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18th European Conference on Thermoelectrics

ABSTRACT BOOK

POSTER SESSION 1

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CNM Centro Nacional de Microelectrónica IMB – CSIC

IREC 10 years – Shaping Energy for a Sustainable Future

ECT'22

Emerging topics

ID: 04990
Type: Poster
Topic: Emerging topics

The ExB Thermoelectric Effect

George Levy[1]

1) Entropic Power

The ExB drift can operate as an efficient thermoelectric effect. In a medium with infinite mobility, when two fields, electric and magnetic are perpendicular, particles drift along cycloid paths perpendicularly to both fields. The drift is only a function of the fields. In contrast with the Seebeck and Nersnt effects, particles drift because of a field configuration, not heat flow drag. With infinite mobility, any return path has the same properties as a forward path and no energy can be extracted because the fields are conservative. However, with finite mobility, the drift becomes a function of dissipative properties such as mobility and concentration. Changing these can turn the drift on and off without changing the conductivity of the material. Therefore, a return path with transport properties different from a forward path, can overcome the limitation of the conservative fields, thereby converting heat in the semiconductor to electrical energy. This effect relies on microscopic asymmetry in the cycloidal thermal motion of carriers, which biases their velocity distribution in the direction of the drift. Unlike other thermoelectric effects which are time-symmetric and rely on unbiased distributions, the ExB effect is CPT symmetric, and not bound by limitations of the H-Theorem.

ID: 05018
Type: Poster
Topic: Emerging topics

Doping by design: Enhanced thermoelectric performance of GeSe-based alloys through metavalent bonding

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For thermoelectrics doping is usually the first step to tailor the charge carrier concentration and concomitant properties. Doping should also turn GeSe, which features intrinsically a low concentration, into a competitive thermoelectric. Yet, elemental doping fails to adjust the charge carrier concentration. Doping with $AgSbSe_2$, on the contrary, works and causes a remarkable enhancement of thermoelectric performance. This improvement is closely related to a change of bonding mechanism, as evidenced by sudden alterations of the optical dielectric constant e?, the Born effective charge Z* and the bond breaking mechanism. These property changes signal the formation of metavalent bonds. These bonds lead to an octahedral-like atomic arrangement and a favorable band structure featuring small effective masses. A quantum-mechanical map distinguishes the different types of chemical bonding. It reveals that orthorhombic GeSe is located in a map region where covalent bonding prevails, while cubic and rhombohedral GeSe are located in the region characterized by metavalent bonding. These assignments are in line with the measured properties and thermoelectric performance of the different phases. Our work thus redefines doping rules and provides a ‘treasure map’ to tailor thermoelectric properties of chalcogenides and related p-bonded materials.

ID: 05117
Type: Poster
Topic: Emerging topics

A solid electrolyte able to significantly enhance the power factor of a thermoelectric oxide film

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1) Universitat Jaume I 2) Solvionic SA

The performance of thermoelectric devices is estimated by the device figure of merit (ZT=S^2?T/?, being S the Seebeck coefficient, ? the electrical conductivity, ? the thermal conductivity, and T the absolute temperature). Recently, large power factor (PF=S^2?) enhancements have been shown in a novel hybrid solid-liquid thermoelectric system, consisting of a porous nanostructured solid material (Sb-doped SnO_2) in contact with diverse liquid electrolytes [1].

In this contribution, we have investigated the nanostructured Sb-SnO_2 film in contact with a solid electrolyte: poly-diallyl dimethylammonium chloride (PDADMAC). It was found more than 2 times improvement in the power factor for the all-solid-state device. This large improvement was due to a ?60% decrease in the electrical resistance of the device accompanied by a slight reduction of less than 10% in the absolute value of the Seebeck coefficient. Impedance spectroscopy analysis was carried out to understand the role of the solid electrolyte in the device performance. This notable power factor improvement paves the way to use polyelectrolytes to enhance the power factor in thermoelectric materials.

References

[1] Márquez-García, L., Beltrán-Pitarch, B., Powell, D., Min, G., García-Cañadas, J. Large Power Factor Improvement in a Novel Solid-Liquid Thermoelectric Hybrid Device. ACS Applied Energy Materials 1 (2), 254–59, (2018)

ID: 05119
Type: Poster
Topic: Emerging topics

How thermo-electrochemical cells work. Explained by an impedance spectroscopy study

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How thermo-electrochemical cells work. Explained by an impedance spectroscopy study

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(Emerging topics, poster)

Thermo-electrochemical cells (or thermogalvanic cells or thermocells) are an alternative technology to solid-state thermoelectrics for the conversion of heat into electricity [1]. These systems are formed by two metal electrodes separated by an electrolyte which contains a redox couple. They are able to produce electricity when a temperature difference is present due to the temperature dependency of the redox species potential. The main advantage of these devices is that show Seebeck coefficient values in the order of mV/K, an order of magnitude higher than solid-state thermoelectric materials. However, their electrical current output is much lower, due to their higher electrical resistance.

The most studied thermocell in the literature is the one formed by two Pt electrodes separated by a 0.4M aqueous solution of potassium ferro/ferricyanide [1]. In this poster, we show how these devices work, describing the processes that govern their performance, by means of an impedance spectroscopy analysis. From this analysis, we have been able to quantify the three main processes that govern the power output of the device: (i) the ionic resistance of the electrolyte, (ii) the charge transfer resistance and (iii) the mass transport resistance. These processes are completely different from those occurring in standard thermoelectrics.

Acknowledgments

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 863222 (UncorrelaTEd project).

References

[1] J. Duan, B. Yu, L. Huang, B. Hu, M. Xu, G. Feng, J. Zhou. Liquid-state thermocells: Opportunities and challenges for low-grade heat harvesting. Joule 5 (2021) 768-779. DOI:10.1016/j.joule.2021.02.009.

ID: 05196
Type: Poster
Topic: Emerging topics

Correlating thermal conductivity, structure and doping in thermoelectric polymers

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Conducting polymers have attracted interest as thermoelectric materials because of their processability, light weight, flexibility, low toxicity and cost. In terms of performance, it is their intrinsically low lattice thermal conductivity (typically 0.2 – 0.5 $Wm^{-1}K^{-1}$) which is of particular interest to the thermoelectric community. However, can we assume that the thermal conductivity is always low in these systems? In addition, doping these systems causes significant morphological changes in order to incorporate the large molecular dopants and because of the polaronic nature of the charge carriers. Do these morphological changes impact the thermal conductivity of polymers? How does this impact zT?

This presentation aims to answer these questions, by investigating the cases of three polymers, poly(3-hexyl thiophene) [P3HT] and poly[6,9-dihydro-6,9-dioxobisbenzimidazo[2,1-b:1?,2?-j]benzo[1mn]phenanthroline-2,12-diyl] [BBB] and poly[17-oxo-7,10-benz[de]-imidazo[4?,5?:5,6]-benzimidazo[2,1-a]isoquinoline-3,4:10,11-tetrayl)-10-carbonyl]) [BBL]. We measure in-plane thermal conductivity of different P3HT morphologies produced by spin-coating, drop casting and aligned by mechanical rubbing. We also compare doped and undoped analogues of these films. We do find an effect of morphology on thermal conductivity in aligned polymer films that we can link to structural changes. However, by far the biggest effect on lattice thermal conductivity comes from electrical doping, which induces a subtle change to the morphology but a significant increase in thermal conductivity. We find thermal conductivity states in the range of 0.2 to > 1 $Wm^{-1}K^{-1}$.[1]

In the case of BBB and BBL we investigate the effect of ladderisation on polymers (BBL being a ladder-type polymer and BBB it’s non-ladder type analogue). Ladder-type polymers should be more planar and more rigid than non-ladder types. Correspondingly, we find that the thermal conductivity in the ladder-type polymers can be >3 times that in the non-ladder-type analogue. When doped the lattice thermal conductivity increases even further to >2 $Wm^{-1}K^{-1}$.

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Thermoelectric devices & applications

ID: 04840
Type: Poster
Topic: Thermoelectric devices and applications

Development of a Thermoelectric Generator for Industrial Waste Heat Recovery at a Zinc Melting Furnace: Operation Conditions and Simulation

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Thermal industrial processes account for a large share of the worldwide annual primary energy consumption. The efficiency of these processes is limited and a lot of the generated heat remains unused. Solely in Europe, the amount of waste heat is estimated to be around 300 TWh per year [1]. This offers a high potential for waste heat recovery and the reduction of the overall CO_2-emissions. The potential is not exploited yet, because most established technologies have either high investment costs or are unable to convert the heat into electrical energy. Thermoelectric Generators offer a solution for this problem. They directly convert heat into electrical energy and are potentially very cost-effective. This research aims to design a Thermoelectric Generator which can be used for waste heat recovery at a zinc melting furnace in an economic way. Therefore, the boundary conditions of an operational plant are measured experimentally in detail. The results are used as input parameters for a novel simulation and optimization method. The method combines empirical macroscopic thermoelectric models, computational thermo-fluid dynamics and economic calculations. The non-linear optimization is performed with an evolutionary algorithm based on key performance indicators such as payback period and total emissions reduction. The described methodical development process and the results are presented here. The results proof the opportunity for the economic application of Thermoelectric Generators for industrial waste heat recovery. Based on these findings, future research plans are to build a functional prototype that validates the simulation and is integrated in the plant to reduce energy costs and emissions in an industrial environment.

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ID: 05022
Type: Poster
Topic: Thermoelectric devices and applications

An experimental approach to flexible thermoelectrics for energy harvesting applications

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Energy harvesting relates to the use of waste energy to produce electric power. Light, electromagnetic radiation, vibrations, thermal gradients, etc. are among these unused energy sources. Nowadays, energy harvesting is expected to play a role in the development of portable, flexible, and wearable electronics that support the concepts of industry 4.0, the internet of things, and the subgroup on internet of medical things. These concepts require the massive deployments of sensors, actuators, etc., which currently depend on chemical batteries, thus presenting limited lifetime, need of periodic recharging, potential environmental pollution, and safety issues. These drawbacks even amplify when remote areas must be covered.

Thermal gradients stand out among the cited waste energy sources, given their ubiquity worldwide. Most of the waste heat take place at low temperature, usually lower than 200 ºC, so that common power generation plants, based on vapor expansion in turbines, are unapplicable.

Thermoelectrics stands out in this context, given that a thermoelectric module can provide this power by harnessing waste heat from a hot spot. Commercial modules are flat and rigid, and their applicability is limited to surfaces of this same condition. Alternatively, we have developed flexible thermoelectric modules (FTM) for application to heat sources with complex geometries. They are composed of rigid semiconductors but flexible substrates, joints, and welds. This combination is the one that offers the greatest efficiency among the possibilities of flexible thermoelectrics.

The objective of this work is the characterization of FTM under real operating conditions. Specifically, the electrical power and efficiency of an FTM will be obtained depending on the temperature difference between its ends, and the load resistance it feeds. Heat sources of different curvature are used to evaluate its influence in the results.

ID: 05036
Type: Poster
Topic: Thermoelectric devices and applications

PERFORMANCE OPTIMIZATION OF VAPOR COMPRESSION SYSTEMS PROVIDED WITH NATURAL REFRIGERANTS BY INCLUDING THERMOELECTRIC SUBCOOLING

Patricia Aranguren[1] , Álvaro Casi[1] , Daniel Sánchez[2] , Miguel Araiz[1] , Irantzu Erro[1] , Ramón Cabello[2] , David Astrain[1]

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The total number of refrigeration, air-conditioning and heat pump systems in operation worldwide is roughly 5 billion units. Consequently, the refrigeration sector (including air conditioning) consumes about the 20 % of the overall electricity used worldwide. Moreover, the International Institute of Refrigeration (IIR) estimates that global electricity demand for refrigeration and air conditioning could more than double by 2050 due to global warming and the increasing of refrigeration demand in numerous sectors. Regarding greenhouse gas emissions, the IIR states that this sector is responsible for the 7.8 % of the global emissions.

In order to reduce the great impact of this sector, this investigation studies the benefits of including thermoelectric subcooling into vapor compression refrigeration cycles provided with natural refrigerants. These devices would be located at the exit of the condenser/gas-cooler producing a reduction in temperature of the refrigerant and consequently increasing the specific cooling capacity of the system, boosting the coefficient of performance (COP) of the refrigeration facility and reducing energy consumption.

Thermoelectric coolers are solid-state refrigeration systems that use electric energy to absorb heat thanks to Peltier effect. These systems need optimized heat exchangers and their operation needs to be carefully studied and performed in order to achieve high thermoelectric COPs that benefit the global application. In this study, optimized thermoelectric coolers are studied to quantify the benefits of including them into vapor compression cycles that include natural refrigerants.

This hybridization of technologies is a perfect match that profits from the benefits of each one of them, the high COPs and cooling capacities of vapor compression systems and the absence of moving parts and refrigerants, reliability, easiness of control and modularity of thermoelectric cooling.

ID: 05039
Type: Indiferrent
Topic: Thermoelectric devices and applications

Development and test results of overheating protection of thermoelectric systems for utilization of radiative waste heat in industrial environments

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The research project InTEGrated (Funded by EU-RFCS Programme, No. 899248) handles amongst others with the overheating protection of thermoelectric systems in industrial applications.
In the steel industry, large amounts of radiant waste heat are generated, especially at the continuous casters and in the hot rolling mill. In the previous research project Therelexpro (Funded by EU-RFCS Programme, No. RFSR-CT-2013-00029), a thermoelectric system for utilizing radiant waste heat was developed and tested in an industrial environment. However, due to strong temperature fluctuations of the radiation source, the prototype was destroyed by overheating during the field tests. Therefore, one goal of the InTEGrated project is to develop solutions for overheating protection of thermoelectric systems and test them in the laboratory and in an industrial environment.
Two ways for overheating protection are investigated: Usage of Phase Change Materials (PCM) in the heat absorber and extraction and transfer of radiant waste heat to the TEGs using heat pipes. To demonstrate the operational feasibility of the targeted solutions, small prototypes are developed and initially tested in the laboratory. Based on the laboratory results and simulations, complete prototypes will be developed and installed for long-term tests at the hot rolling mill of ESF Elbe-Stahlwerke Feralpi in Germany. Prototype designs as well as results of prototype tests and simulation results will be presented.

