Poster Presentation Program

Poster Session 2: Wednesday (Applications, Modules Development and Technology, New Materials and New Materials Discovery, Other Materials, Process and Silicides)

Poster Position	Name of the presenter	Email address	Title of the poster
Applications			
P.1	Araiz Miguel	miguel.araiz@unavarra.es	Passive Thermoelectric Generator for Waste Heat Recovery from a Combustion Chamber
P.2	Aranguren Patricia	patricia.arangureng@unavarra.es	The importance of the assembly in thermoelectric generators
P.3	Attar Alaa	Loattar@kau.edu.sa	Optimum Design of Thermoelectric Cooler Used for Electronic Application
P.4	Bahk Je-Hyeong	bahkjg@uc.edu	Cost-effective metal-based thermoelectric power generator for waste heat recovery from fireplace
P.5	Beltrán-Pitarch Braulio	beltranb@uji.es	Problems and sources of errors in the Harman method identified by impedance spectroscopy
P.6	Boldrini Stefano	stefano.boldrini@cnr.it	Investigation of pulsed thermoelectric performances by impedance spectroscopy
P.7	Garcia Gustavo	ggarcia@centrostirling.com	Development and Experimental Validation of a new off-grid Thermoelectric Fancoil for Domestic Heating
P.8	Heber Lars	Lars.Heber@dlr.de	Thermoelectric Generators for Heavy-Duty Vehicles: A Systemic Approach and Development
P.9	Kim Duckjong	dkim@kimm.re.kr	Novel thermal interface material for high-temperature thermoelectric power generators
P.10	Kim Yong Jun	kyj921@kaist.ac.kr	Self-powered wireless sensor node driven by a flexible thermoelectric generator for industrial environmental monitoring
P.11	Lee Jaewoo	jaewoo@etri.re.kr	Design and Fabrication of Thermoelectric Generator based on BiTe legs for Wearable Device Application
P.12	Lin Yu-Li	yllin@itri.org.tw	Industrial Waste Heat Recovery by Thermoelectric Generators
P.13	Lorenzi Bruno	bruno.lorenzi@unimib.it	Experimental evaluation of wide-gap solar cell thermoelectric hybridization

P.14	Mesalam Ramy	rm467@leicester.ac.uk	The European Am-241 Radioisotope Thermoelectric Generator programme and the effect of cold-side thermoelectric temperature on specific power
P.15	Osipkov Alexey	osipkov@bmstu.ru	Analysis of automobile thermoelectric generator hot heat exchanger design influence on overall vehicle fuel efficiency for urban driving cycles
P.16	Osipkov Alexey	osipkov@bmstu.ru	Applicability limits of a maximum power point tracking controller for thermoelectric generator systems in non-stationary conditions
P.17	Riggio Justin	justin.riggio@mail.mcgill.ca	A Thermoelectric Generator Concept For Waste Heat Recovery
P.18	Snajdarek Ladislav	snajdarek@fme.vutbr.cz	Autonomous power supply for hot water boiler cooling utilizing thermoelectric generators additionally integrated in flue gas duct
P.19	Tabakovic Momir	momir.tabakovic@gmail.com	High temperature thermoelectric generator units in relation to and low temperature Bi_2Te_3 thermoelectric generator unit for direct conversion of waste heat from a wooden pellet stove into electric energy
P.20	Ulibarrena David	david.astrain@unavarra.es	Efficiency Improvement Of A Co_2 Vapour Compression Refrigeration System By Means Of Thermoelectric Subcooling
P.21	Van Nong Ngo	ngno@dtu.dk	A Novel Off-grid Solar-Thermoelectric Desalination System
P.22	Walsh Keith	keith.p.walsh@btinternet.com	Thermoelectric Eddy Current in Bio-Compatible Materials
P.23	Werner Robin	Robin.Werner@uni-bayreuth.de	On the development of a new measurement system for conductivity, Hall constant and Seebeck coefficient
P.24	You Hao-Jen	Haojen.you@gmail.com	Evaluation of Thin-Film Thermoelectric Device Properties and Efficiency by I-V Curves and Simulation
		Modules Development and Technology	
P.25	Amagai Yasutaka	y-amagai@aist.go.jp	Apparatus for Measurement of the Output Power and Efficiency of Flexible Thermoelectric Power Generators
P.26	Bae Sang Hyun	khansh@koreatech.ac.kr	Melt-spinning process effects on enhanced conductivity ratio in $Ce_xFe_3CoSb_{12}$ thermoelectrics
P.27	Chetty Raju	chetty-raju@aist.go.jp	Fabrication of diffusion barriers in Colusite-based thermoelectric elements
P.28	Ferrario Alberto	alberto.ferrario@cnr.it	Matlab modeling of thermoelectric modules including thermal losses

P.29	Garcia Gustavo	ggarcia@centrostirling.com	A Novel Thermoelectric Leg Structure oriented to Cycling Robustness at High Temperature and Low Manufacturing Cost
P.30	Han Seung-Woo	swhan@kimm.re.kr	Radial thin film thermoelectric device for hot spot cooling
P.31	Ikeuchi Satoaki	satoaki_ikeuchi@advance-riko.com	Development of evaluation instrument in thermoelectric module in air
P.32	Kaszyca Kamil	kaszyca@itme.edu.pl	Innovative Segmented Thermoelectric Module for Energy Generation
P.33	Kim Yeongseon	qzerolinep@gmail.com	Development of metallization technique for thermoelectric module using polycrystalline SnSe
P.34	Lin Bin	ben_lin@leizig.com	Solar photovoltaic _ photothermal _ thermoelectric power generation system
P.35	Merkulov Oleg	Merkulov@ihim.uran.ru	Design And Testing Of A Tubular Thermoelectric Module Based On Oxide Elements
P.36	Miyazaki Yuzuru	miya@crystal.apph.tohoku.ac.jp	Design and evaluation of $Fe_2V(Al_{0.9}Si_{0.1})$/Cu tilted-multilayer thermoelectric devices
P.37	Okawa Kenjiro	okawa.k@aist.go.jp	Comparison of Three Accurate Measurement Methods for Measuring the Efficiency in Thermoelectric Modules
P.38	Park Hwanjoo	phwanjoo@gmail.com	Watch strap-shaped flexible thermoelectric body-heat harvester based on inorganic bulk materials
P.39	Ryu Byungki	byungkiryu@keri.re.kr	Design of segmented/graded Thermoelectric Devices based on Beta-Formalism
P.40	Salleras Marc	marc.salleras@imb-cnm.csic.es	Integration of a heat exchanger on an all Si-based thermoelectric micro/nanogenerator
P.41	Satoh Norifusa	SATOH.Norifusa@nims.go.jp	Organic π-type thermoelectric module patterned with photolithographic mold
P.42	Uenuma Mutsunori	uenuma@ms.naist.jp	Flexible TEG using Amorphous InGaZnO Thin Film
P.43	Yoo Chung-Yul	cyoo@kier.re.kr	Interpretation of Frequency Response Analysis in Thermoelectric Modules
P.44	Zhang Zheng	mezzhang@scut.edu.cn	Separation structure and enhanced cooling experiments of a TEM

New Materials and New Materials Discovery			
P.45	Barreteau Celine	barreteau@icmpe.cnrs.fr	From the ab-initio screening of ternary compounds to the synthesis of HfCoP
P.46	Huang Yi	huangyi@crystal.apph.tohoku.ac.jp	Effects of Cu-substitution on Thermoelectric Properties of Pseudogap Ternary Intermetallic Compound TiNiSi
P.47	Kim Ji-Il	k102405@uos.ac.kr	Electronic and thermal properties of Si-doped InSe layered chalcogenides
P.48	Kumagai Masaya	masaya.kumagai@riken.jp	Data-driven materials design from large-scale experimental data
P.49	Ohkubo Isao	OHKUBO.Isao@nims.go.jp	Origin of anomalous anisotropic thermoelectric transport properties in alpha-$NaFeO_2$-type d0-layered complex nitrides
P.50	Ricci Francesco	frankyricci@gmail.com	Metals with band gap as good thermoelectric materials, a High-Throughput approach.
P.51	Sato Yuki	m19b010@akita-pu.ac.jp	Thermoelectric properties of reduced graphene oxide (rGO) prepared under an electric field
P.52	Shi Yixuan	y46shi@uwaterloo.ca	Pnp Conduction Switching and ultralow Thermal Conductivity and Excellent Thermoelectric Properties of Thallium Silver Chalcogenides
P.53	Wang Yunxia	wangyunxia@ms.see.eng.osaka-u.ac.jp	A First-Principles Theoretical Study on the Potential Thermoelectric Properties of MgH_2, CaH_2 and YbH_2
P.54	Witkoske Evan	ewitkosk@purdue.edu	A quality factor limit to zT
P.55	Yang Jiong	jiongy@t.shu.edu.cn	Reliable High Throughput Electrical Transport Calculations and Its Application in Thermoelectrics
P.56	Zhang Tingting	tingitng@whut.edu.cn	Structure and Thermoelectric Properties of 2D Cr_2Se_3-$3xS_{3x}$ solid solutions
Other Materials			
P.57	Ahmed Fahim	AHMED.Fahim@nims.go.jp	Secondary Phase Assisted Enhanced TE properties and Controlled Microstructure in Chalcopyrite-type $CuGaTe_2$
P.58	Aversano Francesco	francesco.aversano@unito.it	Synthesis and thermoelectric properties of (Nb,Ta,V)CoSn Half Heusler alloys

P.59	Balke Benjamin	balke@imw.uni-stuttgart.de	Designing thermoelectric highly efficient Hf-free p-type Heusler compounds via phase separation and nano-composites
P.60	Camut Julia	julia.camut@gmail.com	Thermoelectrics for Lunar Energy Production, development of MgAgSb as a low temperature thermoelectric material
P.61	Cha Ye-Eun	sjscye22@naver.com	Synthesis and Thermoelectric Properties of $(Ce_{1-z}Yb_z)_{0.8}Fe_{4-x}Co_xSb_{12}$ Skutterudites
P.62	Cha Ye-Eun	sjscye22@naver.com	Charge Transport and Thermoelectric Properties of $(La_{1-z}Pr_z)_yFe_{4-x}Co_xSb_{12}$ Skutterudites
P.63	Choi Seongho	shchoi@toyota-ti.ac.jp	Thermal conductivity of Fe_2VAl-based superlattice thin film
P.64	Flipo Sever	sever.flipo@cpfs.mpg.de	Investigation on the Boron-rich compounds in the RE-(Cr, Mo)-B systems
P.65	Flores-Conde Araceli	florcon_ara@hotmail.com	Spark Plasma Sintered $Bi_{1-x}Sb_x$ (x=0.10, 0.14) alloys and their electronic transport properties
P.66	Guélou Gabin	Guelou.gabin@nims.go.jp	Thermoelectric properties of CVD grown ytterbium boride thin films with controlled crystallinity
P.67	Hinterleitner Bernhard	bernhard.hinterleitner@tuwien.ac.at	Bulk and thin film Heulser alloys - alternative moderate temperature thermoelectrics
P.68	Khovaylo Vladimir	khovaylo@misis.ru	Thermoelectric properties of $Fe_2Ti_{1-x}V_xSn$ Heulser alloys
P.69	Le Febvrier Arnaud	arnaud.le.febvrier@liu.se	p-type Al-doped Cr-deficient CrN thin films for thermoelectrics
P.70	Leszczynski Juliusz	juliusz.leszczynski@agh.edu.pl	Performance of amorphous silica-based protective layers on skutterudites in oxidizing atmosphere
P.71	Li Xiaoya	xyli@mail.sic.ac.cn	Effect of Annealing on Sb Doping and Thermoelectric Property of N-type Half-Heusler Compounds
P.72	Masanobu Miyata	m-miyata@jaist.ac.jp	Structural stability and thermoelectric properties of phosphides $NiSi_3P1$ systems
P.73	Meledath Valiyaveettil Suneesh	mvsuneesh@gmail.com	Enhanced thermoelectric properties of Sb doped ternary skutterudite
P.74	Mikio Koyano	koyano@jaist.ac.jp	Contactless temperature measurement of atomic-layered MoS_2 single crystal supported on silicon substrate

P.75	Mohd Said Suhana	smsaid@um.edu.my	Determination of mass transport behavior and electrode kinetic reaction for Spin Crossover (SCO) complexes in thermoelectrochemical cells
P.76	Mona Yuttana	16096008@mmm.muroran-it.ac.jp	Thermoelectric properties of synthesized under high pressure Nd filled $CoSb_3$-skutterudite
P.77	Murata Masayuki	m.murata@aist.go.jp	Evaluation of Galvano-and thermo-magnetic effects in sintered Bi-Sb alloy
P.78	Nishitani Mikihiko	nishitani@pmdp.arl.eng.osaka-u.ac.jp	The Investigation of Mg_2Sn Thin Film Material for Heat Energy Conversion Applications in Room Temperature Range
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P.80	Ricci Fabio	fabio.ricci@uliege.be	Magnetic instability in heavily n-doped Fe-based full-Heusler compounds for thermoelectric applications
P.81	Saito Wataru	wataru.saito.p2@dc.tohoku.ac.jp	Effect of Lattice Defects on the Seebeck Coefficient of Mg_2Sn
P.82	Shimazaki Takeshi	t.shimazaki@aist.go.jp	Cryostat for the measurement of absolute Seebeck Coefficient using high-temperature superconducting reference material and Thomson heat
P.83	Shin Hosun	hshin@kriss.re.kr	Uncertainty evaluation in thermoelectric characterization based on the microdevice technique
P.84	Song Lirong	lirongsong@chem.au.dk	Enhanced thermoelectric performance and high-temperature thermal stability of p-type Ag-doped β-Zn_4Sb_3
P.85	Synoradzki Karol	k.synoradzki@int.pan.wroc.pl	High-temperature thermoelectric properties of the half-Heusler phase ScNiSb
P.86	Tokunaga Yuto	tokunaga@presto.phys.sci.osaka-u.ac.jp	First principles analysis of the power factor in RZnAsO (R=La, Bi, Y)
P.87	Van Der Rest Camille	camille.vanderrest@uclouvain.be	Optimisation of the thermoelectric properties of Heusler Fe_2VAl-based compounds through off-stoichiometry strategies
P.88	Wong Deniz	denizpwong@yahoo.com	Interplay of secondary phases on the thermoelectric properties of ternary skutterudite thin films
P.89	Xia Kaiyang	aoekaiyang@sina.com	Enhanced Thermoelectric Performance in 18-Electron $Nb_{0.8}CoSb$ Half-Heusler Compound with Intrinsic Nb Vacancies

P.90	Hashiba Miri	hashiba0930@gmail.com	Synthesis and characterization of high performance thermoelectric material MgAgSb
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P.91	Castellero Alberto	alberto.castellero@unito.it	Effect of rapid solidification on the thermoelectric properties of (Ti,Zr)NiSn half-Heusler alloys
P.92	Choi Hyeongdo	hdchoi1603@kaist.ac.kr	Fabrication of high performance flexible thermoelectric devices by improving crystallization process of screen-printed material
P.93	Gresslehner Karl	karl.gresslehner@fh-wels.at	Failure analysis of commercial thermoelectric modules by Infrared thermography
P.94	Gucci Francesco	f.f.gucci@qmul.ac.uk	Flash Sintering of thermoelectrics material
P.95	Haïk Dunn Isaac	isaac.haik-dunn@ensicaen.fr	A straightforward 2f technique for the measurement of the Thomson effect
P.96	Hwang Jae-Yeol		Van der Waals epitaxy for High performance thermoelectric 2D chalcogenide films
P.97	Kim Jiwon		Highly (110)-oriented $Bi_2Te_{3-x}Se_x$ films with high thermoelectric power factor via electrodeposition
P.98	Marchal-Marchant Valentin	valentin.marchal@uclouvain.be	Manufacture of TE-modules: joining Fe_2VAl and Cu through several bonding processes.
P.99	Prado-Gonjal Jesus	jpradogonjal@gmail.com	High Pressure Synthesis: An effective approach for tuning thermoelectric properties of filled skutterudites $A_xCo_4Sb_{12}$ (A = K, Sr, Y, rare earth)
P.100	Tan Xiaoming	tellme520@whut.edu.cn	Physical mechanism under the new criterion for self-propagating high-temperature synthesis and its universality
P.101	Wagner Michael	F.M.Wagner@gsi.de	Seebeck coefficient of Bi & Sb nanowire assemblies produced by electrodeposition
P.102	Zeuthen Christian	zeuthen@chem.au.dk	Comparison of Spark Plasma Sintering and Induction Hot Pressing in Preparation of Thermoelectrics
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P.103	Alinejad Babak	16nd114n@vc.ibaraki.ac.jp	Significant Enhancement of Thermoelectric Properties of Nanostructured Mg_2Si via low temperature consolidation

P.104	Ando Ikumi	ikumi.ando.t5@dc.tohoku.ac.jp	Measurements of surface potential of Mg_2Si/M (M = Mg, Al, Ni) interfaces
P.105	Calvi Alessandro Domenico	ac50@hw.ac.uk	Formation of β-$FeSi_2$ nano-inclusions in silicon thin-films by ion-implantation for thermoelectric applications
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P.109	Funakubo Hiroshi	funakubo.h.aa@m.titech.ac.jp	Growth of Mg-Ca-Si thick films by RF sputtering method and their thermoelectric property
P.110	Godlewska Elzbieta	godlewsk@agh.edu.pl	Plasma Electrolytic Oxidation coatings on magnesium silicide
P.111	Isachenko Grigory	G.Isachenko@mail.ioffe.ru	Thermoelectric properties of n-$Mg_2Si_{0.8}Sn_{0.2}$ with complex isovalent doping.
P.112	Kato Daisuke	daisuke.kato2@toyota-boshoku.com	Control of Mg nonstoichiometry δ in $Mg_{2\pm\delta}Si_{1-x}Sb_x$ and its effect on thermoelectric properties
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P.114	Kim Gwansik	kmkk283@naver.com	Improved trade-off between thermoelectric performance and mechanical reliability of Mg_2Si-reduced graphene oxide nanocomposites
P.115	Kim Il-Ho	ihkim@ut.ac.kr	Thermoelectric Properties of Ge-doped Higher Manganese Silicides $MnSi_{1.72\text{-}1.73}$: Ge_m
P.116	Kohri Hitoshi	kohri@cc.kogakuin.ac.jp	Synthesis of tungsten disilicide and its potential as a thermoelectric material
P.117	Koz Cevriye	cevriye@etdyn.com	Process optimization and the effects of process route on thermoelectric properties of n-type doped $Mg_2(Si,Sn)$
P.118	Li Zhiliang	460407475@qq.com	Incorporating a Small Amount of MnS into Higher Manganese Silicide Leading to a Green Thermoelectric Composite with Significantly High Price/performance Ratio

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P.120	Nagai Hiroki	nagai@crystal.apph.tohoku.ac.jp	Effects of Co substitution on crystal structure and thermoelectric properties of melt-grown higher manganese silicides
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P.123	Parasuraman Rajasekar	rajasekarp@iisc.ac.in	Thermoelectric properties of Si/Al-doped β-$FeSi_2$ composites
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P.125	Robbins Mark	mark.robbins@etdyn.com	Silicide Module Development for Automotive Applications
P.126	Sizov Andrey	sizov@chalmers.se	Control of microstructure in magnesium silicide-stannide alloys via heat treatment protocols
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P.129	Symeou Elli	simeou.elli@ucy.ac.cy	$Mg_2(Si,Sn,Ge)$ Thermoelectric Materials by Mechanical Alloying
P.130	Symeou Elli	simeou.elli@ucy.ac.cy	Stability Studies of Magnesium Silicide based Compounds
P.131	Yasseri Mohammad	mohammad.yasseri@dlr.de	Backscattered electron imaging for a rapid screening/determination of composition on inhomogeneous samples: $Mg_2Si_{1-x}Sn_x$ as example
P.132	Yasseri Mohammad	mohammad.yasseri@dlr.de	Studying the miscibility gap in $Mg_2(Si,Sn)$: influence of Mg content
Additional Posters			
P.133	Jiří Hejtmánek	hejtman@fzu.cz	Applications: Potential use of thermoelectric generators in solid waste incineration plant
P.134	Wenbin Li	leewb@bjfu.edu.cn	Applications: A study on forest soil thermoelectric power generation device

P.135	Tiezheng Hu	Modules Development and Technology: Applications: Finite element analysis of temperature and stress fields during the selective laser melting process of thermoelectric SnTe
P.136	Semmar Nadjib	Other Materials: Graphene - Mesoporous Si Or Ge Nanocomposites For Thermoelectric Applications

Passive Thermoelectric Generator for Waste Heat Recovery from a Combustion Chamber

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Abstract

One of the technologies of interest to fight back against the current energy situation is thermoelectric generation which can recover waste heat from many processes and transform it into electric energy. This would increase the efficiency of these processes and would reduce the dependency on fossil fuels. Due to the present state of this technology, it is essential to enhance the performance of thermoelectric generators. This can be done by improving the properties of the thermoelectric materials used and by selecting the proper heat exchangers in charge of keeping a high gradient of temperature between the hot and cold faces of the modules. The work here presented studies a whole passive thermoelectric generator that includes a thermosyphon with phase change used as a cold heat exchanger and a finned dissipater employed on the hot side. The thermosyphon heat exchanger betters the performance of conventional dissipaters due to the lack of auxiliary equipment or moving parts. It works properly releasing the heat into the ambient, and it keeps the robustness of the system. The finned dissipater used for the hot side improves the heat transfer between the heat source, the exhaust gases, and the module faces since it increases the turbulence of the flow and extends the area of exchange. A prototype has been built and installed at the exit flue of a natural gas combustion chamber, and several tests have been carried out in order to, first, prove the proper performance of both heat exchangers, and then, to study the capacity of this technology to become a real mean of power production. The results obtained reveal that it is possible to build a passive thermoelectric generator with no moving parts and that this technology can be used to generate electric energy from waste-heat increasing the efficiency of a combustion process.

Keywords: waste, heat recovery, thermoelectric generator, heat exchanger, thermosyphon, phase change, finned dissipater, heat sink

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The importance of the assembly in thermoelectric generators

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Abstract

Generally, in the optimization of thermoelectric generators, only the heat exchangers or the thermoelectric modules themselves are taken into account. However, the assembly of the generator as a whole is of vital importance since a bad contact or a thermal bridge can waste the performance of an optimal generator. In this sense, this contribution experimentally analyzes the use of different interface materials to reduce the thermal contact resistance between the modules and the heat exchangers, the influence of the pressure distribution in the assembly as well as the effect of different insulating materials in order to reduce the thermal bridge between the exchangers. Thus, it has been demonstrated that a good assembly requires the implementation of thermal interface materials to ensure the microscopic contact between the heat exchangers and the modules, besides a uniform clamping pressure. Nevertheless, since this is normally achieved with screws, they represent a source of thermal bridges in conjunction with the small distance between the heat exchangers. In order to reduce heat losses due to thermal bridges, which can represent up to one third of the incoming heat, an increment of the distance between the heat exchangers and the use of an insulating material is recommended.

Keywords: assembly, pressure distribution, clamping pressure, contact, thermal bridge, thermoelectric generator, thermal resistance

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Optimum Design of Thermoelectric Cooler Used for Electronic Application

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Abstract

It is known that the performance of the microprocessor is proportional to the amount of heat emitted from it; and the technology of the new processors predicts a higher heat to be emitted where the traditional heat sinks won't be sufficient to absorb all heat. In this study, a design of thermoelectric cooler sandwiched between the processor and the heat sink is to be modelled analytically in order to absorb the heat emitted from the processor. With the purpose of reaching the desired rate of heat, thermoelectric ideal equations are being applied where the thermoelectric system's parameters can be optimized. The thermoelectric parameters are being studied simultaneously with the heat sink parameters where the optimum pumping power can be analysed along with the heat sink dimensions in addition to the electrical current and leg length of the thermoelectric module. On the other hand, the system has been simulated numerically in order to validate the analytical model.

Keywords: microprossor cooling, thermoelectric cooler system optimization, electronic application cooling

*Speaker

Cost-effective metal-based thermoelectric power generator for waste heat recovery from fireplace

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Abstract

Metal based thermoelectric materials have high power factors and very low cost. However their high thermal conductivity gives them a low efficiency. Metal thermoelectrics were heavily investigated in the early 1900's, but fell out of favor for new higher efficiency semiconducting thermoelectric materials. They have since only seen use in thermocouples due to their wide temperature range. By lowering their fill factor and making the elements longer, however, the effects of their thermal conductivity could be mitigated to achieve a high power output and a low power cost. In this work, metal thermoelectrics are investigated as a cost effective solution to low-grade waste heat recovery applications. Scale model thermoelectric modules were developed using wire-type metal thermoelectric elements made of constantan and chromel to demonstrate the power output performance with cost analysis in the applications of a small fireplace thermoelectric system. The test module is 10 cm x 10 cm and designed in a scalable way for larger sizes. Module design optimization was performed based on thermal matching prior to the module fabrication using an online simulation tool and a finite element simulation software. A peak power output density of _˜14 W per half square meter was achieved, which corresponds to a power cost as low as 3.4 $/W. This demonstrates that metal thermoelectrics can be a viable technology of generating off-grid power using a small fireplace. Further improvement of performance is discussed with an improved system-level design for enhanced heat transfer.

