bi_{0.5}Sb_{1.5}Te_3$/Fe-50Ni. The material density distribution was optimized for various applications, including generators, coolers, and heat flux sensors. Each optimized TE leg demonstrated a power factor of 8.16×10^−3 W/mK^2, a heat flux sensitivity of 4.39×10^−7 Vm^2/W, and a temperature difference of 40 K, representing improvements of 104%, 115%, and 19%, compared to zT-optimized legs, respectively. These optimized legs were then fabricated using laser powder bed fusion, followed by spark plasma sintering, and their TE performances were experimentally validated for each application. Our study demonstrates that the TO provides application-specific optimization of TTE devices without modifying intrinsic material properties and may serve as a versatile tool for designing high performance TTE devices for various applications.

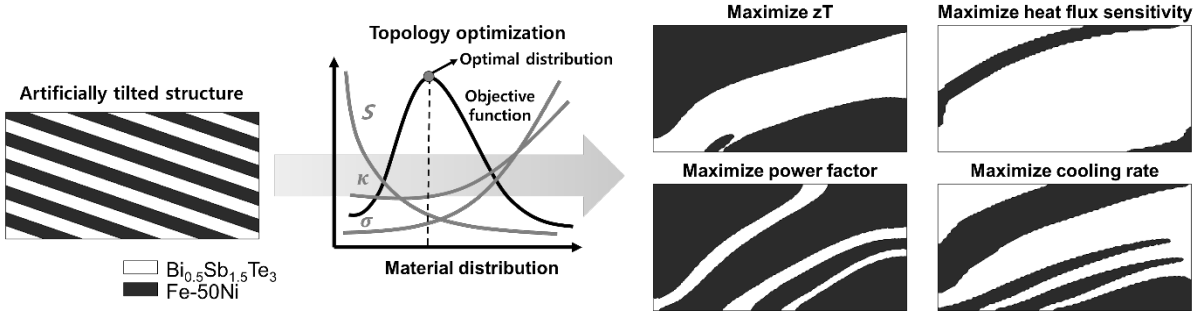


Figure 1. Schematic illustration of binary composite topology optimization process for application-specific transverse thermoelectric

Modelling the lattice thermal conductivity of transverse thermoelectric materials: the case of Re_4Si_7

Elena R. Remesal,[1] Matthew Grayson,[2] Antonio M. Márquez,[1] and José J. Plata[1]

[1]Departamento de Química Física, Universidad de Sevilla, Sevilla, 41009, Spain
[2] Department of Electrical and Computer Engineering, Northwestern University, Evanston, IL, 60208 USA

Modelling the transport properties of transverse thermoelectric materials poses various challenges. Their narrow band gaps require the use of state-of-the-art functionals to properly describe their semiconducting nature. Furthermore, their low symmetry and often large unit cells increase the computational cost of the calculations. Therefore, strategies to combine high-accuracy and reduced computational cost are necessary for the calculation of transport properties of these materials.

In this work, we present a combination of new ab initio methodologies to predict thermal transport properties using machine learning and a high-throughput framework. This approach establishes a solid foundation for the accurate prediction of thermal transport properties of transverse thermoelectric materials. We have applied this strategy to Re4Si7 as a benchmark to test the accuracy of the method. This methodology not only provides a straightforward approach to predict the lattice thermal conductivity as a function of temperature, defects, and anisotropy, but also opens the door to understanding the physicochemical phenomena governing the low lattice thermal conductivity of this compound.

Acknowledgments

This work was funded by Spanish MICIN/AEI/10.13039/501100011033 and by “European Union Next Generation EU/PRTR” (grants PID2022-138063OB-I00 and TED2021-130874B-I00).

Electronic band structure and thermoelectric performance of $SnBi_2Te_4$

K. Pryga[1], I. Terzi[2], B. Wiendlocha[1], P. Levinský[3], S. El Oualid[2], S. Migot[2] , J. Ghanbaja[2] , C. Gendarme[2] , T. Schweitzer[2], B. Malaman[2], G. Le Caër[4], B. Lenoir[2] and C. Candolfi[2]

[1] AGH University of Krakow, Faculty of Physics and Applied Computer Science, Aleja Mickiewicza 30, 30-059 Krakow, Poland
[2]Institut Jean Lamour, UMR 7198 CNRS – Université de Lorraine, 2 allée André Guinier-Campus ARTEM, BP 50840, 54011 Nancy Cedex, France
[3] FZU – Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10/112, 162 00, Prague 6, Czech Republic
[4] Institut de Physique de Rennes, UMR UR1-CNRS 6251, Université de Rennes I, Campus de Beaulieu, 35042 Rennes Cedex, France

$SnBi_2Te_4$ belongs to the class of layered chalcogenide semiconductors which have been a fruitful area for designing efficient thermoelectric materials, as members of this group possess low lattice thermal conductivity and multivalley electronic band structure. While there have been several studies of this material, no detailed investigation on the low-temperature transport properties has been reported so far.