ID: 05069
Type: Poster
Topic: Thermoelectric devices and applications

Fabrication of planar micro-thermoelectric generators integrating a 2.5D thermopile topology

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In this work, we have developed a family of planar micro-thermoelectric generators (µTEGs), integrating a novel 2.5D thermopile topology periodically folded and distributed onto a multi-membrane, capable of converting heat directly into useful electrical energy. This novel kind of thermopile presents a high integration density, and uses thermocouples based on metallic thermoelectric materials (Chromel and Constantan) that are electrically associated either in series or in parallel. All these characteristics allows to reduce drastically the internal electrical resistance compared to our former family of µTEGs (by a factor of 1/1000, down to a hundred Ohms). A 3D thermal modelling in COMSOL Multiphysics® was used to design the optimal dimensions of the modules so they would deliver the maximum output power. The fabrication of these devices is made by CMOS-compatible processes. The harvesting of one Watt of heat leads to thermo-generated electrical powers of a few hundred microwatts.

ID: 05076
Type: Poster
Topic: Thermoelectric devices and applications

Comparison of design concepts for ceramic oxide thermoelectric multilayer generators

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Multilayer thermoelectric generators are a promising perspective to the conventional ?-type generators. Ceramic multilayer technology is well established for production of microelectronics and piezo-stacks. Key features of ceramic multilayer technology are full-automation, cost-effectiveness, and the co-firing of all materials in one single step. This requires similar sintering temperatures of all used materials. The development of multilayer thermoelectric generators is a subject of current research due to the advantages of this technology. One of the challenges is the compatibility of the different materials with respect to the specific design.

The presented study compares three different designs of multilayer generators based on a given set of material properties. Dualleg, unileg and transverse multilayer generators are compared to conventional ?-type generators., the designs are evaluated regarding the expected maximum output power and power density using analytical calculations and FEM simulations. Additionally, the complexity of the production process and material requirements are assessed and design optimizations to simplify production are discussed.

Besides the theoretical aspects, unileg multilayer generator prototypes were produced by tape-casting and pressure-assisted sintering. These prototypes are compared to other multilayer generators from literature regarding the power factors of the used material system and the power density. Improvements of the power output by design optimizations are discussed.

ID: 05089
Type: Poster
Topic: Thermoelectric devices and applications

Batteryless IoT for smart monitoring in ATEX and energy demanding industries

DR. RAUL ARAGONES ORTIZ[1] , DR. JOAN OLIVER MALAGELADA[2] , ROGER MALET MUNTE[1] , DRA. MARIA OLIVER PARERA[2] , PROF. DR. CARLES FERRER RAMIS[2]

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Lelieveld et al. remarks the high exposition for humanity to suffer cardiovascular diseases due to our poisonous air, killing yearly 7M inhabitants worldwide and reducing 2.2 years our life expectancy.

Besides, most of the gases that human activity emits into the atmosphere are due to the industrial processes that require a lot of energy for the transformation of the raw material. Additionally, a large part of this energy is lost in form of waste heat. As a clear example, in the EU27, it is estimated the 21% of the yearly energy needs are lost in industrial waste heat.

This paper presents novel long-range wireless and battery-less industrial Internet of Things device (IIoT) powered by waste heat for measuring and predicting machinery vibrations. These self-powered devices will help energy demanding industries (chemical, petrochemical, oil refineries, paper, iron&steel, rubber, aluminium, etc.) to become more environmentally friendly and profitable in their digitalization transition towards Industry4.0.
Moreover, due to the lack of batteries, new long-range wireless protocols may be adopted such as LoRaWAN, eliminating all the wireless infrastructure in the facility.

Additionally, the edge-computing concept is introduced in this device reducing up to 98% the cloud computation and its GHG emissions.
Finally, the first preliminary results of a Pilot will be presented in the result section. Four all-in-one vibration monitors were installed in the lubricant factory in ILBOC, Cartegena, Spain.

This project has received funds from the European Commission EIC Acceleration, project INDUEYE grant agreement¡ 946845.

ID: 05104
Type: Poster
Topic: Thermoelectric devices and applications

Evaluation of cooling effect of simulated PA MMIC device using peltier cooler

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GaN-based RF power devices generate a large amount of heat due to power loss, so MMIC device and module-level packaging technology that considers heat dissipation design are simultaneously required. In the case of a high-power RF device, it has a heat flux of several hundred W/cm^2 at the package level, so it is important to substantially lower the heat flux (heat flux conversion) by applying heat diffusion technology.

In this study, it is assumed that most of the power lost in the RF power device is converted to heat, and the thermoelectric cooling effect was evaluated by fabricating a simulated device having the same level of heat generation. As for the amount of heat flux, an Au thin film micro heater was manufactured so that heat of about 30 W was generated in an area of 0.3X4 mm^2.

The size of the manufactured micro-heater is 5x5 mm^2, and after bonding it to the metal carrier substrate using solder, a water-cooled Cu block maintained at 20 °C. The surface temperature was measured with a infrared camera, and the thermoelectric cooler was placed between the water-cooled Cu block and the metal carrier to which the heating-simulating device was bonded to compare the surface temperature. The cooling performance of the used thermoelectric element is Imax 6.1 A, Vmax 24.9 V, dTmax 70 K, Qmax 94 W. In the case of direct cooling of the simulated device with a water-cooled Cu block to which no thermoelectric element was applied, the temperature change before and after heating was from 20 °C to 49.5 °C. On the other hand, when the thermoelectric cooler was applied, the temperature was as high as 91.8 °C in the device off state, but the temperature was relatively lower at 38.5 °C in the Imax state of the thermoelectric element.

ID: 05115
Type: Poster
Topic: Thermoelectric devices and applications

Experimental investigation of heat losses and energy balance of a commercial condensing boiler with thermoelectric generators (TEG)

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The presentation presents the results of an ongoing research and development project aimed at designing and optimizing natural gas-fired condensing boiler for commercial use with connected thermoelectric generators. The idea of â€‹â€‹the project is to provide the base load of single-family homes of around 300 W. The thermoelectric generators are connected to an electronic load that simulates an electrical consumer. The reason for this is the assumption that it is more economical to use the electricity yourself than to feed it into the grid. The device includes a commercial burner of a condensing boiler as a heat source, special coolers for the TEG, a heat exchanger for the exhaust gas and the typical periphery of a condensing boiler as well as some conventional thermoelectric generators (TEG) for usage at low temperatures (< 200°C). Furthermore, there are a set of glass plates to simulate a high-temperature TEG with an application temperature of 500°C on the hot side.
The presented design is the result of a manual calculation based on previous studies. The aim of the design is to ensure constant power generation by the TEG with flexible burner capacity in order to facilitate the electrical connection and to verify important parameters for a CFD simulation of the system such as wall temperatures, exhaust gas temperatures, gas consumption and exhaust gas composition depending on the combustion heat output. Cooling capacity, pressure loss and heat losses are investigated and calculated at different burner capacities. A manually operated bypass valve regulates the wall temperature. Performance, handling and measurement results of temperatures and energy balance lead to a different design in ongoing research. The reasons for this are presented, and discussed under scientifically and commercial points.

ID: 05116
Type: Poster
Topic: Thermoelectric devices and applications

Long-term autonomous volcanic surveillance powered by thermoelectric generators

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The recent eruption in La Palma (Canary Islands, Spain) has exposed the importance of volcanic surveillance, which is able to predict when volcanic eruptions are going to occur. Nonetheless, despite its importance, there is still a challenge to be solved: the power supply of the necessary equipment (seismographs, gas sensors…), since volcanoes are normally at remote locations, with access difficulties, lack of power grid, as well as climatological adverse conditions.

The present work demonstrates how thermoelectric generators have the potential to solve the former challenge, being a better solution than PV panels. The presence of fumaroles, hot gases that emerge from the ground, is one of the characteristics of active volcanoes. Transforming this heat into electricity by means of thermoelectric generators suppose a continuous, robust, compact, scalable, and reliable autonomous power supply. These advantages have been demonstrated with a prototype that has been in operation since December 2019 in an 83.5°C fumarole at Teide volcano (Canary Islands, Spain). The prototype is made of high-efficiency heat exchangers based on phase change that maximize power generation with no moving parts. With only two Bi-Te thermoelectric modules, the prototype generates enough energy to measure different variables and emit them to a center located 14 km away, leading to a completely autonomous monitoring station. For this purpose, it has been of utmost importance to reduce power consumption to a minimum, for which Internet of Things (Iot) technologies, such as LoRa, have been key. Taking into account that the device has been steadily working for almost three years without maintenance, the viability and durability of the proposed solution have been demonstrated, arising as a promising application of thermoelectric generators.

ID: 05120
Type: Poster
Topic: Thermoelectric devices and applications

Heat Fluxmeter in Silicon technology with low thermal resistance

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Heat flow measurements have become essential in all sectors of industry as energy, chemicals, automotive, aerospace, environment, medicine and food industry, etc... On one hand, it allows to quantify heat losses through a part of a system surface, on the other hand it also permits to get some information from inside the studied system. Moreover, these measurements allow to predict or follow in real time the system fluctuations to external thermal disturbances and this, well before any temperature sensor would have detected the lesser change. However, these heat flow measurements are very delicate and difficult/harsh to implement. Metrological quality needs heat fluxmeters (ie heat flux sensors, HFs) that diplay accuracy, stability and that are not intrusive. Generally, such devices are built up onto polymer substrates[1].

In this context, we have developed an original heat flux microsensor (µHFS) based on Si technology, which has a high sensitivity and a low thermal resistance. It relies on the use of mesoporous Silicon boxes locally etched into a Si-(100) wafer by anodic chemical, method, such a way to make thermal dissymetries[2]. This Si anodisation allows reducing drastically the Silicon thermal conductivity from 140 W/m/K to some 1W/m/K in the porous areas (boxes). The sensitive component of the µHFS is a planar Gold/polySilicon based thermopile made up with a large number of plated thermocouples associated in series (up to 500 cells) distributed on the periodical distribution of Si-porous boxes. This kind of devices present responsivities ranging up to 260 mV/W with electrical resistance lower than a hundred kW. This presentation will describe the fabrication process of these sensors and their operating principle and the main results will be discussed.

References :

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[2] K. Ziouche and al. “Quasi-monolithic heat flux microsensor based on porous silicon boxes,” Sens. Actuator A-Phys., 164, pp. 35-40, 2010.

ID: 05121
Type: Poster
Topic: Thermoelectric devices and applications

EXPERIMENTAL PERFORMANCE STUDY OF MULTISTAGE THERMOELECTIC HEAT PUMPS USED FOR THERMAL ENERGY STORAGE

Irantzu Erro[1] , Patricia Aranguren[1] , Patricia Alegría[1] , Leyre Catalán[1] , Álvaro Casi[1] , Álvaro Martinez[1] , David Astrain[1]

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The current need to carry out an energy transition towards a 100 % renewable horizon places the energy storage as the key, since it is capable of solving the natural intermittency of renewable energies. Regarding different technologies to keep the exceeding renewable power, the thermal energy storage has the potential to be an optimal technology presenting low costs. Electrical resistors are the current technology used to transform the exceeding electrical energy into thermal energy by heating an air flux and obtaining a coefficient of performance (COP) of one.

In this work, the use of novel multistage thermoelectric heat pumps is proposed to improve the COP of the transformation of energy. Different multistage configurations have been designed using efficient heat exchangers, specifically two types of intermediate heat exchangers between stages have been developed in order to optimize thermal transfer between stages. The first one is based on a conventional aluminium block, while the second one is a novel heat exchanger based on phase change. Experimental characterization has concluded that the novel heat exchanger outperforms the aluminium block, obtaining a 50 % reduction in its thermal resistance.

Air-to-air multistage thermoelectric heat pump prototypes have been built and experimentally studied. The ratio of voltage supply between stages and airflow inlet temperature have been modified and tested. It is demonstrated how the use of efficient heat exchangers improve multistage thermoelectric heat pump performance, where the use of phase change internal heat exchangers improves the heating COP of the system by a 20 %, compared to the conventional technology, obtaining COP values between 2 and 5. These values show the great potential of thermoelectric technology in order to improve the performance of thermally storing energy.

ID: 05123
Type: Poster
Topic: Thermoelectric devices and applications

New thermoelectric generator with no moving parts nor environmental impact for high temperature geothermal energy

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The installed capacity of renewable energies is rising due to the efforts of several countries. Geothermal energy has a great potential and is totally stable, independent of the weather conditions. Nevertheless, this source has been left behind in terms of installed power due to its lack of scalability, long payback time, big environmental impact and high initial investment.

The political declaration on clean energy for EU islands provides a long-term framework to help islands generate their own sustainable, low-cost energy. These islands, although having access to renewable sources, depend highly on expensive fossil fuel imports for their energy supply. For example, primary energy dependence on fossil fuels in Canary Islands is 98%. Thus, it is important to develop technologies that take advantage of the characteristic conditions of these islands: their geothermal activity.

Thermoelectricity has been identified as one of the key technologies to leverage this geothermal potential, but the only geothermal thermoelectric generators studied in the literature include fans or pumps to move a fluid, losing the intrinsic advantage of thermoelectricity: the absence of moving parts.

In this work, a geothermal thermoelectric generator without moving parts thanks to phase change heat exchangers has been developed to harness the high temperature geothermal anomalies in Lanzarote (Canary Islands, Spain). It has no environmental impact and is cost-effectively for high and low powers. Prototypes have been tested in laboratory and successfully installed in field. The device has 8 thermoelectric modules and has been operating in field with a maximum generated power of 36 W (4.5 W per module). The generated energy per year is of 253 kWh. This study has experimentally demonstrated the feasibility of geothermal thermoelectric generators, thus laying the foundations for a future larger-scale installation and for transforming Lanzarote into a more sustainable island.