Keywords: metal thermoelectric, waste heat recovery, cost effective, fireplace

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Problems and sources of errors in the Harman method identified by impedance spectroscopy

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Abstract

The Harman method is extensively used for the characterization of the dimensionless figure of merit ZT of thermoelectric materials and devices, although in many cases this method has high errors associated. The original Harman method consists of performing two measurements, one applying a constant current pulse and the other using an ac current of high frequency. From the ac measurement the electrical resistivity of the sample can be extracted, since only the ohmic resistance is considered to be present. From the current pulse the Peltier effect introduces a Seebeck voltage in addition to the ohmic contribution, which is used to determine ZT.

Despite the simplicity of the method, there are some critical points that must be taken into account when this method is employed, such as the requirement of fully adiabatic conditions, a negligible Joule effect, a homogeneous Peltier effect at the junctions, etc. Impedance spectroscopy has been shown as a promising tool to characterize thermoelectric materials and devices. This technique, in contrast to the Harman method, measures a wide range of frequencies, allowing a better understanding of the processes occurring in the device.

In this study, by using impedance spectroscopy we have evaluated the accuracy of the Harman method in a sample with known thermoelectric properties, which has led to the identification of different sources of errors and possible problems that have not been clearly identified before and can lead to inaccurate results in the Harman method, such as the use of Ag paints and the selection of the right amplitude for both the ac and pulsed currents. Only accurate results are obtained if these identified problems and sources of errors are carefully minimized.

Keywords: Impedance spectroscopy, Harman method, figure of merit ZT

*Speaker

Investigation of pulsed thermoelectric performances by impedance spectroscopy

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Abstract

A widespread use of thermoelectric technology usually collides with their limited efficiency. Efforts to overcome this limitation face the difficulties in decoupling the thermal conductivity from the electrical conductivity (because of Wiedeman-Franz law) and to obtain simultaneously high values of electrical conductivity and Seebeck coefficient (because of Pisarenko realtion). Some efforts to circumvent partially these limitations have been oriented to non-equilibrium solution. This have been proved for cooling [1] and in the last decade have been proposed as a mean to increase power conversion from time varying thermal gradients [2, 3]. Another possibility that have been explored is the enhancement of thermal conversion efficiency obtained by periodically modulating the electronic load applied to a thermoelectric generator [4-6]. Using impedance spectroscopy and pulsed loads applied to thermoelectric modules under adiabatic and non-adiabatic test conditions, we explored the role of several experimental parameters on the output power and conversion efficiency. We discuss operating limits and realistic perspectives of thermoelectric pulsed load application.

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Keywords: Pulsed thermoelectric, Impedance spectroscopy, Conversion efficiency increasing

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Development and Experimental Validation of a new off-grid Thermoelectric Fancoil for Domestic Heating

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Abstract

Conventional heating systems are based either on radiators or on fan coils and the heat transfer process is carried out by convection phenomena in both cases, but with some fundamental differences. Traditional radiators can be considered less efficient compared to fancoils due to the fact that their performance relies on natural convection, a less efficient heat transfer process than forced convection. However, in contrast to fan coils, conventional radiators can operate without the need for mains supply. In this paper, a new heating device based on thermoelectricity, that combines the advantages of both radiators and fancoils, is presented. This new system exploits the heat coming from the heating system to generate 18W of electricity, which is consumed in-situ to power a fan, eliminating the need of a nearby wall outlet. For this purpose, analytical and numerical simulations have been carried out and a laboratory scale prototype has been built. The performance of the system has been validate by means of experimental laboratory tests.

Keywords: Thermoelectric Generator, Power generation, energy harvesting, thermal simulation, heat sink, heat exchanger, Domestic Heating, energy efficiency.

*Speaker
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Thermoelectric Generators for Heavy-Duty Vehicles: A Systemic Approach and Development

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Abstract

At the automotive development the major challenges are the achievement of the required reduction of CO2 emissions and the reduction of the fuel consumption for internal combustion engines (ICE). Therefore, it is necessary to investigate all potential technologies to improve efficiency. Regardless of whether a passenger car or a heavy-duty truck concept with a modern conventional ICE is considered, approximately 2/3 of the fuels chemical energy dissipates as waste heat roughly in equal shares in the exhaust and coolant system. The heavy-duty market is expected to be dominated by ICE for a long-time period, due to the need for energy density in propulsion of larger vehicles and low Total Cost of Ownership (TCO). Specifically, the waste heat of the exhaust gas provides through its high temperature level and semi-stationary characteristics the highest potential as secondary energy source.
The technology of thermoelectric generators (TEG) is very promising for automotive application and under investigation for several years in the research field of alternative energy converter at the DLR Institute of Vehicle Concepts (DLR-FK). It offers a low complexity without moving parts and provides advantages in terms of installation space, weight and a competitive cost to benefit ratio as an exhaust heat recovery system.
In this work the methodical development of a TEG suitable for a modern Euro VI heavy duty vehicle is presented. The boundary conditions are analyzed by using real driving data of road tests and of a representative reference cycle. The necessary systemic approach is given which demonstrates the interactions and effects of a TEG with the vehicle engine, coolant and on-board electric system.

Keywords: Thermoelectric Generator, Waste Heat Recovery, Heavy, Duty Vehicle, Systemic Approach

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Novel thermal interface material for high-temperature thermoelectric power generators

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Abstract

Waste heat at high temperature ranges has high potentiality, but most of it is currently dumped into the environment without being used in any reasonalbe way. Particularly, huge amounts of waste heat energy are generated from inefficient internal combustion engines of vehicles. Thermoelectric generator is expected to be a useful energy harvestor for the waste heat recovery, but there is still much room for improvement to be used in the field. In order to make the thermoelectric generator a commercially-viable technology for automotive waste heat recovery, thermoelectric generators need to be able to operate at exhaust temperatures above 500 ∘C, and stable thermal contacts between the thermoelectric generator and the heat source/sink shoud be guaranteed to maximize the temperature difference across the thermoelectric materials, leading to maxmized output power. For stable thermal contact between the thermoelectric generator and the heat source at high temperature ranges, thermal interface material having both of high thermal conductivity and high-temperature stability is necessary. To meet the requirements, we present a new thermal interface material consist of hybrid fillers based on multi-walled carbon nanotubes functionalized with silver nanoparticles and silver flakes, and polyimide which has high temperature stability. We are going to show thermoelectric power output improvement driven by the use of the thermal interface material and its high-temperature stability.

Keywords: thermal interface material, high temperature, waste heat recovery

*Speaker

Self-powered wireless sensor node driven by a flexible thermoelectric generator for industrial environmental monitoring

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Abstract

In industrial environments, a wireless sensor network is considered to be one of the crucial technologies for efficient and safe operation of the factory. In recent years, self-powered wireless sensor nodes (WSN) using energy harvesting technology have been actively studied to save manpower as well as maintenance costs for replacing batteries. In this work, we demonstrate a self-powered WSN driven by a flexible thermoelectric generator (f-TEG) that can wrap around a heat pipe. As a result of the device optimization study, we harvested a power of about 270 mW from the fabricated 140×113mm2 f-TEG attached to the heat pipe of 70. We also evaluated the performance of the fabricated WSN powered by the f-TEG. The WSN can monitor the temperatures of the heat pipe and ambient, humidity, and concentrations of CO2 and volatile organic compounds (VOCs) in real time and transfer the data using LoRa communication. The outdoor test showed that the WSN powered by the f-TEG was capable of wireless monitoring up to at 500 m distance.

Keywords: flexible thermoelectric generator, energy harvesting, self powered, wireless sensor nodes, fill factor, flexible TEG optimization

*Speaker

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Design and Fabrication of Thermoelectric Generator based on BiTe legs for Wearable Device Application

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Abstract

For the power supply of the wearable device, thermoelectric generator based on BiTe thermoelectric materials was designed, fabricated and characterized. The electrical properties of the n/p type BiTe thermoelectric materials was characterized by using ZEM-3 test set-up to measure Seebeck coefficient and electric conductivity. The thermal resistance of the thermoelectric generator was one of the important factors to select thermoelectric leg dimension, porosity, substrate size, etc. To apply the power generation with body heat, the thermal resistance was impedance matched with the measured human thermal resistance, such as, wrist. In this work, the designed module area size was 10*18 mm2 and the number of legs was 30 pairs. The expected power output voltage and power were several tens of mV and a few hundreds of uW under body heat condition.

Keywords: Thermoelectric generator, thermal resistance, wearable device

*Speaker

Industrial Waste Heat Recovery by Thermoelectric Generators

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Abstract

The thermoelectric generator (TEG) is regarded as a potential technology for the industrial waste heat recovery, but the practical applications remain limited due to the performance, cost, and system design issues. In this study, we established different TEG models for several types of industrial waste heat sources, including flue gas, process saturated steam and thermal radiation etc., to investigate the design strategies of the heat exchangers to capture different types of heat. For the flue gas from the combustors, the heat pipe is suitable due to its high heat transfer capability and low pressure drop requirement during the utilization of the chimney flue gas. For the saturated steam which is a mixture of gas and liquid, the conventional fin-type heat exchanger is feasible and has relatively lower cost to the heat pipe to exhibit higher cost-performance. For the high-temperature thermal radiation, the thermoelectric module can contact the thermal radiation through an absorption interface directly, or using a working fluid, ex. water or heat oil, to process the heat exchange between the fluid and the thermal radiation in advance and transfer the fluid to a TEG system afterward. This depends on the magnitude and stability of the thermal radiation and the characteristics of the working environment.

Keywords: thermoelectric generator (TEG), heat pipe, fin, thermal radiation

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Experimental evaluation of wide-gap solar cell thermoelectric hybridization

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Abstract

It is known that up to the 90% of the losses occurring in photovoltaics (PV) generates heat. Solar cells are thus in principle a natural target for the implementation of heat recovery strategies. Thermoelectric generators (TEGs) may consequently be used to hybridize solar cells with the aim of increasing their efficiency.
Recently, several experimental works have been published on Hybrid Thermoelectric-Photovoltaic (HTEPV) systems, reporting in some cases unphysically large efficiency improvements. Actually, these works have been affected by incorrect experimental procedures such as the implementation of very optimistic cold side temperatures, and the combination of PV and TEG output contributions not normalized upon their active areas.

In this communication we report a rigorous experimental procedure aiming at the determination of the efficiency of a system composed by a thin film Copper Gallium Selenide (CGS) solar cell, with a Bismuth Telluride (Bi2Te3) TEG.

The results showed an absolute efficiency gain of 3% corresponding to $\approx$ 35% of the sole PV efficiency. These results, which are in very well accordance with theoretical estimations, are expected to further increase with optical concentration.

The key of this improvement was found to be the use of a wide-gap solar cell, therefore with small temperature sensitivity, and the implementation of thermal strategies able to prevent heat dissipation towards the environment.
This experimental evaluation demonstrated in an accurate fashion the real potential of thermoelectric hybridization of solar cells.

Keywords: thermoelectrics, photovoltaics, hybrid, solar

*Speaker

The European Am-241 Radioisotope Thermoelectric Generator programme and the effect of cold-side thermoelectric temperature on specific power

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Abstract

The University of Leicester is leading development of European radioisotope thermoelectric generator (RTG) system prototypes under contract to ESA and with academic and industry partners throughout Europe [1]. Future deep space and planetary surface exploration is critically dependent on power sources that are solar-independent. Since 2013 the programme has designed, built and tested a 5 We (nominal) lab breadboard and most recently a prototype flight design of nominally 10 We. European systems have selected americium-241 as the radioisotope fuel. Relatively low system operating temperatures with this fuel drive the use of bismuth telluride thermoelectrics. The programme has developed thermoelectrics with improved mechanical characteristics whilst maintaining, and better characterising, thermoelectric performance [2,3] however a key system optimisation challenge is the trade-off of cold-side temperature. This effects the radiator area required to achieve maximum specific power (We/kg). The latter is a key performance metric for spacecraft power systems. This oral presentation will firstly provide an overview of the Am-241 prototype development and testing conducted at the University of Leicester. The system-level modelling approach and trade-off results will then be presented, with drivers for thermoelectric materials development that may have wider implications for terrestrial applications of thermoelectric highlighted.

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Keywords: radioisotope thermoelectric generator (RTG), bismuth telluride, protoype testing, system performance modelling

*Speaker

Analysis of automobile thermoelectric generator hot heat exchanger design influence on overall vehicle fuel efficiency for urban driving cycles

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Abstract

Automobile thermoelectric generator (ATEG) application is proved to be a solution for increasing vehicle fuel economy by exhaust gas waste heat recovery. The overall efficiency of ATEG system highly depends on its hot heat exchanger design. The main heat exchanger functions are maximization of absorbed heat power energy and transferring it to thermoelectric modules in order to increase generated electrical power. In this purpose, the inner sides of ATEG heat exchangers commonly modified by ribs with different geometry. However, this solution can increase a reverse aerodynamic pressure, which negatively affects engine performance and leads to overall automobile specific power reduction. Several ATEG hot heat exchangers with different inner sides geometry are designed for analyzing a conflict between the generated electrical output power and the reverse pressure. In previous works the behavior of engine-ATEG system was modeled under various stationary conditions. Examined hot exchangers had demonstrated different fuel economy peak value positions according to engine operation speeds. Investigation of the total fuel economy with different hot heat exchangers for the modern urban driving cycles is a subject for actual research.

Keywords: Automobile thermoelectric generator, heat exchanger geometry, fuel economy, reverse pressure, driving cycles

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†Speaker

Applicability limits of a maximum power point tracking controller for thermoelectric generator systems in non-stationary conditions

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Abstract

Non-stationary operating conditions of thermoelectric generator (TEG) lead to its output energy losses, due to a mismatch between TEG resistance and electric load resistance. One potential solution to this issue is a maximum power point tracking (MPPT) method. MPPT controllers allow harvesting maximum power from the TEG under all operating conditions with high processing speed and accuracy. In this way, MPPT application is required for thermoelectric systems with a variable heat flow. However, any MPPT controller has its own conversion losses which affect overall TEG system efficiency. Consequently, there are conditions, when a direct TEG connection to an electric load is more efficient than in the MPPT usage case. This paper discusses MPPT applicability limits for the TEG. Furthermore, the ways of increasing energy transfer from the TEG to electrical consumers by the MPPT controller with a modified schema and working principle are presented. The article describes a test bench designed for TEG characteristics measuring and an experiment of comparing the new MPPT controller efficiency to the MPPT controller efficiency without modification.

Keywords: thermoelectric generator, maximum power point tracking, MPPT, nonstationary conditions

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A Thermoelectric Generator Concept For Waste Heat Recovery

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Abstract

The thermoelectric generator presented is based on the 3C's concept. It uses heat pipes to capture (1st C) and concentrate (2nd C) the waste heat and coupled with thermoelectric modules to convert (3rd C) some of the concentrated heat to electricity. A bench-top prototype was designed and built for a modular concept to recycle waste heat into electricity for industrial systems. The experimental testing of one section involves the measurement of power output of one section of this modular system when varying key input parameters such as volumetric flow rate and temperature of the exhaust gas. A 1-D steady state model using a thermal resistance network was developed to verify and validate the experimental data obtained. The tests are undergoing and the results will be soon available for discussion.

Keywords: "heat pipes", "waste heat", "thermoelectric modules"

*Speaker

Autonomous power supply for hot water boiler cooling utilizing thermoelectric generators additionally integrated in flue gas duct

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Abstract

Modern automatically fed hot water boilers are equipped by combustion control systems providing low emission profiles in wide range of working conditions. Consequently boilers have higher efficiency but on the other hand they must be connected to electrical grid. Thermoelectric generators (TEG) utilizing the flue gas waste heat offer possible solution for autonomous operation of the boilers. This concept is not commonly used due to high cost and technical limitations of thermoelectric power generating systems. The aim of this study is a complex analysis of possible utilizing of a small TEG as an alternative power supply of a boiler. A TEG is considered as an autonomous power supply for powering low power circulation pump and boiler cool unit. This alternative is designed for safety operation in cases of electrical grid failure. Mathematical model of the TEG and hot water boiler was created. The model involves affecting of the combustion device by the TEG, namely cooling of flue gas, rising of additional pressure losses, change of boiler efficiency. Mathematical models of TEGs published previously by different authors substitute TEG as a thermoelectric module with heat exchangers on the hot- and cold-side of the module. The proposed model widen the description by inclusion of detail behaviour of combustion device, flue gas duct and chimney construction. In this point of view, the model considers affecting of TEGs power output by the chemical composition of fuel composition and by the technical parameters of the gas duct and chimney. The carried out complex study provides an identification of minimal power output of the TEG necessary for cooling down the selected boiler or steady operation of the boiler. On the other hand, the study identifies the realistic TEG power production in a particular configuration under different operation parameters.

Keywords: thermoelectric generator, waste heat, boiler cooling

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†Speaker

High temperature thermoelectric generator units in relation to and low temperature Bi2 Te3 thermoelectric generator unit for direct conversion of waste heat from a wooden pellet stove into electric energy

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Abstract

Achieving the sustainable development goals will require a comprehensive portfolio of technologies and policy measures. Modern bioenergy plays an essential role in the International Energy Agency (IEA) 2∘C Scenario. Burning harvested organic matter – biomass – provided most of mankind's energy needs for millennia. Modern technologies can convert this organic matter to solid, liquid and gaseous forms that can more efficiently provide for energy needs and replace fossil fuels. But the modern biomass needs electrical power for the heating pump, control system, regulation. Availability of electricity is essential. In the case of isolated houses used at certain times of the year, such as second homes, the grid connection can be very expensive for occasional occupants. A thermoelectric generator could work against this issue and produce the electric energy for the biomass stoves. In case of black-outs but also to eliminate the dependence of the electrical grid and to meet the auxiliary energy demand through the independent production of electrical energy. This thesis contributes to the research by characterizing, modeling and assessing the performance of a TEG, where thermoelectric modules are integrated on the chimney pipe chamber of a biomass log boiler, to keep structural changes minimal and the temperature difference large. For the measurement, a prototype is developed based on a real stove. Additional high temperature TEG, which are still not available for a moderate price, are simulated. The propose is to show the technical potential of these modules for the future, with the adaptation that the price of such these modules are going down. Results from the measurement, calculation and testing will be presented.

Keywords: waste heat harvesting, high temperature module, prototype, testing, simulation

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EFFICIENCY IMPROVEMENT OF A CO2 VAPOUR COMPRESSION REFRIGERATION SYSTEM BY MEANS OF THERMOELECTRIC SUBCOOLING

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Abstract

Nowadays, due to the increasing climate change problem, the existing regulation in the refrigeration market is leading to an intense research on systems that use CO2 as an efficient alternative to fluorinated substances. In these systems, whose operation implies high working pressures, it has been demonstrated that the performance of transcritical cycles considerably improves when an additional subcooling is introduced after the gascooler. This work presents a vapour compression refrigeration system that operates with CO2 and which utilizes thermoelectric technology in order to provoke the subcooling. To that purpose, a computational model has been developed including, not only the vapour compression system, but also the subcooling system formed by a thermoelectric cooler. The obtained results show that the global COP of the system can be improved up to the 13.3 % and increments of 28.5 % in the cooling power can be achieved by means of thermoelectric subcooling.

Keywords: Cooling, CO2, thermoelectricity, COP, subcooling, computational model

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A Novel Off-grid Solar-Thermoelectric Desalination System

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Abstract

One-third of the world residents currently undergo severe water stress and the percentage keeps increasing. World water resources are mainly salty (97.5%) and freshwater (2.5%). Therefore, one of the most promising solution to overcome the water shortcoming is desalination. A number of humidification/dehumidification (HDH) devices based on conventional vapor compression technology are currently available. However, these devices have a number of inherent problems such as high noise levels, compressor vibration and excessive weight and size, which are hard to be solved by employing traditional technology. In this work, a novel off-grid thermoelectric-photovoltaic (TE-PV) desalination concept is proposed. In our method, photovoltaic technology is used to generate electrical power from the sun, while thermoelectric technology is applied to simultaneously vaporize/condense water. This combination will not only overcome the problems of a conventional HDH system, but it also brings many additional advantages such as being off-grid, having less moving parts, easy to install, less maintenance, and on top being environmentally friendly. Some highlight results will be presented in this report.

Keywords: Thermoelectric cooling and heating, Photovoltaic, Desalination

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Thermoelectric Eddy Current in Bio-Compatible Materials

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Abstract

This poster presentation describes some recent research efforts in establishing the thermoelectric characteristics of materials intended for use in bio-compatible applications. In particular it focuses on the requirement to ensure that materials and devices implanted in the human body do not give rise to any unforeseen thermoelectric effects, such as unintended levels of thermoelectric eddy current, which may have an adverse effect on surrounding tissue and organs.
In recent years medical science has seen a rapid increase in the range of materials and devices used for monitoring, regulating and enhancing natural biological functions. For instance, by using advanced electromagnetic measuring techniques it has become possible to monitor human neurological activity extremely accurately and in great detail. It is recognised also that similar techniques could now also be applied to monitor the size of any thermoelectric effect arising from bio-materials in common use, and for physically detecting any influence that they may have on natural biological tissue in their immediate vicinity.

Areas where due diligence is required are identified, not only in the development of new bio-metric devices and materials, but also where long-established clinical practices can be re-evaluated and brought up-to-date with respect to the bio-compatibility of the materials that they use.
In general, the principal is established that with the continual introduction of new technologies and capabilities which afford us the opportunity to re-asses and re-verify the benefits of both new and established medical practices, then the field of medical science bears a responsibility to act on any such opportunity to the full.

Keywords: thermoelectric, eddy, bio, engineering, dental, amalgam

*Speaker

On the development of a new measurement system for conductivity, Hall constant and Seebeck coefficient

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Abstract

It is of increasing importance in materials characterization to know the electrical transport properties like the electrical conductivity, the Hall constant, and the Seebeck coefficient for high temperature applications. However, high temperature measurements require specific devices in order to avoid electrical, thermal or geometrical errors.
We report on the current state of the development of a new measurement system that combines the electrical conductivity, Hall constant and Seebeck coefficient measurements in a temperature range from -150∘C up to 800 ∘C in different gas atmospheres. The use of only one sample holder with the need for only one sample facilitate the handling and assures the same experimental conditions of the measured parameters.

The new system consists of a gas floated measurement chamber and two permanent magnet yoke systems of opposite polarity. The magnets with a magnetic flux density of +/- 760 mT are placed on a moveable sled to change the polarity of the magnetic field in the fixed measurement chamber. The sample holder, based on alumina substrate, can be easily mounted in the chamber. On the front side are four electrodes located allowing Hall and resistivity measurements according to van der Pauw's method. On the reverse side a screen-printed Platinum structure for Joule's heating was placed. To guarantee a homogenous temperature distribution within the sample, the new holder was designed by FEM analysis.
For future measurements of Seebeck coefficient the sample holder will be equipped with an additional heater and thick-film thermocouples.

Keywords: thermal analysis, high temperature measurement, Hall constant, Seebeck coefficient, charge carrier density, charge carrier mobility

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Evaluation of Thin-Film Thermoelectric Device Properties and Efficiency by I–V Curves and Simulation

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Abstract

Traditionally, the property of thermoelectric devices can be measured at either constant temperature difference or at the constant thermal input. Due to the increasing interests in thin-film thermoelectric devices, we applied the above-mentioned techniques to such devices and determined their thermoelectric property via I-V measurement. Both GeSbTe and Co-GeTe thin films have been measured to confirm the validity of this technique. There has early paper already showed the way to measure the normal thermoelectric device property by I–V curves systems. The kind of technique never applies in the thin-film device. Owing to new technological advances, the thin-film thermoelectric device has gained becomes more popular. Thus, we demonstrate the measurement system was designed and constructed which enables both types of I–V curves to be obtained automatically. The power and conversion efficiency of a thermoelectric module was determined by using this system and comparing with the simulation at different ranges of temperature difference. The results confirm the validity of the proposed technique and increasing the possibility of application.

Keywords: Thermoelectric, Thin, Film, Device, High ZT Value, Measuring System

*Speaker

Apparatus for Measurement of the Output Power and Efficiency of Flexible Thermoelectric Power Generators

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Abstract

Flexible thermoelectric power generators (f-TEGs) are widely recognized as a promising candidate for power source of self-powered sensors, which is necessary for realizing the next-generation smart network monitoring system in the Internet-of-Things (IoT) era. For this reason, a variety of flexible thermoelectric modules have been fabricated owing to their outstanding potential for use as arbitrary heat-source shapes [1], [2]. However, the output power of these TEGs is not yet sufficient. To improve the output power of f-TEGs, we have integrated sintered bulk bismuth telluride chips on a thin flexible printed circuit using a high-speed surface mounting technology. To evaluate this f-TEG, an experimental apparatus for measurement of the output power and efficiency of f-TEGs has been developed in the present study. Employing an arch-shaped heater and inverted arch-shaped heat sink, this apparatus can measure the output power of f-TEGs at several bending radii between 50 and 200 mm. In contrast to other existing apparatus, the proposed apparatus allows us to measure the efficiency in heat flow [3] and adiabatic modes [4], which makes measurement-accuracy confirmation easier. The results from these experiments will be presented in the International Conference on Thermoelectrics 2018. We expect that this apparatus will be a useful tool to characterize f-TEGs, which can be extended to current IoT applications of thermoelectric modules.