Here we perform calculations of electronic band structure for $SnBi_2Te_4$ using the all-electron full-potential linearized augmented plane wave (FP-LAPW) method, as implemented in the WIEN2k package as well as transport properties via the BoltzTraP code.

Electronic band structure calculations reveal that $SnBi_2Te_4$ is a p-type, narrow-band-gap semiconductor with a multivalley valence band structure that has a strong asymmetry between the valence and conduction bands. Antisite defects play a key role in understanding the transport properties, as their existence leads to the onset of bipolar conduction near 300 K due to band gap reduction and modification of the band structure. Both electrical resistivity and thermopower exhibit anisotropy for the in-plane and trigonal magnetic field directions. The combination of low thermal conductivity and relatively high power factors lead to peak ZT values of 0.32 at 350 and 400 K for $Sn_{0.95}Bi_2Te_4$ and $SnBi_2Te_4$, respectively.

References

[1] A. Saxena, N. K. Karn, M. M. Sharma, and V. P. S. Awana, Journal of Physics and Chemistry of Solids **174**, 111169 (2023).

Flexible Talbot Lithography for Fast-Response Heat Flux Sensors Using the Transverse Seebeck Effect

H. Reith[1] O. Rabin[2] and K. Nielsch[1,3,4]

[1] Institute for Metallic Materials, Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

[2] Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA

[3] Institute of Materials Science, Dresden University of Technology, 01062 Dresden, Germany

[4] Institute of Applied Physics, Dresden University of Technology, 01062 Dresden, Germany

Fast-response heat flux sensors with <1 msec resolution are crucial for monitoring electro-optical system power and studying aerospace systems under hypersonic conditions. Achieving such fast response requires minimizing the sensor's thermal mass and maximizing heat dissipation. Thin-film devices utilizing the transverse Seebeck effect offer a promising solution, though controlling the crystallographic orientation of the thin film relative to heat flux remains a challenge. Current approaches, which depend on epitaxial growth on miscut single crystal substrates, face limitations in temperature range and substrate compatibility.

We propose a novel and flexible manufacturing process that leverages displacement Talbot lithography to pattern large-area substrates with nanoscale precision. This method enables the creation of periodic “sawtooth” surface topographies, providing controlled tilt angles for textured thin film growth. Unlike traditional epitaxial methods, Talbot lithography offers scalability, compatibility with a wide range of thermoelectric materials, and flexibility in substrate selection. Our preliminary results with antimony films on patterned silicon wafers demonstrate the potential for achieving controlled grain orientation and enhanced sensor performance, paving the way for broader applications.

Hierarchical phonon scattering from nano to macro scale in Bismuth Telluride bulk composites and cost-effective module structure

Jong Soo Rhyee*, Kwan Young Lee, Pooja Rawat, Anil Kumar

Department of Applied Physics, Integrated Education Institute for Frontier Science and Technology (BK21 Four) and Institute of Natural Sciences, Kyung Hee University, Yong-In 17104, Republic of Korea

We study the thermoelectric properties of a p-type Bi0.4Sb1.6Te3.4 (BST) composite with Ag nano-particle decorated TiO2 microparticles (Ag/TiO2). The dispersion of Ag/TiO2 particles, synthesized by an ultrasonication (US) and spray coating (SC) methods, into the matrix effectively decreases lattice and bipolar thermal conductivity. These reduced grain sizes, alongside nano-particle decorated microparticles dispersed throughout the matrix, scatter phonons effectively from long to short wavelength phonons and subsequently decrease lattice thermal conductivity. The significant suppression of lattice and bipolar thermal conductivity has led to an increase in the maximum zT value. We designed and fabricated new thermoelectric module with cost-effective methods. The new module design does not significantly deteriorate the module performance but have many merits such as high mechanical property, easy fabrication, and significant cost down. Therefore the promising new thermoelectric module structure using the performance enhanced thermoelectric composites can expand the practical applications with low cost and stable mechanical properties.

