Understanding Transport Processes on the Nanoscale for Energy Harvesting Devices

719. WE-Heraeus-Seminar

8 - 9 March 2021
ONLINE

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 719. WE-Heraeus-Seminar:

Energy harvesting devices are required for applications in the Internet-of-Things, autarkic sensors, or highly integrated electronic devices. With ever advancing number of autonomous electronic components the demand for delocalized supply of small amounts of electric energy increases. It is therefore an emerging topic in science and research to design, advance and tailor energy harvesting devices making use of a variety of energy sources and harvesting concepts. A deep understanding of energy transfer and transport processes forms the basis of this development. The relevant lengths scales of many of those energy transfer and transport processes is in the order of only a few nanometers, and today's nanotechnology therefore enabled the improvement of conversion efficiency, power output and reliability of many energy harvesting devices. This seminar will therefore address both, fundamental understanding of energy transfer and transport processes on the nanoscale, as well as different energy harvesting concepts that make use of these energy transfer and transport processes. Topics include fundamental studies, materials design and device design for the optimization of energy harvesting employing the thermoelectric, thermoionic, thermophotovoltaic, piezoelectric, electrochemical and pyroelectric effect.

The seminar is dedicated to a specialized public among which there are around 15 invited speakers, as well as poster presentations. Emphasis is set on giving young investigators at the PhD or PostDoc level the opportunity to participate.

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Program

Program

Monday, 8 March 2021

Thermomagnetic and magnetocaloric harvesting devices

08:55 – 09:00	Gabi Schierning	**Opening Remarks**
09:00 – 09:45	Sebastian Fähler	**Thermomagnetic harvesting of low grade waste heat**
09:45 – 10:30	Luana Caron	**Fundamentals of magnetocaloric materials**
10:30 – 10:40	*Offline- COFFEE BREAK*	
10:40 – 11:00	*Online- Mingling, in virtual meeting room (Networking)*	

Tunneling devices in temperature gradients

11:00 – 11:45	Dietrich Wolf	***Tutorial*: Irreversible Processes in Quantum Mechanics**
11:45 – 11:55	*COFFEE BREAK*	
11:55 – 12:40	Timo Kuschel	**Impact of thermal conductivity in oxide tunnel barrier materials on thermally induced spin currents**
12:40 – 13:25	Mark Baxendale	**Quantum-tunnelling controlled thermoelectricity in polymers**
13:25 – 13:30	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
13:30 – 15:00	*LUNCH BREAK*	
15:00 – 16:00	**Online Poster Session I**	

Fundamentals of transport

16:00 – 16:45	Peter Zahn	**Universal Limits of Thermopower and Figure of Merit from Transport Energy Statistics**
16:45 – 17:30	Johannes de Boor	**The single parabolic band for electronic transport modelling: usage, limitations and applicability to advanced thermoelectric materials with complex band structures**
17:30 – 18:15	Mona Zebarjadi	**Thermal and Electrical Transport in Layered Materials**

Program

Tuesday, 9 March 2021

Onsager's reciprocity relations: application and limits

11:15 – 12:00	Philipp Bredol	**Rectifying Small Currents with Mesoscopic Devices**
12:00 – 13:00	**Online Poster Session II**	
13:00 – 15:30	*LUNCH BREAK*	

Synthesis of thermoelectric materials

15:30 – 16:15	Stephan Schulz	**Thermoelectric Material Synthesis - From Nanoparticles to Epitaxial Thin Films**
16:15 – 17:00	Dave Johnson	**Optimization of Thermoelectric Properties Through the Synthesis of Compounds with Designed Nanoarchitecture**
17:00 – 17:10	*Offline- COFFEE BREAK*	
17:10 – 17:30	*Online- COFFEE BREAK in virtual meeting rooms*	

Thermoelectric materials and devices

17:30 – 18:15	Zhifeng Ren	**Thermoelectric Cooling vs. Power Generation**
18:15 – 19:00	Javier Garcia	**Fabrication and cooling performance characterization of μ-thermoelectric coolers**
19:00 – 19:10	*Offline- (COFFEE) BREAK*	
19:10 – 19:30	*Online- (COFFEE) BREAK in virtual meeting rooms*	
19:30 – 20:15	Lane Martin	**Pyroelectric Energy Conversion – Overview and Demonstration of Novel Thermal-Energy Conversion**
20:15 – 20:20	Gabi Schierning	**Closing Remarks**

End of seminar

Posters

Posters

1	Lamya Abdellaoui	**Thermoelectric Materials: a methodology for defects characterization**
2	Ruben Bueno Villoro	**Effect of grain boundaries on electrical conductivity in Ti(Co,Fe)Sb half Heusler thermoelectrics**
3	Julia Camut	**Overcoming asymmetric contact resistances in Al-contacted Mg2X thermoelectric legs**
4	Fafa Chiker	**Thermoelectric properties of ternary chalcopyrite absorbers $AgInS_2$ and $AgInSe_2$ for solar cell energy conversion**
5	Aditya Savitha Dutt	**Micro-Peltier Coolers towards Applications**
6	Jafar Ghazanfarian	**A Variable-angle Piezo-electric Harvester for Offshore Applications**
7	Leonie Gomell	**Understanding the Microstructure-Property-Relationship in thermoelectric materials – Can we optimize the performance by 3D printing techniques?**
8	Ran He	**Unveiling the phonon scattering mechanisms in half-Heusler thermoelectric compounds**
9	Kazuki Imasato	**Microstructure and Band Engineering for the high performance of n-type Mg_3Sb_2-Mg_3Bi_2 alloys near room temperature**
10	Sepideh Izadi	**Interface-dominated topological transport in nanograin bulk Bi_2Te_3**
11	Rishikesh Kumar	**Numerical Simulation and Fabrication of Unicouple Thermoelectric Generator**

Posters

12	Andreas Kunzmann	**The role of electrons during the martensitic transformation in shape memory alloys**
13	*Cancelled*	
14	*Cancelled*	
15	Léo Millerand	**Optimizing the thermoelectric properties of MgAgSb by adjustment of the Mg content**
16	Mohammad Mostafa Mohammadi	**Harnessing energy from water waves by ore-shaped piezoelectric energy harvesters, and experimental study based on response surface methodology**
17	Harshita Naithani	**Apparatus for Measurement of Thermoelectric Properties of a Single Leg under Large Temperature Gradients**
18	Prasanna Ponnusamy	**On the Peltier-Thomson balance in thermoelectric performance estimation**
19	Heiko Reith	**In-Plane zT-Characterization of Electrodeposited Materials and its Application in Micro Thermoelectric Devices**
20	Lauritz Schnatmann	**Transport properties of $Co_{1-x}Fe_xSi$ from 0% to 20% Fe**
21	Caroline Schwinge	**Seebeck Mapping of Doped Si and SiGe Thin Films**
22	Sergey Sobolev	**Heat conduction across 1D nano films: effective thermal conductivity and extrapolation length**
23	Eugenio Sebastian Suena Galindez	**Electrochemically Exfoliated Graphene Oxide for Thermoelectric Applications**