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Keywords: Measurement, flexible Thermoelectric module, Efficiency, Output power

*Speaker

Melt-spinning process effects on enhanced conductivity ratio in CexFe3CoSb12 thermoelectrics

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Abstract

Thermoelectric figure of merits (ZT) in a CexCoFe3Sb12 (x=0.80, 0.85, 0.90) skutterudite system was investigated by using a conductivity ratio control approach. CexCoFe3Sb12 (x=0.80, 0.85 and 0.90) skutterudite specimens were produced by a melt-spinning and a spark plasma sintering process. The thermoelectric properties of the specimens were measured in the temperature range from 323K to 723K. We found the optimum amount of Ce-filler (x = 0.85) in the CexCoFe3Sb12 system based on the thermo-electronic property measuring and microstructural analysis. The maximum ZT value of 0.81 was obtained at 723K in the La0.85CoFe3Sb12 composition. We discussed our results on the basis of the charge compensation theory to explain different optimum filler amount between a La ratter system and this result. A charge difference between Ce- and La-filler can cause the different optimum filling amount between this system and the LaxCoFe3Sb12 skutterudite system.

Keywords: filled skutterudite, p, type, melt spinning, nanostructure, conductivity ratio

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Fabrication of diffusion barriers in Colusite-based thermoelectric elements

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Abstract

Colusites Cu26A2E6S32 (A = V, Nb, Ta and E = Ge, Sn) are promising candidates as environmentally friendly thermoelectric materials. Their complex crystal structure leads to low thermal conductivity and high thermoelectric figure of merit [1,2,3]. In this study, we developed the diffusion barriers for colusite-based thermoelectric elements, facilitating their use in thermoelectric devices.
Samples of Cu26Nb2Ge6S32 were first prepared by mixing the stoichiometric amount of pure elements Cu, Nb, Ge, S in evacuated and sealed quartz tubes at 1323 K for 12 h. The samples were then hot-pressed with metals (Ti, Pt, Ni, Co and Au as diffusion barrier) at 973 K for 1 h under 70 MPa. Scanning electron microscopy equipped with energy dispersive X-ray spectroscopy was used for studying the interface between diffusion barriers and colusite. The coefficient of thermal expansion (CTE) of Cu26Nb2Ge6S32 was measured between 293 K and 573 K. Output electrical power and efficiency was investigated on the element between 293 K and 573 K.

The mismatch in CTE between Ti and colusite and Pt and colusite leads to the formation of cracks at their junctions. Impurity phases are formed at the junctions between Ni and colusite and Co and colusite. A good CTE match between Au and colusite forms a crack-free junction. Moreover, no impurity phases are found at Au-colusite junction. Therefore, the Au-based diffusion barrier provides reduced electrical and thermal contact resistances, leading to enhanced thermoelectric conversion efficiency.

This work is supported as part of the International Joint Research Program for Innovative Energy Technology funded by the Ministry of Economy, Trade, and Industry (METI), Japan.
K. Suekuni et al., Appl. Phys. Lett, 2014, 105, 132107; [2] Y. Kikuchi, M. Ohta et al., J. Mat. Chem. A, 2016, 4, 15207; [3] Y. Bouyrie, M. Ohta et al., J. Mat. Chem. C, 2017, 5, 4174.

Keywords: Thermoelectrics, Colusite, diffusion barrier, thermal expansion, power generation

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Matlab modeling of thermoelectric modules including thermal losses

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Abstract

The development of thermoelectric modules and their applications required accurate modeling of their performances. Usually, in applications or device testing only applied temperatures are known. Simple calculations which ignore the thermal losses on parasitic elements can overestimate the performances. However, the calculations of internal temperatures generate recursive equations (heat flux, temperature difference and material properties) which can be numerically resolved, often with a finite element approach.
In this work, an accurate and fast model of thermoelectric modules is developed in Matlab with an iterative procedure, avoiding domain discretization (e.g. finite element analysis). The model takes into account the passive components which lead to temperature drops inside the device. It provide a correct evaluation of the effective cold and hot side temperatures on the thermoelectric materials, which are used in the materials properties integral, with an iterative method, improving at each sequence the approximated solutions. Open circuit potential, current, power, heat fluxes and maximum efficiency are evaluated as a function of temperature. Results show that temperatures drops can be tens of degree Celsius and efficiency overestimation can reach 15% at high temperature range. The convergence of the algorithm is demonstrated within few iterations.
The comparison of results with the experimental data from electrical characterization of commercial TEMs, confirms the reliability of the developed numerical analysis. Moreover, a complete Graphical User Interface has been developed, with the possibility to simulate each type of material and geometry.

Keywords: thermoelectric module, module simulation, iterative algorithm

*Speaker

A Novel Thermoelectric Leg Structure oriented to Cycling Robustness at High Temperature and Low Manufacturing Cost

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Abstract

One of the key advantages of thermoelectric power generation systems is that they are solid-state devices with no moving parts, resulting directly in high reliability. However, for high temperature applications, especially when several thermal cycles occur during the system life, the structure is not robust enough to overcome thermal stress. The aim of this work is to present a novel leg structure for UNILEG based thermoelectric generators. The design of this structure has been focused on reliability and robustness but taking into account the cost of the final thermoelectric module. The semiconductor material that has been used for this design is a P-type Ca3Co4O9 because of its chemical stability at high temperatures and easy machinability. Thermomechanical computations have been carried out in the design and optimization process of this structure shape.

Keywords: UNILEG, Oxides, Thermoelectric Generator, thermal stress, Power generation, thermal simulation, energy efficiency.

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Radial thin film thermoelectric device for hot spot cooling

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Abstract

Due to electronic devices continuously shrink in size, the "high flux of hot spots" in localized areas become a main issue in recent years. Planar thin film thermoelectric device is great choice to solve the hot spot problem in electronic devices. In this study, we design radial thermoelectric model with p and n legs to rapidly spread heat from hot spots.
An array of thin film TE legs is deposited in effusion co-cell vacuum thermal evaporation method with shadow mask. We choose Sb2Te3 and Bi2Te3 for p-type and n-type legs, respectively. The thin film TE legs show special columnar grains grown perpendicular to the substrate. The composition and microstructure of the film are studied by X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy dispersive X-ray spectrum (EDX). We also select 1 μm Cu for electrode to build up open circuit.

The optimization design of geometrical dimension and length of TE legs are conducted via finite element method on the basis of the above TE legs properties. According to the optimized radial thin film TE device, we have successfully achieved the high performance of thermoelectric cooling systems.

Keywords: radial, thin film, thermoelectric device, hot spot

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Development of evaluation instrument in thermoelectric module in air

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Abstract

The development of the thermoelectric module is rapidly advanced. To product the thermoelectric module, not only the performance evaluation but also the durable evaluation is demanded. ADVANCE RIKO Inc., has been developing to evaluate the power generation and the power generating efficiency in thermoelectric module (Mini-PEM, PEM-2 and F-PEM). For Mini-PEM, the power generation and the power generating efficiency can be evaluated in thermoelectric device and module below 10 mm square in vacuum. For PEM-2, the power generation and the power generating efficiency can be evaluated in thermoelectric device and module above 20 mm square in vacuum or inert gas. Recently, we developed F-PEM for the purpose of carrying out the durability test of the thermoelectric module in air. F-PEM has the function of keeping the temperature of the high temperature side in long time and cycling between two temperatures. To evaluate the performance in F-PEM, we measured by F-PEM and PEM-2 in thermoelectric module. In this presentation, we compare with the measurement result between F-PEM and PEM-2, and report the change in the power generation in thermoelectric module obtained by keeping test and cyclic test using F-PEM.

Keywords: Evaluation instrument in thermoelectric module, Power generation, Cyclic test

*Speaker

Innovative Segmented Thermoelectric Module for Energy Generation

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Abstract

One of the main issues related to the design of thermoelectric modules is optimization of their working parameters. Due to the temperature correlation of semiconductor's physico-chemical properties (e.g. Seebeck coefficient, electrical conductivity) there is an idea of usage of different materials, matching operating temperature range to their optimum. Usage of segmented thermoelectric elements can also increase the maximum temperature of modules hot side, resulting with enhancement of efficiency and power density.
We have constructed and characterized a TEG module based on segmented Bi2Te3/Sb2Te3 and CoSb3 n-type and p-type thermocouples. The methodology of dimensions optimization, process of materials fabrication, properties of used materials and elements assembly procedure will be presented. The electrical properties (open circuit voltage, short circuit current internal electrical resistance, thermal resistance, power density, and efficiency) were determined as a function of Tc and Th.
Presented work was supported by the National Centre for Research and Development under the project "Innovative thermoelectric modules for energy harvesting" (PBS3/A5/49/2015).
This scientific work has been partially financed as a research project no. UMO-2016/23/D/ST8/02686, National Science Centre, Poland.

Keywords: Segmented Thermoelectric Module, TEG module optimization, TEG module fabrication

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Development of metallization technique for thermoelectric module using polycrystalline SnSe

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Abstract

Single-crystal SnSe that showed high figure of merit of 2.6 was reported in 2014 [1]. Afterward, many studies about polycrystalline SnSe materials were followed for a practical application of thermoelectric generation [2,3]. Despite of the development of polycrystalline SnSe materials, there have been no SnSe thermoelectric module reported so far, due to the lack of metallization technique that can make good electrical contact and prevent elemental diffusion.

In this work, several approaches to fabricate SnSe thermoelectric module from metallization to bonding with electrodes are demonstrated. Regarding the characteristics of polycrystalline SnSe material, various metal layers are studied including Ag, Ni, Ti, and other metal layers. Several fabrication methods are experimented including sputtering, powder hot pressing, and spark plasma co-sintering. The interfaces between metallization layers and SnSe are investigated using energy dispersive spectroscopy and transmission electron microscopy to analyze the intermetallic compounds that are formed during the metallization process. The electrical contact resistances of each metallization layer are measured, and characteristics of SnSe thermoelectric module are simulated using finite element method. Based on this developed metallization technique, the polycrystalline SnSe thermoelectric module is fabricated and its characteristics are investigated.

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Keywords: Thermoelectric module, Metallization, SnSe, Interfaces

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Solar photovoltaic _ photothermal _ thermoelectric power generation system

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Abstract

ABSTRACT: System is abbreviated as PV/TE. When solar energy is converted to electricity, heat is collected by the refrigerant of the heat collecting device, which is used by thermoelectric power generation components, thus the solar radiation energy is fully utilized. The system greatly improves the photovoltaic conversion efficiency, thermoelectric power generation components output more power, the temperature of the refrigerant of the heat collecting component is also reduced, so that the entire power generation system remains stable. The heat-absorbing plate structure of the carbon nanotube/black silicon structure is used in the heat-collecting component. By using the Ag-assisted chemical etching method to obtain the single-crystal black silicon microstructure-silicon nanowire structure under different H2O2 concentration, etching temperature and etching time. Carbon nanotubes is embedded in black silicon nanowire microstructure. The larger aspect ratio of the carbon nanotubes increases the number of times the incident light is absorbed in the silicon nanowires, resulting in an increase in the amount of heat absorbed, and systematically studied the impact of this structure on the surface reflectance. This structure is applied to the light radiating plate, through the radiant plate circulating refrigerant medium, absorb the radiation board heat is used in semiconductor thermoelectric power generation. The experimental results show that the black silicon microstructure reduces the reflectivity, the average reflectivity is less than 5%, the thermal energy absorption rate is greatly increased, and the entire system based on the original photovoltaic system power generation efficiency increased by 15%. In addition, In addition, the PV/TE photovoltaic panels are cooler in temperature and extend the useful life of the product.

Keywords: PV/TE, carbon nanotubes, semiconductor power generation

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DESIGN AND TESTING OF A TUBULAR THERMOELECTRIC MODULE BASED ON OXIDE ELEMENTS

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Abstract

Motor vehicles are particularly attractive for the development of thermoelectric devices. Their internal combustion engines are characterized by high–up to 40%–loss of heat energy that is being discarded to the environment. Thermoelectric converters can provide heat recovery from exhaust systems and contribute to fuel saving, as well as reduced emissions of greenhouse gases and other harmful substances into the air.
Although the thermoelectric efficiency of oxides is relatively low, this class of materials has significant advantages compared to traditional thermoelectric compounds based on alloys: oxides can consist of non-toxic elements; they are stable across a wide temperature range; and have good durability in oxygen. Two main approaches seem to be important for the development of car-implemented thermoelectric converters: the use of stable oxides as functional materials and the design of an effective tubular arrangement.

This work was focused on the design, modeling, testing, and performance analysis of a tubular thermoelectric converter based on oxide materials. The fabricated module included 24 functional oxide elements synthesized by conventional methods. Elements of p- and n- type were made of cobalt-based oxide Ca2.7Bi0.3Co4O9 and manganese-based oxide CaMn0.95Ta0.05O3, respectively. The module was assembled using silver paste and clamping mechanisms, with the thermoelectric elements electrically connected in series by metal plates and placed around the hot tube. The output power of 138 mW was achieved under a temperature gradient of 430∘C with a hot side temperature of 514∘C. The tested module is characterized by an advantageous manufacturing factor of 0.87 at the contact resistance of 0.44 , but a relatively low output power density per volume and per mass.
The reported study was funded by RFBR according to the research project 17-08-01395.

Keywords: Thermoelectric module, oxide thermoelectric, electrical conductivity, Seebeck coefficient, power factor.

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Design and evaluation of Fe2V(Al0.9Si0.1)/Cu tilted-multilayer thermoelectric devices

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Abstract

Recently, tilted-multilayer thermoelectric (TE) devices have attracted considerable attention. The devices consist of a potential TE material and a metal tilted to the temperature gradient. Due to the tilted structure, electric field is generated perpendicular to the temperature gradient. In this combination, power factor PF is enhanced owing to a higher Seebeck coefficient S and a lower electrical resistivity r derived from a TE material and a metal, respectively.

In this study, we designed and evaluated the high performance tilted-multilayer TE devices consisting of Fe2VAl- based full-heusler TE material, that has a high PF, and Cu as a metal. We calculated off diagonal TE properties S_cal, r_cal and PF_cal with changing parameters a and d. The parameter a is the relative thickness of Fe2V(Al0.9Si0.1) and Cu in multilayer, $a = t$_cu / (t_cu + t_TE), and d is the tilt angle. With increasing a , r gradually decreased and PF gradually increased. Under the condition of $d = 30\circ$ and $a = 0.9$, the highest PF_cal = 8.7mW/mK2 can be theoretically obtained.

We fabricated Fe2V(Al0.9Si0.1)/Cu tilted-multilayer TE devices that have $d = 30\circ$ and $a = 0.9$ using Spark Plasma Sintering and measured its S, r, and PF. We obtained PF = 0.21 mW/mK2 which was only 2% of PF_cal. From the SEM observation, Cu was scattered in thin TE layers. Hence, we attributed such a reduction of PF to the electric conduction paths caused by the scattering of Cu powders. We modified devices with thicker layers of TE material $a = 0.5$ and 0.7 to reduce the effect of Cu scattering. As a result, we obtained PF =4.38 mW/mK2 with $a = 0.7$ at dT = 30.1K, which is roughly comparable to that of pi-type Bi2Te3-based modules.

Keywords: tilted, multilayer devices, module, Fe2VAi

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Comparison of Three Accurate Measurement Methods for Measuring the Efficiency in Thermoelectric Modules

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Abstract

To disseminate thermoelectric power generation using waste heat, the establishment of a standard measurement technique for characterizing thermoelectric modules (TEMs) is required. Three typical measurement techniques, (i) the heat flow method, (ii) the guarded heater method, and (iii) the Harman method, have been described in Ref [1]. In the heat flow method, the input heat flux into the TEM is measured by a heat flow meter. In the guarded heater method, the input heat flux is measured from the heater power using the guarded heater block. The Harman method can estimate the dimensionless figure of merit through AC and DC voltage measurements. However, there are only a few studies on the comparison experiments between methods for characterizing TEMs [2-5]. In particular, the comparison between techniques (i) - (iii) using a single TEM has not been reported.
Here, we perform a comparison of the different measurement methods for characterizing TEMs using the uniform modules. To estimate the thermoelectric efficiency when using these methods, we developed an experimental apparatus using methods (i) - (iii). The measurements were performed using the commercial Bi2Te3-based TEM. In each method, the obtained value of thermoelectric efficiency was in the comparable range at the temperature gradients across the hot and cold sides of TEM (dT _˜ 100 K). We will discuss the details of our results and the measurements using other TEMs in the conference.

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Keywords: Module measurement, Heat flow method, Guarded heater method, Harman method

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Watch strap-shaped flexible thermoelectric body-heat harvester based on inorganic bulk materials

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Abstract

This paper represents the watch strap-shaped thermoelectric body-heat harvester based on bulk inorganic thermoelectric materials. The device contains the flexible thermoelectric module as well as the fin-type heat sink. The structural design is presented for high flexibility so that it can fit well on curved surfaces. The device successfully generates 6.97 μW/cm2 output power density on a person's wrist while the subject is walking. The theoretical analysis based on simplified human thermoregulatory model (Journal of Physics D: Applied Physics **51**, 055401 (2018)) is demonstrated, which suggests that the output power density can be further enhanced by modulating the size of the thermoelectric elements or by reducing the thermal contact resistance. This work suggests the possibility for the usage of body-heat as an alternative energy source for wearable devices.

Keywords: Thermoelectric, body heat harvesting, flexibility

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Design of segmented/graded Thermoelectric Devices based on Beta-Formalism

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Abstract

The energy-conversion-efficiency is critical for application of thermoelectric technology. Thus, many material research works have been focused on increasing peak-zT of materials, believing that zT is a good figure of merit for efficiency.
However, the classical zT formula is developed with the assumption that material properties are temperature/position-independent and the efficiency formula contains error. Moreover, due to the non-local and non-linear nature of thermoelectric equation of temperature, the classical method based on peak-zT becomes useless especially when designing the segmented or graded devices.

In this work, we develop the new formalism called **"Beta-Formalism" to overcome the temperature/position-dependency of material properties** and to predict the thermoelectric performances precisely. We find **hidden parameters** which can describe the temperature dependency of material properties. Using hidden parameters in addition to redefined average parameter Z, we develop the **analytical thermoelctric equation for power, heat, and efficiency.**

We successfully apply our "Beta-Formalism" to find and optimize the thermoelectric devices especially for **segmented or graded** thermoelectric devices with and without contact resistance, using **pykeri** code we have made. We design the 5 to 7 segmented power or efficiency-devices among 18 candidate materials for wide temperature application from 300 K to 1200 K. We also design the graded devices using Bi2Te3 materials with various doping-concentrations.
We believe that our "Beta-Formalism" opens a new way to design thermoelectric materials, devices, and systems.

Keywords: figure of merit, thermoelectric device, design, segmented, graded

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Integration of a heat exchanger on an all Si-based thermoelectric micro/nanogenerator

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Abstract

Maximizing materials' zT by optimizing the thermoelectric coefficients is not enough to have an efficient thermoelectric generator. Under harvesting operations, it is very critical to have large temperature gradients across the device to obtain reasonable power output, which is usually not the case for microgenerators. This work focuses on the enhancement of the performance of a thermoelectric microgenerator by increasing the temperature gradient between the hot and cold sides of the generator, which is achieved integrating a heat exchanger.

An all-Si unileg thermoelectric microgenerator has been fabricated in a SOI substrate using the process described in [1]. Since the proposed thermoelectric microgenerator has a planar layout built around a suspended microplatform, the heat sink cannot be directly placed on top of this fragile platform. In this work, different routes have been designed for the integration of a heat exchanger onto such a microgenerator to maximize the power output. Simulations of the temperature distribution across the assembly as well as the power generated, are evaluated to compare the performance of these two approaches. Harvesting measurements are performed on mock-up assemblies to be able to investigate the enhancement reached with the integration of a heat exchanger. An increase in the power output of up to three orders of magnitude is measured comparing the cases with and without heat sink, as a result of the reduction of the thermal resistance between the cold side of the device and the ambient.

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Keywords: thermoelectric micro/nano generator, Si micro/nanostructures, heat exchanger, MEMS

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Organic π-type thermoelectric module patterned with photolithographic mold

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Abstract

Thermoelectrics (TEs) have the potential to capture usable energy from waste heat in the environment [1]. The largest amount of heat are wasted in the low temperature region _˜ 150◦C [2], because the conventional systems lost the recovery power for such low temperature heat. TEs, however, can maintain the energy convergent efficiency to exceed the conventional systems in the efficiency for the low temperature region [3]. In addition to the technical advantage, organic materials can provide an additional value for TEs: flexibility. The TE figure of merit has been dramatically improved to 0.42, recently [4]. The Seebeck effect, yet, generates only several ten μV/K. To drive electric devices, we need to pattern and connect more than one hundred TE legs as a TE module.
Herein, we fabricated π-type TE modules via fulfilling p-type and n- type TE materials into photolithographic molds to maintain the temperature difference in TE legs. To achieve 250 mV to drive a booster circuit, we designed a module pattern, 13 $\times$ 13 legs in 40 $\times$ 40 mm2. for the single π unit showing 3 mV. To reach the output voltage, we optimized p-type and n-type TE materials based on poly(3,4-ethylenedioxy thiophene) polystyrene sulfonate [4] and tetrathiafulvalene 7,7,8,8-tetracyanoquinodimethane salt [5], respectively. Overall, we attempt to re-arrange the well-established fabrication processes, such as photolithography, fulfilling, and electrode deposition, to emergently fabricate the organic π-type TE modules. In the presentation, we report the details of the optimized TE materials and the module performances.
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Keywords: contract resistance, flexible thermoelectric sheet, mass production

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Flexible TEG using Amorphous InGaZnO Thin Film

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Abstract

Amorphous-InGaZnO is n-type semiconductor material and has enormous potential such as a transparency and a flexible application owing to a low temperature sputtering process. In this study, we demonstrated flexible TEG using a-InGaZnO and ITO electrode on PEN substrate. The flexible TEG with heat guide was designed with 625 pairs of a-InGaZnO and ITO uni-leg structure with heat guides. The heat guides were formed using KMPR photoresist. The heat guide formed a temperature gradient in the in-plane direction of the thin film and generated electrical power.

Keywords: flexible, oxide, thin film

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Interpretation of Frequency Response Analysis in Thermoelectric Modules

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Abstract

Recently, impedance spectroscopy based on frequency response analysis has been employed to unambiguously elucidate the thermoelectric module properties under a practical operating condition [1, 2]. Analysis of the impedance spectrum enables the determination of the thermoelectric module figure of merit, while enabling extraction of three key parameters-the Seebeck coefficient, thermal conductivity, and electrical conductivity by employing a one-dimensional heat equation. Furthermore, the resistive and capacitive processes of thermoelectric elements can be identified and quantitatively compared from the impedance spectrum for different thermoelectric modules to investigate thermoelectric carrier diffusion properties.
Here, we present systematic investigations on the thermoelectric properties of Bi2Te3- and skutterudite-based modules using impedance spectroscopy followed by the analysis of distribution of relaxation time and equivalent circuit analysis. The effects of temperature and thermoelectric elements on the impedance spectroscopy data of thermoelectric modules are also discussed in detail. Some of remaining challenges are outlined for the further research.

J. García-Cañadas and G. Min, J. Appl. Phys., 116, 174510 (2014).
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Keywords: Bi2Te3, skutterudite, impedance spectroscopy, thermoelectric properties, frequency response analysis

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Separation structure and enhanced cooling experiments of a TEM

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Abstract

A thermoelectric generator (TEG) that uses fluid as a heat source and cold source, the cooling mechanism of its thermoelectric modules (TEMs) is often more complex than the structure of its high temperature components. In order to enhance the heat transfer process of the TEG, maintain the compactness of its structure and the uniformity of the TEMs temperature distribution, a new separate thermoelectric module (STEM) is proposed to co-operate with the TEG. The STEM still uses electrodes made of BiTe, whose hot nodes and cold nodes are connected by metal conductor, the circuit adopts series-parallel optimal connection. These measures can not only reduce its resistance, but also allow its cold end to be cooled in a more efficient way. In this paper, the basic principle of centralized and enhanced cooling for the cold end of STEM is studied, and the influences of structure parameters and cooling water temperature on its temperature are analyzed. The results show that although STEM can't improve the efficiency of thermoelectric conversion on TEG, it can enhance the cooling effect and make the working temperature difference even more uniform.