ID: 05129
Type: Poster
Topic: Thermoelectric devices and applications

Critical thermal stress between high / intermediate temperature thermoelectric elements and passive layers: a finite element evaluation

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In thermoelectric modules operating at intermediate temperature, critical stress and potential failure likely occur at the interface between thermoelectric legs and passive elements. In particular, the insertion of ceramic substrates with lower coefficient of thermal expansion than the thermoelectric elements may reduce the strength of the module because of localization of high thermal stress. Such stress may also affect the assembly reducing its ultimate mechanical strength, resulting in an assembly failure or an operating life time reduction. The evaluation of potential failure mechanisms has to be done considering suitable failure criteria for the elements of the module, identifying ductile and brittle components. In the first case, a yield criterion, based on maximum distortion or shear stress, has to be chosen, whereas in the latter case a failure / strength criterion based on maximum compressive / tensile stresses must be considered. In this work, both yield and failure criteria have been implemented in a Finite Element environment to evaluate the maximum admissible thermal stress in Mg_2Si and HMS based thermoelectric modules as a case study. This work shows the results of the Finite Element simulation which can lead to feasible strategies for brazing thermoelectric materials, connectors and ceramic substrates and eventually for the realization of the entire module.

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Topic: Thermoelectric devices and applications

Novel thick film thermoelectric devices for heat sink-free energy harvesting applications

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Current thermoelectric solutions for energy harvesting systems for remote sensors and IoT applications, tend to be heavy, expensive and require a range of adaptor plates for different heat sources. Although the power requirements for these devices depend heavily on the application, they typically vary from microwatts for very low power sensing with low update rates to milliwatts for more frequent or complex sensing including remote communication. We demonstrate a novel BiTe- thick film thermoelectric device with integrated heat sink for energy harvesting applications which produces 400 ?W at a ?T=46 °C between a hot surface and air. Such a device is demonstrated to be able to power off the shelf energy harvesting boards to give a stable 3V output.

This is accomplished by using thick film technology and advanced assembly techniques to reduce thermal losses from interfaces, maximise voltage output and minimise use of thermoelectric material. This allows a low weight device while producing a high voltage output, up to 0.7 mV/g·K, which is 7 times higher than achieved with a conventional device. High voltage outputs enable simpler integration with electronic systems. The sensitivity to the surrounding airflow is also tested, with a power increase of 145 % observed as the air speed increases from zero to 1.5 m/sec.

ID: 05140
Type: Poster
Topic: Thermoelectric devices and applications

Experimental transcritical carbon dioxide refrigeration cycle working with a thermoelectric subcooler and an internal heat exchanger

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The use of carbon dioxide in transcritical state has become one of the most used solutions to comply with F-Gas directive and reduce greenhouse gases emissions from refrigeration systems. For low-medium power units, the commonly used solutions to improve the efficiency such as the ejector, multiple compressor arrangements, mechanical subcooler etc. are too high and complexity of the refrigeration facility, which is not practical for small units.

For low-medium power units, the use of an internal heat exchanger (IHX) is one of the simplest solutions to increase the COP of the installation. It subcools the refrigerant at the outlet of the gas-cooler, thus increasing the specific cooling power, and the energy consumption of the compressor rises. Another alternative that has been the focus of recent studies is the inclusion of a thermoelectric subcooler (TESC). The system subcools the refrigerant at the outlet of the gas-cooler enhancing the specific cooling capacity while adding an electrical power consumption. If properly managed the system is able to enhance cooling capacity and the efficiency of the system.

This study brings a complete research in which both solutions have been tested in an experimental transcritical carbon dioxide refrigeration facility. The technologies are compared for a wide range of working conditions. This work focuses on the real performance of both systems and discusses the strengths and weaknesses of using an internal heat exchanger or a thermoelectric subcooler.

ID: 05141
Type: Poster
Topic: Thermoelectric devices and applications

Flexible multilayer graphene-based devices for large-area thermoelectric sensing applications

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Emerging applications in areas such as wearable electronics and internet-of-things require devices that are lightweight, flexible and consume a minimal amount of power. Recent progress in flexible thermoelectrics has brought up promising material candidates, which in addition to above characteristics, can be fitted into scalable fabrication processes suitable for large production volumes.

One such material is multilayer graphene, which can be produced via a liquid-phase route. Here, we demonstrate a large-area, flexible thermoelectric sensor device exploiting the properties of a thin film made of multilayer graphene flakes [1]. The films are fabricated from multilayer graphene containing ink, which we further deposit by spray-coating onto flexible substrates to produce electrically conductive films covering large-areas. The exceptional mechanical properties and thermoelectric character of these films are then utilized to realize thermocouple arrays allowing for passive detection of temperature gradients.

The resulting sensor devices are demonstrated in example applications of touch sensing, detection of heated objects and sensing temperature distributions of surfaces on which the sensor is fixed. The low-cost and scalable ink route used to produce the thermoelectric film is inherently suitable for a range of large-scale deposition methods, such as gravure printing, thus promoting integration into industrially manufactured devices for practical applications.

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ID: 05150
Type: Poster
Topic: Thermoelectric devices and applications

Thermoelectric Generators for Waste Heat Recovery in Heavy-Duty Vehicles

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Modern heavy-duty vehicles have to fulfill the highest demands in terms of economy and ecology, i. e. reduction of total cost of ownership, fuel consumption and pollutant emissions. A holistic technically and economically optimized waste heat recovery system in the form of a thermoelectric generator, which takes into account mechanical, electrical, thermoelectric and thermodynamic as well as economic aspects, can contribute to the achievement of these objectives.

Two application scenarios are considered, heavy-duty vehicles with conventional diesel engines and with stoichiometric natural gas engines. Thermoelectric generator concepts were developed that combine high electrical power (peak power of about 3000 W for the natural gas heavy-duty vehicle) with low negative impact on the overall vehicle.

As a result of this research study significantly higher fuel savings are achieved compared to the state of the art. For the diesel vehicle fuel reductions in dynamic driving scenarios are between 0.5 - 1.5 %, CO_2-emission reductions are between 4 – 15 gCO2/km and the minimum amortization period is 1.4 years. The economic use of the system is demonstrated considering the total cost of ownership. Better results are obtained for natural gas vehicles due to the higher exhaust enthalpy. These are 1.8 - 2.8%, 13 - 35 gCO2/km, and 0.7 years.

A functional model has successfully validated the simulation environment with an average deviation of less than 6 %. An electrical output power of up to 2700 W was measured under the boundary conditions of the natural gas engine. The results obtained increase the technological maturity level, which has been low to date, and contribute significantly to getting thermoelectrics closer to series maturity in technological and economic aspects.

ID: 05156
Type: Poster
Topic: Thermoelectric devices and applications

Geothermal thermoelectric generators: a promising alternative for hot dry rock fields

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Thermoelectricity applied to geothermal energy has great future potential due to its robustness, reliability and its lack of auxiliary consumption. However, the efficiency of a thermoelectric generator highly depends on heat exchangers.

In this work, a thermoelectric generator has been developed which transforms the heat in the ground of the Timanfaya National Park (Lanzarote, Canary Islands) into electricity. Therefore, passive heat exchangers were designed and built specifically for this application. These transport the heat with the maximum possible efficiency from the well (hot side) to the thermoelectric modules. The heat that is not transformed into electricity was dissipated into the environment through very effective cond side heat exchangers. The principle of operation of all these exchangers is phase change.

Different configurations of heat exchangers were evaluated, the prototype was built and it was finally experimented in the laboratory under different convection conditions, temperatures and heat flows. The prototype was finally installed in a well in the Timanfaya National Park, where it generated until 40 W (22.35W of a prototype with 10 modules and 17.64W with 6) with temperature difference between the hot source and the ambient of 154 ?C, with an average wind speed of 14 km/h.

With this research, the viability of thermoelectric generators to harness hot dry rock fields that nowadays cannot be exploited has been demonstrated. They permit to generate electricity in an environmentally friendly way and improve the implementation of renewable energies as the geothermal one, moving us closer to achieving the sustainable development goals.

ID: 05159
Type: Poster
Topic: Thermoelectric devices and applications

Estimation of the thermal breakdown voltage of Al2O3 anodic layer for thermoelectric module substrate

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In this study, we presented an original idea of a thermoelectric module construction where an anodized aluminium oxide (Al_2O_3) thin layer is used as a dielectric substrate. Al_2O_3 coatings were produced on aluminium (Al) alloys by the electrochemical anodization method and investigated by a range of techniques, including scanning electron microscopy, X-ray diffraction and energy dispersive spectroscopy. The thermal conductivity of the anodic oxide layer was defined on the base of the thermal properties of the Al_2O_3/Al heterostructural substrate measured by the laser flash analysis method. The temperature-dependent breakdown voltage of the Al_2O_3 anodic layer was estimated as a key parameter which defined the thermoelectric module's workability. The analytical calculus of the breakdown voltage was performed using the Walter-Fock theory of thermal breakdown of solid dielectrics in application to thin electrical insulating layers. The breakdown voltage measurement was carried out over a temperature range of 500–300 K by the developed temperature-controlled testing setup. The obtained results indicated the negative temperature influence on aluminium oxide dielectric properties leading to the decrease of breakdown voltage level. The maximum breakdown voltage values of approximately 300 V and 100 V were achieved for a 10 ?m layer thick at 300 K and 500 K temperatures, respectively. Considering Seebeck voltage the required thickness of the Al_2O_3 layer was defined to prevent the destruction of the dielectric substrate during the thermoelectric module operation. The application of the presented results can significantly contribute to the development of the long-life, robustness, and high-reliability thermoelectric energy converters.

ID: 05192
Type: Poster
Topic: Thermoelectric devices and applications

Efficiency and thermal stability of silicide-based thermoelectric modules

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The feasibility and reliability of a thermoelectric module at intermediate/high temperature is key point in heat harvesting. In this work, we report the development and characterization of thermoelectric modules (TEMs) based on abundant silicide materials. TE modules are assembled in order to avoid high temperature mechanical stresses. Different electrodes, substrates and brazing materials were tested. Contact resistivity measurement of the silicide/metal brazed electrode and finite element analysis of thermal induced stress are presented, to guide the design of TE modules. Measurements of output power and conversion efficiency were performed. Moreover, thermal stability of thermal and electrical properties in the 400 °C – 550 °C was evaluated.

For the characterization of module efficiency and performances a custom-built apparatus has been developed. The testing apparatus is based on the heat flow meter method at the cold side of the module and it is conceived to test TE modules (single or in cascade) with a footprint up to 60x60 mm^2. The system works from room temperature up to about 900 K, under vacuum or inert atmosphere.

ID: 05253
Type: Poster
Topic: Thermoelectric devices and applications

Model-based Design of Thermoelectric Generators for Waste Heat Recovery from Marine Engine Exhaust Gases

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The Internal Combustion Engines (ICE) of commercial or passenger ships waste significant amounts of energy through their exhaust gases, at high temperature, which are released to the environment. Thermoelectric generators can diminish this problem by converting this otherwise wasted thermal energy into useful electrical energy. The aim of this study is to propose a thermoelectric generator system to recover energy from the exhaust gases of ships. The proposed thermoelectric device uses the outside area of the ship's ICE manifold as the hot side of the thermoelectric module, while the cold side is maintained at a low temperature through the flow of water. This thermoelectric generator is designed through modeling and simulation and systematic analysis. Design and analysis are performed with the use of modeling and simulation using a commercial software to study 3-dimensional fluid flow coupled with heat transfer. A parametric design analysis is carried out to detect the parameters with the highest contribution to energy recovery. Design parameters are also studied using the Latin Hypercube methodology for better and efficient exploration of the design space. The analysis shows that significant energy of the exhaust gases can be converted into electric power with the use of an optimized heatsink, which creates the highest temperature difference between the two sides of the thermoelectric module.

ID: 05258
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Topic: Thermoelectric devices and applications

Printed thermoelectric generators wirelessly powered by high-power laser beam

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Herein, we present an innovative system that combines two fast-rising fields - Energy Harvesting and Wireless Energy Transfer.
The proposed system consists of a flexible radial thermoelectric generator, powered by a high power laser beam, focused on the centre of the device, generating a temperature gradient. The device was fabricated by screen-printing. Commercial silver ink was used for the electrical contacts. The TE ink was developed with a base of a polymer matrix of PVA (Polyvinyl Alcohol) doped with phosphoric acid (16.4%wt) mixed with PEDOT:PSS (poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate)) (16.4%wt), and combined with commercial Bi-Te microparticles (67.2%wt), adapted from a previous study[1]. Transport properties analyses were performed for the printed film. The TE film presents a Seebeck coefficient of 33 µVK-1 and electrical conductivity of 7.32 Sm^{-1}, thus leading to a Power Factor (PF=S?^{2}) of 7.97 $\mu Wm^{-1}K^{-2}$.

The characterization of the developed device was performed under vacuum at room temperature, with an incident laser beam with a wavelength of 1500 nm and a variable power (0.5–2 W). To increase the generated temperature gradient, the presence of a light collector in the centre of the device was considered, and a comparative analysis was carried out. A maximum output voltage of 16 mV and a maximum power density of 25 ?Wm^{-2} were achieved with the collector and a laser power of 2 W. The temperature and pressure effect on the output was also evaluated, and an increase of 25% and 230%, respectively, was observed.