References

[1] Pooja Rawat, Anil Kumar, Jae Hun Yun, Seokyeong Byeon, Hyungyu Jin, Jong-Soo Rhyee* / Hierarchical phonon scattering from nano to macro scale in Ag-nano/TiO2-micro particle decorated p-type Bismuth Telluride bulk composites using ultrasonication, ACS Applied Materials & Interfaces **15,** 58487-58496 (2023)

[2] Anil Kumar, Saurabh Thoravat, Hong Jong Jin, Junyoung Park, Hyungyu Jin, Pooja Rawat, Jong-Soo Rhyee / Hierarchical nano-/micro-architecture phonon scattering of p-type Bismuth Telluride bulk composites with Ag-TiO2 nano particles synthesized by fluidized bed spray coating method, Journal of Alloys and Compounds **979**, 173503 (2024)

[3] Anil Kumar, Saurabh Thoravat, Hong Jong Jin, Junyoung Park, Hyungyu Jin, Pooja Rawat, Jong-Soo Rhyee / Enhancement of Thermoelectric Properties of p-type Bismuth Telluride bulk composites with Ag-TiO2 nano particles spray coating and Hot deformation process, in press Journal of Materiomics

Characterization of the Anisotropic Nernst Effect in Antiferromagnetic $YbMnSb_2$ and $YbMnBi_2$

Katherine A. Schlaak[1], Shuo Liu[2], Chenguang Fu[2], Sarah J. Watzman[1]

[1]*Department of Mechanical and Materials Engineering, University of Cincinnati, Cincinnati, USA*

[2]*School of Materials Science and Engineering, Zhejiang University, Hangzhou, China*

E-mail: schlaaka@mail.uc.edu

This work characterizes thermomagnetic transport properties of antiferromagnetic topological semimetals $YbMnSb_2$ and $YbMnBi_2$ which have been shown to exhibit highly anisotropic behavior in their single-crystalline form as a result of their exotic magnetic structures [1,2]. For $YbMnSb_2$, emphasis will be placed on the orientation-dependence of the Nernst effect as the temperature gradient, induced electric field, and externally applied magnetic field are aligned along each crystallographic axis. Preliminary results show that the Nernst effect is maximized in $YbMnSb_2$ when the externally applied magnetic field is aligned with the c-axis, which is expected to also be the direction of Mn magnetic moments, but the full orientation-dependent study will reveal the optimized orientation for transverse thermomagnetic transport. This project will be extended to $YbMnBi_2$, where previous work has revealed large anomalous thermomagnetic effects in single-crystalline $YbMnBi_2$ when the applied magnetic field is parallel to the material's Berry curvature [2]. In this work, polycrystalline $YbMnBi_2$ is synthesized for the first time with the motivation of determining whether the anisotropic transport properties are removed in a polycrystalline sample such that enhanced thermomagnetic effects might remain in any given orientation.

References

[1] Y. Pan et al. Adv. Mater. 33, 2003168 (2021).
[2] Y. Pan et al. Nat. Mater 21, 203-209 (2022).

This work is supported by the U.S. Department of Energy under Award No. DE-SC0020154 and the National Science Foundation Graduate Research Fellowship Program under Grant No. 2035701.

Low-temperature thermoelectric properties of p-type $Sb_2Se_xTe_{3-x}$

Shailja Sharma[1], Vicente Pacheco[2], Kornelius Nielsch[1], Nicolas Perez[1]

[1]Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

[2]Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Winterbergstr. 28, 01277 Dresden

Bi_2Te_3 and its-based alloys $(Bi,Sb)_2(Se,Te,S)_3$ have been widely used as commercial thermoelectric materials near-room temperature applications for decades.[1] In this study, a series of $Sb_2Se_xTe_{3-x}$ ($0.3 \leq x \leq 2$) single crystals were synthesized and investigated for their electronic transport and thermoelectric properties. Sb_2Se_3 crystallizes in an orthorhombic (*Pnma*, 62) structure, while Sb_2Te_3 crystallizes in a rhombohedral structure (*R-3m*, 166).[2] It is particularly interesting to tune the physical properties of Sb_2Te_3 by substituting Se, forming $Sb_2Se_xTe_{3-x}$ solid solution. Composition upto $x = 2$ are expected to remain isostructural to Sb_2Te_3 whereas a phase separation was predicted for $2 < x < 2.75$.[3] The temperature and composition-dependent electronic conductivity, thermal conductivity and Seebeck coefficient were measured using thermal transport option of PPMS in the temperature range of 2-380 K. These materials exhibited low thermal conductivity across the measured temperature range, attributed to the heavy atomic masses and layered crystal structure. Additionally, a composition and temperature regime were identified where the Hall coefficient is positive, while the Seebeck coefficient is negative. [4] This sign anomaly is distinct from what has been observed in other ternary systems such as $Bi_2(Te,Se)_3$, $(Bi,Sb)_2Te_3$ studied so date.[5] These p-type materials show promise for thermoelectric applications.