24	Weidong Tang	**Enhanced stability and thermoelectric performance for thermally evaporated $CsSnI_3$ thin films**
25	Siyuan Zhang	**Dislocation networks impede phonon transport in PbTe thermoelectrics**
26	Tianhui Zhu	**Thermoelectric Transport Measurement of Supported Holey Silicon Thin Films across a Broad Temperature Range**

Abstracts of Lectures

(in alphabetical order)

Quantum-tunnelling controlled thermoelectricity in polymers

M. Qiu and M. Baxendale

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Thermoelectric energy conversion within a homogeneous conductor is governed by the charge carrier mobility and the density of electronic states, intrinsic trades-off limit efficiency. Heterogeneous conduction created by the spatial variation of disorder is considered undesirable because it is conceptually difficult and not easily reproduced. However, could it be the basis for unique, exploitable thermoelectric effects? Here we show that the heterogeneous conduction typically found in conducting polymer films can result in thermoelectricity governed by only quantum mechanical tunnelling of charge carriers through nanoscale Coulomb barriers at order-disorder boundaries. We conclude this to be the basis of a new category of thermoelectric system centred on heterogeneous conductors or conducting networks. We show that thermoelectricity of this origin can be engineered without doping or intrinsic trades-off. Our findings point to a wide range of alternatives to the doped inorganic semiconductor paradigm [1].

References

[1] M. Qiu and M. Baxendale, Organic Electronics **78**, 105553 (2020)

Rectifying Small Currents with Mesoscopic Devices

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Rectifiers that work with small excitations are an important building block for possible energy harvesting devices. For their fabrication, it is desirable to avoid complex layer stacks or doping profiles, to facilitate process integration with the fluctuating energy source to be harvested.

We present numerical and experimental evidence for nonreciprocal electron transport, which is realizable by simply patterning a conducting material. This effect occurs in the transition regime between quantum mechanics and classical physics, where quantum-mechanical effects are still visible, but interactions with the environment cause significant decoherence [1].

In this transition regime, the conductance of asymmetric two-terminal devices usually depends on the direction of the current flow. Exploring the magnetotransport properties of asymmetric Aharonov-Bohm rings, we observe that the Aharonov-Bohm oscillations generally depend on the direction of the current through the rings. This provides direct evidence that the transport across such samples is directional, i.e. the structures act as rectifiers, although the samples consist of one material only.

References

1. P. Bredol, H. Boschker, D. Braak, J. Mannhart, arXiv: 1912.11948 (2019).

Fundamentals of magnetocaloric materials

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The magnetocaloric effect (MCE) presents itself as the change in temperature of a system due to the variation of an externally applied magnetic field. It was first observed by Weiss and Piccard in Ni in 1917 [1], with the first application using paramagnetic salts to achieve extremely low temperatures (the so-called adiabatic demagnetization) being proposed soon after by Debye [2] and Giauque [3].
Although the idea of using phase transitions, where the effect is maximum, for cooling gained some momentum during the 1970's, it was only with the discovery of the giant MCE in $Gd_5(Ge_2Si_2)$ around room temperature in 1997 [4], that the field has seen a true renaissance. Not only have the discovery of many other materials systems followed, but also applications have become feasible. The two main applications of the magnetocaloric effect are refrigeration and power generation.

In this talk I will focus on the fundamental aspects of the magnetocaloric effect and the properties we look for in materials for magnetocaloric refrigeration applications. I will, in particular, take a closer look at the Fe_2P-based family of compounds, which are, to date, one of the most promising for applications.

References

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The single parabolic band for electronic transport modelling: usage, limitations and applicability to advanced thermoelectric materials with complex band structures

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Due to the complex interplay between composition, synthesis parameters and performance of thermoelectric materials the optimization of thermoelectric materials needs to be complemented by modelling. A relatively simple and thus popular approach is the so called single parabolic band model, which allows for an efficient optimization of the material properties and a benchmarking of different materials based on relatively few, well available experimental results. I'll discuss typical usage of the SPB but also limitations of this approach, in particular with respect to materials with complex band structures [1, 2]. These are common for high performance materials and the single parabolic band modelling is also employed to those material systems even though the underlying assumptions are not well fulfilled. The consequences of this will be analyzed[3].

References

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2. Kamila, H., et al., *Analyzing transport properties of p-type Mg2Si–Mg2Sn solid solutions: optimization of thermoelectric performance and insight into the electronic band structure.* Journal of Materials Chemistry A, 2019. **7**(3): p. 1045-1054.
3. de Boor, J., *On the applicability of the single parabolic band model to advanced thermoelectric materials with complex band structures.* Journal of Materiomics, 2020.

Thermomagnetic harvesting of low grade waste heat

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Thermomagnetic materials are a new type of magnetic energy materials, which enable the conversion of low temperature waste heat to electricity by three routes: Thermomagnetic motors, oscillators, and generators. Taking our work on thermomagnetic generators with different magnetic field topologies (TMG) [1] as a starting point, in this talk we also analyse the material requirements for a more energy efficient and affordable conversion.

We present experiments of our TMG using different thermomagnetic materials (La-Fe-Si-Co with different transition temperatures and Gd). We compare the suitability of these materials and from this derive a generalized approach to evaluate the suitability of different thermomagnetic materials, which is different compared to magnetocaloric materials. We show that the thermodynamic efficiency of the best thermomagnetic materials outperforms thermoelectric materials when harvesting low temperature waste heat. Furthermore, the low raw materials cost results in a price per watt more than one order of magnitude lower than today's power plants and thermoelectrics, which makes them also economically competitive. As summary, we present a materials library which allows selecting the best available thermomagnetic materials in two Ashby plots as figures of merit and gives guidelines for future development of this material class [2]. At the end of this talk, approaches towards micro systems for harvesting low temperature waste heat are given.

References

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Fabrication and cooling performance characterization of μ-thermoelectric coolers

J. García[1,3], G. Li[2,3], D. Lara-Ramos[3,4,5], V. Barati[3,4], N. Pérez[3], I. Soldatov[3], H. Reith[3], G. Schierning[3] and K. Nielsch[3,4].

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Electronics, optoelectronics and integrated semiconductor technologies in general suffer of internal energy losses that, in fact, turns out into heat[1]. Such phenomenon can provoke malfunctioning of the systems ranging from an unusual high energy consumption to a severe damage of different components. Optimized thermal management of such devices could improve both, the energy efficiency and performance of a specific device which, among others, is specially critical in photonic integrated circuits[2]. Thermoelectric devices have been used for many years as solid-state coolers (TEC) making used of the well-known Peltier effect. However, due to miniaturization and high compactness of modern technologies, the implementation of such TEC´s around specific components of integrated circuits remains challenging. Thus, it becomes clear the need of an optimized TEC´s fabrication procedure that fulfils all requirements for its successful implementation. In that sense, electrochemical deposition in combination with photolithographic techniques offer the possibility to grow, in a cost-effective manner, a wide range of materials and dimensions, all of this compatible with standard semiconductor technology[3,4]. In this work, a fabrication process of a microstructured TEC based on the electrodeposition of $Bi_2(Te_xSe_{1-x})_3$ (n-type) and pure Te (p-type) thermoelectric materials is presented. Furthermore, cooling performance and reliability of such devices are also discussed, showing rapid response (~1ms), good cycling performance (~10 million cycles) and time stability (>1 month).