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ID: 05263
Type: Poster
Topic: Thermoelectric devices and applications

Boosting Thermoelectric Power Generation Coupling NIR absorbers for Wireless Power Transfer

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Architected system such as micro-thermoelectric (TE) materials will take advantage of converting a concentrated thermal energy source, and the external temperature of the system gives rise to an enhanced thermal gradient. One of the strategies to boost the thermal gradient in the thermoelectric generators (TEGs) can be through the use of collectors or/and plasmonic systems [1]. In the present work, the influence of several screen-printed collectors will be used to study their impact on the output of the TEGs. Several TEGs were produced by screen-printing and using p-type Bi-Te-based inks, as reported in [2], in a radial configuration. In this TE configuration, the heat will be made from the center of the device by using a laser with a ? of 1500 nm. Additionally, commercial carbon black, TiN, ZnO, and Bi_2O_3-based inks were screen printed in the center of the TEG. To better analyze the impact of the produce collectors in the TEG, a complete characterization of the production devices was performed before and after the application of each collector. The printed collectors with a thickness between 80 to 100 µm were analyzed by UV-Vis-NIR reaching an absorbance higher than 90%. With the present work, we will demonstrate that implementing a collector increased the generated temperature gradient by 50%, leading to an overall performance increase of ~ 47%.

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ID: 05269
Type: Poster
Topic: Thermoelectric devices and applications

Powering Wearable Electronics with Modular Thermoelectric Generators – Material Optimization to Device and System Demonstration

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Designing thermoelectric generators (TEG) for powering wearable electronics requires careful control over various parameters, from material properties to device and system integration. We present results highlighting some challenging trade-offs observed while fabricating a 9-TEG modular device that can be integrated with a shirt and a smartwatch. This device includes TEGs composed of n-type and p-type Bismuth Telluride (Bi_2Te_3) based nanocomposites tuned to achieve a near-peak thermopower and minimized thermal conductivity at room temperature, which is more critical than zT for increasing the wearable device performance. Since the thermal gradient is only a few degrees in most wearables applications, the TEGs have been fabricated with legs cut into high aspect ratios to increase the thermal resistance. The metalized Bi_2Te_3 legs are fabricated into TEGs using a homemade compression bonder and then assembled in a modular fashion. The performance of the modular device is characterized by three different boost-converters that are integral components of any energy harvesting device meant to power wearable systems. Based on this test, the optimum TEG and boost converter combination is tested under conditions that mimic the body heat harvesting scenario. These TEGs were also tested for powering a smartwatch platform for measuring electrocardiographs, photoplethysmographs, and acceleration signals for wearable health monitoring systems.

ID: 05348
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Topic: Thermoelectric devices and applications

Maximizing Vehicle Thermoelectric Generator Output through Thermal control: simulations and concept validation

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The thermoelectric (TE) recovery of the energy lost through the exhaust of vehicles has long been studied as a promising technology to improve vehicle efficiency and sustainability, especially now that hybrid powertrains can better utilize the electricity produced onboard to extend the electric range of the vehicle.
However, high costs per unit power produced and the difficulty of optimizing the TEG under real world driving, with its highly variable exhaust power and temperature, has made the use of TEGs in vehicles not viable so far.
New affordable TE materials are helping to overcome the cost issue. Materials such as magnesium silicide and tetrahedrites, which the authors have bee exploring, have proven to achieve efficiencies comparable to existing materials, but at a fraction of the cost.
Additionally, the use of thermal control, such as the concept proposed by the authors on previous publications, allows to achieve an optimal thermal distribution of the heat across the TEG irrespective of engine regime, so that it is possible to maximize heat absorption from the exhaust while still avoiding both thermal dilution or overheating. This is done by spreading excess heat from hotter to cooler regions of the heat exchangers through liquid/vapour phase change done at a controlled temperature.
The present poster highlights the latest developments of the use of this concept, namely illustrating its potential when used in Heavy Duty Vehicles (HDVs) during long haul driving cycles, the use of vapour chambers and high performance wavy fin heat exchangers and showing the validation of the concept with experimental tests illustrating its temperature control and heat spreading characteristics.

ID: 05349
Type: Poster
Topic: Thermoelectric devices and applications

Enabling Large-Scale Waste Heat Recovery Applications using Thermoelectrics: Affordable materials, geometries and methods sutable for upscaling

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Thermoelectric (TE) generators (TEGs) have two notable advantages when compared against other thermal machines: if carefully designed, TEGs can be installed and (almost) forgotten. This is a notable advantage in situations where low-to-no maintenance is intended. TEGs are also modular and therefore highly scalable.
Until recently, the use of TEGs for large-scale applications could not be viable due to the cost of commercially-avaliable TE materials and the geometric configuration of commercially-available TEG modules, which is suited for small-scale applications. In fact, these modules are built and assembled with a large number of tiny elements that need to be cut, soldered and assembled with tight tolerances and expensive methods.
The advent of affordable TE materials allows to cut down TEG cost. However, manufacturing costs and complexity must also be reduced to enable a viable large-scale TEG.
The authors propose a concept based on using large TE elements made of affordable n-magnesium-silicide and p-tetrahedrite, which are materials they have been developing.
The big advantages of using large elements is the radical reduction of the number of elements per unit power produced (and thus, cuttings, solders, etc). Larger element modules tend to generate lower overall voltages and larger currents. While this might be a problem for small-scale applications, it may become manageable in large-scale applications: the overall voltage is no longer low and the large currents can be handled with robust power electronics that would be impractical for small-scale systems. Also, coarser tolerances, higher thermal expansions, and simpler assembly and bonding methods are possible with large element TEGs.
The authors illustrate the influence of element size on the performance of a TEG using multiphysics analyses and discuss thermal management solutions. Finally, they assess this concept with a case study based on the recovery of the heat from the air flow of a clinker cooler from a cement industry.

Thermoelectric materials & materials processing

ID: 04917
Type: Poster
Topic: Thermoelectric materials and materials processing

Epitaxial growth and thermoelectric properties of Mg3Bi2 thin films deposited by magnetron sputtering

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Mg_3Sb_2-based thermoelectric materials attract attention for applications near room temperature. Here, Mg-Bi films were synthesized using magnetron sputtering at deposition temperatures from room temperature to 400 °C. Single-phase Mg_3Bi_2 thin films were grown on *c*-plane-oriented sapphire and Si(100) substrates at a low deposition temperature of 200 °C. The Mg_3Bi_2 films grew epitaxially on *c*-sapphire and fiber-textured on Si(100). The orientation relationships for Mg_3Bi_2 film with respect to the *c*-sapphire substrate are: (0001) Mg_3Bi_2||(0001) Al_2O_3 and [11$\underline{2}$0] Mg_3Bi_2||[11$\underline{2}$0] Al_2O_3. The observed epitaxy is consistent with the relatively high work of separation, calculated by density functional theory, of 6.92 J m^{-2} for the Mg_3Bi_2 (0001)/Al_2O_3 (0001) interface. Mg_3Bi_2 films exhibited an in-plane electrical resistivity of 34 µ?m and a Seebeck coefficient of +82.5 µV K^{-1}, yielding a thermoelectric power factor of 200 µWm^{-1} K^{-2} near room temperature.

ID: 05001
Type: Poster
Topic: Thermoelectric materials and materials processing

Reducing the thermal conductivity of nanocrystalline CuNi alloys

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

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ID: 05004
Type: Poster
Topic: Thermoelectric materials and materials processing

Going further and towards sustainability: magnesium-based materials for space applications

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The alarming global energy and environmental crisis that we are living in today requires a fast and suitable response. In that sense, thermoelectrics, which possess the ability to directly convert heat into usable electrical energy, emerges as a possible solution for the mitigation of this issue.

In the past two decades much research has been made to discover new suitable thermoelectric materials to replace the conventional ones, that either possess toxic or expensive elements. Hence, magnesium-based thermoelectrics arise as a more sustainable alternative, displaying a competitive performance when compared to conventional materials.

In this work, fast production using unconventional methods, such as induction furnace heating and hot-pressing, were employed to produce MgAgSb, Mg_3Sb_2 and Mg_2X (X=Si, Sn) materials, to develop p and n-type (respectively) legs for novel devices to be employed in space applications.

The idea behind it is to use these materials in original devices for small satellites. Thermoelectric generators (RTG) are already used to power space probes, as Voyager or Cassini, but the materials employed are the conventional ones (mostly Si-Ge based). Moreover, if successful, the new thermoelectric devices may be employed for other purposes (mostly focusing on space), as in lunar bases or other remote locations where waste-heat recovery can be used as a power source supply.

However, these materials exhibit additional challenges: Mg losses during the process, propensity to oxidation and persistency of secondary phases for MgAgSb, hence additional efforts must be made to overcome these issues.

Hitherto, characterization, using XRD and SEM/EDS have been made on samples based on the MgAgSb, Mg_3Sb_2 and Mg_2X (X=Si, Sn) materials, changing the composition, using distinct doping elements and testing different production conditions. Thermoelectric properties, such as the Seebeck coefficient and electrical resistivity, were measured at room temperature on selected samples, with good results for the pristine Mg_2Si compound.

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Type: Poster
Topic: Thermoelectric materials and materials processing

Enhancement in Thermoelectric Efficiency of n-type Yb-Filled Co4Sb12 via Incorporation of InSb and Carbon-Coated Nano-Boron

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Thermoelectric (TE) materials, which can produce electricity from harvested waste heat, are an up-and-coming option as next-generation renewable energy solutions. Co_4Sb_{12}-based TE materials composed of non-toxic and relatively abundant elements offer adequate thermoelectric efficiency at mid-temperatures with good thermal and mechanical stability. This study deals with synergetic Yb filling and utilization of a nano-structuring approach with carbon-coated nano-boron (CnB) and InSb in the n-type $Yb_{0.4}Co_4Sb_{12}$ skutterudite phase to enhance its thermoelectric efficiency. A combination of solid-state synthesis, high-energy ball milling, and spark plasma sintering techniques was employed to obtain $Yb_{0.4}Co_4Sb_{12}$ + *x* wt.% InSb (*x* = 2, 3 and 4) and $Yb_{0.4}Co_4Sb_{12}$ + *y* wt.% $(CnB)_y$ (*y* = 0.1 and 0.2) nanocomposites. Nanosized InSb or CnB particles decorating the grain boundaries of the large $Yb_{0.4}Co_4Sb_{12}$ matrix combined with the anharmonicity introduced by the filler Yb atoms in the structure were responsible for achieving the highest *zT* value of 1.5 in this study for $Yb_{0.4}Co_4Sb_{12}$ + 2 wt.% InSb at around 773 K. The obtained zT value accounts for a 25% increment with respect to pristine $Yb_{0.4}Co_4Sb_{12}$. Besides the enhancement in zT values, mechanical properties were also enhanced with the additions of CnB or InSb to the $Yb_{0.4}Co_4Sb_{12}$ matrix which can enhance the potential usage of Co_4Sb_{12}-based n-type legs in thermoelectric modules.

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Type: Poster
Topic: Thermoelectric materials and materials processing

Significant influence of microstructure on the thermoelectric performance of Mg3+xSb1.49Bi0.49Te0.02 (x=0.2, 0.3, 0.4)

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Tellurium doped n-type Mg_3Sb_2-Mg_3Bi_2 solid solutions are excellent candidates for medium-range (RT-700K) thermoelectric (TE) applications due to the high figure of merit (peak zT value of 1.6 at 650K) and cost-effective constituent elements. The observed high zT values is attributed to presence of favourable features of the conduction band edge which improve the TE power factor. In this work, we show that an additional factor contributing to the high zT values is microstructural features which lower the lattice thermal conductivity. Compositions of $Mg_{3+x}Sb_{1.49}Bi_{0.49}Te_{0.02}$ with varying nominal Mg content were prepared for this study and its TE properties were measured as a function of temperature. The results show very similar power factor values for all the compositions but an influence of the nominal Mg content on the lattice thermal conductivity. This results in a peak zT value variation between 1-1.4 amongst the compositions. In this talk, the reason behind this observed difference in the lattice thermal conductivity values will be presented based on microstructural and thermoelectric property studies.

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Topic: Thermoelectric materials and materials processing

Lattice dynamics and thermoelectric properties of Ca-Si alloys

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A drawback of the best-performing thermoelectric materials (TEM) is their toxicity, scarcity, and/or costs of the chemical elements they are synthesized from. For this reason, alkali-earth silicides have attracted high interest as they are made of abundant, cheap, and non-toxic elements. Among their many compounds, semiconducting Ca_3Si_4 [$P6_3/m$, No 176] and $Ca_{14}Si_{19}$ [R-3c, No167] meet all the requirements to be the next generation TEMs[1] as their narrow energy bandgaps are favorable for large power factors. According to the "phonon glass-electron crystal" concept, their complex structures should also favor very low thermal conductivities. Ab initio studies of thermoelectric transport in Ca_3Si_4 also conjectured that large anharmonic motions of Ca chains could contribute additionally to reduce thermal transport[2]. Despite these promising prerequisite properties for excellent TEMs, so far only a few experimental studies have been carried out to shed light on the phonon properties of Ca_3Si_4 and $Ca_{14}Si_{19}$.

In the present study, we investigate the structure-function relationship of these compounds on a microscopic scale by ab initio lattice dynamics calculations, neutron and x-ray diffraction, and inelastic neutron scattering experiments. We examined the structural and phonon properties over a wide temperature range (2-950 K) to establish their ground state properties and in particular their dynamical response to heat treatment in the temperature regime of potential applications. The experimental data are supported by density functional theory calculations to scrutinize the microscopic origin of the vibrational properties and thus the reduced heat transport. The aim of the work is to improve the thermoelectric properties of these materials.