References

[1] I. T. Witting *et al.* Adv. Electron. Mater. **5**, 1800904 (2019).
[2] W. Procarione, C. Wood, Phys. Status Solidi B, **42**, 871-878 (1970).
[3] T. L. Anderson, H. B. Krause, Acta Cryst. B, **30**, 1307-1310 (1974).
[4] S. Sharma *et al.* to be submitted.
[5] B Ramachandran *et al.* J. Phys. D: Appl. Phys. **50** 025302 (2017).

Thermoelectric transport in atomically thin van der Waals cuprate superconductors

***Sanaz Shokri*[1,2], *Michele Ceccardi*[3,4], *Tommaso Confalone*[1,2], *Christian N. Saggau*[1,5,6], *Yejin Lee*[7,1], *Mickey Martini*[8,1], *Ilaria Pallecchi*[4], *Genda D. Gu*[9], *Valerii M. Vinokur*[10], *Kornelius Nielsch*[1,2,11], *Federico Caglieris*[4] *and Nicola Poccia*[1,12]**

1 Institute for Metallic Materials, IFW Dresden, Dresden,Germany, IFW Dresden, Helmholtzstraße 20, Dresden, 01069, Saxony, Germany.

2 Institute of Applied Physics, Technische Universit¨at Dresden, 01062 Dresden, Germany.

3University of Genova, Department of Physics, Via Dodecaneso 33, 16146 Genova, Italy

4 CNR-SPIN Institute, Corso Perrone 24, 16152 Genova, Italy

5 DTU Electro, Department of Electrical and Photonics Engineering, Technical University of Denmark, Lyngby, Denmark

6 Center for Silicon Photonics for Optical Communications (SPOC), Technical University of Denmark, Lyngby, Denmark

7 Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

8 Swabian Instruments GmbH, Stammheimer Str. 41, 70435 Stuttgart, Germany

9 Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, USA

10 Terra Quantum AG, 9400 Rorschach, Switzerland

11 Institute of Materials Science, Technische Universit¨at Dresden, 01062 Dresden, Germany

12 Department of Physics, University of Naples Federico II, Via Cintia, Naples 80126, Italy

**E-mail: s.shokri@ifw-dresden.de*

Type of presentation: Poster

Here we report the effects of finite size on the dissipation mechanisms of the Nernst effect in the optimally doped $Bi_2Sr_2CaCu_2O_{8+x}$ high-temperature superconductor, down to the atomic length limit.

Magnetotransport in $(Bi_xSb_{1-x})_2Te_3$ nanoparticles and the challenges of data analysis

M. Staiger[1,2], S. Izadi[1,2] and G. Schierning[1,2]

[1] Institute for Energy and Materials Processes Applied Quantum Materials, University of Duisburg-Essen, 47057 Duisburg, Germany
[2] Research Center Future Energy Materials and Systems, Research Alliance Ruhr, 44780 Bochum, Germany

This study investigates the influence of doping Bi_2Te_3 with Sb in regard to the protected topological state. It can be shown that the addition of Sb to the system drastically decrease the electron phase coherence length. Additionally, the challenges of data analysis are presented and their influence on the observed physical properties are investigated.

Preparation and characterization of 2D molybdenum dichalcogenides for thermoelectric applications

T. Tavrina[1,2] and S. Linden[1]

[1]Rheinische Friedrich-Wilhelms-Universität, Bonn, Germany
[2] National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine

In the last decade, a novel class of two-dimensional (2D) transition metal dichalcogenides (TMDCs) has attracted large attention due to their unique layered structure, outstanding mechanical, electrical, and optical properties, and device functionalities [1]. The theory predicts significant enhancement of thermoelectric (TE) efficiency in TMDC flakes with less than five layers [2,3], and some experiments have revealed that a MoS_2 bilayer has the highest TE power factor among all TE materials. Nevertheless, the present experimental data exhibits significant variations [4-6], and a systematic experimental investigation of the TE properties of 2D TMDCs is still missing. This work is motivated by finding 2D TMDCs with better TE properties than conventional TE materials, taking into account the possibility of optimizing the TE properties by reducing film thickness. A mechanical exfoliation followed by stacking with a dry transfer technique was used to fabricate high-quality samples based on 2D MoS_2 and $MoSe_2$ with different number of layers. Laser cutting technology has been developed and utilized to electrically separate monolayers from the transferred bulk material. Characterization of the samples in terms of their morphology, microstructure, thickness and number of layers was performed using optical microscopy, reflectance measurements, scanning electron microscopy, and atomic force microscopy. Two-step electron beam lithography, deposition, and lift-off techniques were used to make contact probes, heater, and micro-thermometers. The fabrication of micro-devices will allow us to perform independent measurements of two- or four-probe electrical conductivity in addition to the Seebeck coefficient in dependence on thickness and temperature. This will allow us to recommend suitable MoS_2 and $MoSe_2$ mono- and multilayer for TE applications.

References

[1] D. Li, Y. Gong, Y. Chen, et al., Nano-Micro Lett. **12**, 36 (2020).
[2] W. Huang, X. Luo, C.K. Gan, et al., Phys. Chem. Chem. Phys. **16**, 10866 (2014).
[3] D. Wickramaratne, F. Zahid, and R.K. Lake, J. Chem. Phys. **140**, 124710 (2014).
[4] M. Buscema, M. Barkelid, V. Zwiller, et al., Nano Lett. **13**, 358 (2013).
[5] J. Wu, H. Schmidt, K.K. Amara, et al., Nano Lett. **14**, 2730 (2014).
[6] K. Hippalgaonkar, Y. Wang, Y. Ye, et al., Phys. Rev. B **95**, 115407 (2017).

Engineering Tin Chalcogenides Thermoelectric Materials for Power Generation

Tessera A. Wubieneh[1] and Yang-Yuan Chen[2]

[1]Bahir Dar University, Bahir Dar, Ethiopia
[2] Institute of Physics Academia Sinica, Taipei, Taiwn

Abstract:
In recent times, the single crystal SnSe has garnered significant attention owing to its remarkably high zT value of around 2.6, sparking interest in exploring its polycrystalline counterparts through effective doping. Polycrystalline $(Sn_{1-x}Ge_x)Se$ samples were fabricated via melting and spark plasma sintering (SPS) techniques to enhance the thermoelectric performance and mechanical characteristics of the pristine SnSe material. This research systematically delved into the doping effects of Ge and examined the anisotropic behavior influencing the thermoelectric properties of SPS-sintered $(Sn_{1-x}Ge_x)Se$ samples. The study revealed that Ge doping not only significantly boosted the Seebeck coefficient but also lowered the thermal conductivity of the $(Sn_{1-x}Ge_x)Se$ series. All Ge-doped compounds exhibited reduced thermal conductivity, primarily attributed to phonon scattering from disordered dopant atoms and the strong anharmonic bonding characteristics of SnSe. As a result, a peak zT value of 0.77 was achieved at 800 K for $(Sn_{0.99}Ge_{0.01})Se$, representing an approximate 40% enhancement compared to the pristine polycrystalline SnSe (zT = 0.56). Therefore, $(Sn_{1-x}Ge_x)Se$ emerges as a promising contender for highly efficient thermoelectric materials for power generation.

Enhancing transverse thermoelectric performance using topology optimization combined with laser powder bed fusion

Hyun Yu*, Junyoung Park *, Hyungyu Jin*

* Department of Mechanical Engineering, Pohang University of Science and Technology (POSTECH), Pohang 37673, South Korea.

Transverse thermoelectric (TE) generators have demonstrated potential as thermal energy harvesting devices owing to their superior device architecture. Consequently, enhancing their power generation performance is expected to facilitate innovative energy harvesting. This paper proposes topology optimization (TO) combined with laser powder bed fusion (LPBF) (TO-LPBF) to enhance the TE transverse output power while using single-material TE legs. The optimized shape of the TE leg modifies the temperature distribution, and consequently generates a non-zero temperature difference across the transverse direction. The modified temperature distribution enables the optimized TE shape to exhibit a power density of 3.3 μW/mm^2 and an effective transverse TE coefficient of 23.3 μV/K, which is 1097 and 12.7 times higher than that in case of a non-optimized shape. Furthermore, a compressive test indicates negligible changes in electrical resistance up to a yield strength of 90 MPa, thereby satisfying the mechanical stability requirements for practical applications. Moreover, the applicability of TO-LPBF to various shapes of heat source is demonstrated, accompanied by a significantly enhanced TE transverse output power. TO-LPBF is a new strategy for designing TE legs in transverse TE devices, and can be utilized in practical energy harvesting applications.