References

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Optimization of Thermoelectric Properties Through the Synthesis of Compounds with Designed Nanoarchitecture

David C. Johnson

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Major limitations to discovering new compounds include the lack of synthetic routes to compounds that are metastable, the inability to predict structure of likely unknown compounds, and the challenge of predicting the energy landscape around local free energy minima to assess potential metastability. Solid state synthesis approaches are typically diffusion limited, producing thermodynamic products as a result of high reaction temperatures and long reaction times. Fluid phase synthesis approaches are nucleation limited with high diffusion rates enabling a large part of the energy landscape to be explored. We have developed a third approach, controlled by nucleation but diffusion limited, based on controlling the composition of an amorphous intermediate on a nanoscale. The low diffusion rates limit the extent that the energy landscape is explored, enabling many new compounds to be synthesized with structure close to that of the precursor. Emergent properties (electrical, thermal and magnetic) vary systematically with nanoarchitecture. Our goal is to discover the design rules to predict how emergent properties change with nanoarchitecture and understand why. The optimization of thermoelectric properties thorough nanoarchitecture will be used to illustrate some advantages of our approach.

Impact of thermal conductivity in oxide tunnel barrier materials on thermally induced spin currents

Timo Kuschel

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Spin currents generated from thermal gradients in magnetic tunnel junctions (MTJs) via the tunnel magneto-Seebeck effect (TMS) [1-3] have high potential for future nano-electronic devices [4]. The TMS effect can be enhanced by proper choice of barrier [5] and electrode [6] materials. However, quantitative determination and comparison of the TMS coefficients require accurate knowledge of the temperature drop across the insulating tunnel barrier. The key property here is the thermal conductivity, which determines the temperature drop. However, the thermal conductivity of oxide materials and especially of tunnel barriers is experimentally difficult to access.

In my contribution, I will introduce the TMS within the related research field: spin caloritronics [7]. Furthermore, I will discuss the role of the thermal conductivity in oxide tunnel barriers of an MTJ in a TMS device. Additionally, I will present two experimental approaches to obtain quantitative values for the thermal conductivity in these barrier materials. These are laser-induced TMS in combination with finite-element modeling [8] as well as time-domain thermoreflectance and time-resolved magnetooptic Kerr effect thermometry [9]. Here, we extract values of the thermal conductivity for MgAl2O4 and MgO barrier materials in half-MTJ stacks with Co-Fe-B electrode. The results are in nice agreement with theoretical predictions for ultra-thin oxide barriers [10].

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Pyroelectric Energy Conversion – Overview and Demonstration of Novel Thermal-Energy Conversion

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The need for improved utilization of energy resources is abundantly clear. In the United States, for example, nearly 70% of all energy produced (from all sources, renewable or otherwise) are lost due to inefficiencies in energy transport, device operation, etc. The vast majority of this lost energy is dissipated as heat or thermal losses. Harvesting even a small fraction of this energy would dramatically impact one of the most pressing societal challenges today. In this spirit, a number of direct thermal-to-electric energy conversion technologies have been proposed and explored with thermoelectric energy conversion being the most common and widely studied. One additional (and complementary) approach to thermal-to-electric energy conversion is so-called *pyroelectric energy conversion* (PEC) in which a solid-state heat engine transforms temporally-varying thermal signatures into electrical current. PEC is based on the *pyroelectric effect* which is the variation of remnant polarization P of a material as a function of temperature T at constant electric field E [$(\partial P/\partial T)_E$]. Efficient PEC requires operating the material using thermal-electrical cycles to produce sustained pyroelectric generation of electricity.

Here, I will introduce the concept of PEC and provide a foundation for understanding what it takes to create high-performance pyroelectric materials and PEC devices. We will explore the fundamentals of the field- and temperature-dependent response of ferroelectric materials which are known to exhibit large pyroelectric response. We will examine recent insights into material design algorithms that can allow us to maximize PEC potential via control of both electrical/dielectric and pyroelectric responses that determine the figure of merit for such applications. Additionally, we will explore recent work wherein control of prototypical relaxor $0.68PbMg_{1/3}Nb_{2/3}O_3$-$0.32PbTiO_3$ (PMN-PT) thin films has enabled the realization of large pyroelectric coefficients and suppression of dielectric response under applied fields; in turn, yielding unprecedented figures of merit for PEC and devices exhibiting energy densities, power densities, and efficiencies of 1.06 J cm^{-3}, 526 W cm^{-3}, and 19% of Carnot, respectively. Future prospects will also be explored.

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Thermoelectric Cooling vs. Power Generation

Zhifeng Ren

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Bi_2Te_3-based p-type $Bi_{0.5}Sb_{1.5}Te_3$ and n-type $Bi_2Te_{2.7}Se_3$ have been the only materials used for thermoelectric cooling for more than five decades. Even though the progress on advancing the thermoelectric figure-of-merit (ZT) has been significant especially the materials with peak ZT at high temperatures, materials with high ZT around room temperature are very rare. Up to now, besides Bi_2Te_3-based ones, the only reported is p-type MgAgSb with ZT of ~0.8 at room temperature. There is no report on any n-type material exhibiting high ZT at around room temperature. In this talk, I will present a new n-type material that has a ZT of ~0.7 at room temperature, and the cooling performance coupled with p-type $Bi_{0.5}Sb_{1.5}Te_3$, and also power generation performance coupled with either p-type $Bi_{0.5}Sb_{1.5}Te_3$ or p-type MgAgSb.

Zhifeng Ren, M. D. Anderson Chair Professor of Physics at the University of Houston and Director of the Texas Center for Superconductivity. He received his PhD from the Chinese Academy of Sciences, His research has been on thermoelectrics, BAs for high thermal conductivity, enhanced oil recovery, water splitting for H_2 generation, carbon nanotubes, solar absorbers, flexible transparent conductors, superconductors, etc. He is a fellow of the American Physical Society, the American Association for the Advancement of Science, and the National Academy of Inventors. He won the Edith and Peter O'Donnell Award in Science from The Academy of Medicine, Engineering & Science of Texas (TAMEST), Humboldt Research Award, *etc*. He is also a highly cited researcher in Physics.

Thermoelectric Material Synthesis - From Nanoparticles to Epitaxial Thin Films

S. Salloum, G. Bendt, and S. Schulz

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The development of efficient thermoelectric generators TEG and thermoelectric coolers have attracted considerable attention. Radioisotope thermoelectric generators (RTG) are known since the 1950´s, but their low thermoelectric efficiency as given by the dimensionless figure of merit ZT= ($\alpha^2\sigma/\lambda$)T (α = Seebeck coefficient, σ = specific electrical conductivity, λ = thermal conductivity = sum of electronic λ_{el} and lattice λ_{la} contribution, T = absolute temperature [K]) inhibited their broad technical application. Nanostructuring has been proven to be a promising method for increasing the thermoelectric efficiency (zT) of a given material due to an efficient phonon scattering at boundaries and interfaces, resulting in a decreased thermal conductivity, and a simultaneously increased Seebeck coefficient due to both quantum confinement effects and the modification of the electronic band structure.
We will report on the synthesis of tetradymite-type - Sb_2Te_3, Bi_2Te_3, $(Bi_xSb_{1-x})_2Te_3$ - nanoparticles[1] and thin films[2] by use of different solution-based and gas phase-based processes and discuss the role of the synthesis pathway, material composition and material processing on the resulting thermoelectric properties.