[1] Adrien Moll et al, Acta Materialia 125, 490 (2017)

[2] Shin Yabuuchi et al, Physical Review Materials 1, 045405 (2017)

ID: 05050
Type: Poster
Topic: Thermoelectric materials and materials processing

High Performance Tin Sulfide Thin Films Prepared by Aerosol Assisted Chemical Vapor Deposition

Yu Liu[1] , Paul D. McNaughter[1] , Feridoon Azough[1] , Xiaodong Liu[1] , David J. Lewis[1] , Robert Freer[1]

1) University of Manchester

To date, most of studies on tin sulfide (SnS) thermoelectrics focus on bulk materials. With the developing requirement for wearable and portable thermoelectric devices, thin film thermoelectrics have attracted increasing interest. In this work, SnS thin films were prepared by a low-cost, aerosol assisted chemical vapour deposition (AACVD) technique using the single source precursor dibutyl-bis(diethyldithiocarbamato)tin(IV) $[Sn(C_4H_9)_2(S_2CN(C_2H_5)_2)_2]$ with a range of deposition temperatures (375, 397, 418 and 445 °C). The effects of flow rate and solution concentration were also evaluated. The resulting films were characterised by XRD, SEM, TEM and Raman spectroscopy. The temperature dependence of the electrical transport properties (Seebeck coefficient, electrical conductivity and power factor) for the SnS films were measured; the effect of deposition temperature and other deposition parameters on thermoelectric performance of SnS films was investigated. The maximum power factor increased as deposition temperature increased. The highest power factor of ~0.22 ?W·cm^{-1}·K^{-2} at 570 K was achieved for SnS films deposited at 445 °C. This power factor value is higher than most of published values for SnSe and SnS films measured at temperatures up to 540 K. SnS films are good candidates for thermoelectric applications, and AACVD is a promising technique for the preparation of high performance thermoelectric films.

ID: 05051
Type: Poster
Topic: Thermoelectric materials and materials processing

Evolution of the microstructure and thermoelectric performance of strontium titanate-graphene materials

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Modulating polycrystalline thermoelectric oxides via graphene-based materials is a robust method to achieve high thermoelectric performance. Here we seek to understand the effect of the type and amount of graphene addition on the thermoelectric performance of $SrTiO_3$ doped with 15 % Nb. Ceramic powders were prepared by the standard mixed oxide route and calcined at 1200 C for 12 hours in air. To the mixed powders we introduced 0 – 1 wt. % of electrochemically produced graphene oxide (eGO). The as-prepared eGO yields a low oxygen content of 3.2 at. % after reduction and the value is close to the pristine graphite. Ceramics were sintered at 1427 C for 24 hours in a reducing atmosphere. The high quality products exhibited maximum *zT* values of 0.25 at ~ 600 C. We will first show how the microstructure and thermoelectric performance of these materials depend on the amount of eGO added. By comparing with the results for a range of $SrTiO_3$ ceramics (including electron-doped and pristine) prepared with additions of other forms of graphene (including graphene nanosheet (G), graphene oxide (GO), and reduced graphene oxide (rGO)) we will evaluate the effects of the different forms of graphene on the thermoelectric performance of $SrTiO_3$ ceramics. It is clear that the processing route and type of graphene have controlling effects on thermoelectric performance of these oxides.

ID: 05053
Type: Poster
Topic: Transport phenomena

Mobility-enhanced thermoelectric performance in textured nanograin Bi2Se3, effect on scattering and surface-like transport

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We report on the effect of artificially generated textures of Bi_2Se_3 in thermoelectric performance and low-temperature magnetoresistance [1]. A set of texturized nanograined Bi_2Se_3 samples was investigated, ranging from predominantly *c*-axis texture to random texture. *c*-axis oriented layered domains rendered the samples highly conducting due to drastically enhanced mobility, up to 1600 $cm^2V^{-1}s^{-1}$ at low temperature, and enhanced both carrier concentration and electrical conductivity. The largest power factor of 800 $\mu Wm^{-1}K^{-2}$ and highest ***zT ?*** 0.14 both at 300K were observed in a sample with a predominantly layered and *c*-axis oriented texture. The carrier scattering mechanism in the samples changed from mostly electron-phonon interaction at in the predominantly layered microstructure, to disorder-related scattering as the texture became random. The weak antilocalization effect was observed predominantly in the random textured samples, pointing towards enhanced surface-like transport channels. The phase coherence length evaluated using the Hikami-Larkin-Nagaoka model resulted in a high value of roughly 600 nm regardless of the texture. In the *c*-axis oriented layered Bi_2Se_3 oxidic insulating inclusions from either Fe_3O_4 or SiO_2 were incorporated. Both insulating phases reduced mobility. However, finely dispersed Fe_3O_4 secondary phase in Bi_2Se_3 resulted in a further increase of ***zT ?*** 0.2 due to much increased electrical conductivity. The combined effect of layered texture and Fe_3O_4 secondary phase resulted in an overall increase of ***zT*** around 50% compared to a non-textured polycrstal.

Reference

[1] S. Bayesteh *et al.*, Mat. Today Physics **24** (2022) 100669, DOI: 10.1016/j.mtphys.2022.100669.

ID: 05064
Type: Poster
Topic: Thermoelectric materials and materials processing

Optimizing the thermoelectric performance of nanocrystalline Si thin films by à la carte B doping using sputtering co-deposition

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The thermoelectric performance of semiconductors is strongly dependent on the charge carrier concentration. For example, it has been found that high boron doping levels produce a simultaneous increase in electrical conductivity and Seebeck coefficient in nanocrystalline Si films [N. Neophytou *et al.* Nanotech **24**, 205402 (2013)]. This way, exceptional power factors have been obtained in nanocrystalline Si films highly doped with B using ion implantation [D. Narducci *et al.* APL **119**, 263903 (2021)]. However, this doping technique is expensive, time-consuming and may cause structural damage when large doses are required.

Sputter deposition is a well-established, inexpensive, and very versatile technique for the fabrication of a wide variety of films with all kinds of compositions, which can be highly controlled by the simultaneous use of several magnetrons with the different elements to conform the desired film. In the present work, we achieve a high control of boron doping and, consequently, of the carrier concentration on Si nanocrystalline films grown by sputtering co-deposition. Starting from thin films deposited from an individual B-doped Si target, we can enrich them with different amounts of B by simply changing the B magnetron power in a co-deposition configuration.

We observe a continuous increase in carrier concentration from 10^{19} to 10^{21} /cm^3 and, consequently, in the electrical conductivity for B magnetron power, ranging from 10 to 60 W. Along with this, there is a steady decrease in the Seebeck coefficient from 500 to 100 ?V/K. These values result in power factors that present a marked maximum of around 5 mW/K^{2}m for a carrier concentration around 10^{21} /cm^3.

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ID: 05072
Type: Poster
Topic: Thermoelectric materials and materials processing

The influence of nanocrystalline grains in the amorphous Silicon matrix on the Power Factor of hot wire chemical vapor deposited silicon films

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At present, bismuth tellurium is a primary thermoelectric (TE) material in the low to medium temperature range but it is rare and toxic. Silicon which is an earth-abundant and environment-friendly material has been thought of as an alternative, but it has a very low figure of merit (ZT). One of the possible solutions to increase the ZT value is to increase the power factor (PF) of amorphous silicon (a-Si) without affecting the thermal conductivity. In this work, we report the deposition of hydrogenated nanocrystalline silicon (nc-Si: H) thin films by Hot-Wire Chemical Vapor Deposition (HWCVD). These nc-Si: H thin films have nanocrystalline grains in the amorphous Silicon matrix which is confirmed by Raman spectroscopy. The power factor enhancement in nc-Si: H is achieved by two processes - one is by introducing nanocrystalline Si grains in an amorphous Si matrix and the other is by introducing phosphorous as an N-type dopant. The Seebeck coefficient (S) of the deposited n-type nc-Si: H thin films is found to be ~150 µV/K, which is very close to the S value of bismuth tellurium (160 µV/K). The Power Factor of doped nc-Si: H films is improved without any post-annealing treatment. These results, along with the fact that these films can be fabricated using well-established technology, open up a new opportunity to use Si films as an alternative TE thin-film material.

ID: 05081
Type: Poster
Topic: Thermoelectric materials and materials processing

OXIDE COMPOSITES FOR HIGH TEMPERATURE THERMOELECTRIC POWER GENERATION

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Thermoelectric material, which has potential to convert waste heat energy into electricity without any carbon foot print has been drawing increasing attention as promising renewable energy sources in the last decade due to global energy crisis and environmental challenges. However, they are not yet commercialized at a large scale mainly due to the concern of poor high temperature stability and poor thermoelectric performance. Oxides such as doped $SrTiO_3$ are preferred as thermoelectric materials over conventional chalcogenides due to its high temperature stability and environmental benignity. However, dopped $SrTiO_3$ has been found to be critically suffering from Anderson localization of electrons resulting in poor electrical conductivity even after bearing large electron concentration. It also suffers from large thermal conductivity compared to chalcogenides resulting in poor thermoelectric performance. In the present study, we have fabricated carbon based (graphite, graphene oxides) composites with doped $SrTiO_3$. In one of our very recent works, we have obtained maximum *ZT* of 0.68 in La and Nb co-doped $SrTiO_3$ (LSTN)+graphite composite which is around 423% larger value than that of pristine LSTN. We have also obtained *ZT* of 1.42 in Nb doped $SrTiO_3$ +graphite composite which is a ground breaking result for n-type oxide thermoelectrics. Graphite has been found to be acting as a momentum booster in $SrTiO_3$ based matrix causing an order of magnitude increase in weighted mobility which otherwise suffers from Anderson localization of electrons. Lattice thermal conductivity in graphite composite is also suppressed especially at elevated temperature due to enhanced Umklapp scattering as confirmed by Debye-Callaway fitting. Finally, we have also constructed a 4-legged thermoelectric device in uni-leg configuration where we have achieved milli-watt level of power output. This remarkable power output is unattainable up until now in the context of oxide thermoelectrics.

ID: 05088
Type: Poster
Topic: Thermoelectric materials and materials processing

Point Defects and Thermoelectric Properties of Melt-grown Mg2Ge Single Crystals

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Recently, our research group found that Mg_2Sn single crystals (SCs) melt-grown under Ar atmosphere contained Mg vacancies (V_{Mg}) as a point defect, leading to lower thermal conductivity *?* and higher electrical conductivity *?* than Mg_2Sn polycrystals (PCs) [1,2]. Motivated by this study, we aimed to V_{Mg}-incorporated Mg_2Ge SCs, which has the same crystal structure as Mg_2Sn, to achieve higher thermoelectric (TE) properties than Mg_2Ge PCs. Mg_2Ge SCs were prepared by the melting method. Mg and Ge starting materials were enclosed in an alumina tube. The alumina tube was further enclosed in a quartz tube under Ar atmosphere. This ample was heated up to 1443 K for melting, and then cooled down to 1343 K over x hours (x = 6, 12, 24, and 36). From the Laue X-ray diffraction (XRD), prepared samples were found to be a PC for x = 6 and SCs for x =12, 24, and 36. As for the point defect, SC-XRD revealed that all samples contained V_{Mg}: the V_{Mg} fraction was about 3% independent of x. The *?* of the prepared Mg_2Ge SCs were higher than that of a Mg_2Ge PC reported in a previous study [3]. To reduce *?*, the V_{Mg} fraction should be increased further by optimizing the preparation conditions. The Mg_2Ge SC for x = 24 h showed the maximum zT = 0.15 at T = 700 K, which was larger than that of the Mg_2Ge PC [3]. In the presentation, we will present the other TE properties, comparing with those of the Mg_2Ge PC [3].

[1] W. Saito *et al.*, *Sci. Rep.*, **10**, 2020 (2020).

[2] W. Saito *et al.*, *ACS Appl. Mater. Interfaces*, **12**, 57888 (2020).

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ID: 05098
Type: Poster
Topic: Thermoelectric materials and materials processing

Using graphite as mobility boaster in La and Nb co-doped SrTiO3 for enhanced thermoelectric performance

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One of the greatest challenges of 21th century is global warming and escalating energy demand at the same time. Search of clean and sustainable energy source is one of the prominent concerns for scientific community. About two third of the energy produced in manufacturing industries, automobiles are wasted in the form of heat energy. Thermoelectric generator (TEG) has ability to convert this waste heat into useful electrical energy. Perovskite oxides are one of the promising materials for TEG with respect to conventional chalcogenides mainly due to their environmental benignity and high temperature stability. In this work, graphite composite with La and Nb co-doped $SrTiO_3$ (LSTN) are formed for high temperature power generation application in TEG devices. Electrical conductivity of pristine LSTN is found to be significantly supressed due to Anderson localization of electrons resulting poor figure of merit. However, it is posited that graphite works as a mobility boaster in LSTN matrix causing an order of magnitude increase in weighted mobility exceeding even the single crystal weighted mobility. Debye-Callaway model has been implemented to study the phonon transport mechanism where lattice thermal conductivity at elevated temperature has been found to be supressed after graphite incorporation due to dominating effect of Umklapp scattering. As a result, maximum ZT of 0.68 is obtained in LSTN+G composite which is more than 291% than that of pure LSTN. In addition, A module with four n-type legs (of LSTN+G) has been fabricated which is the first module to the best of our knowledge in polycrystalline $SrTiO_3$ system. The maximum power-output of 2.5 mW has been obtained with maximum open circuit voltage of 294mV. This remarkable power output is unattainable up until now in the context of oxide thermoelectrics. This also demonstrates a new strategy to design oxide thermoelectrics for better thermoelectric performance.

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Type: Poster
Topic: Thermoelectric materials and materials processing

Polycrystalline samples showing axis-dependent conduction polarity and investigation of new materials

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Most thermoelectric materials are not anisotropic in carrier polarity, with either holes (p-type) or electrons (n-type) as the primary carriers. However, several materials that exhibit axis-dependent carrier polarity have been reported so far, such as Mg, Zn, Cd, Re_4Si_7, and $NaSn_2As_2$ which have the unique property that holes are the main carriers in the interplane direction and electrons in the in-plane direction. By processing such materials in such a way that the layers are inclined with respect to the temperature difference, they could be applied to modules that utilize thermoelectric conversion (transverse thermoelectric conversion), in which the direction of the current and heat flow are different. However, the sample used in this report is a single crystal, so it is assumed that it would be difficult to fabricate a large sample to construct a transverse thermoelectric device. However, since the samples used in these reports are single crystals, it is difficult to fabricate large samples, and the performance index ZT is one order of magnitude smaller than that of conventional thermoelectric devices, making practical application of lateral thermoelectric devices difficult.