Keywords: thermoelectric generator, enhanced cooling, experiment, module, separation structure

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From the ab-initio screening of ternary compounds to the synthesis of HfCoP

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Abstract

Novel high performance and cheap materials are needed for developing thermoelectric devices and extend them to a mass market. One way to answer this need is to improve the figure of merit of thermoelectric materials which are already known. Another approach focuses on identifying new materials which could exhibit promising properties. In our work, we decided to follow the second approach by combining first-principles calculations and experiments, in order to screen a large number of compounds. We thus investigated ternary *TMX* intermetallic compounds, with *T* a transition metal, a rare earth or an alkaline earth metal, *M* an element from the first line of the transition metal and *X*, a metalloid. A systematic study of crystal databases allowed us to identify four main structural prototypes for this composition: **TiNiSi** (*Pnma*, 62), **MgAgAs** (*F-43m*, 216), **BeZrSi** (*P63/mmc*, 194) and **ZrNiAl** (*P-62m*, 189). In order to screen among these four structural prototypes all the possible *TMX* configurations (*T* (13) * *M* (9) * *X* (5)), we have used first-principles calculations to identify those which are predicted as thermodynamically stable and semiconducting. For these 570 configurations, the most stable structure among the four prototypes was determined. In a second step, we looked more specifically at the **TiNiSi** structure-type, which has been so far reported to display only metallic properties. Nonetheless, this screening helped us identify one compound, HfCoP which does not present a metallic band structure. HfCoP was thus synthesized by melting the elements (a = 6.272 Å, b = 3.669 Å, c = 7.116 Å). Its electrical resistivity indeed displays a semi-conducting behaviour and confirms our theoretical work.

Keywords: First, principles calculations, Intermetallic

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Effects of Cu-substitution on Thermoelectric Properties of Pseudogap Ternary Intermetallic Compound TiNiSi

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Abstract

A material with a pseudogap at the Fermi-level in the density of states (DOS) has been considered as a promising candidate of thermoelectric (TE) material which can operate around room temperature. For instance, a full-Heusler Fe_2V(Al_1-xSi_x) compound with a pseudogap shows a large power factor about 5.5×10ˆ-3 W/mKˆ2 around room temperature (1). According to Landrum and Hoffmann's report (2), a pseudogap can be identified from the calculated DOS of TiNiSi with an orthorhombic structure. Hence, it is expected that the TiNiSi compound could be a hopeful TE material which can be used around room temperature. In this work, the effects of Cu-substitution for Ni-sites on TE properties of TiNiSi are investigated.

Polycrystalline samples of Cu-substituted Ti(Ni_1-xCu_x)Si (x = 0, 0.05, 0.10, 0.15, 0.20) compounds were synthesized by combining arc-melting and spark plasma sintering methods. The crystal structure of the compounds was investigated by Rietveld analysis of powder X-ray diffraction data. The electrical conductivity, Seebeck coefficient, and thermal conductivity were measured in the temperature range from 300 K to 800 K. The Hall coefficient was measured at 300 K.

With increasing the Cu content, the TE properties of TiNiSi compound were improved; the absolute value of the Seebeck coefficient and electrical conductivity both increased. Although the thermal conductivity increased, the dimensionless figure-of-merit, zT, was enhanced by the Cu-substitution. The highest zT was achieved about 0.037 at 700 K for the 15% Cu-substituted compound.

In the conference, the detailed results and discussion on the TE properties of Ti(Ni_1-xCu_x)Si (x = 0, 0.05, 0.10, 0.15, 0.20) compounds will be presented.

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Keywords: thermoelectric material, pseudogap, intermetallics

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Electronic and thermal properties of Si-doped InSe layered chalcogenides

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Abstract

Layered metal chalcogenide materials have been paid attention for potential thermoelectric materials due to their intrinsic low thermal conductivity due to their weak atomic boning between layers. Indium selenide InSe crystal is known to have low thermal conductivity in range of _˜0.37 – 1.2 Wm-1K-1, while their intrinsic carrier concentration is quite low as _˜10ˆ14 cm-3 due to the relatively large bandgap of 1.2 eV. Therefore, InSe-based materials can be good candidates for thermoelectric materials, if the carrier concentration can be increased by proper doping. Here, we investigated the electronic and thermal properties of the series of Si-doped InSe, In1-xSixSe polycrystalline samples. The cation substitution of Si increased electrical conductivity, while decreasing activation energy for the electrical conductivity. The negative Seebeck coefficient increased as Si doping increases, resulting in large enhancement in power factor. The slight reduction of thermal conductivity was also observed by the doping. As results, the thermoelectric figure of merit zT value was expected to higher than 0.2 at high temperature, which can offer possibility for InSe-based thermoelectric materials. The improvement of thermoelectric properties is related with simultaneous increase of σ and S with Si doping, which will be discussed based on the interrelationship between two kinds of electrons contributing to charge transport in InSe; (1) high mobility electrons in the conduction band and (2) low-moblity electrons in the 2D electric subbands.

Keywords: InSe, doping

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Data-driven materials design from large-scale experimental data

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Abstract

Experimental data published in papers are seeds for materials informatics. However, most of published experimental data are in plot images, and digitization of such data is difficult by automatic programs.
In this study, we developed a web system named *Starrydata*, to collect the digitized experimental data from plot images. Although this system relies on manual data collection, our user interface dramatically improved the data collection speed. Our database contains over 2,300 samples, and 500 samples are added in each month. The target datasets were temperature (T) dependences of Seebeck coefficient S, electrical conductivity σ (or resistivity ρ), thermal conductivity , power factor PF, figure of merit ZT and carrier density n. Sample composition were manually collected from text.

Digitization of plot data enables evaluation of missing parameters, such as ρ from σ, and Z from ZT and T. Pisarenko (S-n) plot and Jonker (S-lnσ) plot were generated, using many more samples than past studies.

Combination of first-principles calculation and experimental data enables evaluation of more parameters. Electron relaxation time
*taue*l was evaluated by dividing experimental σ by calculated σ/
*taue*l. We found that
*taue*l is strongly dependent on samples, and longer
*taue*l results in high ZT.
We carried out machine learning of the digitized data by using neural networks, to predict the values of S, σ, and n from chemical compositions. Our prediction of S achieved ±10% of accuracy, for 90% of the samples. This allows us to predict promising compositions to achieve high ZT.

Keywords: thermoelectric materials, materials informatics, database, machine learning

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Origin of anomalous anisotropic thermoelectric transport properties in alpha-NaFeO2-type d0-layered complex nitrides

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Abstract

Layered crystals exhibit various properties that make them suitable as thermoelectric materials. For example, layered chalcogenides, layered oxides, and misfit layered compounds are promising materials for high-efficiency thermoelectric conversion. [1] There are several layered complex nitrides, but they remain quite underdeveloped. Recently, we have evaluated the thermoelectric transport properties of d0-layered complex nitrides, AMN2 (A = Sr2+, Ba2+, Na1+, Cu1+, M = Ti4+, Zr4+, Hf4+, Nb5+, Ta5+) by density functional theory calculations.[2-6] Among them, unusual isotropic or anisotropic electronic transport properties were found in alpha-NaFeO2-type d0-AMN2.[3,5,6] Despite the alpha-NaFeO2-type layered crystal structure, all materials had three-dimensional electronic structures. SrZrN2 and SrHfN2 exhibited isotropic electronic transport properties because of the contribution of the Sr 4d orbitals to the conduction band minimums (CBMs) in addition to that of the Zr 4d (Hf 5d) orbitals. NaNbN2 and NaTaN2 showed weak anisotropic electronic transport properties due to the main contribution of the Nb 4d (Ta 5d) and N 2p orbitals to the CBMs and no contribution of the Na orbitals. Origins of the isotropic or anisotropic thermoelectric transport properties in the alpha-NaFeO2-type AMN2 will be discussed.

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Keywords: Layered complex nitrides, Density functional theory calculations

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Metals with band gap as good thermoelectric materials, a High-Throughput approach.

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Abstract

Most of the research in thermoelectrics is focused on small band gap semiconductor. They usually show high Seebeck coefficient and can reach via doping high values of conductivity in order to get a high power factor (PF) value.

On the other hand, metals are generally considered as bad thermoelectric materials. However, among them some exceptions like La3Te4, Yb14MnSb11, NbCoSb are well known. Indeed, looking at their band structure, all these materials are metals with Fermi level crossing some bands, but a gap is present somewhere little above or below it. This key feature makes these metals comparable to degenerate semiconductors and suitable for TE applications.

Usually these few exceptions steamed from studying single semiconductor phases chemically
linked to them. Nowadays, though, High-Throughput (HT) DFT calculations allow to have access to a large quantity of computed properties for thousands of materials. This allows for large scale investigations screening materials according specific features.

In this work, exploiting the power of HT computational screening and using the band structures and the transport properties available in Materials Project database, we searched for metallic compounds (i.e., with a Fermi level crossing bands) but with a band gap close to this Fermi level. We will show that thousands of metals have this feature, part of them have a decent value of the PF and many of them can reach very high values of PF as soon as the chemical potential is tuned through doping. We will discuss the identified compounds and show that our approach opens a new way to search for high performance thermoelectric materials within computational databases.

Keywords: metals, bandstructure, highthroughput, database, computation, dft, boltztrap

*Speaker

Thermoelectric properties of reduced graphene oxide (rGO) prepared under an electric field

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Abstract

Graphene, graphene oxide (GO) and reduced graphene oxide (rGO) are of great interest as two-dimensional (2D) thermoelectric materials. Recently, Li et al. synthesized rGO film with a reduction treatment at 3300 K and attained a extremely high conductivity and power factor. On the other hand, we reported that applying an DC electric field during dry process of GO solution increasd intensity ratio of G/D bands in Raman spectrum of rGO films.
In the present work, we studied the effect of an external electric field during film formation on thermoelectric properties of rGO films with various thickness. Firstly, GO aqueous suspension was spin-coated on UV ozone-treated SiO2 substrate at spin coating speed between 500 and 3000 rpm. The substrates with GO solution were dried at room temperature for 30 min under an electric field up to 1.1 kV/cm. Next, the reduction treatment was carried out in ethanol vapor at 950 ∘C for 30 min. Film thickness was estimated by means of SEM analysis and turned out to be 300-30 nm.
Electrical conductivity and Seebeck coefficient S were measured at room temperature. It was found that S did not change with increase of electric field Edry applied during dry process. This suggests small change in carrier density. Meanwhile, increased significantly with increase of Edry. This tendency becomes more evident for the thinner film. The highest value was attained to be 2300 S/cm for the film coated at 3000 rpm and dried under 1.1 kV/cm. These results can be explained as below. The directions of GO molecules could be aligned under DC electric field due to the molecular polarization. The effect of DC field on GO solution become more effective for thinner film. Therefore, crystallinity of thinner rGO films synthesized under high DC field could be improved drastically which results in high electrical conductivity.

Keywords: graphene, reduced graphene oxide, electric field, thermoelectric

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Pnp Conduction Switching and ultralow Thermal Conductivity and Excellent Thermoelectric Properties of Thallium Silver Chalcogenides

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Abstract

Among the materials under thermoelectric investigation, thallium tellurides are bestowed with extraordinarily low thermal conductivity. Here we report on our newest results in the Tl-Ag-*Q* systems with Se and Te, specifically on variants of the Zr2Fe12P7 structure type. Tl2Ag12Se7 crystallizes in a $\sqrt{3}$ x $\sqrt{3}$ x 1 super cell, while the corresponding telluride forms an incommensurately modulated composite cell. As prepared, both materials exhibit small deficiencies on the Ag positions, and the telluride comprises a Te excess with regards to the 2-12-7 stoichiometry. Thusly, the formulae are best expressed as Tl2Ag12–xSe7 and Tl2Ag12–xTe7+y. In accord with our electronic structure calculations, both materials are narrow gap *p*-type semiconductors with ultralow thermal conductivity. The latter is especially true for the telluride because of its incommensurate modulation. While the selenide's thermoelectric performance is inhibited by its low electrical conductivity, the telluride achieved figure-of-merit values in excess of unity above 500 K.

Keywords: pnp switch, thermal conductivity, thallium chalcogenides

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A First-Principles Theoretical Study on the Potential Thermoelectric Properties of MgH2, CaH2 and YbH2

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Abstract

Most TE materials studied till now are around traditional systems and cannot meet the requirements of application due to their low efficiencies or toxicity. Therefore, it is still under urgently need to explore new kinds of TE materials, especially those with nontoxic and earth-abundant elements considering the practical applications. Metal hydrides have been studied for their potential as promising hydrogen storage candidates for the last 20 years but the TE properties of these compounds have been rarely studied on calculations or by experiments. According to previous studies, some of the hydrides are semiconductors. It is desirable to predict the individual thermoelectric parameters and develop a fundamental understanding of heat and charge transports in these compounds. In this paper, we studied the thermal and electronic transport properties of MgH2, CaH2 and YbH2 systematically as examples using first-principles calculations, Boltzmann transport properties, and a modified Slack's model. Our theoretical study showed that these hydrides could be potential thermoelectric materials.

Keywords: First, principles calculations, Hydrides, Thermal properties

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A quality factor limit to zT

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Abstract

Recent years have witnessed steady increases in the thermoelectric (TE) material figure of merit, zT driven by engineering materials to lower the lattice thermal conductivity, but wider applications require still higher zT's. Three of the four parameters in zT are electronic transport coefficients, and complex TE materials and electronic structure engineering may offer possibilities for increasing zT. We present a computational technique for identifying promising materials. It provides a strong filter that can help identify especially promising research directions as well as unpromising ones. The widely-used TE quality factor (the B-factor) is based on an effective mass approximation. We generalize the B-factor (and refer to it as the b-factor) so that it applies directly to complex TE materials with no need to extract effective mass parameters. In the absence of bipolar effects, zT is a function of the b-factor alone. Using a parabolic band reference, we compute the maximum zT (for optimized doping) and plot it vs. the b-factor at the maximum zT. Large b-factors are always beneficial, but we ask the question: "At a given b-factor, are there complex TE materials that offer a zT that is higher than that of a simple parabolic energy band?" We then numerically compute the peak zT vs. b-factor characteristics for a number of complex TE materials. Remarkably, all results are essentially identical to that of a simple parabolic energy band. We also examine TE performance in 1D, 2D and for a single energy channel, and show that these approaches provide no benefit. We do not, however, believe that this behavior is fundamental. Identifying materials that exceed this apparent parabolic band limit would open up new possibilities to increase zT.

Keywords: Figure of merit, Quality factor, B, factor

*Speaker

Reliable High Throughput Electrical Transport Calculations and Its Application in Thermoelectrics

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Abstract

In recent years, high throughput (HT) material screenings, represented by the materials genome initiative proposed in 2011, have been ever important in the search of novel functional materials. The key issues of successful HT prediction are two-fold, one is the application of big data, the other is the proper HT algorithm for functional properties. In thermoelectric (TE) field, several groups have made HT attempts on the predictions of electrical transport properties. These pioneering works focus mostly on the big data results; the improvements of the HT algorithm are, however, basically ignored. In this talk, we will briefly review the current HT works on electrical transport properties, and then present our solution on HT electrical transport properties. Our method, Transoptic, considers both the momentum matrix method for accurate group velocities and the evaluations for carrier relaxation times. The former ensures the accuracy when dealing with large cells, and the latter improves the accuracy of carrier mobilities. The applications of this method on several types of materials are demonstrated, and very accurate results can be seen in TE chalcogenides with diamond-like structures.

Keywords: thermoelectrics, electrical transport properties, relaxation time, group velocity

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Structure and Thermoelectric Properties of 2D Cr2Se3-3xS3x solid solutions

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Abstract

Chromium selenide (Cr2Se3), consisting of earth-abundant elements, is a new cost-efficient thermoelectric material. In this study, a series of Cr2Se3-3xS3x (x = 0–0.1) solid solutions was synthesized by solid-state reaction combined with the spark plasma sintering (SPS) process. The correlation between sulphur substituted on selenium sites, the structure, and the thermoelectric properties of Cr2Se3-3xS3x solid solutions was systematically investigated. The solubility limit of S in Cr2Se3-3xS3x is about 10%. Through S substitutions, the band gap has been increased, the Seebeck coefficient has been effectively increased, and the lattice thermal conductivity has been substantially decreased. Mainly due to the remarkable decrease in the lattice thermal conductivity, the ZT values of Cr2Se3-3xS3x (x = 0–0.1) solid solutions have been increased. The maximum ZT value of 0.29 has been achieved at 623 K for the Cr2Se2.7S0.3 compound, which is by 32% higher than the ZT value of pure Cr2Se3.

Keywords: Cr2Se3, 3xS3x, 2D materialthermoelectric properties

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Secondary Phase Assisted Enhanced TE properties and Controlled Microstructure in Chalcopyrite-type CuGaTe2

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Abstract

Novel materials and concepts are being investigated to try to develop viable thermoelectrics [1]. Chalcopyrite family is well known for its high thermoelectric performance [2-4]. In our recent research we discussed high power factor in CuGa1-xMnxTe as a result of interactions between magnetic moments of Mn and charge carriers [4]. In this research work we synthesized polycrystalline samples with composition CuGa1-xFexTe2 with x = 0.0 to 0.05 by spark plasma sintering method [5]. Structural, thermal and thermoelectric transport properties were measured and analyzed for all nominal compositions up to 870 K. Solubility of Fe in CuGaTe2 was found to be very small, and other phases like FeTe2 and CuTe were identified. These secondary phases assisted in tuning thermoelectric properties within the certain limit. EPMA revealed secondary phase FeTe2 has grain sizes of a few micro meters, and is distributed at the grain boundaries for $x \leq 0.02$. On the other hand, for $x \geq 0.03$ the grain sizes of the FeTe2 phase develops to the order of 10 mm, comparable to the grain sizes of the chalcopyrite-type phase. This microstructural change greatly influenced on thermal conductivity. Thermal conductivity showed a significant decrease with the addition of Fe up to x = 0.02, which started to increase for $x \geq 0.03$. ZT peak value of 0.92 is recorded for x = 0.02 at 870 K, which corresponds to an enhancement of 60% from that of non-doped CuGaTe2. We will present how controlling microstructure can be crucial in enhancing thermoelectric properties.

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F. Ahmed, N. Tsujii and T. Mori, J. Materiomics (2018). https://doi.org/10.1016/j.jmat.2018.02.002

Keywords: Chalcopyrite, Composite, Microstructure, Thermal conductivity, Thermoelectricity

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Synthesis and thermoelectric properties of (Nb,Ta,V)CoSn Half Heusler alloys

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Abstract

Half Heusler alloys are intermetallic compounds with general formula ABX, where A is a highly electropositive transition metal, B is a less electropositive transition metal and X is a main group element. These materials include families with 8 and 18 valance electrons per formula unit. According to ab-initio calculations [1], the stability of half-Heusler phases was predicted for different combination of elements respecting the count of 18 valence electrons. The focus of this work is on the family (V,Nb,Ta)CoSn, where VCoSn is predicted to be unstable while NbCoSn and TaCoSn are predicted to be stable, as confirmed by experimental data [2,3].

The formation of the terminal half-Heusler phases (VCoSn, NbCoSn, TaCoSn) was studied both in equilibrium and metastable conditions using different processing routes (arc melting, rapid solidification, mechanical alloying). It was found that VCoSn is not an equilibrium phase, while the NbCoSn and TaCoSn phases can be synthesized by arc-melting and mechanical alloying, respectively. In both cases, pure single phase was obtained after annealing.

Isoelectronic partial substitution of the site A was also performed in (V,Nb,Ta)CoSn in order to obtain substituted or immiscible half-Heusler phases with enhanced phonon scattering.

Selected (V,Nb,Ta)CoSn were sintered by Spark Plasma Sintering (SPS) starting from different precursors to evaluated the effect of different processing routes on thermoelectric properties.

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Work financed from Grant N. CSTO162398 (A. Castellero)

Keywords: Half Heusler alloys, Thermoelectric, microstructure

*Speaker

Thermoelectrics for Lunar Energy Production, development of MgAgSb as a low temperature thermoelectric material

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Abstract

MgAgSb is a high performance thermoelectric (TE) material for harvesting energy from heat sources at temperatures between 300 and 573K. While the research performed has yielded very good results in terms of thermoelectric performance, the synthesis method used in the publications are not suited to industrial production, and the heat treatment needed to temper the material is too long to be viable in a large scale production process.
We attempt to produce a material of comparable quality with industrial production capacity. We use melting, ball milling and hot pressing to produce the material. The results gradually improve as we adjust various parameters such as composition, melting temperature, ball milling parameters and several others. Only one of the samples makes a true breakthrough and gets on par with desired properties, comparable to those published by Zhao et al. (*High thermoelectric performance of mgagsb-based materials. Nano Energy, pages 2211–2855*; PF=2.0E-3 W/mK^2 ZT=0.8K at 300K ; PF=2.2E-3 W/mK^2 ZT=1.2K at 500K). The next step in the study of this process is the doping of the material with Te, for which the first attempt gives a PF comparable to the previous values and a slightly lower ZT.
A second manufacturing procedure is studied, with the material being synthesized in two steps: first magnesium and silver are reacted together in a gas atomizer, leading to the formation of MgAg precursor. This compound is then mixed in a ball mill with pure antimony and additional magnesium and pressed to form the final product. It has been notices that this method gives equivalent properties to Zhao and al.'s publication when small amounts of alumina (impurities) is found in the microstructure. The next step is to study the influence of alumina on the microstructure and the properties by changing the amount we voluntarily add to the ball-milling step.

Keywords: MgAgSb, thermoelectric, process, development, energy production, ball, milling, hot, pressing, melting, gas atomisation

*Speaker

Designing thermoelectric highly efficient Hf-free p-type Heusler compounds via phase separation and nano-composites

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Abstract

Half-Heusler compounds are one of the most promising candidates for thermoelectric materials for automotive and industrial waste heat recovery applications. In this talk, we will give an overview about our recent investigations in the material design of thermoelectric half-Heusler materials. Since the price for Hafnium was doubled within the last 2 years, our research focusses on the design of half-Heusler compounds without Hafnium. We will present a recent calculation on ZT per and efficiency per for various materials followed by our very promising results for n-type half-Heusler compounds without Hafnium resulting in 20 times higher ZT/ values, which reduces the cost of TE materials used in a commercial TEG by 90%, entering an economical meaningful scenario. We will show how we adapted our knowledge from the n-type materials to design p-type Heusler compound without Hafnium exhibiting similar thermoelectric properties. We will present how we used phase separation to design thermoelectric highly efficient nano-composites of different single-phase materials. Since any high temperature TE material will only be suitable for the mass market if the material production and the module production is industrial upscalable, we will comment on various upscaling approaches, their challenges, and how one could tackle these challenges.

Keywords: Heusler compounds, phase separation, Hf, free

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Synthesis and Thermoelectric Properties of (Ce1-zYbz)0.8Fe4-xCoxSb12 Skutterudites

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Abstract

Skutterudite is one of the promising materials for thermoelectric power generation because it exhibits superior thermoelectric performance in the intermediate temperature range and has both n-type and p-type materials. Thermoelectric properties for the filled skutterudite can be improved through compositional optimization by filling and substitution: optimized carrier concentration and charge compensation. In this study, p-type skutterudites were prepared with the partial double filling of Ce-Yb and the partial substitution Co for Fe. (Ce1-zYbz)0.8Fe4-xCoxSb12 (z = 0.25-0.75 and x = 0-1) were synthesized by using encapsulated melting at 1323 K for 10 h. Ingots were annealed at 873 K for 24 h and then hot-pressed at 873 K for 1 h. Thermoelectric and transport properties were examined and discussed.

Keywords: thermoelectric, skutterudite, double filling, substitution

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Charge Transport and Thermoelectric Properties of (La1–zPrz)yFe4–xCoxSb12 Skutterudites

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Abstract

Filled skutterudite is a thermoelectric material that reduces lattice thermal conductivity by phonon scattering due to the rattling effect of atoms filled in the voids. Co4Sb12-based n-type filled skutterudites have high thermoelectric performances but Fe4Sb12-based p-type filled skutterudites have relatively lower thermoelectric properties. Fe4Sb12 has only 68 valence electrons with a deficiency of 4 valence electrons and thus it is unstable. However, it can be stabilized as R4+[Fe4Sb12]4– and Co or Ni charge compensation is sometimes employed to improve the thermoelectric performance and to stabilize the electronic structure. Many studies have been conducted to enhance the thermoelectric properties of p-type filled skutterudites. In particular, double- or multiple-filling reduces the lattice thermal conductivity through a wider range of phonon scattering by filling two or more rare-earth elements in the voids. In this study, La/Pr-partially-double-filled and Co-substituted (La1–zPrz)yFe4–xCoxSb12 were prepared, and their thermoelectric and charge transport properties were examined.