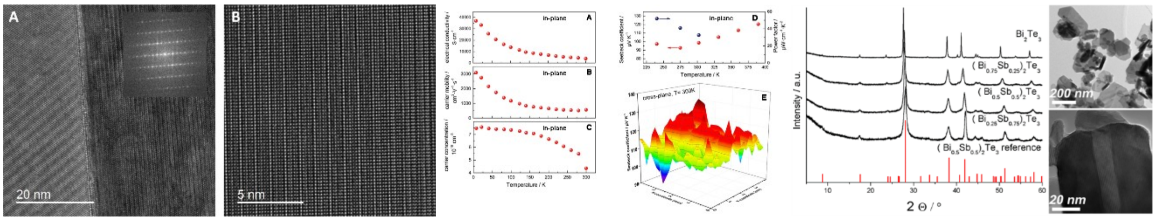

Figure: HRTEM of Sb_2Te_3 thin films (left) and their thermoelectric properties (middle); XRD and REM of Sb_2Te_3, Bi_2Te_3 and $Bi_xSb_{1-x})_2Te_3$ nanoparticles.

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Universal Limits of Thermopower and Figure of Merit from Transport Energy Statistics

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The search for new thermoelectric materials aims at improving their power and efficiency, as expressed by thermopower S and figure of merit ZT.

By considering a very general transport spectral function $w(\varepsilon)$, expressions for S and ZT can be derived, which contain the statistical weights of an effective distribution function only, see Ref. [1]. The assumption of a Lorentzian peak of width k_BT resulting from the phonon bath allows estimating upper limits of S and ZT. These do not depend on the microscopic transport mechanisms. The limit of |S| is **1.88** in units of k_B/e, which is about 160 μV/K, and the limit for ZT is about **1.11**, see the red dots in the figure. Furthermore, the general case of a band gap material will be discussed.

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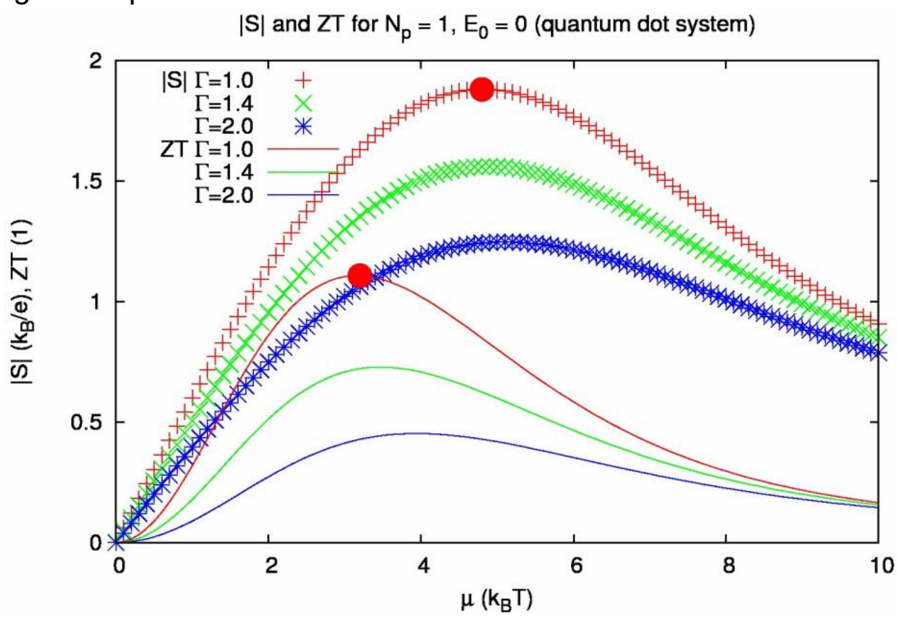

Figure: Thermopower |S| and Figure of merit ZT for a quantum dot system with a Lorentzian transport spectral function of width $\Gamma=n*k_BT$ centered at $E_0=0$, μ is the chemical potential.

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Abstracts of Posters

(in alphabetical order)

Thermoelectric Materials:
a methodology for defects characterization

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Converting thermal energy into electricity through thermoelectric materials can be made more efficient by introducing defects into the lattice reducing the lattice thermal conductivity. Chalcogenide compounds are promising thermoelectric materials with a high efficiency, suitable for thermoelectric power generation in the low-to mid-temperature range (e.g. 600-800 K). The conversion efficiency is indicated by the dimensionless figure of merit, zT. Attempts to optimize zT require reducing the thermal conductivity κ, while maintaining relatively high values of the electrical conductivity σ and the Seebeck coefficient S.

The lattice thermal conductivity can be reduced by crystallographic defects such as planar faults and dislocations. In this work, we investigated various microstructural features in the as-quenched δ-phase of $Ag_{16.7}Sb_{30}Te_{53.3}$ [1-3]. We applied a scale bridging methodology from the millimeter scale down to the atomic scale. We used electron contrast channeling imaging (ECCI) in a scanning electron microscope, high angle annular dark field (HAADF) imaging in an aberration corrected scanning transmission electron microscope and atom probe tomography [1-3] to study the planar faults density and distribution together with their atomic arrangement and chemical composition. The material showed a distinct mosaic microstructure with abundant low angle grain boundaries, where planar fault networks are accumulated [1]. We found a high density of 1.6×10^{8} m^{-1} at grain boundaries. In addition, we observed a change in stoichiometry within the planar faults compared to their adjacent bulk regions, similarly a dislocation network on PbTe based TE is studied using the same methodology [3] is discussed.

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Effect of grain boundaries on electrical conductivity in Ti(Co,Fe)Sb half Heusler thermoelectrics

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Thermoelectric materials have excellent potential for energy harvesting by converting heat gradients into electricity. Half Heusler are ternary intermetallic phases with broad design spaces to search for cheap and non-toxic combinations. For thermoelectric applications, they offer flexibility in n- and p-type doping to optimize transport properties and hence thermoelectric performance.

Ti(Co,Fe)Sb half Heusler samples with different grain sizes were synthesized and investigated. The transport properties were found to be very sensitive to the grain size. Therefore, the structural and chemical characteristics of grain boundaries were studied down to the atomic resolution using scanning electron microscopy, transmission electron microscopy and atom probe tomography. Grain boundary segregation was observed at different grain sizes.

Moreover, special experimental setups were developed to study the effects of grain boundaries on the local electrical conductivity and to stablish a correlation between bulk and local properties.