Therefore, in this presentation, 2 points will be reported: 1) an oriented polycrystalline sample of $NaSn_2As_2$ single crystal by uniaxial pressurized hot press sintering, which maintains the single crystal feature of anisotropic carrier polarity, and 2) first-principles calculation predicts that the axis-dependent conduction polarity emerges in EuCuAs upon heavily hole doping (approximately 0.1 holes per formula unit) because of their anisotropy in effective mass. Synthesis and measurement of transport properties of each sample, and even a prototype of a measurement device for transverse thermoelectricity will be presented.

ID: 05106
Type: Poster
Topic: Thermoelectric materials and materials processing

Adjustement of carrier concentration and texturation processing on thermoelectric silicide – Higher Manganese Silicide (HMS) and CrSi2

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We will present our recent results on silicide materials ($CrSi_2$ and MnSi?) which were selected for their low cost and/or advantageous properties. For example, the Nowotny-chimney ladder compounds MnSi? (? ~ 1.73)[1] is particularly interesting as it exhibits sufficiently high ZT values (? 0.5 at 500 °C) in a wide temperature range, which is an advantage for stable electricity production. These advantages render them ideal candidates for the development of industrial prototypes. $CrSi_2$ is also an interesting p-type alternative materials with similar structural features to above mentioned one, and we will present here recent results on the improvement of its thermoelectric properties through a slip-casting process under a strong magnetic field[2].

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ID: 05111
Type: Poster
Topic: Thermoelectric materials and materials processing

CMOS compatible silicon based thin films on 300 mm wafer level for thermoelectric applications

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The ever-increasing integration densities in nano- and microelectronics require innovations in thermal management strategies to meet industry requirements. Thermoelectric based temperature sensing, cooling as well as energy harvesting could be useful methods to achieve a reliable device performance and design energy efficient devices. This approach requires optimized CMOS compatible thin films. In this work, we characterized silicon, silicon germanium and silicides thin films fabricated in a 300 mm CMOS compatible cleanroom. For the thermoelectric characterization, we used a custom build setup to determine both Seebeck coefficient and sheet resistance. The results are benchmarked with established methods. For the sample preparation, we used physical and chemical vapor deposition (LPCVD and PVD) with *insitu* doping and subsequent rapid thermal annealing (RTA) on 300 mm wafers. Thin film properties such as film thickness (15-250 nm), elemental composition, crystallinity and microstructure are studied via spectroscopic ellipsometry, XPS, XRD and SEM. Further electrical transport properties like hall mobility and charge carrier concentration are determined via Hall measurements. The silicon based thin films reach Seebeck coefficients up to 1.5 mV/K in transition metal silicides. All examined layers are ready for industrial use and can be integrated into existing CMOS process flows. Thermoelectric approaches such as sensors, peltier coolers or energy harvesters depending on the characterized chemical and electronic properties of all films are discussed and represent a good possibility for thermal management of various electronic devices.

ID: 05138
Type: Poster
Topic: Thermoelectric materials and materials processing

Powder-Aerosol deposited (PAD) calcium manganate as n-type thermoelectric material

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Currently, calcium manganate $CaMnO_3$ and calcium cobaltite $Ca_3Co_4O_9$ are being investigated as n-type resp. p-type semiconducting materials as oxidation- and temperature-resistant thermoelectric materials for oxide multilayer thermoelectric generators (TEGs). In order to manufacture multilayer TEGs, pressure-assisted sintering processes at high temperatures are necessary to achieve optimal thermoelectric material properties. To realize TEGs in planar film technology, another method to obtain dense ceramic layers directly from the synthesized starting powders without a subsequent high temperature step is emerging recently: the powder aerosol deposition (PAD) method. In the present work, it is investigated whether PAD is suitable to produce dense ceramic films from Sm-doped $CaMnO_3$ and $Ca_3Co_4O_9$ powders. The resulting thermoelectric properties are characterized as a function of temperature.

$CaMnO_3$ powder could successfully be processed by PAD with resulting layer thicknesses of 5- 6 µm without any high-temperature sintering steps of the films. The electrical conductivity and the Seebeck coefficient of the films were determined in-plane from room temperature to 600 °C in air. The results show a Seebeck coefficient of around -200 µV/K, which is comparable to results of pressed and sintered bars. At 400 °C, the electrical conductivity corresponds to the conductivity of the bar. At higher temperatures the conductivity is better than with the reference. Below 400°C, the electrical conductivity is somewhat lower than that of the reference sample, a mild thermal treatment of the PAD layer improves it. It is expected that the thermal conductivity of the PAD film will be lower compared to the bars due to the nano-crystalline film morphology. This should result in a significantly increased ZT value for the PAD layers and a higher efficiency of the TEG.

The work shows that both $CaMnO_3$ and $Ca_3Co_4O_9$ can be successfully processed by PAD, and the PAD films show comparable thermoelectric properties.

ID: 05144
Type: Poster
Topic: Thermoelectric materials and materials processing

Application of MXene reinforced nanocomposites for thermoelectric power generation

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To recover waste heat and generate electricity thermoelectric materials have shown great potential. Energy conversion efficiency of these materials have been improved by making their nanocomposites. In the present work new generation 2D material MXene have been used to synthesize the nanocomposites with perovskite oxide ($SrTi_{0.85}Nb_{0.15}O_3$) and silicide ($Mg_2Si_{0.3}Sn_{0.7}$). $Ti_3C_2T_x$ MXene has been synthesized by selective etching of Al from Ti_3AlC_2 MAX phase using a low-cost processing technique. Nanosized layered sheets of MXene have been incorporated as inclusion in the matrix of thermoelectric materials by Spark Plasma Sintering (SPS) method. Seebeck coefficient, electrical conductivity and thermal conductivity of these nanocomposites have been measured in the temperature range from 323 K to 921 K and 323 K to 723 K for $SrTi_{0.85}Nb_{0.15}O_3$ and $Mg_2Si_{0.3}Sn_{0.7}$, respectively. These novel nanocomposites have shown significant improvement in the thermoelectric power factor (PF) and figure of merit (ZT). Further, transport properties of these composites have been analyzed in correlation with XRD, SEM, XPS and Raman spectra.

ID: 05147
Type: Poster
Topic: Thermoelectric materials and materials processing

Room Temperature Thermoelectric Performance of n-type Multiphase Pseudo-Binary Bi2Te3 – Bi2S3 Compounds

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The state-of-the-art thermoelectric material for the low temperature range (< 500K) is still based on Bi_2Te_3 alloys. Despite significant advances in the efficiency of *p*-type Bi_2Te_3-based materials through engineering the electronic band structure by multiple bands convergence, the *n*-type pair still suffers from poor efficiency due to lower number of electron pockets near the conduction band edge than the valence band, failing to take advantages of the power factor, , enhancement through engineering of the electronic band structure by multiple bands convergence. Therefore, a new approach is required to tackle its persistent low *z*T.

Recently, multiphase thermoelectric materials have attracted the attention of the thermoelectric research community due to higher degrees of freedoms that these materials provide to design high performance compounds through phonon scattering at interfaces, energy filtering, modulation doping, and potentially benefiting from incorporating magnetic interaction.

Here, we have fabricated multiphase pseudo-binary – compounds to take advantages of phonon scattering and energy filtering at interfaces, enhancing the efficinecy of these materials. These compounds contain and phases. (~0.28 eV) has higher band gaps than (~0.15 eV). The energy barrier generated at the interface of secondary phase of in the matrix resulted in higher Seebeck coefficient and consequently higher power factor in multiphase compounds than the single-phase alloys. This effect was combined with low thermal conductivity achieved through phonon scattering at the interfaces of finely structured multiphase compounds and resulted in relatively high thermoelectric efficiency of ~0.7 over 300-550K temperature range for multiphase sample of *n*-type $Bi_2Te_{2.75}S_{0.25}$, doubled the efficiency of single phase .

ID: 05152
Type: Poster
Topic: Thermoelectric materials and materials processing

Establishing synthesis-structure-property relationships for enhanced and reproducible MgAgSb thermoelectric properties

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Thermoelectric materials can directly convert thermal energy into electricity and vice versa. For high performance between room-temperature and 300 °C, ?-MgAgSb is a promising p-type thermoelectric (TE) material to produce the next generation of thermoelectric generator that could be used for a future lunar habitat. However, while the material certainly has attractive TE properties $zT_{average} > 1$) it is also known to be highly sensitive to small variations during the synthesis process often resulting in the formation of impurities (such as Ag_3Sb, Mg_3Sb_2, Ag, Sb). These likely deteriorate the TE performance and limit the reproducibility of the synthesis and hence, eventually its practical applicability.

We have established an improved synthesis procedure consisting of the following steps: inspired by literature, it starts with 8 hours of high energy ball mill to mechanically alloy Mg with Ag. This step is followed by a hot pressing at 673K for 8 minutes and a cleaning of the ball mill jar to avoid residues and limit compositional variation. Afterward, Sb is added to the MgAg precursor and ball milled for 5 more hours. The last step to complete the reaction is a sintering at 573K under 85MPa for 8 minutes.

We can show that the added cleaning step enhances the synthesis control, resulting in zT_{max} of 1.3 and a high batch-to-batch reproducibility. The impact of overall material composition and secondary phases on the TE properties is also analyzed, aiming to establish a synthesis-structure-property relationship for MgAgSb. It appears that the combination of Mg_3Sb_2 (p-type TE material) and Sb impurities do not affect the TE properties as much as Mg_3Sb_2 (n-type semiconductor) combined with Ag, identified to be highly detrimental. Hence, through the research, it is clear that $MgAg_{0.97}Sb_{0.995}$ is the best effective composition giving rise to the highest zT.

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Type: Poster
Topic: Thermoelectric materials and materials processing

Discovery of new thermoelectric copper-based sulfides

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Among the various possibilities offered by the periodic table, copper-rich sulfides represent a formidable source for the discovery of low cost and environmentally benign thermoelectric materials. Copper-rich sulfides form an important class where univalent copper is the dominant element, giving the possibility of creating hole carriers in the conductive “Cu–S” network for the generation of p-type thermoelectrics, as exemplified by bornite Cu_5FeS_4, germanite derivative $Cu_{22}Fe_8Ge_4S_{32}$,stannoidite $Cu_8Fe_3Sn_2S_{12}$, colusites $Cu_{26}T_2M_6S_{32}$ (T = V, Cr, Nb, Mo, Ta, W; M = Sn, Ge), synthetic Cu_2SnS_3, kesterite Cu_2ZnSnS_4, and tetrahedrites $Cu_{12}Sb_4S_{13}$. On this poster, recent advances in synthetic minerals and new sulphide compounds will be shown. Some peculiar structural features in connection with chemical bonding, such as the existence of metal complexes within the matrix and/or structural disorder, were carefully examined to establish rules and correlations between the crystal structures, electronic structures, vibrational and thermoelectric properties.

ID: 05217
Type: Poster
Topic: Thermoelectric materials and materials processing

On the enhancement of thermoelectric properties of Bi2-xYxO2Se ceramics

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Oxygen-containing compound Bi_2O_2Se due to its high thermal and good chemical stability along with its predicted promising semiconducting properties have attracted an extensive interest of thermoelectric research mainly as a perfect n-type thermoelectric counterpart of state-of-the-art p-type BiCuSeO materials. In this contribution, a concentration series of Yttrium-doped Bi2O2Se ($Bi_{2-xY}xO_2Se$) polycrystalline samples was prepared by the powder-metallurgy method within range of 0?x?0,2 and their transport and thermoelectric properties were investigated. The observed changes of the measured properties are discussed within terms of compositional purity of the studied samples and the changes in point defect structure as well. The enhancement of the power factor (~ 0.45 W.m-1.K-2 at 570 K for $Bi_{1.9}Y_{0.1}O_2Se$ sample) and the ZT parameter (~ 0.45 at 620 K for $Bi_{1.9}Y_{0.1}O_2Se$ sample) is presented.

ID: 05218
Type: Poster
Topic: Thermoelectric materials and materials processing

Influence of implantation induced defects on the thermoelectric properties of ScN

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In this work, noble gases were implanted to highlight only the role of defects on the thermoelectric properties of ScN and in particular to increase the phonons scattering. Indeed, ScN is known to have a relatively high power factor but its thermal conductivity is too high, 10-12 $W.m^{-1}.K^{-1}$ [1]. In this work, Ar ions were implanted into n-type ScN at room temperature in a high damage regime (5-6 dpa, at a low concentration < 0.3% Ar concentration) and then annealed at high temperature (1500 K, 10 min). The ScN (111) / Al_2O_3 (0001) thin films were synthesized by magnetron sputtering at 800°C. These 240 nm thick films were then characterized by different techniques such as XRD, Ellipsometry, Seebeck measurements, van der Pauw method for the electrical conductivity and TDTR for thermal conductivity. The implanted samples show an increase in resistivity from 1.64×10^{-4} ?.cm to 1.41×10^{-3} ?.cm at 300K but also a decrease in carrier mobility from 16 $cm^2.V^{-1}.s^{-1}$ to 4 $cm^2.V^{-1}.s^{-1}$. Post-implant annealing allows a partial restoration of the initial electric conductivity (restored at 90%). Similarly, the Seebeck coefficient is found to increase (by a factor of 3 at 600 K) with the introduction of defects and is roughly restored by the post-implant annealing leaving the power factor almost unchanged. However, the electrical, optical and structural characterization show that several defects are still present in the film even after annealing and would improve the *ZT* value. These leads to the reduction of the thermal conductivity in particular after implantation the value of *k* is divided by 3. Annealing partially restore the thermal conductivity via the reduction and evolution of defects. Furthermore, TEM observations are in progress to study the as-formed defects according to the gas implanted.