Keywords: thermoelectric, skutterudite, partial double filling, charge compensation

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Thermal conductivity of Fe2VAl-based superlattice thin film

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Abstract

Fe2VAl-based compound ($L2_1$-type Heusler phase) has been widely investigated as one of the most promising "practical thermoelectric materials" due to the large power factor reaching 6.5 mWm-1K-2 which is even larger than that of Bi2Te3-based thermoelectric materials. Besides, Fe2VAl-based compounds are composed of non-toxic and abundant elements and characterized by good mechanical strength and strong resistance both for oxidation and corrosion. These characteristics let us strongly believe that Fe2VAl-based compounds are suitable for practical applications. Unfortunately, however, the figure of merit is still much less than unity due to the high thermal conductivity. [K. Renard et al., *J. Appl. Phys.* **115**, 033707 (2014); S. I. Kim et al., *Science* **348**, 109 (2015)]
We tried, in this study, to fabricate the artificial superlattice thin film in order to effectively reduce the thermal conductivity, and investigated the phonon scattering mechanism in the Fe2VAl-based thin films.
The epitaxially grown thin film samples were prepared by the radio frequency magnetron sputtering technique on the MgO (001) single crystalline substrate. The deposited films were characterized by high-resolution X-ray diffraction, scanning transmission electron microscope. We also employed the reciprocal space mapping around the 202 spot from the Mo-layers and FeVAl-layers in Ta-doped FeVAl/Mo superlattice using hard X-ray synchrotron radiation with 12.4 keV photon energy (wavelength is 0.1 nm) at BL15XU, SPring-8. The thermal conductivity was evaluated using pico-seconds time-domain thermo-reflectance measurements with the rear-heating front-detection configuration (PicoTR, PicoTherm Ltd.). The effects of periodicity in superlattice, impurity scattering, boundary scattering on thermoelectric properties will be discussed at the presentation.

Keywords: Fe2VAl, Heusler, thermoelectric, reciprocal space mapping, time, domain thermo, reflectance

*Speaker

Investigation on the Boron-rich compounds in the RE-(Cr, Mo)-B systems

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Abstract

Since years, Boron-rich compounds arouse a strong interest in the thermoelectric field, in particular in the extremely high temperature range for power generation, due to the very high melting point of such compound. [1]
Among them, the compound YCrB4 (Pbam, a=5,972 Å, b=11,46 Å, c=3,461 Å [2]) were of a special interest because of the semiconducting behavior. Interestingly YMoB4 has an electrical resistivity with one more order of magnitude, a lightly more important thermopower but a better power factor over 900 K. [3]

It would be interesting to dope this system with some rare-earth element (Y1-xRExCrB4) to see how will evolve those properties, with the investigation of RE-(Cr, Mo)-B systems by first, achieving the synthesis of a single phase and then proceed to the physical measurements.

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Keywords: YCrB4, Ternary boride, Boron rich

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Spark Plasma Sintered Bi1-xSbx (x=0.10, 0.14) alloys and their electronic transport properties

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Abstract

In this work, the electronic transport properties of polycrystalline Bi1-xSbx *(x=0.10, 0.14)* alloys were studied in the temperature range of 20-300 K. The alloys were prepared by Ball Milling and transformed into pellets by Spark Plasma Sintering (SPS). The prepared samples displayed a negative Seebeck coefficient, indicating their n-type conductivity, and the magnitude depends on the composition.
The temperature dependence of transport parameters, scattering coefficients and Fermi level, were determined assuming that prepared alloys are non-degenerated semiconductors in the temperature range where they displayed such one characteristic.

Outstandingly, the Bi0.86Sb0.14 alloy displays a semiconducting behavior in the entire 20-300K temperature range, whereas, the Bi0.90Sb0.10 alloy exhibits metallic conductivity at low temperatures (20-120 K) and semiconducting one at (160-300 K) temperature range. The metal-like character of the Bi0.90Sb0.10 sample was attributed to the electron conduction trough the surface gapless states.
The thermoelectric properties such as, Seebeck Coefficient, electrical resistivity and power factor for the Bi0.90Sb0.10 sample exhibited encouraging, FP= 1 W/mK2, S=-120 μV/K and ρ=3$\mu\Omega$-m, in agreement with those have been reported for the state of the art .

Keywords: Bi1, xSbx alloys, Fermi Level, scattering coefficient, gapless states

*Speaker

Thermoelectric properties of CVD grown ytterbium boride thin films with controlled crystallinity

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Abstract

In parallel with the recent developments regarding bulk thermoelectric materials,[1] thin film thermoelectrics offer new perspectives for different applications such as microsensors. While some materials like Bi-Sb-Te derivatives or organic thin films have already shown promising results at low temperature, there is a dearth of suitable high-temperature resistant films. In this context, the general ability of boride materials to withstand such high temperatures and the encouraging thermoelectric properties in SrB6 thin films are highly promising prospects.[2,3]
Here, we report the rapid chemical vapor deposition of high-purity ytterbium boride thin films with controlled crystallinity and their thermoelectric properties. An excellent power factor of ≈200 μW m-1 K-2 at 573 K was measured on a highly orientated YbB6 thin film.

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Keywords: Boride, Thin, film, CVD

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Bulk and thin film Heulser alloys - alternative moderate temperature thermoelectrics

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Abstract

Fe2VAL-based Heusler systems are promising thermoelectric materials in the range of 70 to 300∘C, due to their large power factor. The base material exhibits a gap in its electronic density of states near the Fermi energy. Since the Fermi energy is located towards the valence band, a hole-dominated transport is observed. By various means, like substitution and doping, as well as by off-stoichiometric sample preparation, which results in small shifts of the Fermi level, optimised p- and n-type materials have been prepared, exceeding the power factor of Bi2Te3-based systems substantially. To reduce the thermal conductivity, which is around a magnitude higher as in commonly used thermoelectric materials, metals of group 6, like tungsten, were used for substitutions. Besides, depositing these materials as thin films on different substrates, presumably reduce the overall thermal conductivity, too [1]. Magnetron sputtering under reduced argon atmosphere was used for the coating process. The resulting thin films were then heat treated at different temperatures and durations. Afterwards, the structure was analysed by X-ray diffraction. The temperature dependent electric resistivity, Seebeck coefficient and thermal conductivity were measured in order to characterise the physical behaviour. Here, we report on results of p- and n-type thin films deposited on different substrates and summarise the thermoelectric properties of these systems. In fact, the thermoelectric performance turns out to be significant enhanced.

Furuta, Yukihiro, et al. "Fe2VAl-based thermoelectric thin films prepared by a sputtering technique." Journal of Electronic Materials43.6 (2014): 2157-2164

Keywords: Heulser, thin film, thermoelectric

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Thermoelectric properties of Fe2Ti1-xVxSn Heulser alloys

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Abstract

Theoretical calculations [1] have predicted that a large (up to -300 μV/K) Seebeck coefficient can be achieved in Si or V doped Fe2TiSn alloys due to the change of the band structure of the host compound. The aim of the present work is experimental and theoretical investigation of the influence of vanadium on thermoelectric properties of Fe2TiSn. Polycrystalline ingots of Fe2Ti1-xVxSn (0 £ x £ 0.2) were prepared by arc melting method in protective argon atmosphere. The obtained ingots were annealed in vacuum at 1073 K for 10 h. X-ray diffraction revealed that all the alloys crystallize in the L21 Heusler structure. Measurements of electrical resistivity r, Seebeck coefficient S, and thermal conductivity k performed in a temperature interval 300 – 973 K showed that *i*) r demonstrates behaviour typical for semiconductors and non-monotonously depends on the V doping level; *ii*) contrary to the theoretical predictions [1], V doping was found to have an immaterial impact on the enhancement of S which did not exceed 30 /K in the studied temperature interval; *iii*) thermal conductivity increases with increase in temperature. This increase is conditioned by the charge carrier subsystem. Results of theoretical calculations of transport properties performed in the framework of Boltzmann transport theory for the stoichiometric composition are in qualitative agreement with the experimental results.

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Keywords: Heusler alloys, transport properties, Seebeck coefficient

*Speaker

p-type Al-doped Cr-deficient CrN thin films for thermoelectrics

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Abstract

Thermoelectric properties of chromium nitride (CrN) based thin films grown on c-plane sapphire and MgO substrate by dcreactive magnetron sputtering were investigated. CrN is well known as a degenerate n-type semiconductor. In this work, aluminum doping was introduced in CrN using co-sputtering deposition. Under the present deposition conditions, over-stoichiometry in nitrogen (CrN1+x) is obtained in the epitaxial rock-salt structure. Structural, morphology and electrical characterization were performed on the different Cr-deficient CrN films. The thermoelectric properties of the films depends on the substrate nature and also on the aluminium content. The over-stoichiometry in nitrogen combined with aluminum doping lead to a p-type semiconductor behavior of CrN, with promising thermoelectric properties. For example, the Cr0.96Al0.04N1.17 film exhibited a Seebeck coefficient of +140 micro.V/K and a power factor of 0.3 mW/(m.K) at 300 ∘C. The control of the semiconductor behavior of CrN films can be tailored by controling of the stoechiometry and/or aluminum doping. These results are a starting point for designing p-type and n-type thermoelectric materials based on chromium nitride thin film, a material cheap and routinely grown at industrial scale.

Keywords: film, nitride, p type semiconductor, stoichiometry

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Performance of amorphous silica-based protective layers on skutterudites in oxidizing atmosphere

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Abstract

Abstract

A common issue of most thermoelectric materials designed for working at high temperatures is their stability. Beside the structural and microstructural stability and durability against separation of host atoms and dopants, which are necessary conditions to be met for a particular material for application, chemical stability of interface of the TE material with surrounding environment (air, vacuum, interconnectors) is the main challenge for materials scientists. Skutterudites are well developed thermoelectrics with many beneficial properties, which makes them good candidates for TE generators fabrication. However, pure CoSb3 depending on the chemical environment undergoes decomposition or oxidation at temperatures as low as 650K, thus it needs surface protection.

In our study we have used silica-based layers for surface protection of n and p-type skutterudites. Various thermal analysis techniques and SEM observations were used in order to examine layer stability, sample-coating interface and material durability under long-term annealing in the air. We show applicability range of this type of layers on skutterudites and their further perspectives.

Acknowledgments

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Keywords: skutterudites, oxidation, stability, protective layers

*Speaker

Effect of Annealing on Sb Doping and Thermoelectric Property of N-type Half-Heusler Compounds

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Abstract

Sb doping n-type half-Heusler thermoelectric materials Zr0.25Hf0.25Ti0.5NiSn1-xSbx by direct arc melting method may cause problems such as uncontrollable doping amount and unstable thermoelectric performance. A practical way was developed to combine high temperature annealing and quenching according to the study on the effect of quenching temperature and cooling rate on the microstructure and thermoelectric properties of the Sb doped Zr0.25Hf0.25Ti0.5NiSn1-xSbx materials. By this method, the doping amount of Sb is controlled and the lower melting point second phase is suppressed effectively, which leads to a more stable thermoelectric performance of Sb doped Zr0.25Hf0.25Ti0.5NiSn1-xSbx materials.

Keywords: N, type Half, Heusler, annealing temperature and cooling rate, Sb doping, thermoelectric performance

*Speaker

Structural stability and thermoelectric properties of phosphides NiSi3P4 systems

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Abstract

In recent years, the computational performance increases more and more. The exploration of novel thermoelectric (TE) materials using computational method is attracted as an economically-efficiently material design. However, TE materials screened by the computational methods focusing on only TE properties tend to have the difficulty for its synthesis or carrier doping in general.
We selected the mother phases of crystal structures experimentally reported in the Crystallography Open Database. The structural stability of the substitution systems was evaluated by comparison between total energy of the substitution systems and that of decomposed systems using density functional theory (DFT) calculation. The possibility of doping carriers was evaluated from the shift of the chemical potential between the mother phase and the substitution systems. After that, we chose the phosphides NiSi3P4 and the Ga substitution NiSi3-xGaxP4 as a typical example of carrier tuning under consideration of the structural stability.

The density of states (DOS) of NiSi3-xGaxP4 (x = 0, 0.042) was calculated using the OpenMX software package based on DFT. For the DOS of $x = 0$, the chemical potential locates in a forbidden band. For $x = 0.042$, the shape of the DOS is not so changed compared to that of $x = 0$, and the chemical potential is shifted to the top of valence band.

We experimentally investigated the TE properties of NiSi3-xGaxP4 (x = 0, 0.042). The polycrystalline samples were synthesized using fusion method. When the x increases; the electrical resistivity at 300 K decreases less than five-tenth of that of $x = 0$. These experimental and theoretical results indicate that the hole doping is occurred by the Ga substitution. This material design under consideration of a structural stability for doping carriers using DFT calculation develops the exploration of the novel TE materials.

Keywords: phosphides, DFT calculation, experiment

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Enhanced thermoelectric properties of Sb doped ternary skutterudite

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Abstract

Substituting Ge and Te elements on the pnictogen site in the CoSb3 skutterudite structure yields a class of ternary CoGe1.5Te1.5 compounds, in which Ge and Te form an ordered ring structure. Analysis of the X-ray diffraction data reveals that CoGe1.5Te1.5 adopt a rhombohedral skutterudite-related structure. Due to the structural complexity as compared with the binary skutterudite, the pnictogen substituted compound exhibit low thermal conductivity (1.56 W/mK at 723K). However, due to low carrier concentration and bipolar conduction in the n-type ternary compound, the zT was found to be low at high temperature. To overcome this issue Sb-doped CoGe1.5Te1.5 was synthesized by conventional ball milling method. By introducing Sb into the system, we are able to optimize the carrier concentration, which resulted in two order improvement in electrical conductivity without reducing the Seebeck coefficient. The Sb-doped CoGe1.5Te1.5 also exhibited low thermal conductivity (2.1 W/mK) and a maximum zT value of 0.48 was obtained at 723K.

Keywords: Skutterudite, Thermoelectric properties, thermal conductivity

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Contactless temperature measurement of atomic-layered MoS2 single crystal supported on silicon substrate

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Abstract

Thermoelectric (TE) power generation attracts much attention as one of energy harvesting technologies for utilizing low-scale energy. Improvement of TE performance of TE materials holds the key to success of the utilization. The recent trend of increase in ZT is the suppression of the lattice thermal conductivity by the introducing phonon scattering centers into the TE material specimen. In order to give a clear picture of the thermal conductivity suppression, we require the information of themal conduction and temperature distribution in the nano-scale which is the same as phonon mean free path. From this point of view, we have performed the temperature measurement of atomic-layered MoS2 single crystal by using Raman scattering spectroscopy.

We prepared thin flakes of MoS2 single crystals with thickness ranging from 10 to 700 nm by using mechanical exfoliation. These samples were mounted on a silicon substrate. We have measured the Raman scattering spectrum by using Horiba T64000 spectrometer and excitation laser with 532 nm. The temperature at the laser-spot on the MoS2 is calculated by the ratio of the anti-Stokes and Stokes scattering intensities.

The laser spot temperature T increases linearly with rising laser power P. The maximum T reaches ~600 K when P=200 mW in the case of 90 nm in thickness. The slope of T-P line strongly depends on the MoS2 thickness. This result indicates that this method gives information of thermal conduction through the thin MoS2 crystal. We will discuss the thermal conduction in nano-scale based on the contactless temperature measurements.

Keywords: Contactless temperature measurement, atomic, layered MoS2, Raman scattering

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Determination of mass transport behavior and electrode kinetic reaction for Spin Crossover (SCO) complexes in thermoelectrochemical cells

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Abstract

The thermoelectrochemical Seebeck effect (Se) is analogous to the solid state thermoelectric Se. In thermo-electrochemical cells (TECs), a potential arises when the potential equilibrium between the electrolyte and two working electrode surface in a solution containing a redox active material is disturbed by the temperature gradient. The capability to tune the electrochemical bandgap of the SCO material through manipulation of its spin state as a function of temperature makes it valuable as an optimization strategy for designing high power output TECs material. Three octahedral ionic complexes with N-donor ligands and benzoate counter ion were synthesized and dissolved in solvent and supporting electrolyte TBATFB for 0.1mM electrolyte solution. The spin states of the metal complexes determine both (i)the mass transfer characteristic (diffusion rate) of the TECs system, as defined by its diffusion coefficient; (ii) the electrochemical bandgap energy. Both information can be deduced by Cyclic Voltammetry (CV) and related back to the spin states and Se of the metal complexes. For example, the Fe complex solution is able to produce a Se of (-0.9mV/K) at 328 K. This is due to the fact that the Diffusion rate of the Fe complex is highest, as well as possessing the lowest electrochemical bandgap. In particular, the diffusion rate of the complex shows two distinct gradients which represent the two stable molecular conformations corresponding to the LS and HS states at the lower and higher temperatures respectively. In summary, we have demonstrated the potential of tuning the Se depending on the choice of metal centre if similar octahedral SCO metal complexes. Its application in practice TECs can be extended by utilizing positive and negative Se solutions as potential "p" and "n" type materials for TECs energy harvesting devices.

Keywords: Thermoelectrochemical cells, Spin crossover, Seebeck polarity, P, type, N, type

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Thermoelectric properties of synthesized under high pressure Nd filled CoSb3-skutterudite

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Abstract

Thermoelectric properties of NdxCo4Sb12 ($0 \leq x \leq 1.0$), synthesized using high-pressure techniques, have been studied. Although the binary skutterudites are known for their large Seebeck coefficients and high hole mobilities, the lattice thermal conductivity is too high. However, the partially filling of the voids with foreign atoms loosely bound produces "rattling" and consequently, reduces the lattice thermal conductivity. As partially void filling atoms, rare earth ions are effective in reducing the lattice thermal conductivity, while preserving both of the Seebeck coefficient and the electrical conductivity. A preparation of high-quality sample of Nd-filled CoSb3-skutterudite compound is quite difficult because of the low melting temperature and high vaper pressure of Sb. Furthermore, this causes impurity phases easily. High-pressure synthesis technique is one of the best technique to prepare high-quality samples of filled skutterudite compound. Moreover, the high-pressure technique increases filling limit of foreign ions in CoSb3-skutterudite structure. In this study, we report the thermoelectric properties of NdxCo4Sb12, with high filling ratio, prepared under high pressure.

Keywords: High, Pressure Synthesis, CoSb3, Skutterudite, Thermoelectric Properties, Thermal conductivity, Rattling effect.

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Evaluation of Galvano-and thermo-magnetic effects in sintered Bi-Sb alloy

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Abstract

Bi-Sb alloys show a strong thermomagnetic effect such as the magneto-Seebeck effect and Nernst effect. Wolfe *et al.* reported high dimensionless figure of merit ZT of 1.28 at 220 K in 1.7 T using a single crystal of Bi88Sb12 alloy [1]. We also reported the experimental results of the magneto-Seebeck coefficient in a sintered Bi90Sb10 alloy, and it was successfully explained by the theoretical calculation [2]. As a next step, this study focuses on the Galvano-and thermo-magnetic effect in a sintered Bi-Sb (Sb 23 at.%) alloy. A sintered Bi-Sb pellet was prepared by Spark Plasma Sintering (SPS) method. The electrical resistivity, Hall coefficient, Seebeck coefficient, Nernst coefficient and thermal conductivity in the magnetic field are evaluated.
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M. Murata et. al., Magnetic-field dependence of thermoelectric properties of sintered Bi90Sb10 alloy, *Journal of Electronic Materials*, **45**, 1875 (2016).

Keywords: Galvano, magnetic effect, thermo, magnetic effect, Bi, Sb

*Speaker

The Investigation of Mg2Sn Thin Film Material for Heat Energy Conversion Applications in Room Temperature Range

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Abstract

The various wearable devices for real time monitoring of vital information are researched, and part are being put to practice use. In this study, we especially focused on the Mg2Sn material to be able to expect a high TE characteristic shown in Room Temperature (RT) range, and carried out the research of the thin film process to fabricate the TE device on the glass substrate or other flexible substrate. We have the high quality single phase (cubic crystal) Mg2Sn thin film with the conventional magnetron sputtering process at 550C on the glass substrate followed by the deposition of very thin metal layer of Ag at RT with the sputtering which we introduce to try to control the conduction type ; Ag as a p-type dopant. The thickness of the Ag film was less than several 10 nm and the sintered Mg2Sn compound target was used in this sputtering process. We confirmed the single phase of the Mg2Sn films with XRD measurement, and the almost uniform distribution of the dopants (Ag) in the Mg2Sn films with the depth profile measurements of XPS. We speculate that the existence of Ag metal thin layer on the glass substrate controls the stacking of the film growth in the initial stage and then the dopants Ag are diffused into the film during the following growth process. Electrical p-type conductivity (σ) is increased with the doping of Ag. In the case of the Mg2Sn film doped 5 atomic% of Ag, ten times higher compared with undoped one. Despite the prediction from the theoretical point of view, Seebeck coefficient (S) is slightly increase on the Mg2Sn film with the 5 atomic% content of Ag, compared with the undoed one. Power Factor (= S*S σ) of the Ag doped film shows about 3x10-4 W/K2/m at around 300K. Further improvements will be expected by co-doping such as Co, Ni and Cu. So far, we have the result that the co-doping Co with Ag for Mg2S thin film is much effective to enhance the Power Factor.

Keywords: Mg2Sn, thin film, Ag, doping, co, doping

*Speaker

Morphology control of colloidal gropu(IV) nanoparticles via low-temperature synthesis from benign organogermanium halide reagents

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Abstract

Group IV semiconductor nanoparticles (NPs), such as Si, Ge, or SiGe, are gaining increasing interest in many fields, including batteries, photovoltaics, and thermoelectrics due to the size dependence of their properties that arise in the quantum confinement regime. Through nanostructuring and controlling stoichiometry, we aim to gain a higher degree of control over the electrical and thermal conductivity, in addition to being able to tune features such as the band gap energy and its position. One critical scientific goal is to enhance the performance of these materials via engineering their structures at the nanoscale. However, it has proven challenging to synthesize group (IV) nanomaterials with high quality and low cost, in addition to concerns revolving around synthetic scalability, safety, and environmental impact. We have been investigating a new synthetic scheme that combines benign reagents such as sulfur and primary amines to promote the reduction of Si(IV) and Ge(IV) organometallic precursors to form NPs at low temperatures (300 ∘C). We have elucidated the reaction mechanism and examined the effects of different variables, including the temperature, the solvating species, the Si and Ge precursor materials and their relative concentrations, among others, on the resulting morphology. These variables allow for control over the particle size and crystalline or amorphous nature of Ge, Si, and SiGe NPs. Ultimately, we aim to use these materials as high-temperature thermoelectrics with controlled properties.

Keywords: Nanoparticles, Amorphous, Crystalline, Germanium, Silicon, Sulfur, Colloidal synthesis

*Speaker

Magnetic instability in heavily n-doped Fe-based full-Heusler com-pounds for thermoelectric applications

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Abstract

Fe2YZ full-Heusler compounds were recently predicted from density functional theory (DFT) simulations to exhibit very large thermoelectric power factor (PF), promising for thermoelectric applications [1]. Their fundamental property is the simultaneous "flat-and-dispersive" character [2] of the Fe eg bands that can be engineered to increase PF under n-doping [3]. However, the consequences of explicit n-doping in these compounds has not been carefully investigated yet. Here, we study Fe2YZ1-xAx (Y=V, Ti, Ta, Nb, Z=Al, Si, Sn, Ga and A=Si, P, Sb, Ge) doped compounds from DFT using both Hybrid Functionals and GGA+U methods, and highlight in some cases the appearance of a Stoner instability inducing a half-metal ferromagnetic phase. This transition is shown to be strictly linked to the Fe-eg and Y-site eg orbital hybridization and to have an electronic origin, which does not depend on the nature of dopants. In fact, using a model exploring different relative positions of those Fe-eg and Y-site eg levels, we rationalize that different regimes (non-magnetic or magnetic) can be activated by electronic doping. Although the magnetic phase exhibits a lower PF, reducing the number of carriers available at the Fermi level, its value can remain promising for thermoelectric applications. In addition, we elucidate how to engineer the band structure of these compounds searching for a good compromise among the eg states arrangement at the conduction band, the carrier density and the appearance of the ferromagnetic phase. Finally, the Stoner instability in these materials could provide useful half-metallic ferromagnetic systems with coupled thermomagnetic responses. Work supported by FEDER and Walloon Region through the project LoCoTED. References [1] Phys. Rev. B 83, 205204 (2011). [2] Proc. Natl. Acad. Sci. USA 93, 7436 (1996). [3] Phys. Rev. Lett. 114, 136601 (2015).

Keywords: Heusler, Full, Heusler, DFT, Theory, Doping

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Effect of Lattice Defects on the Seebeck Coefficient of Mg2Sn

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Abstract

Recently, we succeeded in analyzing lattice defects in Mg2Si: a small amount of Mg existed at an interstitial site of Mg2Si. In this study, we focused on Mg2Sn that has an identical crystal structure with Mg2Si. The Seebeck coefficient (S) of Mg2Sn measured at room temperature (R.T.) ranges from -250 to 300 μV/K depending on researchers. Although it is believed that lattice defects in Mg2Sn affect the S value, their amounts and effects on S were not fully understood yet. Hence, we investigated the relation between lattice defects and S of Mg2Sn by using single-crystal X-ray diffraction and measuring S at R.T. Mg2Sn single crystals were prepared by using the melt growth method under (A) vacuum and (B) Ar 1.3 atm. Furthermore, Mg2Sn polycrystalline samples were prepared by using the spark plasma sintering method, and subsequently annealed at 100, 200, 300, 400∘C for 1h. The S values of the single crystals (A) and (B) were 11 μV/K and 138 μV/K, whereas that of polycrystalline samples gradually decreased in its absolute value from —-230— μV/K to —-204— μV/K with increasing annealing temperature. From the results of single-crystal XRD, it was found that Mg deficiency at a (1/4 1/4 1/4) regular site (VMg) existed in all samples. The amount of VMg of the single crystals (A) and (B) were 6.0(13) % and 7.8(17) %, respectively. For the polycrystalline samples, the amount of VMg gradually increased from 1.4(11) % to 3.3(17) % with increasing annealing temperature. Since VMg is an accepter-type defect, it is considered that the hole carrier concentration increases with increasing the amount of VMg. The increase in hole concentration results in a change of the sign of S, being consistent with the dependence of S on the amount of VMg of the prepared samples. Thus, it is concluded that the S value of Mg2Sn can be controlled by tuning the amount of VMg.