Overcoming asymmetric contact resistances in Al-contacted Mg2X thermoelectric legs

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Magnesium silicide-stannide Mg2(Si,Sn) are high performance thermoelectric (TE) materials with the advantage of being composed of light, cheap and abundant elements. Therefore, they are especially attractive for the conversion of remnant heat into electricity in fields like the automotive or aerospace industry. It has recently been shown that aluminum is a compatible and very promising electrode for this material system [1], making one more step towards the development of high performance Mg2(Si,Sn)-based thermoelectric generators (TEG). However, the contacting of the Al electrode to the TE material is found to be challenging, as samples can sometimes show highly asymmetric electrical contact resistivities on both sides of a leg (eg. 10 μΩcm² and 200 μΩcm²). The origins of this behavior are investigated and it is shown that the stable oxide layer on the Al foil as well as the dicing of the pellets into legs are the two main factors at play. In order to avoid any oxidation of the foil, a thin layer of Zn is sputtered after etching the Al surface; this method proves itself quite effective in keeping the contact resistivies of both interfaces equally low (<10 μΩcm²), with little impact on the TE properties of the leg. The efficiency measurements of a TEG built using this method are displayed.

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Thermoelectric properties of ternary chalcopyrite absorbers $AgInS_2$ and $AgInSe_2$ for solar cell energy conversion

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The thermoelectric and electronic properties of ternary chalcopyrite absorbers $AgInS_2$ and $AgInSe_2$ have been investigated by theoretical calculations, using the first principles density functional calculations implemented in the full potential linear augmented plane wave (FP-LAPW) method. The important application of the chalcopyrite-type compounds includes the energy conversion and serve as thermoelectric and photovoltaic energy converters. Our calculated band structure both without and including spin orbit coupling of these compounds using the Tran-Blaha modified Becke-Johnson potential (TB-mBJ), shows the direct band gap semiconductors around 1.63eV and 1.14eV for both $AgInS_2$ and $AgInSe_2$ respectively) in good agreement with the available experiment data. Further they show more dispersive bands at the valence band maximum which indicates that these compounds may be a promising material for generating thermoelectricity. In order to study the thermoelectric properties of these two ternary chalcopyrite semiconductors, transport properties are calculated within Boltzmann transport theory, based on the electronic structure using Boltztrap code implemented in the WIEN2k code. All calculated thermoelectric properties like thermopower, electrical conductivity scaled by relaxation time are calculated as a function of carrier concentrations at different temperatures, and show reasonable characteristics for a desirable thermoelectric material like Seebeck Coefficient > 100 μV/K, thermal conductivity ~ 10 W/m.K.s, and High Temperature Capability. Finally the efficiency of thermoelectricity generated by this method is specified by a large value of the figure of merit (ZT) for both studied compounds.

Compound	**Seebeck Coefficient** S (μV/K)		**Electrical Conductivity** σ/τ $10^{20}(\Omega ms)^{-1}$		**Thermal Conductivity** k^0 10^{15} (W/mKs)	
	p-type	n-type	p-type	n-type	p-type	n-type
$AgInS_2$	172.171	-3547.516	2.313	8.717	3.675	6.549
$AgInSe_2$	169.831	-2762.035	2.842	0.105	4.497	7.820

Table 1: The calculated thermoelectric parameters of *p* and *n* type $AgInS_2$ and $AgInSe_2$ compounds at 300K.

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Micro Thermoelectric Coolers towards Applications

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Summary

Thermoelectric devices can be used for cooling, power generation or in sensor applications. Here, we fabricate µTEDs using optimized geometry and improved thermoelectric material deposition combined with a novel packaging technique that is fully compatible with on-chip integration.

Therefore, we developed a process flow for the fabrication of micro thermoelectric coolers (µTECs) with vertically free-standing leg pairs without top plate. For the stability of the device, it is crucial to embed our µTECs with a filling material that builds a flat surface at the top level. Photoresist is a good choice as filling material because of its low thermal conductivity. The µTECs with and without photoresist were characterized by thermoreflectance thermal imaging technique to study the cooling efficiency of devices and the influence of the photoresist matrix on the performance.

A Variable-angle Piezo-electric Harvester for Offshore Applications

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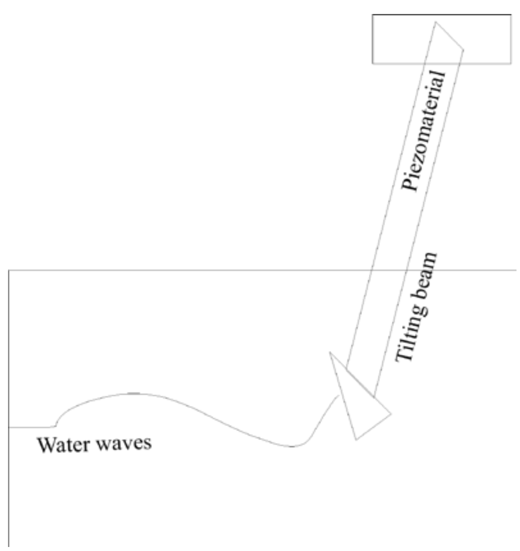
Abstract

The most challenging part of design of piezo-harvesters is the low efficiency of the process of energy extraction [1]. In order to increase the efficiency of waste energy conversion into the electrical energy, a novel structure of a piezo-harvesting device has been proposed. The new structure can increase the output voltage of the harvesting device based on strengthening the interaction of the water waves with the beam. The tip geometry of the beam will be extended to increases the momentum exchange between the free-surface water waves and the piezo-beam. Different geometrical shapes will be tested using an experimental setup with respect to the added mass concept and the angle of impact of the waves with the beam.



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Understanding the Microstructure-Property-Relationship in thermoelectric materials – Can we optimize the performance by 3D printing techniques?

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The microstructure influences the thermoelectric properties because it affects phonon and electron scattering processes in the material. While this is common knowledge to some, the specific relationship between the microstructure and the properties is mainly unknown, which hinders performance optimization by microstructure design.
Here, we use a correlative method to investigate the microstructure and local properties of Heusler-phase Fe_2VAl [1]. The microstructure is analyzed on different length scales using scanning electron microscopy and atom probe tomography. On the same sample, we measure the electrical resistivity using a local *in-situ* 4-point technique.
We use laser surface remelting to manipulate the microstructure of bulk Fe_2VAl. Laser surface remelting belongs to the arsenal of additive manufacturing techniques. It ensures a high solidification rate, making it ideal for generating complex microstructures on the micrometer scale.
We observe elongated grains, separated by low-angle grain boundaries. These grains grow (nearly) epitaxially from the surrounding material. Within the grains, a high density of dislocations is found. Using atom probe tomography, segregation of nitrogen and carbon towards these defects is revealed. The grain boundaries lead to an increase of the electrical resistivity. However, the relative increase is lower at low-angle grain boundaries within the remelted area compared to high-angle grain boundaries of the cast sample
Our results suggest that grain boundary or defect engineering can be used to optimize thermoelectric properties, and that laser-melting approaches can be used to manipulate the microstructure on a fine scale.