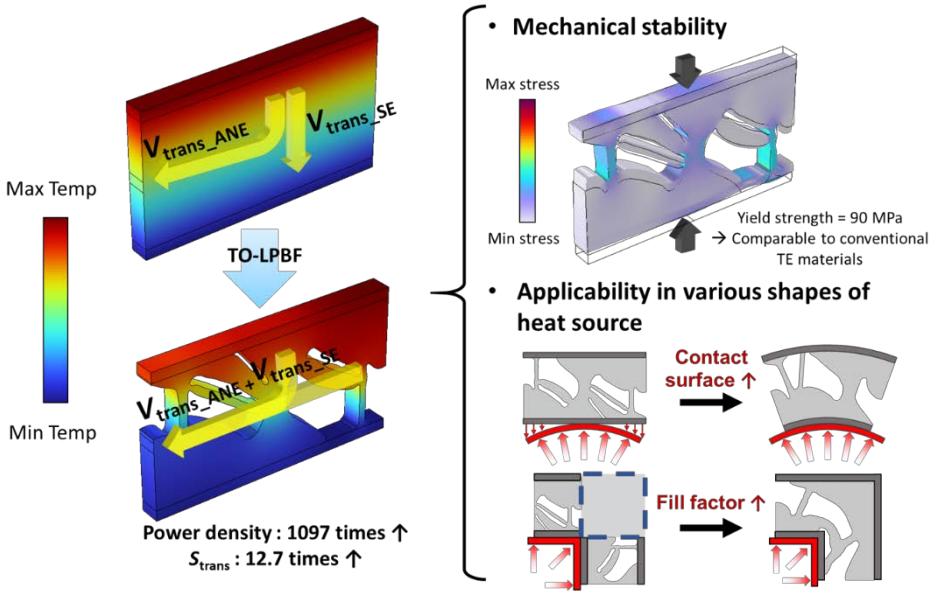


Figure 1 Enhanced TE transverse performance with sufficient mechanical stability and applicability by TO-LPBF

Giant pyroelectric polarization ripples in transverse thermoelectrics

Y. Zhou[1], C-W. Qiu[1], J. He[2] and G. W. Ho[1]

[1]Department of Electrical and Computer Engineering, National University of Singapore, Singapore, Singapore
[2]Department of Physics, Southern University of Science and Technology, Shenzhen, China

Pyroelectricity originates from spontaneous polarization variation, promising in waste heat recovery. Particularly, changing spontaneous polarization via longitudinal heat perturbations has been shown in conventional thermoelectrics. However, these approaches present unequivocal inefficiency due to spatially coupled temperature change intensity and duration along the longitudinal direction. Here we demonstrate unconventional giant pyroelectric polarization ripples in transverse thermoelectrics, without increasing the net thermal input, into electricity with an efficiency of 5-fold of conventional longitudinal counterparts. The inhomogeneous graded temperature variation arises from decoupled heat localization and propagation, leading to anomalous transverse heat perturbation (29-fold) and enhanced thermal disequilibrium effects. This in turn triggers an augmented polarization ripple, fundamentally enabling unprecedented electricity generation performance. Notably, the transverse device generates a power density of 38 mW/m^2 at consistent thermal flux, which is competitive with that of solar thermoelectrics. Our findings provide a viable paradigm, not only for universal practical waste heat recovery but also for flexible manipulation of transverse heat transfer towards sustainable energy harvesting.

References

[1] Y. Zhou, T. Ding, J. Guo, G. Xu, M. Cheng, C. Zhang, X. Wang, W. Lu, W. L. Ong, J. Li, J. He, C-W. Qiu, G. W. Ho, Nature Communications **14**, 426 (2023)
[2] Y. Zhou, T. Ding, G. Xu, S. Yang, C-W. Qiu, J. He, G. W. Ho, Nature Reviews Physics **na**, in press (2024)
[3] Y. Zhou, T. Ding, Y. Cheng, Y. Huang, W. Wang, J. Yang, L. Xie, J. He, G. W. Ho, National Science Review **10**, nwad186, (2023)