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ID: 05231
Type: Poster
Topic: Thermoelectric materials and materials processing

Impact of oxygen deficiency on thermoelectric properties of Bi2O2Se

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Bismuth oxyselenide, Bi_2O_2Se, is a promising low thermal conductivity thermoelectric material. While extensive research of this material goes on for over a decade, understanding of defects, vacancies, and the role of doping is inconsistent within the literature. To evaluate existing doping studies with a non-stoichiometric Bi_2O_2Se, we prepared oxygen-deficient Bi_2O_2Se. Polycrystalline samples with the composition $Bi_2O_{2-x}Se$ are synthesized by solid-state reaction and compacted using a hot-pressing technique. Thermoelectric properties in the temperature range of 300 to 780K are studied. We compare the measured results with previous theoretical and experimental results to further assess the role of non-stichometry in Bi_2O_2Se properties in the frame of thermoelectric performance. The study also includes various synthesis methods.

ID: 05239
Type: Poster
Topic: Thermoelectric materials and materials processing

Thermoelectric properties of Mg(Si, Sn) prepared by different grades of Si-kerf from PV manufacturing

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Nowadays, silicide-based thermoelectric (TE) materials are very promising for heat-electricity conversion devices at medium temperatures, due to their low cost, abundance, as well as their non-toxicity. At the same time, recycling approaches have been applied in the fabrication process of TE, by using silicon from the photovoltaic industry, as more than 50% of materials end up as kerf, upon the cutting procedure of the Si wafer. In this work, we use Si-kerf to fabricate high-quality Bi-doped Mg(Si, Sn) TE materials. The synthesis method employed is ball milling, followed by hot pressing to sinter the TE samples and provide suitable shapes and dimensions for the oncoming thermoelectric measurements. The captured figure-of-merit is very compatible with the case of using pure crystalline Si and other similar studies using Si-kerf. The use of Si-kerf for the synthesis and fabrication of TE elements and modules is of high importance for a green transition, as it adopts a circular approach by using recycled materials.

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

ID: 05241
Type: Poster
Topic: Thermoelectric materials and materials processing

Laser Processing of Zn4Sb3 Thermoelectric Powders

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Fast sintering of thermoelectric powders is a powerful strategy used to achieve a nanostructured bulk sample. The nanostructure obtained by fast sintering processes like spark plasma sintering or open die pressing starting from nanopowders, showed improved materials performance also in bulk form. However, thermal stability of the microstructure produced, reproducibility of the performance or effects of the nanostructuring on the resistance to oxidation are limiting factor to industrial exploitation.

The increasing interest on additive solutions for 3D building of complex structures suggests an opportunity to grow thermoelectric devices via layer-by-layer sintering of a powder bed. Up to date, such a possibility has been mainly investigated by LeBlanc et al. who realised a built element of chalcogenide through selected laser melting (SLM) The technique used was only partially effective due to the geometrical characteristics of the chalcogenide powder which didn’t match the technological needs for SLM processing. At the same time, some groups are developing a laser processing with the target of a simultaneous synthesis and sintering of thermoelectric pellets starting from pressed precursors powders.

In this work we present the preliminary results of a laser processing of Zn_4Sb_3 powders. An investigation on the development of the thermoelectric powders to be processed is presented. The main target, is related to achieve a powder fitting the laser processing needs in terms of morphology without involving atomization process. An experimental setup has been designed to investigate the effects of different combinations of laser parameters on the obtained microstructure. Sintering dynamics in the thermoelectric powders have been investigated by SEM and EDS analyses. The thermal effects observed have been used to design a continuous line sintering.

Our work aims to understand the laser processing mechanisms in different operating conditions for the development of an effective additive approach, a new perspective for thermoelectric micro-device fabrication.

ID: 05274
Type: Indiferrent
Topic: Thermoelectric materials and materials processing

Silicon-alloy thermoelectric nanostructured fibers

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The tremendous increase in energy demand and interest in expanding the internet of things (IoT) to build more sustainable cities and communities led to a much-needed boost in energy sources for low-power microelectronics. Thermoelectric (TE) materials present a versatile and environmentally beneficial option to harvest energy from ambient waste heat to power this transition. Moreover, thanks to nanostructurization, commonly poor TE materials (i.e., silicon) have remarkably enhanced their TE properties; this is the case for nanowires and Si-based fabrics made of nanotubes. Nonetheless, the scalability of Si-based nanostructured materials remains a challenge.

In the present work, Silicon-alloys (SiGe and silicides) nanotubes were studied due to their easy integrability in the electronics industry, abundance, and low extraction environmental impact. Most importantly, the fabrication of TE nanotubes was up-scaled to large areas. The nanotubes were fabricated in a multistep process, including an electrospun fiber template and chemical vapor deposition (CVD).

Different strategies to improve Silicon-alloys performance as TE materials were explored to optimize their *Figure of Merit* $ZT = ?\ S^2/?$. The thermal conductivity *?* was tuned by fast thermal treatments employing Laser Flash Measurements; the Seebeck coefficient was modified by varying the ratio between silicon and the alloying elements (Mg, Ge). We have also studied the change of *?* by controlling the material’s doping and the thickness of the nanostructures. Likewise, a complete morphological and compositional characterization was performed using electron microscopy techniques, EDX, and XRD.

To conclude, the suitability of electrospinning and CVD to fabricate large-area and flexible TE materials were successfully accessed. Furthermore, the TE properties were investigated, and steps to optimal morphology and compositional conditions of the Si-alloy materials were found.

ID: 05282
Type: Poster
Topic: Thermoelectric materials and materials processing

Thermoelectric performance of Y-doped CaMnO3-based oxides processed by ball milling

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$CaMnO_3$-based oxides offer a good combination between thermal and electronic transport properties; their charge transport is dominated by hopping of small polarons, which couple charge carriers with lattice polarization [1]. Earlier studies have shown that Y doping of Ca_2MnO_4 compounds enhances charge carrier mobility by up to 2.5 times compared to the case of La doping, while maintaining similar charge carrier concentration [2]. Here, we use ball milling (BM) to examine optional ways to improve thermoelectric (TE) performance of Y-doped $CaMnO_3$ materials. Employing characterization techniques such as x-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive x-ray spectroscopy (EDS), we investigate how BM energy and duration affect bulk density, microstructure, chemical composition, and electronic transport. We find that relative bulk density and electrical conductivity of samples processed at 250 RPM for 15 min. increase by 15 and 230 %, respectively, compared to samples produced from manually milled powder. Our work suggests that bulk density and TE performance of $CaMnO_3$-based materials can be enhanced using low energy and short duration BM powder processing.

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ID: 05343
Type: Indiferrent
Topic: Thermoelectric materials and materials processing

Refractory Metal Inclusions and Their Impact on the Thermoelectric Performance of La3-xTe4 Composites

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Lanthanum telluride (La3-xTe4) has recently emerged as a high-efficiency n-type thermoelectric material. The performance of the La3-xTe4 system arise from a complex defect thorium phosphide (Th3P4) crystal structure, where La3+ vacancies control a wide range of carrier concentrations from degenerately to intrinsically semiconducting. Optimizing the carrier concentration leads to a large power factor (?S2) that, combined with the intrinsically low lattice thermal conductivity, allow La3-xTe4 to achieve a ZT of 1.2 at 1275 K.

Previously, our group has demonstrated a 25% increase in ?S2 of La3-xTe4 with the addition of 12-15 vol% Ni inclusions on the order of 2-3 microns. The enhancement in ZT is a result of composite-assisted funneling of electrons (CAFE), where the inclusions form a charge funneling network that reduces the electrical resistivity of the composite while leaving the thermal conductivity and thermopower virtually unchanged. Further improvements to the ZT of these La3-xTe4-Ni composites have also been demonstrated using nanoscale Ni inclusions, at an equivalent volume fraction, leading to a 60% improvement in over baseline La3-xTe4 from a further increased ?S2 and lower thermal conductivity. Here we will investigate the use of other metallic inclusions to improve the thermoelectric performance of La3-xTe4. Varying volume fractions of refractory metal inclusions were combined with La3-xTe4 and then compacted using spark plasma sintering. The temperature dependent electrical resistivity, thermopower, and thermal conductivity data of the sintered compacts will be presented

Transport phenomena

ID: 05057
Type: Poster
Topic: Transport phenomena

Dynamic instability of higher manganese silicides

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Higher manganese silicide (HMS) based materials exhibit remarkable refractory and thermoelectric transport properties. Being an incommensurate composite, HMS embodies unusual spacing and orientational anomalies, which are amplified at higher temperatures. We demonstrate the structural-property modulations at higher temperatures for the highly oriented $MnSi_{1.74}$ single crystal synthesized employing the Bridgman method. A labile Si-sublattice and inter-evolutions within the commensurately prevailing HMS phases were observed which can be correlated to an irrepressible and hysterical deviation in the electrical transport measured during a thermal cycle at temperature ~ 500-800K. These observations pave the way for understanding the inherent thermodynamic instability of HMS phases which is associated with an unusual hysteresis in the electrical transport at higher temperatures.

ID: 05063
Type: Indiferrent
Topic: Transport phenomena

On the phonon and magnon drag thermopower

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Bosons that exchanges momentum with the system of charge carriers may introduce a drag contribution to the thermoelectric power. As a consequence, besides the diffusive mechanism, thermoelectric power can be also generated via the so called drag mechanisms. A more familiar phonon drag contribution (S_{ph}) is eminent when phonons, diffusing along the direction of the thermal gradient like charge carriers, are thermalized by scattering preferentially with charge carriers. Consequently, S_{ph} is observed in pure and defectless materials at low temperatures as in highly disordered materials and/or high temperatures phonon relaxation is dominated by different processes.

The magnon drag contribution (S_{mag}) to the Seebeck effect is reminiscent to the phonon drag effect; proportional to the magnon specific heat C_m and the characteristic scattering parameter reflecting the magnon-carrier scattering rate with respect to any other relaxing mechanism (magnon-grain boundary, magnon-defect, magnon-phonon, magnon-magnon,...). The typical temperature window, where magnon-drag manifests significantly, is shifted to higher temperatures with respect to phonon drag due to the different dynamics of the magnons. Moreover a more complex situation can occur in case of magnon drag when the effect of magnon decay, characterized by the Gilbert damping parameter, prevails over the viscous hydrodynamic S_{mag} naturally strengthening the diffusive thermopower. In such a case the drag governed by the magnon decay acts in the opposite direction.

Considering the characteristic time and length scales of phonon/magnon drag, depending on electron-phonon/magnon interaction, respective specific heat and group velocity we will exemplify and discuss our experimental data where above mentioned drag effects are observed.

ID: 05065
Type: Poster
Topic: Transport phenomena

Thermoelectric and magnetic properties of Co2ZrSn and Co2HfSn Heusler alloys

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

In this work, Co_2ZrSn and Co_2HfSn Heusler alloys were studied by combining experimental and ab-initio investigations in order to accurately estimate their electronic density of states in proximity of the Fermi level and to measure their transport properties over a wide range of temperatures. The effect of secondary phases which are typically present in this type of alloy was also taken in account. The thermoelectric properties were determined both for compounds in which the amount of such impurities is negligible and for samples with secondary phases content up to 20% in weight. The effect of these on the transport properties is discussed in detail. In particular, an increase of electrical conductivity was observed for the spurious alloys, which translates on an increase of power factor. On the contrary, the Seebeck coefficient is overall not greatly influenced by the presence of impurities.

ID: 05068
Type: Poster
Topic: Transport phenomena

Determination of transport properties of a electrochemically deposited polycrystalline SnSe thin film on Au-substrate by spectroscopic ellipsometry

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In this work we investigate the transport properties at room temperature of electrochemically deposited polycrystalline SnSe thin film on Au-substrate by spectroscopic ellipsometrie (SE). The electroplating experiments were conducted in a three-electrode cell configuration: a KCl-sat. AgCl/Ag reference electrode, a Pt wire counter-electrode and an Au-coated glass working electrode. The bath was defined as $SnCl_2.2H_2O$ and $Na_2SeO_3.5H_2O$ as precursors of Tin and Selenide respectively in presence of oxalate salt as stabilizing reagent, operated at 50°C and continuously deaerated by an Ar flux. The films were obtained in potentiostatic pulse mode by applying a potential step of -0,55 V.

Due to the electrically conductive Au-substrate the conventional Hall effect cannot be used to determine the transport properties of the sample. Therefore measurements were carried out by spectroscopic ellipsometry in the IR photon energy range for three angles of incidence (AOI) 65°, 70° and 75° respectively. Ellipsometry uses the fact, that the polarization state of light changes when it is reflected from a surface of a solid material. Ellipsometry does not directly measure optical constants, it measures change in light polarization expressed as the ellipsometric angles Psi and delta. From these, one obtains by model fitting the real and imaginary part of the dielectric function e_1 and e_2 respectively as a function of photon energy.

A successive steps evaluation of the SE data in the photon energy range 0.10 eV to 0.35 eV finally evidenced a Drude compatible fitting model.

Based on the literature the carriers were assumed to be *p*-type and the transport parameters of the SnSe film were estimated by p = 1.22 × 10^{20} cm^{-3} and the mobility by ? = 60 $cm^2V^{-1}s^{-1}$.

ID: 05090
Type: Poster
Topic: Transport phenomena

Transverse thermoelectric properties of CuCr2X4 (X=S, Se and Te), experiment and ab-initio calculation

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We present a combined experimental and theoretical study of the transverse thermoelectric properties, namely anomalous Nernst effect, of ferrimagnetic spinels $CuCr_2X_4$ (X=S, Se, Te).

The $CuCr_2X_4$ phases exhibit long range ferrimagnetic ordering below T_C?380, 430 and 325 K for X=S, Se, and Te, respectively, with saturated magnetic moment at low temperature around 5 µB. It was found that the behavior of anomalous Hall (AHE) and anomalous Nernst (ANE) effects in $CuCr_2Se_4$ corresponds to the intrinsic mechanism explained by Karplus-Luttinger theory and its modern generalization based on the Berry-phase approach. We assumed that the same approach can be applied for $CuCr_2S_4$ and $CuCr_2Te_4$.