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Anomalous reduction of lattice thermal conductivty in half-Heusler ZrCoSb

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The reduction of lattice thermal conductivity (κL) can be realized by introducing large mass contrast through atomic substitution within pristine compounds. Such process are usually termed as “point-defect scattering” and has been proved effective to improve the thermoelectric figure-of-merit (zT). Recently we synthesized two sets of half-Heusler compounds: ZrCoSb1-xSnx and Zr1-yTiyCoSb, and compared their lattice thermal conductivity with respect to the substitution level. Contrary to the general concept that larger mass difference are more effective in phonon scattering, we find a much lower κL in compounds with Sn substitution as the Sb site than the ones with Ti substitution at the Zr site. The origin of phonon scattering in the Sn-containing compounds will be discussed in great detail through transport property measurement and structure characterization. Our work propose a novel strategy for increasing phonon scattering without large mass contrast so that a high carrier mobility might be preserved.

Microstructure and Band Engineering for the high performance of n-type Mg3Sb2-Mg3Bi2 alloys

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We demonstrate that the Mg_3Sb_2-Mg_3Bi_2 alloy can overcome the performance of commercial Bi2Te3 around room temperature, which will be a significant progress for the energy harvesting applications of thermoelectric materials. The main mechanisms of this improvement are optimization of the band structure and microstructure. Our annealing and grain size study shows, the reduction of low temperature electrical resistance leads to a multi-fold improvement in the thermoelectric performance zT at room temperature. By investigating the effect of Bi content on the effective mass and grain size, the optimized composition of the alloy, achieves *zT* of 1.0-1.2 at 350 K -500 K. The understanding of these mechanisms are crucial to the cooling and wasted heat recovery applications of Mg_3Sb_2-Mg_3Bi_2 alloy. Considering the limited number of state-of-art n-type thermoelectric materials for the low-grade heat recovery and cooling technology, the further development of Mg_3Sb_2-Mg_3Bi_2 alloys is a significant step towards the commercial application of thermoelectric materials.

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Interface-dominated topological transport in nanograin bulk Bi2Te3

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Three-dimensional (3D) topological insulators (TI) host surface carriers with extremely high mobility. However, their transport properties are typically dominated by bulk carriers that outnumber the surface carriers by orders of magnitude[1]. We herein present a new concept to overcome the problem of bulk carrier domination by using highly pure 3D TI nanoparticles, which were compacted by hot-pressing to macroscopic nanograined bulk samples. Bi_2Te_3 nanoparticles that are well known for their excellent thermoelectric[2] and 3D TI properties[3] serve as our model system. As key enabler for this approach, we applied a specific synthesis that creates nanoparticles with a low level of impurities and surface contamination[4]. The compacted nanograined bulk contains a high number of interfaces and grain boundaries. Here we show that these samples exhibit metallic-like electrical transport properties and a distinct weak antilocalization. THz time-domain spectroscopy revealed a dominance of the surface transport at low frequencies with a major contribution to the direct current (DC) transport with a mobility of above $10^3\,\mathrm{cm^2V^{-1}s^{-1}}$ even at room temperature. These findings clearly demonstrate that nanograined bulk Bi_2Te_3 features surface carrier properties that are of Jeongimportance for technical applications, e.g. thermoelectricity.

The role of electrons during the martensitic transformation in shape memory alloys

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Shape memory alloys (SMAs) are used for multiple applications like actors, valves, bio-medical applications. Amongst the variety of materials, nickel-titanium (Ni_xTi_{100-x}) based alloys are industrially most important and a model system because of the simple crystallographic structure, textbook-like microstructure and the well-accessible temperature range. However, while the martensitic phase transformation is structurally well-studied, the role of electrons in this transformation is not concludingly understood. Here we show how alloy composition and microstructure affect the contribution of the electronic entropy during the martensitic transformation. We find that the electrons form a charge density wave (CDW) phase in the martensite. Martensitic start temperature and misfit factor directly scale with the increase of electronic entropy change. Therefore, we suggest that the CDW phase uses the real structure distortion of the martensite that is introduced by microstructural elements, specifically misfit dislocations. Because of the requested relation between the wave vector of the lattice distortion and Fermi wave vector for the CDW to form, this corresponds to a specific condition of arrangement for these microstructural elements, closely related to the macroscopic shape memory. Our study suggests a general mechanism that a free electron gas in a real-structure metal can reduce its entropy by condensing at specific lattice defects.

Optimizing the thermoelectric properties of MgAgSb by adjustment of the Mg content

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Thermoelectric materials have the capacity of directly converting thermal energy into electricity and vice versa. The MgAgSb-ternary system has been identified as good *p-type thermoelectric material* from room temperature up to 500K and has been considered as a potential material for TEGs in future lunar habitat. More precisely, α-MgAgSb structure has been proven by *Kirkham and al.* to be the most promising crystal structure for building thermoelectric generator [1]. The efficiency of heat-to-electricity conversion based on thermoelectric effect is directly calculated by the figure of merit $\mathrm{zT} = \frac{S*\sigma^2}{\kappa} * T$, where S, σ, κ and T are the Seebeck coefficient, the electrical conductivity, the thermal conductivity and the absolute temperature.
However, MgAgSb synthesis is tricky because of its narrow window in the ternary diagram. Furthermore, the commonly observed secondary phases have a direct negative impact on thermoelectric properties and are quite stable and persistent.
This project has aimed to reproduce literature results by using the previously identified “optimized stoichiometry $MgAg_{0.97}Sb_{0.995}$. Furthermore, based on the observed impurities, we have tried to adjust the nominal stoichiometry, in particular by varying the magnesium content.

The 2-step synthesis is composed of a first consolidation of MgAg precursor by 8 hours of high energy ball milling followed by a hot pressing at 673K for 8 minutes. A second- high energy ball milling of MgAg+Sb initiates a partial formation of MgAgSb. This is followed by a sintering at 573K to form a pellet and finish the reaction. The process permitted to reach a zTmax = 1 at 563K using the literature stoichiometry, however we also found repeatedly Mg3Sb2+Allargentum as impurity phases. Adjustment of the nominal stoichiometry to Mg0.98Ag0.97Sb0.995 resulted in zTmax = 1.1 at 563K and reduced impurities.

A certain reproducibility of results has been proven by making different batches. The reasons for differences between our optimum stoichiometry and the literature results lie in the synthesis routine and will be discussed as well as the influence of further compositional adjustments.

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Harnessing energy from water waves by ore-shaped piezoelectric energy harvesters, and experimental study based on response surface methodology

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Abstract. An ore shape cantilever based piezoelectric energy harvester is developed for harnessing energy from water waves. Experiments have been conducted to investigate the effect of different design parameters on the output electric power. Such parameters include the longitudinal distance of the cantilever beam from the wave-maker (L), the angle of spatial orientation (ɵ), and the depth of the beam below the free-surface (h). These experimental inputs are represented in Fig 1.

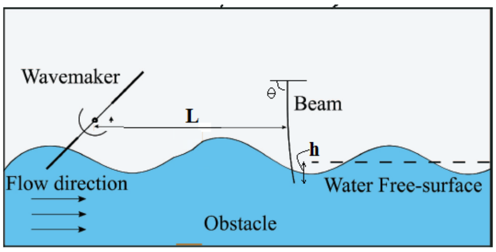

Fig.1. input parameters of the experimental study

The experiments are designed via central composite design (CCD) method in response surface methodology (RSM). Table. 1 represents the design layout of the experiments.