Keywords: Mg2Sn, Mg deficiency, Single crystal X ray diffraction

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Cryostat for the measurement of absolute Seebeck Coefficient using high-temperature superconducting reference material and Thomson heat

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Abstract

Seebeck coefficient is one of the properties that characterize the thermoelectric material and is used to evaluate the performance of the material. We have developed a cryostat for measurement of absolute Seebeck coefficient of bulk material sample. The cryostat has a capability to measure the Seebeck coefficient of materials using a superconducting material as a reference material. It is also capable to measure the Thomson heat. By combining those capability, the absolute Seebeck coefficient can be obtained for wide temperature range. The cryostat can be operated with liquid helium or liquid nitrogen or without those liquid cryogen depending on the operational temperature. The range of the operational temperature is designed to be from near 1 K to 320 K. Currently, the cryostat is mainly operated with liquid nitrogen. For Thomson heat and precise Seebeck coefficient measurements, highly stabilized sample temperature control is required. The sample stage in the cryostat is surrounded by temperature-stabilized double thermal shield. The temperature stability at the sample stage of an order of mK can be obtained at 90 K for example. The configuration of the sample stage can be modified depending of the measurement requirements by changing the sample holder unit. When a high-temperature superconductor is used as a reference material, the absolute Seebeck coefficient of the sample can be directly measured below its superconducting transition temperature [1, 2]. Above the superconducting transition temperature, the sample holder was configured for Thomson heat measurement and then the absolute Seebeck coefficient was calculated. Detailed configuration of the cryostat, characteristics and basic measurement results will be discussed in this paper.

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Keywords: Cryostat, absolute Seebeck Coefficient, Thomson heat, temperature control, high, temperature superconducting reference material

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Uncertainty evaluation in thermoelectric characterization based on the microdevice technique

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Abstract

Nanostructures are used to improve the thermoelectric figure-of-merit by phonons scattering at interfaces without scattering of charge carriers. Since thermoelectric characterization for nanostructured materials are challenging due to their dimensions, various approaches have been proposed, such as microdevice technique, Raman spectroscopy, TDTR, SThM, etc. However, these methods require specific conditions and assumptions to determine the thermoelectric parameters from meausrement results, which may lead to a large uncertainty. In this work, the thermoelectric properties of black phosphorus nanosheet were measured using a suspended-type microdevice. We evaluated the uncertainty of the Seebeck coefficient, electrical conductivity, and thermal conductivity according to the law of uncertainty propagation.

Keywords: Uncertainty analysis, microdevice technique, black phosphorus

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Enhanced thermoelectric performance and high-temperature thermal stability of p-type Ag-doped β-Zn4Sb3

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Abstract

β-Zn4Sb3 is a well-known thermoelectric material in the intermediate temperature range (400-700 K), showing excellent TE performance as well as nontoxic, earth-abundant and cheap chemical elements. Here we present that the thermoelectric properties of bulk β-Zn4Sb3 can be improved by Ag doping at the Zn sites in the range 300-575 K [1]. Proper Ag doping leads to decreased electrical resistivity and increased Seebeck coefficient, thus resulting in a large improvement in power factor. Owing to Ag doping, the figure of merit, zT, has a considerable enhancement although the thermal conductivity is slightly increased. (Zn0.9925Ag0.0075)4Sb3 exhibits a promising zT of around 1.2 at 575 K, which is superior to most previously reported p-type doped Zn4Sb3 materials. Furthermore, the high-temperature thermal stability is studied in detail. The (Zn0.9925Ag0.0075)4Sb3 bulk sample does not decompose even when the temperature is elevated to 793 K in vacuum. When the bulk sample is heated to 573 K in air, (Zn0.9925Ag0.0075)4Sb3 is also stable, unlike undoped Zn4Sb3 where Zn whiskers come out of the surface. In-house *in situ* powder X-ray diffraction (PXRD) and multi-temperature synchrotron PXRD (up to 793 K) reveal that the undoped Zn4Sb3 powder sample starts decomposing into ZnSb at 473 K if exposed to the air and it is fully decomposed into ZnSb, ZnO and Sb after cooling down from 793 to 300 K. Nevertheless, there is about 24 wt.% Zn4Sb3 preserved in the (Zn0.995Ag0.005)4Sb3 powder sample after the same heat treatment, while only about 6 wt.% Zn4Sb3 remains in (Zn0.99Ag0.01)4Sb3. The above results indicate that proper Ag doping leads to enhanced high-temperature thermal stability in β-Zn4Sb3.

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Keywords: Ag doped Zn4Sb3, enhanced thermoelectric performance, in situ XRD, synchrotron PXRD, improved thermal stability

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High-temperature thermoelectric properties of the half-Heusler phase ScNiSb

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Abstract

Half-Heusler (HH) phases with rare-earth constituents have recently been recognized as possible candidates for thermoelectric materials, applicable at high temperatures. In this work, we studied the thermoelectric properties of the HH antimonide ScNiSb that previously was investigated only below 400 K. A single-phase sample was obtained by arc-melting pure elements. In the next step, the ingot was hand-milled to the fine powder and compacted using spark plasma sintering technique at 950 oC and uniaxial pressures 100 MPa. The so-prepared bulk specimen was examined by X-ray diffraction and scanning electron microscopy with energy-dispersive analysis. No phase decomposition or structural transformation of the MgAgAs-type single-phase material was found. Measurements of the thermopower, electrical resistivity, and thermal conductivity were performed in the temperature range 350-950 K. The material is *p*-type conductor with a positive values of the Seebeck coefficient with a remarkably enhanced magnitude of about 240 mV/K near 450 K. On the other hand, the measured electrical resistivity values are relatively high (83 mWm at 350 K) resulting rather small values of the power factor (less than 0.9 × 10-3 Wm-1K-2) in the temperature range examined. Furthermore, the thermal conductivity is high with a local minimum about 6 Wm-1K-2 near 600 K. Altogether, the dimensionless thermoelectric figure of merit of our ScNiSb sample was below 0.1 in the entire temperature range studied. This work was supported by the National Science Centre (Poland) under research grant no. 2015/18/A/ST3/00057.

Keywords: ScNiSb, half, Heusler

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First principles analysis of the power factor in RZnAsO (R=La, Bi, Y)

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Abstract

Good thermoelectric materials have high efficiency evaluated by the dimensionless figure of merit ZT = (σS2/)T, where σ, S, , and T are the electrical conductivity, Seebeck coefficient, thermal conductivity, and temperature, respectively. Recently, it has been found that BiCuSeO has a high dimensionless figure of merit ZT _˜ 1.1 at 923K [1]. Thermoelectric properties of BiCuSeO are characterized as low thermal conductivity _˜ 0.5 Wm-1K-1 at around 900K while the power factor σS2 _˜ 6 μWcm-1K-2 is moderate [1]. The experimental results are well explained within the first principles calculations [2,3].
In the present study, we theoretically study the thermoelectric performance of RZnAsO (where R is one of La, Bi, and Y) from the band structure point of view. BiCuSeO and RZnAsO are isotypic with tetragonal ZrCuSiAs (space group: P4/nmm), therefore RZnAsO can be a promising candidate for a thermoelectric material. RZnAsO has a crystal structure with alternating conducting ZnAs layers and RO layers. It is found that the anisotropy of the valence band structure of BiZnAsO and YZnAsO around the Fermi level is larger than that of LaZnAsO, and the highest valence band of BiZnAsO and YZnAsO has the "pudding mold type" band structure, which was discussed in a thermoelectric material NaxCoO2 (ZT > 1) [4]. We also found that the conduction band of YZnAsO has a multi-valley band structure, and the power factor of YZnAsO with electron doping is comparable with that of YZnAsO with hole doping. We will discuss the band structure and the power factor of RZnAsO in detail.

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Keywords: First principles calculations, Boltzmann equation, ZrCuSiAs structure

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Optimisation of the thermoelectric properties of Heusler Fe2VAl-based compounds through off-stoichiometry strategies

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Abstract

Using the thermoelectric technology for large scale applications requires thermoelectric (TE) materials that are efficient but also abundant, non-toxic, and cheap. Fe2VAl-based compounds fulfil these requirements in a temperature range that is suitable for many industrial energy harvesting applications (RT-600K). The Seebeck coefficient of such compounds can be tuned from positive to negative values by doping or by applying departures from the stoichiometric composition. Indeed, p- and n-type materials are needed in order to build TE modules. In the present work, off-stoichiometric Heusler Fe2VAl-based compounds are explored in order to find the optimised Fe-V-Al compositions for a given application, i.e. in a targeted range of temperatures. It has been shown that describing the evolution of the Seebeck coefficient as a function of the concentration in valence electrons (VEC) is not appropriate as rigid-band shift behaviours do not apply for any type of off-stoichiometry. We suggest here to represent the Seebeck coefficient as a function of the actual composition on ternary diagrams, for a given temperature. It brings the opportunity to have a quick overview of the best compositions, but also of the effect of specific off-stoichiometry strategies on the TE properties. It is worth noting that, in addition to the Seebeck coefficient, it is of primary importance to take into account the electrical conductivity and thermal resistivity when optimising the composition.

Keywords: Heusler compounds, Fe2VAl, offstoichiometry strategies, ternary diagrams, Seebeck coefficient, power factor

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Interplay of secondary phases on the thermoelectric properties of ternary skutterudite thin films

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Abstract

Materials with skutterudite structure are potentially useful for thermoelectric applications due to their novel transport properties. In this study, ternary skutterudite Sb-doped Co-Ge-Te has shown to possess large power factor due to the tuning of the amount of secondary phases present in the films. By depositing our film on different substrate, we are able to produce films with varying composition of these secondary phases, which has shown to affect its thermoelectric transport properties. Using x-ray diffraction analysis, we were able to distinguish the amount of phases in the films and correlate to the existing electronic transport property. Furthermore, the temperature-dependent Hall measurement, which provide information on our carrier concentration and mobility, also corroborates the effect of the secondary phases in our thermoelectric properties. Lastly, using transmission electron microscope, we were able to demonstrate the distribution of secondary phases in our system.

Keywords: skutterudite, secondary phases, thin films

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Enhanced Thermoelectric Performance in 18-Electron Nb0.8CoSb Half-Heusler Compound with Intrinsic Nb Vacancies

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Abstract

Typical 18-electron half-Heusler compounds, ZrNiSn and NbFeSb, are identifed as promising high-temperature thermoelectric materials. NbCoSb with nominal 19 valence electrons, which is supposed to be metallic, is recently reported to also exhibit thermoelectric properties of a heavily doped n-type semiconductor. Here for the frst time, it is experimentally demonstrated that the nominal 19-electron NbCoSb is actually the composite of 18-electron Nb0.8+δCoSb ($0 \leq \delta < 0.05$) and impurity phases. Single-phase Nb0.8+δCoSb with intrinsic Nb vacancies, following the 18-electron rule, possesses improved thermoelectric performance, and the slight change in the content of Nb vacancies has a profound effect on the thermoelectric properties. The carrier concentration can be controlled by varying the Nb defciency, and the optimization of the thermoelectric properties can be realized within the narrow pure phase region. Benefting from the elimination of impurity phases and the optimization of carrier concentration, thermoelectric performance is remarkably enhanced by ≈100% and a maximum zT of 0.9 is achieved in Nb0.83CoSb at 1123 K. This work expands the family of half-Heusler thermoelectric materials and opens a new avenue for searching for nominal 19-electron half-Heusler compounds with intrinsic vacancies as promising thermoelectric materials.

Keywords: half Heusler, thermoelectric, NbCoSb, nonstoichiometry, vacancies

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Synthesis and characterization of high performance thermoelectric material MgAgSb

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Abstract

Over a half-century, the compound that exhibits the highest thermoelectric performance at room temperature is Bi2Te3 system. Although the record has not been rewritten yet, the performance has been drastically improved at a temperature region of around 500 K. Particularly, MgAgSb exhibit maximum ZT value of $ZT = 1.4$ at 525 K [1]. Great interest has been attracted in MgAgSb because of its high performance, though only a few groups has reported its thermoelectric properties. Synthesis of its high purity polycrystal is difficult because it is a low temperature phase appearing below $T = 560$ K with the space group of *Ic2*. We, thus, try to establish reproducible synthesis method of α-MgAgSb.
We synthesized α-MgAgSb samples by using melting method followed by hot press. Optimum condition was explored to eliminate impurity phases. Thermoelectric properties of the obtained samples were examined. Details will be discussed in the conference. [1] Zihang Liu et al., Acta Mater., 128, 227 (2017).

Keywords: MgAgSb, melting method

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Effect of rapid solidification on the thermoelectric properties of (Ti,Zr)NiSn half-Heusler alloys

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Abstract

Thermoelectric (Ti,Zr,Hf)NiSn half-Heusler compounds reveal high Seebeck coefficient and electrical conductivity, that lead to high power factor. However, high values of thermal conductivity reduce overall performance. To reduce lattice thermal conductivity, development of point defect or grain boundary scattering was suggested, leading to increased phonon scattering [1].
In this work, we investigated the effect of rapid solidification on the microstructure refinement of TiNiSn and ZrNiSn and the solubility limits in (Ti,Zr)NiSn with the aim to enhance phonon scattering.

Master alloys were prepared by arc melting of pure elements. Rapid solidified ribbons were obtained by planar flow casting with different wheel speeds (10, 20, 30 m/s). Rapid solidified ribbons were crushed into powders and sintered in pellets. As a reference, bulk materials were prepared by annealing the arc melted ingots.

In as quenched TiNiSn, the fraction of half-Heusler phase, obtained by X-ray diffraction, progressively increases with increasing wheel speed, suggesting that formation of primary TiNi2Sn is hindered by undercooling of the liquid.

ZrNiSn half-Heusler phase is obtained directly by solidification due to congruent melting.

Both rapidly solidified and annealed (Ti,Zr)NiSn samples show the miscibility gap between ZrNiSn and TiNiSn. However, rapid solidification causes Ti supersaturation in Zr-rich (Ti,Zr)NiSn.

Sintering promotes formation of equilibrium phases and allows to obtain dense pellets with refined microstructure that originates from the as quenched ribbons. Thermoelectric properties were correlated to the final microstructure.

H.-H. Xie, C. Yu, T.-J. Zhu, C.-G. Fu, G.J. Snyder, X.-B. Zhao, *Appl. Phys. Lett.* **100** (2012) 254104
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Keywords: half Heusler, rapid solidification, phonon scattering

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Fabrication of high performance flexible thermoelectric devices by improving crystallization process of screen-printed material

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Abstract

The screen printing technique in the fabrication of flexible thermoelectric generators (f-TEGs) is useful in large-scale mass production of the TEG module, because the screen-printed thermoelectric materials (sp-TEs) can be quickly formed on a large area through a simple printing process. In order to fabricate high performance f-TEGs with a good manufacturability, the crystallization process of sp-TEs must be carefully optimized. The crystallization process determines the mechanical and thermoelectric (TE) properties such as density, surface morphology, carrier concentration and preferred orientation of the sp-TEs. In this work, we present a new sintering process for sp-TE. This new process uses excess Te in the TE paste and adopts a simplified/unified crystallization process of various steps which were used in the previous works. Through this simplified process, the deviation of the performance, caused from the accumulation of the non-uniformities of the various process steps, could be minimized. The densities of BST and BTS sp-TEs were increased from 5.22 g cm-3 to 6.23 g cm-3 and 5.18 g cm-3 to 6.43 g cm-3, respectively, and the average surface roughness decreased from 8.1 μm to 2.2 μm. In addition, when more than 200 sp-TEs were crystallized, the carrier concentration deviations of p- and n-type sp-TEs were also reduced from ± 0.22 × 1019 cm–3 to ± 0.06 × 1019 cm–3 and from ± 0.29 × 1019 cm–3 to ± 0.09 × 1019 cm–3, respectively. As a result, the output power of fabricated f-TEG module were improved by 130 % and achieved 5.02–5.43 mW/cm2 at a temperature difference of about 25 K.

Keywords: Screen printing, Te, Process, Flexible, Thermoelectric generator

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Failure analysis of commercial thermoelectric modules by Infrared thermography

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Abstract

In this work we investigate commercially available thermoelectric modules (TEM) by infrared (IR) thermography. IR thermography is a non-destructive method which can be applied in practically any processes where temperature is an indicator of abnormal operation of an object. As demonstrated in an earlier work with this method subsurface defects of the multilayered TEM structure can be detected. Additionally, advantages of IR thermography are, that several TEM's can be analyzed simultaneously (typically up to 10, depending on their dimensions) and the analyzing time lies in the range of several seconds.
TEM's can be classified in failure free or faulty ones having a 'weak' or 'hard' failure. Weak failure means, that the TEM is principal operable but the electrical resistance is increased compared to a failure free TEM (e.g. by an increased contact resistance). A hard failure means that the TEM is inoperable because no current can flow (e.g. due to opens).

For IR imaging the TEM must be thermally excited. In the case of a weak failure, this is preferably done by electrical sourcing (internal joule heating) or alternatively by an external source (e. g. flash lamp or laser). In the case of a hard failure, the TEM must be thermally excited by an external source.
Investigating a TEM with a weak failure, typical parameters of electrical sourcing are a pulsed sine wave with a frequency of appr. 1 Hz, a peak voltage of appr. 5 – 6 V and a peak current of appr. 1 – 2 A. At positions, where a failure is located (e. g. by increased electrical resistance), a hot spot occurs. To get information on the physical cause of this failure, a metallographic cross section was carried out and the failure region was inspected by optical microscopy and / or SEM analysis.

Keywords: thermoelectric, IR thermography, failure analysis

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Flash Sintering of thermoelectrics material

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Abstract

Electric current assisted processing techniques, such as Spark Plasma Sintering (SPS) have been used widely used to densify thermoelectric powders. The reason for this is that the rapid heating rate (typically > 50 ∘C /min) enables dense, nanostructured materials to be prepared in minutes. A more recent development is flash-SPS, in which by direct electrical heating of the material heating rates of $>$ 5,000 ∘C /min have been achieved and materials have been densified in seconds. The process is dieless and requires a pre-sintered sample, therefore powders cannot be directly processed. At the high current densities involved and heating rates there is the possibility of additional effects, including disorder and point defects that might contribute to improved thermoelectric performance. Up to now only two papers have investigated the thermoelectric properties of flashed samples, leaving the effect of high heating rate almost unexplored.

In this work, a new derivative of SPS was developed, a thin stainless steel die was used to constrain the powder/sample and still achieve very rapid heating (7500 ∘C/min). In contrast with other flash work, the process is more controlled and reproducible. The rapid heating allowed samples of Ni0.15Co0.85Sb3 to be synthesised and sintered simultaneously from elemental powders. High density ($> 95\%$) was achieved and the samples were nearly single phase. But most remarkably the rapid heating, combined with rapid cooling produced a sample with significantly reduced (30%) thermal conductivity, while the electrical properties were not significantly modified. This resulted in sample with a peak ZT of 0.81 at 500 ∘C while samples produced by conventional SPS reached only 0.54.

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Keywords: Sintering, skutterudite, microstructure, flash sintering, rapid heating

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A straightforward 2f technique for the measurement of the Thomson effect

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Abstract

We present a simplified rapid, and accurate method for the measurement of the thermoelectric Thomson coefficient by the dynamical heating of a suspended wire by an alternating current. By applying a temperature gradient across the wire, we find that the response at the second harmonic of the excitation frequency is directly proportional to the Thomson coefficient. The absolute thermoelectric coefficient of a single material can therefore be extracted by a phase sensitive detector with arbitrary precision.

Keywords: thomson coefficient, dynamical heating

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Van der Waals epitaxy for High performance thermoelectric 2D chalcogenide films

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Abstract

Demands on high-quality layer structured two-dimensional (2D) chalcogenide films are growing due to the findings of remarkable physical properties and potentials for device applications. However, the difficulties in controlling epitaxial growth with defect density and the poor understanding of van der Waals epitaxy (vdWE) for 2D chalcogenide film on the substrate have been major obstacles for the further advances of these materials. In this research, we demonstrate new approaches enabling the vdWE of 2D chalcogenide epitaxial films on 2D and 3D substrates, individually. As a proof of concept, highly oriented crystalline bismuth antimony telluride thermoelectric films were epitaxially grown on 2D (graphene) and 3D (α-Al2O3) substrates by pulsed laser deposition exploiting the surface reaction of the substrate with chalcogen and the growth mechanism of these films on 2D and 3D substrates *via* vdWE were elucidated. In particular, this peculiar vdWE renders the high-quality 2D chalcogenide film with high carrier mobility and low defect density comparable to single crystal. Furthermore, exceptionally low thermal conductivity were observed in these vdWE films.

Keywords: 2D chalcogenide, van der Waals epitaxy, graphene, α, Al2O3, defect

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Highly (110)-oriented Bi2Te3-xSex films with high thermoelectric power factor via electrodeposition

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Abstract

A simple process of electrodeposition is shown to produce highly (110)-oriented thin film of Bi2Te3-based alloys with improved composition controllability. The potential-current co-adjusted pulse electrodeposition (PCP-ED) by the control of zero current during the off-time period enables the fabrication of highly dense Bi2Te3-xSex thin film with (110)-oriented grains. The power factor of the PCP-ED thin film was much higher than that of the Bi2Te3-xSex thin film fabricated by conventional d.c. electrodeposition due to the simultaneous enhancement of electrical conductivity and Seebeck coefficient. Additionally, significantly enhanced power factor of _˜2000 μW/mK2 at room temperature, which is the best value among the reported n-type Bi2Te3-based thin films, was obtained after low temperature annealing at 200oC by triggering the compositional modulation for improved crystallinity and optimized carrier concentration.

Keywords: electrodeposition, Bi2Te3, thin film, orientation, crystallinity

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Manufacture of TE-modules: joining Fe2VAl and Cu through several bonding processes.

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Abstract

Fe2VAl-based thermoelectric modules are very promising for large scale applications such as industrial energy harvesting since its constituent materials are abundant, non-toxic and low cost. However, the assembly of modules based on Fe2VAl compounds requires to properly bond this thermoelectric material with high electrical conductivity material such as copper. Two types of process have been investigated in the present work: copper metallization directly on Fe2VAl and brazing. Copper metallization has been performed either by diffusion bonding under pressure, physical vapor deposition or electrodeposition. Brazing has been studied by using both low and high temperature (from 300K to 700K) brazing materials in order to enlarge the application field. Very promising results have been obtained for several of those processes in terms of contact resistance measurements ($< 10\mu\Omega$cm2), element diffusion (highlighted by SEM and EDX) and mechanical resistance. Moreover, for silver-based brazing, a thin reactive layer has been observed at the surface of Fe2VAl. This layer appears owing to chemical reaction between the brazing material, copper and Fe2VAl. This phenomenon was never observed before and is supposed to have a positive effect on the contact resistance and thus on the module efficiency, as long as it does not involve too large scale elemental diffusion.

Keywords: Fe2VAl, Module assembly, bonding process, brazing, diffusion bonding, electrodeposition, physical vapor deposition

*Speaker

High Pressure Synthesis: An effective approach for tuning thermoelectric properties of filled skutterudites AxCo4Sb12 (A = K, Sr, Y, rare earth)

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Abstract

High pressure is an effective tool for the preparation of new CoSb3-based skutterudites. The high hydrostatic pressure (HP) favors the formation of short and strongly covalent chemical bonds. Furthermore, pressure helps to increase the coordination numbers and it favors the denser phases. [1]
CoSb3 skutterudite shows high carrier mobility, high electrical conductivity and a notably good Seebeck coefficient. Nevertheless, its high thermal conductivity hinders the optimization of the thermoelectric figure of merit. In order to enhance the thermoelectric properties of CoSb3-based skutterudites, nanostructuration and filling part of the structural cavity with guest atoms are the common approaches used to modify the electrical and thermal transport properties. [2] [3] In our work, we have explored the effects of high pressure synthesis to tune the thermoelectric properties of a plethora of unfilled and filled CoSb3-based skutterudites (fillers: K, Sr, Y, rare earth). We show that this method produces an effect of strain-field scattering of high-energy phonons, dramatically reducing the lattice thermal conductivity of the studied materials.