The observed ANE is negative at room temperature for all phases. The highest absolute value up to ~1.5 µV/K is observed for $CuCr_2Te_4$, but at room temperature it is exceeded by ANE of $CuCr_2Se_4$ due to lower T_C of $CuCr_2Te_4$. A sign change of ANE to positive is observed at 285 K for $CuCr_2S_4$ and at 65 K for $CuCr_2Se_4$. The trend of ANE is reproduced by Berry phase approach using the band structures obtained by calculations based on Density Functional Theory (DFT), however, for better agreement the renormalization of the bands has to be taken into account. In principle, the strong correlation effects of d-electrons yield bandwidth renormalization, namely narrowing of the bands, which cannot be evaluated by the DFT approach.

For the possible thermoelectric applications it is interesting that the magnitude of the ANE displays the same trend as the electrical conductivity, i.e. they both increase from X =S to Te, and thus both enhance the “transverse” power factor $P_{xy}= S_{xy}^2 \cdot ?_{yy}$. However, the possible application of the Nernst effect of $CuCr_2Te_4$ is limited by a rather low critical temperature of the long range magnetic ordering.

ID: 05157
Type: Indiferrent
Topic: Transport phenomena

Bipolar transport in Bi-Sb alloys

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The Bi-Sb alloy space contains the best materials for low temperature cooling applications, exhibiting excellent mobility and Seebeck as well as a maximum zT near 0.5 at 200K. This extremely low-temperature maximum arises from a reported band gap of less than 100 meV. In a device, a significant fraction of each thermoelectric leg operates within the bipolar regime. Bipolar electronic transport behavior is not often analyzed in literature, but a robust bipolar analysis is an effective tool for understanding and optimizing thermoelectric performance. We have developed a framework for bipolar analysis which unites low temperature experimental measurements with high accuracy first-principles calculations. Several unique assumptions are applied to allow for deeper analysis of fundamental transport coefficients (band gap, effective mass, Fermi level, and scattering rate) and their evolution with temperature.

Using well-established alloy modeling techniques including special quasi-random structures (SQS) and effective band structure (EBS), we obtained alloy effective masses and band gaps from first-principles calculations. Polycrystalline samples of Bi-Sb alloys were melt-synthesized and hot pressed to produce samples. Seebeck, resistivity, and Hall measurements were taken from 2K to 473K; semiconducting Bi-Sb alloys are natively n-type. Before the transition to bipolar behavior around 150K, this data is analyzed using a single parabolic band model. At higher temperatures, the experimental data is fit to the bipolar equations for Seebeck and Hall coefficients, and band gap, hole effective mass, and temperature dependent Fermi level are extracted. The scattering rate ratio is also extracted and combined with conductivity to obtain the absolute scattering rates. Finally, a best fit is determined by comparing the model to the theoretical hole effective mass and band gap. With this methodology established, the model can (i) be extended to understand how changes in chemistry or processing affects thermoelectric transport and (ii) optimize thermoelectric performance of the bipolar regime.

ID: 05165
Type: Poster
Topic: Transport phenomena

Disorder-induced localization for bidimensional thermolectrics optimization

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Early work by Ioffe has developed into the standard thermoelectric optimization paradigm of tuning the electronic carrier concentration in semiconductors. Although the localization theory of electrons by Anderson and Mott has developed in parallel, its potential for thermoelectrics optimization has not been explored. Here, we show that structural-disorder-induced electron localization also provides an effective optimization strategy for thermoelectric materials. By using a transport model that includes the relevant physics of localization, it is shown that the maximum thermoelectric figure of merit can be increased ~20% by tuning both carrier concentration and disorder. The benefit of slight disorder is confirmed in two model Ge-Sb-Te material systems. This work provides a transferable and experimentally verified model that adds to our understanding of charge transport in disordered solids. By including the relevant physics of Anderson-like electron localization with current state-of-the-art methods of thermoelectric material optimization, we demonstrate a new avenue of charge transport engineering in solids. Particularly for highly degenerate semiconductors, this bidimensional optimization strategy provides a new methodology to attain high thermoelectric performance.

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Type: Indiferrent
Topic: Transport phenomena

Highly efficient Monte Carlo simulation method for transport in complex nanostructured thermoelectric materials

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The general method to evaluate thermoelectric (TE) transport in bulk materials is to solve the semi-classical Boltzmann transport equation (BTE). However, in complex nanostructured materials, the use of analytical BTE cannot accurately model the TE coefficients. Typically, Monte Carlo (MC) ray-tracing simulation approach can model transport in nanostructured configurations efficiently in real space, accounting for all the peculiarities of the nanostructured domain. These simulations, however, tend to be overly computationally expensive. Their major issues are- i) the nano-features spanning from macro- to nano-scale (including boundaries, potential barriers, pores, nano-inclusions, atomic defects, etc.), slow down the flow of particles (and thus conductivity) significantly, and ii) the net flux computed by the subtraction of two opposite flowing fluxes, under linear response operation (small fields), is statistically and computationally very difficult. Typical simulations in a micrometer length channel will require 50 million particle simulations and hundreds of CPU hours.

Here, we present a novel MC ray-tracing algorithm with a computational efficiency of at least 2 orders of magnitude compared to existing algorithms. It is specifically ideal for Seebeck coefficient calculations, which present otherwise significant challenges as a transport under temperature gradients that is typically numerically much more challenging and cumbersome compared to the transport under-voltage gradients. Our new method utilizes only a limited number of ray-tracing particles and merges ideas from the calculation of the analytical BTE, allowing it to avoid the statistically challenging subtraction of two opposite going fluxes, but also the application of a driving force altogether, which sometimes leads to different type of numerical issues. We demonstrate the algorithm’s efficiency in accurately simulating large domain nanostructures with multiple defects, and use it to study electronic transport in highly complex nanostructured materials. We believe our work provides a more efficient and user-friendly algorithm, which will enable the proper study of nanostructured TE materials.

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Topic: Transport phenomena

Measurement of ionic Seebeck coefficient of Cu2-?Se at the phase transition

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Copper selenide undergoes a superionic phase transition. Since the mobile Cu+ ions are present in the structure, there exists a thermoelectric effect related to those carriers. The transport part of the ionic Seebeck coefficient was measured by Balapanov, at temperatures significantly above the transition, e.g. [1]. There exist one report [2] about ionic thermodiffusion at the phase transition temperature, but it was performed in untypical conditions.

A method of measurement of the ionic Seebeck coefficient of copper selenide has been developed. The desired temperature range required the preparation of Cu+ electrolyte; a $C_6H_{12}N_4CH_3I$+CuI mixture was chosen. A sandwich-like assembly of the investigated material and electrodes was used. In the steady-state conditions, the total ionic Seebeck coefficient was measured, according to Wagner’s paper [3]. Values were found to be on the order of millivolts per Kelvin, increasing from low- to high-temperature phase. The temperature range, in which the change occurs agrees with the mixed-phase composition range.

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ID: 05225
Type: Indiferrent
Topic: Transport phenomena

Thermoelectrical properties and EPR in Sb2-xCuxTe3 single crystals

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Sb_2Te_3 is a thermoelectric material for room temperature applications [1]. However, the efficiency of a thermoelectric material is limited by its low value of figure of merit, $ZT=S^2T/rk$, where r is the resistivity, S is the Seebeck coefficient and k is the thermal conductivity. Tuning of the transport properties, viz., r, S and k by doping of thermoelectric materials such as Sb_2Te_3 are important and effective [2-4]. It is clear that to increase the value of ZT, it is important to increase the mobility and *n* of charge carriers.

In this study, we investigate the influence of doping with copper on the thermoelectrical properties at 77<T<330K and concentration of holes (using Shubnikov–de Haas effect) in $Sb_{2-x}Cu_xTe_3$ (0?x?0.1) single crystals. In addition, we investigate the influence of doping with copper on electron paramagnetic resonance of *p*-$Sb_{2-x}Cu_xTe_3$ single crystals. EPR measurements show that the copper atoms in the studied samples are most likely in the spinless Cu^{+1} state.

We obtained that Seebeck coefficient in $Sb_{2-x}Cu_xTe_3$ single crystals decreases with addition of copper. Heat conductivity of the samples with copper was slightly higher than of the pristine Sb_2Te_3. Electrical resistance decreases with doping. As a result, the thermoelectric figure of merit ZT decreases at 77<T<300 K and increases with increasing the Cu content at T=330 K. Thus, doping by copper is promising for fabrication of a new effective thermoelectric material based on bismuth-antimony telluride because Cu increases its electrical conductivity without essential change in the thermal conductivity and thermopower.

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Type: Poster
Topic: Transport phenomena

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

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High-entropy oxides (HEOs) are a new class of multicomponent oxides stabilized by configurational entropy. When various elements occupy one site in a crystal structure, the neighborhood of each cation is different. This leads to a strong lattice strain that distorts the atom positions [1-2]. Triple conducting oxides (TCOs) belong to a group of mixed ion-electron conductors which may contain three mobile charge carriers - electrons, protons, and oxygen ions. We propose that the combination of high configurational entropy and mixed oxygen ionic, protonic and electronic conductivity (HEOs-TCOs) of selected high-entropy perovskites may render them interesting thermoelectric and electrochemical materials [3].

This work is related to the systematic description and understanding of the thermoelectric and electrochemical properties of different $(Sr,Ba)(Ce,Zr,Y,Ti,Sn,Fe,Co,Bi)O_3$ oxides that are protonic, oxygen ionic and electronic conductors. The structure and microstructure of these materials will be analyzed with the use of X-ray Diffractometry (XRD) and Scanning Electron Microscopy (SEM). Electrochemical measurements will be performed both by DC four-wire technique and Electrochemical Impedance Spectroscopy (EIS) as a function of temperature and water vapour or oxygen partial pressures. The temperature dependence of the Seebeck coefficient and Figure of Merit (ZT) will also be measured as a function of pH_2O and pO_2.

The results of preliminary measurements done for different samples: $BaCe_{0.6}Zr_{0.2}Y_{0.2}O_{3-?}$, $BaCe_{0.6}Zr_{0.2}Y_{0.1}M_{0.1}O_{3-?}$, (M=transition metals like Pr,Tb and Fe) and $BaZr_{0.1}Hf_{0.1}Sn_{0.1}Ti_{0.1}Ce_{0.1}Y_{0.1}Fe_{0.1}Co_{0.1}Bi_{0.1}Zn_{0.1}O_{3-?}$ shown the great influence of number of elements in the materials and the presence of protonic defects in the samples on the both electrical conductivity and Seebeck coefficient.

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Topic: Transport phenomena

Thermal conductivity in BiSb alloys

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Bismuth-antimony alloys are among the most efficient thermoelectric materials for low-temperature applications. Despite relatively simple crystal structure, their lattice thermal conductivity is known to be strongly suppressed, with values below 1 W/mK at 300 K for Bi-rich samples. In the current study, we address origin of this important feature. Bulk polycrystalline samples were studied by means of thermal conductivity, Seebeck coefficient, electrical resistivity, heat capacity and sounds velocity measurements. The experiments were supported by ab-initio calculations of phonon dispersion and electron density distribution. Suppression of phonon transport in BiSb alloys is found to occur due to combination of (i) extremely soft bonding, (ii) large anharmonicity, and (iii) efficient point-defect scattering of phonons due to strain field. Soft character of chemical bonding is quantified in pure bismuth by the lowest sound velocity among state-of-the-art thermoelectric materials (v_s = 1284 m/s), small Debye temperature, and low values of the calculated elastic moduli. Its phonon dispersion comprises relatively low-lying optical modes, signatures of which are detectable via Einstein peaks in heat capacity. Sizable anharmonicity is confirmed by experimental Gruneisen parameter, $?_G$ = 2.04. Its origin is resonant character of the atomic interactions for Bi, as indicated by ab-initio calculations. Last but not least, for Bi-Sb alloys we report on intense scattering of phonons on strain fields resultant from point defects. Efficiency of this scattering mechanisms stems from disparity of elastic properties for the parent elements — bulk, shear, and Young’s moduli as well as Poisson ratio show variation up to 85% between Bi and Sb. The presented conteptual framework can be useful for understanding low thermal conductivity in novel functional alloys.

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Topic: Transport phenomena

Bonding pattern and atomic disorder vs. thermoelectric properties in Ga3Fe-type intermetallic semiconductors

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The intermetallic compounds with composition $Tr_3T^{(8)}$ (Tr = Ga, In; $T^{(8)}$ = Fe, Rh, Os) and tetragonal crystal structure of the Ga_3Fe-type (Space group $P4_2/mnm$, Pearson symbol t*P16*) are semiconductors. Thereby, their thermoelectric properties have been the object of numerous studies, including their substitution derivatives, aiming optimization of the transport properties by band-gap tailoring [1].

The crystal structure of Ga_3Fe, built on the basis of corner-sharing tetracapped trigonal double prisms *ttdps*, results in a unit cell with the composition $Ga1_4Ga2_8Fe_4$ and a valence electron count of 68 ve/uc. This atomic arrangement presents an electronic structure of higher complexity. The detailed bonding analysis shows the presence of three-center Fe-Ga-Ga' bonds, which at the same time have a direct influence on the Fe-Fe bonding in the dumbbell [2]. This results in a structuring of the electronic density of states appropriate for electronic transport property tuning.

In addition, the crystal structure of isotypic compounds show the singular common feature of large and anisotropic atomic displacement parameters (ADPs) for the gallium atoms. The temperature dependency of the ADPs has been studied for Ga_3Fe and *ht*-Ga_3Ir, the latter being a rather unexpectedly semiconductor. The rather low lattice thermal conductivity observed in *ht*-Ga_3Ir can be assessed to a complex local atomic disorder [3].

We discuss the relation between the lattice thermal conductivities, bonding pattern and the static or dynamic nature of the atomic disorder reflected by the ADPs.

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