Test number	L (cm)	ɵ (degree)	h(cm)	Test number	L (cm)	ɵ (degree)	h(cm)
1	40	20	1.5	11	60	40	0
2	80	20	1.5	12	60	40	6
3	40	20	4.5	13	60	0	3
4	80	20	4.5	14	60	80	3
5	40	60	1.5	15	60	40	3
6	80	60	3	16	60	40	3
7	40	60	4.5	17	60	40	3
8	80	60	4.5	18	60	40	3
9	20	40	3	19	60	40	3
10	100	40	3	20	60	40	3

An empirical model is extracted by RSM for relating the output power of the harvester with the input variables. Analysis of variance (ANOVA) is conducted for evaluating the adequacy of empirical model. Using this empirical model the effect of individual design input variables and also their interactions on the output RMS voltage of the harvester are evaluated. Finally, the input variables are optimized for maximizing the performance of the harvester.

Apparatus for Measurement of Thermoelectric Properties of a Single Leg under Large Temperature Gradients

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Thermoelectric (TE) devices are synthesized after optimization of the properties of their constituent legs. While, TE devices generally operate under large temperature differences, material properties which are used for their optimization, namely, Seebeck coefficient, thermal conductivity and electrical conductivity, are measured under low temperature differences or at a single temperature. These properties are then averaged over the desired temperature range using a suitable averaging method. Due to problems associated with forming proper contact with the electrodes, experimental measurements of material properties over large temperature differences are practically difficult and very few such works are available in literature. In this work, a setup has been designed and assembled to measure the TE properties – Seebeck coefficient, electrical conductivity, thermal conductivity, and power and efficiency of a single leg over a large temperature difference. The sample holder – a unique feature of this design, lowers the contact resistance between the sample and the electrodes. Testing has been done on a metallized $Mg_2Si_{0.3}Sn_{0.7}$ leg synthesized in the laboratory. Transient measurements were carried out for the temperature difference ranging from 50 K to 300 K with the hot side reaching a maximum of 673 K. To simulate practical operating conditions, steady state measurements were also carried out. Separate standard low temperature gradient measurement of material properties was done on a pellet. Data obtained from these measurements were used to calculate theoretical values using temperature averaging, corresponding to the temperature difference across the metallized leg during the transient experiments in the designed setup. Comparison of the theoretical and experimental values indicates that the designed setup is reliable for measuring various thermoelectric generator properties of single TE legs when subjected to temperature differences between 50 K and 300 K.

On the Peltier-Thomson balance in thermoelectric performance estimation

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Theoretically, the efficiency of a thermoelectric generator (TEG) which converts heat into electricity can be easily but roughly estimated using a Constant Properties Model (CPM) suggested by Ioffe. However, material properties in general are temperature dependent and the CPM can yield meaningful estimates only if physically appropriate averages, i.e. spatial averages for thermal conductivity (κ) and electrical resistivity (ρ) and the temperature average for the Seebeck coefficient (α) [1] are used. Nevertheless, even with appropriate averages we find remaining errors which need to be systematically analysed and corrected to reach a rather high precision of efficiency estimate. This remaining deviation is primarily due to the asymmetry in the heat distribution which is not accounted for in CPM. In this regard, to understand the importance of temperature dependence of each property, a study using model materials, i.e. keeping one of the three thermoelectric properties constant and comparing the performance between the general temperature dependent case and the model cases was done. It revealed that the temperature dependence of Seebeck coefficient and that of thermal conductivity are significant for an exact TEG performance estimation, while the temperature dependence of electrical resistivity has only a minor influence in typical highly efficient thermoelectric materials. By studying a linearly increasing α(T) model case, we can see that even though the global Peltier –Thomson heat balance is satisfied between the CPM and fully temperature dependent cases, there is some uncompensated Thomson heat at the hot-side which systematically leads to a deviation in estimation of the heat input in the CPM case. This further leads to a shift in the estimation of the optimum current, thereby leading to an error in power estimation at maximum efficiency in CPM. This deviation can be corrected mainly by calculating the uncompensated heat at the hot side using the temperature dependent α(T) curve of the material. This physically appropriate correction, not only reduces the error with CPM considerably but provides deeper insights into understanding the TEG performance [2].

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In-Plane zT-Characterization of Electrodeposited Materials and its Application in Micro Thermoelectric Devices

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Micro thermoelectric (TE) harvesting or Peltier cooling devices will be prospectively used in a broad range of applications from industry to consumer products. Successful optimization of the thermoelectric figure of merit, zT, is a key enabler for the introduction of these devices to application. Especially, the TE characterization of films grown by electrochemical deposition, which is a common technique for the fabrication of micro TE devices, remains a great challenge. Therefore, we present a platform for the full in-plane zT characterization of electrochemically deposited TE materials, eliminating the electrical shortcut through the conducting seed layer. The transport characterization could be realized using a suspended TE material within a transport device prepared by a combination of photolithography and etching processes. This full in-plane zT characterization provides an inevitable milestone for a materials optimization under realistic conditions in micro TE devices. The TE characterization of electrochemically deposited materials and its application in micro TE devices will be presented.

Effects in the electrical transport of $Co_{1-x}Fe_xSi$ from 0% to 20% Fe

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In condensed quantum matter materials with topological electronic state rose as one of the most exciting discoveries in the past years. Transition metal silicides, crystallizing in B20 cubic structure, are hosting topologically states with non-zero chiral charge, linear dispersion bands with nodal points named Weyl states, in the bulk. Therefore, these silicides belong to material class of topological materials. The electronic structure of Cobalt Monosilicide contains Weyl states close to the Fermi energy with a chiral charge up to ± 4. Thus, the Weyl states can give high contribution to the electrical transport phenomena, which makes cobalt silicide highly attractive to study the correlation between the topological states and the electrical transport.
Here we studied the electrical transport in different magnetic field orientations and analyzed the transport using a semi classical fitting model in different compositions from 0% to 20% Fe. Hereby, we were able to separate different transport contributions related to the chiral anomaly, the weak anti localization and an additional feature which can be related to the potential formation of a charge density wave. These transport contributions were related and analyzed in respect to the Fe composition in the sample, leading to a “phase diagram” showing the different effects in the $Co_{1-x}Fe_xSi$ compositions.

719. WE-Heraeus-Seminar
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Abstract

Title: Seebeck Mapping of Doped Si and SiGe Thin Films

The incessant downscaling of computer chips and the expansion of the Internet of Things (IoT) market require more and more energy-efficient devices. Temperature sensing and manipulation as well as harvesting could be useful for a reliable device performance. For thermoelectric applications, CMOS-compatible thin films are needed and have to be characterized.