Synchrotron x-ray diffraction measurements, SEM, HRTEM, EELS and thermoelectric measurements will be presented and discussed.
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Keywords: Skutterudites, High Pressure Synthesis

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Physical mechanism under the new criterion for self-propagating high-temperature synthesis and its universality

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Abstract

Self-propagating high temperature synthesis (SHS) is a technique for rapid preparation of compounds utilizing the heat released by the exothermic chemical reaction itself. Empirical criterion [1] states that the combustion wave of SHS could only sustain when the adiabatic temperature Tad is over 1800 K. Recently, our group [2] proposed a new criterion for sustainability of the combustion reaction, in which the adiabatic temperature must be higher than the melting point of the elemental component with the least melting point, i.e. Tad/Tm, L> 1. In order to uncover the physical mechanism underlined the new criterion and its universality, we carried out a survey research including 138 binary compounds with the experimental observation and theoretical calculations. Results indicate that, besides the requirement of the new criterion, the enthalpy of the reaction must be larger than the heat needed to raise the reactants to the melting point Tm, L. For vast majority of reactions, SHS can take place only when the melting process occurs during the reaction, which is consistent with the new criterion. On the other hand, SHS processes can be sustainable when preheating is adopted in certain less-exothermic systems, such as Sb2Te3 and Cu2Te. This phenomenon further implies the correctness of the new criterion and its universality. Our work helps broaden the application fields of SHS reaction and provides a highly efficient and economical preparation method for a large number of materials.

Keywords: SHS, new criterion, physical mechanism and universality

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Seebeck coefficient of Bi & Sb nanowire assemblies produced by electrodeposition

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Abstract

The unique properties of bismuth antimony (Bi1-xSbx) nanostructures and the theoretical predictions on their enhanced thermoelectric efficiency two decades ago1 triggered the development of a wide variety of growth and characterization methods aiming at measuring the thermoelectric properties of nanowires. Since then, several groups have studied the properties of Bi1-xSbx nanowires and size dependent effects have been highlighted2-4. However the experimental demonstration of a size dependent thermoelectric efficiency is still challenged by the difficulties to fabricate well-defined nanowire systems and to achieve reliable and stable electrical and thermal contacts.

Here we present the fabrication of Bi and Sb nanowire assemblies, consisting of either parallel arrays or highly interconnected networks, by pulsed electro-deposition in ion track-etched polycarbonate membranes.4-5 The wire diameter is determined by the host channel and was adjusted systematically between 30 nm and 160 nm. The Seebeck coefficient of both parallel and interconnected nanowire assemblies has been measured as a function of the wire diameter and the results will be discussed.

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Keywords: nanowire, bismuth, antimony

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Comparison of Spark Plasma Sintering and Induction Hot Pressing in Preparation of Thermoelectrics

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Abstract

Spark Plasma Sintering (SPS) is a pressing technique often used in preparing thermoelectric samples. Advantages of using the SPS technique include ease of use, rapid heating, high pressures, high compaction degree and low grain growth.1 The advance of the SPS technique has resulted in improved thermoelectric properties and ease of synthesis in many systems.
The SPS process involves high currents, which has been shown to influence materials properties as well as phase formation1. In SPS pressing of the Zn4Sb3 system, zinc depletion on one side of the sample was observed, which the authors attributed to the current.2 The exact influence of the current has not yet been fully established, as the very high heating rate of the SPS process is directly coupled to the current density though the sample. In ordinary hot pressing it is not possible to achieve the rapid heating rates of the SPS process and therefore it has not been possible to distinguish the two effects.
Recently, a new rapid sintering process was published by LaLonde et. al.3 using induction heating. This setup mimics the SPS process closely with very rapid heating rates, high pressures and the same graphite dies, while sending no current through the sample, enabling the distinction between the two effects.
As such, we have compared the two processes using known thermoelectrics such as Zn4Sb3, ZnSb and Mg2Si1-xSnx regarding phase composition, microstructure and physical properties. The samples have been examined by X-ray diffraction, Seebeck Micro Probe and Hall measurements.

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Keywords: SPS, Induction, Spark Plasma Sintering, ZnSb, Mg2Si, Mg2Sn

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Significant Enhancement of Thermoelectric Properties of Nanostructured Mg2Si via low temperature consolidation

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Abstract

Owing to their ability to convert heat directly to electricity, thermoelectric materials are quite unique and promising in recycling the wasted energy. Magnesium silicide seems to be the most qualified compound for mid-temperature thermoelectric applications. However, magnesium is highly oxidable and MgO has an adverse effect on figure-of-merit of the product. The higher the synthesis temperature, the more likely to form MgO. Therefore, decreasing the synthesis temperature not only reduces the energy consumption of the process and makes the product more economic, but also leads to purer and consequently more efficient product.
Silicon grains (99.999%, 2-5 mm) were ball-milled together with bismuth and aluminum at 700 rpm for 1h, using zirconia vials and balls. Then the obtained powder and magnesium (99.9%, < 180 μm) were mixed according to Mg1.98Al0.02Si0.98Bi0.02 stoichiometric proportions at 500 rpm for 40 min. The mixture was then consolidated into pellets at 300 °C under 100 MPa for 5 min. The samples were characterized with scanning electron microscopy and X-ray diffraction. Seebeck coefficient, electrical conductivity and thermal diffusivity were measured from 25 to 550 ∘C.
Synthesis temperature of Mg2Si was reduced from about 600 down to 300∘C by thoroughly activating the starting materials using silicon nano-particles. No evidence for presence of MgO was found in the product. Electronic and thermal transport properties may be manipulated in a wider range by addition of aluminum at magnesium sites. Highest zT for Mg1.98Al0.02Si0.98Bi0.02 was measured to be 1.3 at 550∘C. To elucidate fast reaction of Mg and Si particles at low temperature, a plum-pudding microstructure model was proposed.

Keywords: Activated reactive consolidation, Plum pudding model microstructure, Mg2Si

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Measurements of surface potential of Mg2Si/M (M = Mg, Al, Ni) interfaces

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Abstract

Recently, we have fabricated Mg2Si/X (X = Mg, Al) composite materials where the X metal phase was dispersed in the Mg2Si matrix[1, 2]. The dispersed X metal phase led to an increase in the electrical conductivity of Mg2Si. However, Hayatsu et al[3]., reported the electrical conductivity of a Mg2Si/Ni composite material was lower than Mg2Si. These contrarieties in electrical conductivity are considered to correlate with an interfacial contact state between Mg2Si and dispersed phases. In this study, we fabricated Mg2Si/M (M = MgAlNi) double layered samples as a model structure of composite materials, and measured a surface potential by means of the kelvin probe force microscopy. As for the Mg2Si/Mg sample, the surface potential of Mg2Si phase was found to be higher than that of the Mg phase by 200 meV. This result indicated that the interface of Mg2Si/Mg was an ohmic contact, which accounted for the increase in electrical conductivity of Mg2Si/Mg relative to the Mg2Si. In the cases of Mg2Si/Al and Mg2Si/Ni samples, the surface potential of Mg2Si phase was found to be lower than Al and Ni phase by 250 meV and 400 meV, respectively. Thus, the interface of Mg2Si/Al sample and Mg2Si/Ni sample was a Schottky barrier junction. The difference in the surface potential between Mg2Si and metal phases was about two times higher in the case of Mg2Si/Ni than Mg2Si/Al. Therefore, to enhance the electrical conductivity of Mg2Si, we need to select a proper metal as a dispersion phase that does not form a high Schottky barrier at the interface between the Mg2Si and metal phases. In the conference, we also report a surface potential of the Mg2Si/Al composite.
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Keywords: Mg2Si, composite, surface potential

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Formation of β-FeSi2 nano-inclusions in silicon thin-films by ion-implantation for thermoelectric applications

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Abstract

Elemental silicon is a common, relatively low-cost semiconductor, whose potential use in thermoelectric (TE) applications is known [1-2], however its high thermal conductivity (k) [3] has been identified as a major barrier to commercial development. Recent studies have attempted to reduce silicon's k, with negligible reductions in power factor (PF), via approaches such as creating structures as nanowires, nano-porous thin-films, or by defect-engineering [1-2, 4-6].
Introducing nano-inclusions (NIs) into a host material is a popular way of enhancing the TE properties of said material. This has been demonstrated for a number of material systems, including silicides [7-10], where NIs disrupt the regular crystal structure, leading sometimes to both a reduced k and enhanced PF. Since many silicides are well-known TE materials, the premise of the study was that it is likely that silicide NIs within elemental Si will enhance its otherwise ordinary figure-of-merit.
Ion implantation is a staple technique used in microelectronics manufacturing which offers reliable and repeatable thin-film synthesis. As elements are introduced into a target by a high-energy ion beam, it is well-suited to producing NIs in any thin-film, but is relatively untested for TE material synthesis. In this study, we apply ion implantation and thermal annealing as a novel route to TE thin-film formation, specifically the creation of ß-FeSi2 NIs within single-crystal silicon. In order to pinpoint the experimental conditions that lead to optimal performance a comprehensive multi-variable analysis, with a wide range of temperatures, exposure times, and ion-doses, has been undertaken. These samples have been characterised by both qualitative (SEM, TEM) and quantitative (Seebeck, Raman, thermal and electrical conductivity) measurements showing promising TE performance enhancement.

Keywords: Thermoelectricity, Iron disilicide, silicon, ion, implantation, nano, inclusions

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GLASS-CERAMIC OXIDATION PROTECTIVE COATINGS FOR HIGHER MANGANESE SILICIDE THERMOELECTRICS

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Abstract

Higher manganese silicide (HMS) is considered a promising thermoelectric material to generate electricity from waste-heat recovery. A critical aspect of the success of HMS is the stability over time and the oxidation resistance at temperatures higher than 500∘C. Thanks to the versatility of their compositions and properties, glass-based materials, with low electrical and thermal conductivity, are potentially good candidates as protective coatings.
In this work, a HMS substrate (MnSi1. 74), densified by spark plasma sintering, was coated with a silica-based glass-ceramic material in order to provide oxidation protection above 500∘C. The thermal cycling stability (from room temperature to 600∘C in air) of as-sintered and glass-ceramic coated HMS thermoelectric was studied with respect to changes in the chemical composition and electrical properties. It was found that the formation of a Si-deficient layer (MnSi) on the uncoated HMS surface, due to the reaction between the HMS and oxygen at 600∘C, leads to a higher electrical resistivity and a reduced power factor. The coated samples did not show variations in electrical resistivity, power factor and zT compared to the as-sintered sample, thus demonstrating that the use of a glass-ceramic coating is an efficient oxidation protective system during cyclic working conditions. The self-healing property of the glass-ceramic coating was also demonstrated at 600∘C, by the healing of an indentation mark impressed on its surface.
In addition, a number of novel silica-based glass-ceramic coatings were designed and thermally characterized with the intent to further extend the operational temperature range of thermoelectric devices.

Keywords: Glass ceramic, Coating, Thermoelectric, Oxidation

*Speaker

Effect of Dislocation Lines on Thermoelectric Properties of Si/CrSi2 Nanocomposites Prepared by Liquid-phase Sintering

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Abstract

Recently, we have developed a new method to introduce high density of dislocation lines in Si by liquid-phase sintering of Si/CoSi2 nanocomposite [1]. In this method, Si/CoSi2 nanocomposite synthesized by melt-spinning (MS) technique is sintered by spark plasma sintering (SPS) technique at around the eutectic point of Si and CoSi2 so that the composite partially melts during the sintering by the eutectic reaction. The generated dense dislocation lines were found to effectively reduce the thermal conductivity and enhance *ZT*. The formation mechanism of the dislocation lines is however not understood well. To validate the applicability of this method to other materials and to get insight into the formation mechanism of the dislocation lines, we applied this method to Si/CrSi2 system whose binary phase diagram is similar to that of Si/CoSi2.
The ribbon-shaped samples with nominal composition of (Si0.97P0.03)95Cr5 were prepared by MS method to uniformly disperse CrSi2 nanoprecipitates in the Si matrix. The ribbon samples were sintered by SPS at 1323 K. The thermal conductivity was evaluated by laser flash technique.

The sintered sample showed an over 36% decrease in the lattice thermal conductivity (_˜16 Wm-1K-1 at room temperature, _˜7.4 Wm-1K-1 at 1073 K) compared with the P-doped Si without CrSi2[2]. Since this reduction can be attributed to the presence of high density of dislocations, the liquid-phase sintering seems to be applicable to Si/CrSi2 system too to introduce dense dislocation lines.

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A. Yusufu *et al.*, *Nanoscale* **6,** 13921 (2014).

Keywords: Si, silicide, nanocomposite, dislocation, eutectic reaction, liquid, phase sintering

*Speaker

Effect of sputter conditions on the structural and thermoelectric properties of nanostructured Si80Ge20 thin films

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Abstract

Silicon-germanium (Si1-xGex) alloys are suitable candidates for high-temperature thermoelectric applications. Thermoelectric modules based on Si1-xGex are used with a material figure-of-merit ZT of 0.5 (p-type) and 0.9 (n-type) [1]. Further improvements in ZT have been achieved due to reduction of the phonon thermal conductivity in nanocomposites (ZT of 1.3 at 900 ∘C) [2] or by incorporating nanoparticles (ZT of 1.7 at 900 K) [3]. Here, we use metal-induced crystallization (MIC) as tool to gain nanostructured Si1-xGex films of 200 nm at a reduced crystallization temperature of 600 ∘C. Therefore, amorphous sputtered Si1-xGex on thin metal films is crystallized in a post annealing step. We studied the influence of the deposition parameters, including the sputter power and target-substrate distance. We present the films electrical conductivity, Seebeck coefficient, power factor, charge carrier concentration and mobility in the temperature range between room temperature and 400 ∘C. Further, the influence of the metal layer on the properties of Si1-xGex is considered by variation of the layer thicknesses, the interchange of Al by Au and by different heating processes, which will influence the morphology and microstructure of the resulting film. The microstructure of the samples was characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Finally, the preparation conditions tune the charge charrier density so that transport properties can be tailored.

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Keywords: silicon germanium (SiGe), thermoelectrics, electrical transport, sputter deposition

*Speaker

Growth of Mg-Ca-Si thick films by RF sputtering method and their thermoelectric property

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Abstract

Mg2Si consists of abundant and non-toxic elements, and reported to show good thermoelectric properties in addition to the fact that Mg2Si can realize both *p*- and *n*-type conduction. Expansion of composition system from Mg-Si binary system to the ternary one is one of the promising ways to enhance the thermoelectric properties. Ca is also abundant and non-toxic element and CaMgSi is expected to show the good thermal thermoelectric properties. However, the investigation of the thermoelectric property in Ca-Mg-Si system is limited to the narrow composition region. In the present study, films of Ca-Mg-Si system were prepared by RF magnetron sputtering system and thermoelectric properties were investigated for wide composition region. Investigation using films is fast way to investigate the wide range of composition because composition can be easily change by change the sputtering target.
Films with wide composition range were successfully obtained on (001)Al2O3 substrates at the deposition temperature of 260-340 oC using Mg target with various numbers of Ca and Si chips. Obtained films were post heat treated at 500–700 oC under the 5% H2 included Ar atmosphere.

Conduction type of the films mainly changed by the Si/(Ca+Mg+Si) ratio of the films and *p*-type and *n*-type conductions were observed below 0.6 and above 0.7, respectively. Single phase of CaMgSi and Ca7Mg7.25Si14 were successfully obtained and showed *p*-type. However, they showed low Seebeck coefficient value for the temperature range from 100-500 oC. Maximum power factor of 0.15 mW/(mK2) at 400 oC was obtained for the films with Ca:Mg:Si = 0.2:0.2:0.6.
In our presentation, we show the systematic data of the crystal structure and thermoelectric properties as a function of film composition.

Keywords: Mg, Ca, Si thick films, RF sputtering method

*Speaker

Plasma Electrolytic Oxidation coatings on magnesium silicide

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Abstract

Materials based on Mg2Si are considered as components of diverse energy harvesting and storage devices including thermoelectric modules, batteries or hydrogen storage systems. Numerous advantages of these materials can be mentioned, such as low density (1.99 gcm-3), non-toxicity, as well as abundance in nature and low cost of the main constituents. One of the major problems in diverse applications is high reactivity in the environments containing oxygen. They readily oxidize in air at temperatures exceeding 465 oC. In this work an oxide coating produced by Plasma Electrolytic Oxidation (PEO) technique is proposed for the protection of Mg2Si. The PEO technique, referred to also as micro-arc oxidation (MAO) or spark discharge anodizing, is accessible and relatively simple and widely investigated to develop protective layers on aluminium and magnesium alloys. In the literature no information is available on the possibilities of depositing PEO coatings on Mg2Si. In general, coatings produced by PEO show good mechanical properties and adhesion, high thermal and corrosion resistance, however, they are usually porous. Since the expected effect of coating deposition is to prevent oxidation of the underlying material, it is important to control porosity. In this study multiple attempts were made to produce the PEO coatings on Mg2Si substrates. The influence of the process conditions on coating microstructure was investigated using advanced electron microscopy techniques.

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Keywords: magnesium silicide, protective coatings, PEO

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Thermoelectric properties of n-Mg2Si0.8Sn0.2 with complex isovalent doping.

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Abstract

Mg2Si-Mg2Sn alloys are promising TE materials. The highest ZT> 1.4 achieve in Mg2Sn-rich solid solutions, where the lowest thermal conductivity and optimal bands convergence. However, magnesium stannide has poor stability, and durability such solid solutions stays under question. On another hand, magnesium silicide has ZT about 1, but has a higher melting temperature, is more stable and has the lowest density that makes it more fit material for real TE devices. The disadvantage of Mg2Si is high thermal conductivity, which necessary to be reduced. In this work influence of complex doping by replacing magnesium atom with calcium and/or tin atom with germanium in the solid solution of Mg2Si0.8Sn0.2 on thermoelectric properties were studied. Samples containing Ge and Ca up to 5 % and doped with antimony were prepared. Thermal and electrical conductivity and Seebeck coefficient at temperatures between of 300-800K were measured. It was shown that ZT increases to 1.1 in the Ge doped samples.

Keywords: silicides, magnesium silicide, hot pressing, figure of merit

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Control of Mg nonstoichiometry δ in Mg2±δSi1–xSbx and its effect on thermoelectric properties

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Abstract

Intermetallic compound of Mg2Si and its solid solutions are promising thermoelectric materials. To tune the thermoelectric properties, control of the amount of three types of point defects (dopants, interstitial Mg atoms, and Mg-vacancies) is an important requirement. When a dopant with high solubility in Mg2Si is selected, such as Sb, control of the dopant content is relatively easy. However, the Mg nonstoichiometry, which is related to Mg-vacancies and interstitial Mg atoms, is difficult to control due to the high vapor pressure of Mg.

In this study, an approach to control the Mg nonstoichiometry δ in Mg2±δSi1–xSbx via post annealing under different Mg partial pressures is developed. Annealing under low and high Mg partial pressures ($\leq$ 1×10ˆ–1 Pa and 1×10ˆ1 Pa) leads to low and high carrier concentrations of Mg2±δSi1–xSbx (1.4×10ˆ20 cmˆ–3 and 6.3×10ˆ20 cmˆ–3 for x = 0.10), respectively. The change in the carrier concentration, which corresponds to the change in the Mg content (1.954 < 2±δ < 1.971 for x = 0.10), is reversible and attributed to Mg transfer between the sample and the gas phase. The Mg content range for Mg2±δSi1–xSbx depends on the Sb content x (*e.g.* 1.999 < 2±δ < 2.001 for x = 0.01).

The carrier mobility of Mg2±δSi1–xSbx is significantly reduced around the Mg-poor-limit composition. (*e.g.* 75 cmˆ2 Vˆ–1 sˆ–1 for Mg2.001Si0.99Sb0.01 and 12 cmˆ2 Vˆ–1 sˆ–1 for Mg1.999Si0.99Sb0.01). The low carrier mobility (ca. 10 cmˆ2 Vˆ–1 sˆ–1) is observed regardless of the Sb content, suggesting that the charge carrier is significantly scattered at Mg-deficient grain boundaries. Details of other thermoelectric property evaluation will be presented.

Keywords: Magnesium silicide, Sb doped Mg2Si, Nonstoichiometry, Equilibrium vapor pressure

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High temperature X-ray diffraction study of melt grown MnSiγ

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Abstract

Higher manganese sillicide, MnSiγ, possesses a (3+1)-dimentional composite crystal structure, consisting of two tetragonal subsystems of [Mn] and [Si] (c-axis ratio $\gamma = c\mathrm{Mn}/c\mathrm{Si}$ ~ 1.74). Kikuchi *et. al.* (*J. Alloys Comp.*, **616** (2014) 263.) performed high temperature X-ray difraction (HTXRD) experiments and reported that the γ value remains a constant value of 1.7387(1) from 293 K to 800 K but starts to decrease gradually at $T >$ 800 K. The change in γ corresponds to that in chemical composition of MnSiγ and hence it may influence TE properties. However, the effect of change in γ on TE properties has not been reported.

We prepared single crystal ingots of MnSiγ with fixing the nominal composition of $\gamma = 1.74$. The samples were first prepared by arc melting. The obtained alloys were pulverized and melted in an evacuated quartz tube at 1473 K for 8 h, and gradually cooled down to 1373 K, followed by furnace cooling. Seebeck coefficient (S) and electrical conductivity (σ) were mesured from room temperature to 1000 K. Lattice parameters were refined using Le Bail analysis of HTXRD patterns.

From the Le Bail analysis, a- and cMn-axis lengths were confirmed to change linearly; the lattice parameters did not show any deviations upon thermal history. On the other hand, the cSi-axis length started to change steeply at $T >$ 800 K which causes an irreversible change upon heating and cooling. The cSi-axis length was longer upon cooling. As a result, the γ-value was nearly equal to 1.74239(3) at $T <$ 800 K, while it started to degrease at $T >$ 800 K. Due to the irreversible change in cSi, the room temperature γ-value was smaller than that before the thermal cycle heated above 800 K.

Discussion of TE properties based on the detailed structural change will be also presented at the conference.

Keywords: Higher manganese sillicide, solid solution, thermoelectric properties, chimney, ladder phase, high temperature X, ray difraction

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Improved trade-off between thermoelectric performance and mechanical reliability of Mg2Si-reduced graphene oxide nanocomposites

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Abstract

We prepared hybrid powders of Mg1.96Al0.04Si0.97Bi0.03 and rGO, and fabricated the rGO nanocomposites without agglomeration of nano-phase by precisely controlling sintering process. The prevailing notion is to demonstrate the trade-off relationship between thermoelectric performance and mechanical reliability. By introducing rGO (5 nm) in the grain boundaries, the fracture toughness was significantly increased due to the deflection of crack propagation, bridging and sheet pull-out. In addition, systematic analysis of the effect on the thermoelectric properties and fracture toughness on the shape, dimension, and size of the introduced nano-phase (metal nanoparticles and rGO) were carried out. The introduction of the two-dimensional nano-phase (rGO), expected to have a high interface density, was more effective in improving the trade-off relationship. As a result, optimized ZT value (_˜0.60 @ 873K) and fracture toughness (1.88 MPa m1/2) were obtained at 3 vol% of rGO nanocomposite, and these results emphasized the importance of the trade-off relationship between thermoelectric performance and mechanical reliability.

Keywords: Thermoelectric, Mg2Si, Fracture toughness, trade, off relationship

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Thermoelectric Properties of Ge-doped Higher Manganese Silicides MnSi1.72-1.73:Gem

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Abstract

Higher manganese silicides (HMSs) have been considered as promising p-type thermoelectric materials at temperature range from 500 K to 800 K because of environmental friendliness, high oxidation resistance, and superior thermal stability. Four distinct HMS phases with Nowotny chimney ladder structure have been reported: Mn11Si19 (MnSi1.72), Mn15Si26 (MnSi1.73), Mn27Si47 (MnSi1.74) and Mn4Si7 (MnSi1.75). The substitution of Ge for Si causes a lattice distortion due to the difference in the covalent radius between Ge and Si, which varies the bonding strength and leads to an increase in the carrier concentration. In this study, Ge-doped HMSs were prepared by using solid-state reaction and hot pressing, and the doping effects on the thermoelectric properties were examined.

Keywords: thermoelectric, higher manganese silicide, HMS, solid state reaction, hot pressing

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Synthesis of tungsten disilicide and its potential as a thermoelectric material

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Abstract

WSi2 has received much interest owing to the properties mainly as high heat resistance, hardness and conductivity. Therefore, WSi2 is expected as a high-temperature material. It is known that WSi2 has two phase of stable tetragonal phase and metastable hexagonal phase. The hexagonal WSi2 was reported that this phase was suitable as thermoelectric material at around room temperature by a first principle calculation. On the other hand, the tetragonal WSi2 (t-WSi2) was reported that the Seebeck coefficient of this phase shows 100 x uV/K over above 1000 K. A method for obtaining tetragonal WSi2 by the reduction method has already been reported. However, with this method, it is necessary to remove SiO2 remaining in the sample after the reaction with an aqueous HF solution, and there is a possibility that activated carbon used as a reducing agent may remain in the sample. In addition, since tungsten or sponge titanium is used for the reaction vessel to obtain WSi2 of high purity, the synthesis cost also increases. Therefore, synthesis of tungsten disilicide was attempted by simple synthesis method using reduction method and arc melting method. Moreover, we tried reducing the carrier concentration of WSi2 by element substitution, and the thermoelectric properties of the WSi2 were investigated. Tetragonal tungsten disilicide could be obtained by the reduction method using the graphite container, but it was found that impurity phase such as tungsten carbide was easily formed. Single phase tetragonal tungsten disilicide could be obtained by the arc melting method. It was confirmed that the carrier concentration of tungsten disilicide decreased by substitution of Mn or Cr. The peak temperature of the power factor of the element substituted sample decreased to about 600 K, and the maximum value of the power factor of the Mn-substituted sample was 1 mW / (K2m).