In this contribution we present a fully automated thermovoltage and sheet resistance measurement setup for CMOS-compatibly produced thin films. A LabVIEW-programmed software controls automatically measurement and recording of the thermo-voltages at individually defined temperature set points. So it is possible to measure at different temperature differences between the hot and cold side or average temperatures. With the inversion method we calculate the Seebeck coefficient to eliminate the offset voltage influence [1]. For the sample preparation we use low pressure chemical vapor deposition (LPCVD) with in-situ doping and subsequent rapid thermal anneal (RTA) on 300mm wafers [2]. Different silicon-based samples like doped poly and amorphous silicon or SiGe were deposited. All samples are fabricated in a state-of-the-art 300mm batch furnace with the possibility of simultaneous processing of more than 100 wafers. The SiGe-based samples vary in the ratio of Si and Ge as well as the layer thicknesses and doping concentrations. For selected samples we present a Seebeck coefficient map depending on the temperature difference and average temperature.

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Heat conduction across 1D nano films: effective thermal conductivity and extrapolation length

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Abstract. We analyze the short scale effects on the 1D steady-state heat conduction across a nano film using discrete variable model (DVM). The DVM takes into account the ballistic component of energy transport and the minimum size of the heated region over which a local temperature can be assigned. This implies that the DVM can be used to study far from local equilibrium processes when the characteristic space and time scales of interest are of the order of or even smaller than the mean free path and mean free time of energy carriers, respectively. This is particularly important for the performance evaluation of modern thermal nano systems and microdevices, which usually operate on an extremely short space scale. Local thermal conductivity, overall effective thermal conductivity, thermal conductance and thermal extrapolation length, which are obtained analytically, describe the transition from the diffusive to ballistic heat transport with decreasing film thickness. Thermal extrapolation length and local (position-dependant) thermal conductivity are introduced to virtually eliminate the temperature jump at the boundaries with thermal baths. We also analyze the effects of the film thickness on the bulk effective thermal conductivities and effective boundary conductance to describe the transition from diffusive to ballistic heat transfer with decreasing film thickness. The results are given in a relatively simple analytical form and can be easily implemented for practical experimental conditions or used as an effective tool for rapid calculations to make more elaborated approaches less computationally expensive.

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Electrochemically Exfoliated Graphene Oxide for Thermoelectric Applications

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In this study, thermoelectric properties of electrochemically exfoliated graphene oxide (EGO) were measured. The synthesis process for EGO samples consisted on the sequential process of electrochemical intercalation of perchlorate anions and acetonitrile in (HOPG) graphite, the expansion of the graphite using microwaves to evaporate the trapped acetonitrile, followed by electrochemical exfoliation in DMF and deposition on Nylon membrane to obtain a free standing film. These films were later electrochemically reduced yielding rEGO. The thermoelectric properties were measured for EGO films with thickness of $14 \pm 1\mu m$, prior and post electrochemical reduction treatment. The electrical conductivity was measured using a four point probe and measured at room temperature to be $10 \pm 1\ \mathrm{Scm^{-1}}$ and $225 \pm 10\ \mathrm{Scm^{-1}}$, for the EGO and rEGO respectively. The Seebeck coefficient was measured between $80\mathrm{K} - 400\mathrm{K}$ allowing us to identify the mode of transport, whilst measurements at room temperature resulted in Seebeck coefficients of $32 \pm 2\mathrm{\mu VK^{-1}}$, for both films. Therefore, power factors at room temperature were calculated as $1 \pm 0.1\ \mathrm{\mu Wm^{-1}K^{-2}}$ and $22 \pm 3\ \mathrm{\mu Wm^{-1}K^{-2}}$, for the EGO and rEGO respectively. The power factor was seemed to increase after reduction due to the increase of electrical conductivity while maintaining an adequate Seebeck coefficient. A further study showed a further increase the power factor to $48 \pm 10\mathrm{\mu Wm^{-1}K^{-2}}$ due to a subtle change in morphology, caused by using a different pore size filter.

Enhanced stability and thermoelectric performance for thermally evaporated $CsSnI_3$ thin films

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Tin-based metal halide perovskites have been considered as promising candidates in the field of thermoelectrics due to their ultralow thermal conductivity[1] and considerable electronic conductivity[2]. Its large electrical conductivity is attributed to oxidation of Sn^{2+} to Sn^{4+}. This highly accessible self-doping mechanism raises questions about stability for thermoelectric applications. Here, we report increased stability of sequential thermally evaporated $CsSnI_3$ thin films without any additives. We show that films are quite stable at low temperatures, but that higher temperatures contribute to the oxidation of Sn^{2+} to Sn^{4+}, with an impact on thermal and electrical transport properties. We obtain a figure-of-merit (ZT) of 0.12 for $CsSnI_3$ thin films with much improved stability over previous reports. This work provides more insight into the impact of self-doping on thermoelectric properties and improves the stability of $CsSnI_3$.

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Dislocation networks impede phonon transport in PbTe thermoelectrics

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Dislocations play an important role in thermal transport by scattering phonons. Nevertheless, for materials with intrinsically low thermal conductivity, such as thermoelectrics, classical models require exceedingly high numbers of dislocations (>10^{12} cm^{-2}) to further impede thermal transport [1]. In this presentation [2], significant reduction in thermal conductivity of $Na_{0.025}Eu_{0.03}Pb_{0.945}Te$ is demonstrated at a moderate dislocation density of 1×10^{10} cm^{-2}. Further characteristics of dislocations, including their arrangement, orientation, and local chemistry were shown to be crucial to their phonon-scattering effect and characterized by correlative microscopy techniques. Electron channeling contrast imaging (ECCI) reveals a uniform distribution of dislocations within individual grains, with parallel lines along four <111> directions. Transmission electron microscopy (TEM) shows the parallel networks are edge-type and share the same Burgers vectors within each group. Atom probe tomography (APT) reveals the enrichment of dopant Na at dislocation cores, forming Cottrell atmospheres. The dislocation network was demonstrated to be stable during *in situ* heating in the TEM. By the Callaway transport model, it is demonstrated that both parallel arrangement of dislocations and Cottrell atmospheres make dislocations more efficient in phonon scattering. These two mechanisms provide new avenues to lower the thermal conductivity in materials for thermal-insulating applications.

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Thermoelectric Transport Measurement of Supported Holey Silicon Thin Films across a Broad Temperature Range

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Silicon thin films are compatible with the semiconductor industry and possess a relatively large thermoelectric power factor, indicating their potential as good thermoelectric devices. However, the high thermal conductivity of silicon yields a low thermoelectric figure of merit, *ZT*, which is not desirable for thermoelectric applications. By patterning the silicon thin films with periodic nano-sized holes spaced closer than the phonon mean free path, their thermal conductivity can be greatly suppressed while their electronic properties are roughly maintained. Here, we present a hybrid approach based on thermoreflectance imaging technique and heat spreader method for the in-plane thermal conductivity measurement of the supported holey silicon thin films, which we refer to as heat diffusion imaging method. The thermal conductivity is extracted from the temperature distribution profile measured on the film on the substrate. The measurements do not require film suspension or multiple thermometer deposition. By coupling the thermoreflectance imaging system with a cryostat, we were able to conduct measurements from 40K to 400K. A silicon thin film sample without the holes was measured as a validation for our method. Finally, thermoelectric properties of the holey silicon films understudying were measured, and a *ZT* of 0.09 at room temperature and an estimated *ZT* of 0.29 at 650K are reported.