Keywords: Tungsten disilicide, Arc melting, Reduction method

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Process optimization and the effects of process route on thermoelectric properties of n-type doped Mg2(Si,Sn)

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Abstract

Magnesium silicide stannides, Mg2(Si,Sn), which contain non-toxic and earth abundant elements are attractive thermoelectric materials for practical applications in the temperature range of 500–800 K [1]. High zTmax values of 1.1–1.5 were reported for the n-type doped Mg2(Si,Sn) in laboratory scale [2,3]. Here, we show the importance of process optimization and the effects of process route on the production of n-type doped Mg2(Si,Sn), in order to scale up high performance thermoelectric material. The thermoelectric material was synthesized by mechanical alloying and consolidated by spark-plasma sintering. X-ray diffraction (XRD) and scanning electron microscopy with energy dispersive X-ray spectroscopy techniques (SEM/EDX) were used for characterization of material. Thermoelectric properties were investigated by laser flash analysis, resistivity and Seebeck coefficient measurements. Our process is promising for scaling-up the production of mechanically and thermally stable material with zTmax value of 1.2 to be used for fabricating thermoelectric devices.

Liu *et al.*, Natl. Sci. Rev., **4**, 611 (2017).

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Keywords: magnesium silicide stannide, ball milling, spark plasma sintering

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Incorporating a Small Amount of MnS into Higher Manganese Silicide Leading to a Green Thermoelectric Composite with Significantly High Price/performance Ratio

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Abstract

Thermoelectric materials that can directly convert heat to electrical energy, offers a promising solution for the increasingly global energy crisis. Higher manganese silicide (HMS) is a naturally abundant, eco-friendly, and low-cost p-type thermoelectric semiconductor with high power factor (PF); however, its figure of merit (ZT) is limited by the intrinsically high thermal conductivity (). To effectively enhance the thermoelectric performance of HMS and also avoid the using of some expensive or toxic elements such as Re, Te or Pb, a green p-type MnS, with high Seebeck coefficient (S) and low , was incorporated into the HMS matrix to form MnS/HMS composites. The incorporation of MnS led to a 31% reduction of as well as a 10% increase of S. The ZT value of MnS/HMS composites increased by _˜48% from 0.40 to 0.59 at 823 K. And correspondingly, its price/performance ratio was firstly proposed, and was demonstrated higher than the currently vast majority thermoelectric materials. This study gives a glimpse of boosting the ZT value of HMS as well as reducing the costs, which is also applicable to other thermoelectric materials.

Keywords: Higher Manganese Silicide, Thermoelectric material, Price/performance Ratio

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A Thermoelectric Study Of Thin Film Nanocrystalline Silicon Prepared By Chemical-Vapor Deposition

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Abstract

Silicon is one of the most abundant and environmentally friendly materials on earth. It is also the most widely used semiconductor material that forms the foundation of modern electronics. Although doped bulk silicon possesses a favorable Seebeck coefficient and electrical conductivity, its high thermal conductivity prevents it to become a practical thermoelectric material. In this work, we explore the possibility to use thin film nanocrystalline silicon prepared by chemical-vapor deposition (CVD) as a potential high temperature thin film thermoelectric material. We have reduced its average grain size to below 10 nm, and reach a thermal conductivity that is much smaller than its amorphous limit. We also find that ion implantation and annealing can be used to precisely control and optimize dopant concentration and activation. We examine the thermoelectric power and electrical conductivity of boron-doped CVD nanocrystalline silicon and find that its power factor can reach those of doped nanostructured silicon alloys prepared by other methods. Because of its low thermal conductivity, we find it promising in high temperature thermoelectric applications.

Keywords: nanocrystalline silicon, chemical, vapor deposition, ion implantation, thermoelectric, thermal conductivity

*Speaker

Effects of Co substitution on crystal structure and thermoelectric properties of melt-grown higher manganese silicides

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Abstract

Higher manganese silicide, MnSiγ, has attracted much interest as a promising candidate for thermoelectric (TE) materials owing to the natural abundance of their constituents, low toxicity, and the relatively low thermal conductivity (3 W/mK). MnSiγ consists of Mn- and Si-subsystems, and these subsystems have different c-axis lengths. The ratio of these c-axis lengths, γ is an important value to understand electronic transport properties of MnSiγ because γ relates to valence electron counts (VEC). In MnSiγ, change of carrier concentration can be briefly estimated by VEC. We have reported that melt-grown V-substituted MnSiγ exhibits high power factor (2.4 mW/mK2 at 800 K) owing to the decrease in VEC. In addition, it has been reported that electrical conductivity of sintered MnSiγ increases by Co substitution. In this study, we investigate effects of Co substitution on the crystal structure and TE properties of melt-grown MnSiγ. We prepared Co-substituted samples using an arc melting method. The obtained alloys were pulverized and remelted in an evacuated quartz tube at 1473 K for 8 hours, and slowly cooled down to 1373 K for 100 hours. After the cooling process, the samples were further cooled down to room temperature for 24 hours. The γ value was refined by Rietveld analysis using a powder X-ray diffraction pattern. Calculated VEC for obtained samples decreased from 13.972(1) to 13.921(1) with increasing Co content. From this result, the carrier concentration is expected to increase by Co substitution. Actually, the electrical conductivity and Seebeck coefficient increased and decreased, respectively. Consequently, the maximum power factor greatly increased from 1.1 mW/mK2 to about 2.0 mW/mK2 at 800 K.

Keywords: higher manganese silicides, valence electron counts

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Synthesis and Thermoelectric Properties of Mo-substituted CrSi2 by Reduction-Diffusion Process

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Abstract

Chromium disilicide, CrSi2, is a promising p-type thermoelectric material because of its less toxicity, chemical stability at high temperatures and high power factor. However, the zT value of CrSi2 remains still low due to its high thermal conductivity. Recently, Ohishi et al. fabricated Mo-substituted CrSi2 by arc-melting and reported a reduction of the thermal conductivity owing to the partial substitution of a heavier atom Mo for the Cr sites. (Y. Ohishi et al., J. Phys. Chem. Solids, **87** (2015) 153.) The solubility limit of Mo in Cr1-xMoxSi2 was reported to be $x = 0.30$. To further decrease thermal conductivity of CrSi2, we prepared Cr1-xMoxSi2 samples in the range of $x >$ 0.30 by means of Reduction-Diffusion process. This process uses metal oxides as raw materials, which are reduced by a binary metal hydride and fine powder can be obtained due to the high reactivity of a reductant.
In this study, powdered Cr2O3, MoO3 and Si were mixed with LiH and ground in an Ar-filled glove box, and then pressed into pellets. These pellets were heated at 800°C for 6 h in an evacuated quartz tube. After that, pellets were washed with deionized water to remove byproducts. Finally, obtained powders were sintered by Spark Plasma Sintering at 900°C for 5min under an applying pressure of 50 MPa in vacuum. Bulk samples were identified by powder X-ray diffraction (XRD).
By employing the Reduction-Diffusion process, we have succeeded in expanding the solubility limit of Mo up to $x = 0.40$ in Cr1-xMoxSi2 for the first time. Thermoelectric properties of Mo-substituted CrSi2 samples will be discussed at the conference.

Keywords: Mo substituted CrSi2, metal hydride, Reduction, Diffusion process, fine powder, solubility limit of Mo

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Advanced corrosion protective layers for Mg2Si thermoelectric material

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Abstract

Magnesium silicide is the most promising, environmental friendly thermoelectric material, which has low density (1.99 g·cm-3) and is cheap. These attributes distinguish it from other well-known thermoelectric materials and therefore it is currently intensively studied. The aim of the work was to develop anticorrosive layer for magnesium silicide using silanes-based, amorphous layers. High purity Mg2Si samples were prepared by self-propagating high-temperature synthesis (SHS) and hot-pressing method (Thermal Technology Hot Press). Magnesium silicide samples were covered with selected amorphous layers by dip-coating method and then annealed in various gas atmospheres (O2, Ar) and for different time periods (several hours, days). The obtained layers were characterized using scanning electron microscopy (SEM) and Raman spectroscopy. The structural and phase compositions of the samples were examined by means of the X-ray diffraction (XRD) method and chemical composition analysis by SEM-EDX. The transport properties for Mg2Si samples i.e.: electrical conductivity, the Seebeck coefficient, impedance spectroscopy and the thermal conductivity were studied in temperature range from 300 to 720 K.

Acknowledgments

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Keywords: Mg2Si, corrosion, thermoelectric properties

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Thermoelectric properties of Si/Al-doped β-FeSi2 composites

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Abstract

The composite samples made up of silicon dispersed β-FeSi2 with different aluminium concentrations are synthesized using the eutectoid decomposition of α-Fe2Si5–xAlx ($0 \leq x \leq 0.1$). Silicon phase fractions, microstructure and thermoelectric properties of the composites have been investigated. Al-doping in Si dispersed β-FeSi2 results in increased hole-carrier concentration thereby enhancing the electrical conductivity without compromising the Seebeck coefficient. This results in maximum power factor value of 4.7 μWcm–1 K–2 at 773 K for the sample with x = 0.1 which is significantly higher than that of an undoped sample. We used Debye- Callaway model to understand the various scattering process involved in phonon scattering. From the analysis, it is shown that an increased point defect scattering of phonons with Al-doping in addition to scattering by Si/β-FeSi2 interface lowers the thermal conductivity significantly.

Keywords: Transition metal silicides: Iron disilicide

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The influence of interband electron scattering on thermoelectric properties of transition metal monosilicides.

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Abstract

In the present work we continue the investigation of the thermoelectric properties of cobalt monosilicide and its solid solutions with the B20 cubic noncentrosymmetric crystal structure. These materials demonstrate not only good thermoelectric properties, but, as was revealed recently, they have unconventional electronic topology. In this work, using first principle calculations, we investigate the scattering of charge carriers by phonons and point defects taking into account both interband and intraband transitions. The comparison with the experimental results and calculations in the constant relaxation time approximation is made. It is shown that the account of interband scattering and energy dependence of relaxation time is important for correct description of transport properties of these materials.

Keywords: cobalt monosilicide, ab initio calculations, electron scattering, interband scattering

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Silicide Module Development for Automotive Applications

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Abstract

Researchers focusing on the development of medium temperature thermoelectric generators have predominantly concentrated on a handful of thermoelectric compounds such as half heuslers, skutterudites, lead tellurides and silicides. Silicide materials offer a low cost, environmentally friendly option for medium temperature thermoelectric generation. To produce modules which are attractive to industrial sectors such as the automotive industry, a number of technological issues must be solved. The major challenges lie in the development of scalable and low-cost manufacturing processes for modules which have sufficient performance and lifetime properties to meet the demanding targets from end-users. A particularly difficult requirement is the need for low resistance and strong mechanical joining of the silicide materials to electrical contacts. Furthermore, these properties must be maintained under operating conditions to ensure a long lifetime. European Thermodynamics Ltd has developed a 40mm x 40mm, 66 couple, mid-temperature thermoelectric generator device, comprising magnesium silicide and higher manganese silicide. The module has a maximum power output of 4.94W at a temperature differential of 376oC (measured in air), equating to a power density of 309mW/cm2 for the module. We review the design considerations for a mid-temperature module and present the geometry used for the tested device. Electrical and mechanical performance data is presented for both 7-couple and 66-couple devices and the methods for measurement are explained. The lifetime requirements, the testing procedures and the lifetime data of the presented module are discussed.

Keywords: Silicide, Module, Lifetime, Power, Generator

*Speaker

Control of microstructure in magnesium silicide-stannide alloys via heat treatment protocols

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Abstract

Microstructuring has already proved itself as a reliable approach for enhancement of thermoelectric properties [1]. However, this approach has not been much applied to alloys of Mg2Si1-xSnx possibly due to a high discrepancy among published phase diagrams [2, 3]. The presence of the miscibility gap demonstrated in the current study allows to manipulate the composition as well as morphology in the magnesium silicide-stannide phases. The spinodal decomposition in solid state is of particular interest, since alternating endotaxial phases can be formed creating a large density of interfaces, in which the low frequency phonons are scattered more preferentially than high frequency electrons.
The influence of composition and temperature on the microstructure of Mg2Si1-xSnx in the Si-rich region is investigated in order to identify the critical demixing temperature, which plays a significant role in the formation of lamellae-like arrangement of phases. The judiciously designed protocols made it possible to control the microstructure. Another important parameter, which is responsible for spinodal decomposition, is the cooling rate, the effect of which is also demonstrated.

The formed phases in the Mg2Si-Mg2Sn system were characterized via X-ray diffraction, scanning and transmission electron microscopy. The acquired data of the composition of the phases clarify the behavior of the system as well as reveal details of the miscibility gap, which can be utilized to control the microstructure in the other regions of the quasi-binary phase diagram.

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Keywords: Magnesium silicide, stannide, microstructuring, spinodal decomposition

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Investigating the effect of processing route on the microstructure and thermoelectric properties of higher manganese Silicide

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Abstract

Higher manganese silicide (HMS) has been considered as an environment-friendly thermoelectric material due to the abundant and non-toxic elements it consists of. The technological advances in producing high quality feedstock materials, particularly Si, facilitate large scale production perspectives. In this work, we compare three different approaches for producing HMS samples, namely melt-casting (MC) which is a matured and widely-used industrial process for silicon and other alloy production, spark plasma sintering (SPS) which has been mostly reported for lab-scale fabrication of HMS samples, and hot-pressing (HP) for a small-scale synthesis.
We have made kilogram batches of HMS with nominal compositions of MnSi1.75-xGex, where x= 0.005 and 0.01, and for further SPS and HP processes. The microstructures were investigated by scanning electron microscopy and X-ray diffraction. The Seebeck coefficient, electrical conductivity and thermal conductivity measurements were carried out from room temperature up to 500C.

We show how the peritectic phases dissolve and microstructure changes upon employing different processing approaches at different temperatures. The electrical conductivity and thermal conductivity are strongly dependent on the microstructure, while the Seebeck coefficient shows a dependency on the doping level. It is expected that the outcome of the present study will provide important feedback to the transition from lab-fabrication to industrial production.

Keywords: HMS, synthesis

*Speaker

Transmission electron microscopy of Mg2Si thermoelectric leg subjected to high-temperature oxidization tests under ambient atmosphere

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Abstract

High temperature degradation is an issue of Mg2Si thermoelectric devices operating at 500–800 degC. The authors demonstrated that an enhancement of sintering pressures (Ref. 1) and impurity doping to raw materials (Ref. 2) were effective to improve high temperature durability in spark plasma sintered (SPS) n-type Mg2Si compacts. In this work, cross-sectional transmission electron microscopy (TEM) was carried out to investigate the inner matrix of these compacts subjected to high-temperature tests at 600 degC. TEM observation revealed that the compacts contained surface oxide layers, Mg2Si crystalline, and complexes of MgO and Mg2Si. The sample compacted at lower pressure exhibiting lower density and weaker temperature stability and contained a larger amount of MgO complex, indicating that high temperature stability is attributed to formation of oxides inside body rather than on the surface oxide layer. A sintered sample made from raw Mg2Si powder doped with tungsten (W) and zinc (Zn) impurities contained W and WSi2 particles, which prevented the formation of oxides inside the sample, resulting in longer high-temperature stability.

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Keywords: Mg2Si, Oxidation, Transmission Electron Microscopy

*Speaker

Mg2(Si,Sn,Ge) Thermoelectric Materials by Mechanical Alloying

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Abstract

Silicides have been considered as candidates for high performance thermoelectric materials because they combine relatively high Seebeck coefficients, high electrical conductivities and low thermal conductivities. Recent studies have shown that silicides offer considerable advantages over conventional materials for mass production and scale up due to their low cost, relatively high abundance and availability of raw materials. However, scalable synthesis is a critical issue for this type of materials due to the features of their starting elements (i.e. large difference in melting points, ductile materials etc) that limit the type of techniques that can be applied. In this study, doped Mg2(Si,Sn,Ge) materials were prepared by mechanical alloying in an effort to increase the mass capabilities of the synthetic route compared to the typical solid state reaction. Mechanical alloying and hot pressing conditions were investigated for optimization aiming to achieve good thermoelectric properties, comparable to the promising materials prepared via solid state synthesis. Structural features and thermoelectric properties were studied in detail.

Keywords: Silicides, mechanical alloying, scale up

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Stability Studies of Magnesium Silicide based Compounds

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Abstract

Magnesium silicide related materials have attracted increasing attention for thermoelectrics being promising, environmentally friendly and operated in a medium temperature range. Target applications are related to waste heat recovery from various systems. However, besides their high thermoelectric performance, their high sensitivity to oxidation that leads to poor thermoelectric properties due to the degradation of the compound is also known. Reported works on such materials focus mainly of the thermoelectric properties and the figure-of-merit while reports on stability tests are still limited. In this work, the stability of Mg2(Si,Sn,Ge)-based compounds are investigated under certain conditions. Our recent results on the compositional and structural stability of materials as well as their thermoelectric properties (Seebeck coefficient and electrical conductivity) will be presented.

Keywords: Stability, Magnesium silicide

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Backscattered electron imaging for a rapid screening/determination of composition on inhomogeneous samples: Mg2Si1-xSnx as example

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Abstract

In the field of thermoelectrics, multiphase materials are of considerable interest due to the additional scattering of different phases that can reduce the lattice thermal conductivity and consequently improve the thermoelectric performance of the material. Furthermore, secondary phases can be beneficial for blocking undesired minority carriers in heterostructures; hence suppressing the bipolar part of the thermal conductivity or for filtering the low energy majority carrier, therefore enhancing the power factor. To be able to tune the thermoelectric properties, size, amount, and occasionally, composition of the secondary phases need to be assessed and optimized. SEM-EDX is the state-of-the-art method for such phase analysis. However, it is limited by a low throughput and a relatively poor spatial resolution. Therefore, development of a quick and simple method for phase quantification (in composition and volume fraction) can be useful. In this work, we prove experimentally a simple relation between the grey value of the different points of the backscattered electron images and their respective chemical composition using multiphase Mg2Si1-xSnx as an example for a quasi-binary multi-composition/multiphase thermoelectric material system. Utilizing the grey values of the backscattered electron images, a rapid method for phase quantification in such material systems is introduced. Applying this method on Mg2Si1-xSnx, the Si and Sn content of each individual point of the BSE images can be calculated assuming that Mg2(Si,Sn) is a line phase (i.e. we do not have Mg content fluctuation), based on only two EDX point measurements giving a superior spatial resolution compared with EDX mapping. Through this method, the area percentage of Si- rich secondary phases were calculated in the Mg2Si1-xSnx samples sintered at 700 C for different time durations.

Keywords: Phase quantification, Magnesium silicide stannide, Quasi binary compounds, Thermoelectric, Back scattered electron image, Energy dispersive X ray spectroscopy, Spatial Resolution

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Studying the miscibility gap in Mg2(Si,Sn): influence of Mg content

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Abstract

Mg2Si1-xSnx is a promising thermoelectric material with a high figure of merit (zTmax) of _˜1.1–1.4 for n-type Mg2Si0.4Sn0.6 solid solutions. There is a miscibility gap reported for the Mg2(Si,Sn) compound, though the limits are disputed. A miscibility gap gives a chance for self-assembling and temperature stable nanostructuring; hence, further reduction of the thermal conductivity through additional phonon scattering. Therefore, its understanding is important for a possible further optimization of material performance. In this work, two approaches were taken to investigate thermodynamic stable phases and range of the miscibility gap: interdiffusion experiments of Mg2Si/Mg2Sn couples and long-term annealing on Mg2Si1-xSnx samples with $x = 0.5$ (supposedly inside the miscibility gap). A group of sintered Mg2Si/Mg2Sn diffusion couples together with excess elemental Mg, was annealed at 600 C, 525 C, and 450 C in quartz ampoules. Moreover, three groups of Mg2Si0.5Sn0.5 samples were annealed with and without excess Mg at the aforementioned set of temperatures. The phase evolution of the Mg2Si/Mg2Sn diffusion couples and Mg2Si0.5Sn0.5 samples was studied using SEM/EDAX. The Mg content in the samples can change due to the high vapor pressure of Mg at high temperatures. EDAX results revealed that the Mg- loss has a considerable influence on the preliminary obtained boundaries of the miscibility gap; for the Mg2Si0.5Sn0.5 sample annealed at 600 C (with Mg- loss) the limits of the miscibility gap were determined as $0.25 < x < 0.9$ while for the Mg2Si/Mg2Sn diffusion couple annealed at the same temperature without Mg- loss the range was obtained as $0.2 < x < 0.6$. Differences in Mg content might thus explain why the miscibility range was disputed for decades.

Keywords: Magnesium silicide stannide, Thermoelectric, Miscibility gap, Magnesium loss

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Potential use of thermoelectric generators in solid waste incineration plant

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Abstract

Based on the Roadmap to a Resource Efficient Europe, the European Union should achieve a situation where waste is managed as a resource by 2020 [1]. In this respect, let us underline that in 10 EU states more than 90% of the waste is already recycled [2]. This clearly insinuates the fact that using waste represents one of the EU's key resources.
Due to the fact that not all of the municipal solid waste (MSW) can be properly recycled or composted, another possibility of harvesting MSW is using it as a valuable energy resource via waste to heat technology in incinerator plant [2]. To eventually further improve the efficiency of incineration process, there is a clear demand to analyze in detail the energy balance of waste-to-energy plant. We have performed such analysis for municipal waste incineration factory located in Prague agglomeration, which generates energy in the form of electricity, steam and hot water further sent to a nearby district to heat homes, households, offices and used by the nearby industry. Namely we aimed to target such zones or places, where the application of thermoelectric technology could either improve the energy gain via electric energy generation and/or help to improve the complex control and energy management of modern incineration plant.

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Keywords: waste recovery

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A study on forest soil thermoelectric power generation device

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Abstract

An environmental micro-energy collection device was further perfected and field experiments were carried out under the natural condition for the first time. The device used gravity-assisted heat pipe to transmit heat from shallow soil to the earth surface and thermoelectric generators (TEG) were employed to generate electric by temperature difference between soil and air. During the experiments carried out in natural field, a 3.7 mW electrical power was observed and energy about 128.74 J could be harvested in a single day. The device can be used to generate electric to power the forest wireless sensors in remote forest or other environment, where electricity is unavailable, this work also has a referential significance to acute energy shortage and environmental pollution problem.

Keywords: Environmental microenergy, Thermoelectric device, Soil, Wireless sensors.

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Finite element analysis of temperature and stress fields during the selective laser melting process of thermoelectric SnTe

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Abstract

A three dimensional nonlinear transient thermo-mechanically coupled finite element model (FEM) is introduced to analyze the temperature and stress fields during the selective laser melting (SLM) of thermoelectric (TE) SnTe. Considering the powder-to-solid transition and the latent heats of melting and vaporization, we simulate the temperature distribution near the molten pool and the residual stress inside the printed material at room temperature under different laser processing parameters. The calculated results indicate that vaporization gradually weakens as the laser power decreases and the scanning speed increases. Within the optimum forming window, the residual stress rises with the increasing laser power and decreasing scanning speed. The thermal stress mainly concentrates in the middle of the first scanning track, the terminal of each scanning track, and the edges of the forming surface, which is well consistent with the experimental results. This work has laid a significant foundation for rapid manufacturing of bulk SnTe thermoelectric materials using the selective laser melting process and will serve as a guide for laser processing of other thermoelectrics and perhaps even complete thermoelectric modules.

Keywords: selective laser melting, thermoelectric SnTe, finite element analysis, temperature field, stress field

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GRAPHENE – MESOPOROUS SI OR GE NANOCOMPOSITES FOR THERMOELECTRIC APPLICATIONS

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Abstract

Nanoporous semiconductors such as silicon and germanium have been predicted theoretically to be appealing candidates [1]. A figure of merit of 0.40 for nanoporous silicon is calculated [1]. Moreover, nanoporous germanium presents appealing properties and (ZT)max twice larger than nanoporous silicon [1]. In the two cases, the figure of merit is lower than other materials. However, graphene provides a higher thermal stability for porous materials and a better electrical conductivity so potentially a higher figure of merit than predicted without grapheme. The association of mesoporous semiconductor with a 3D graphene-like coating creates a nanocomposite with hybrid physical properties. In this work, we evaluate the potential of using these composite materials for thermoelectric applications. The nanocomposite are synthesised thanks to electrochemical etching and then carbonization using Chemical Vapor Infiltration (CVI). The chemical and structural properties of these composites are studied by XPS and Raman spectroscopy. Thermal and electrical properties of the nanocomposite are studied by Raman spectroscopy and current voltage measurements respectively. According to the results, the carbon coating structure is graphene-like and enhances electrical conductivity. Indeed, a significant factor is present between the slope for graphene mesoporous silicon nanocomposite and slope for mesoporous silicon. Additionally the thermal conductivity of the nanocomposite is _˜15mW/mK which is similar to the one of initial mesoporous silicon sample. [1] J-H. Lee and J. C. Grossman, Applied Physics Letters, 2009, 95 (1), DOI: 10.1063/1.3159813

Keywords: mesoporous silicon, Graphene, Nanocomposites, thermoelectric effect

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