# Poster Presentation Program

## Poster Session 1: Monday (Chalcogenides (S, Se, Te), Modelling, Organics and Hybrids, Oxides and Zintl)

| Poster Position | Name of the presenter | Email address | Title of the poster |
|---|---|---|---|
| **Chalcogenides (S, Se, Te)** | | | |
| P.1 | Čermák Patrik | patrik.cermak@email.cz | Investigation of stability of doped SnS |
| P.2 | Acharya Somnath | somphys@gmail.com | Effect of Charge Carrier Optimization on Thermoelectric Properties of Mn and Yb Doped SnTe |
| P.3 | Agne Matthias | mt.agne.matsci@gmail.com | Defect engineering and dopability of PbTe using phase boundary mapping |
| P.4 | Back Song Yi | song2b@khu.ac.kr | Enhancement of Thermoelectric Performance in $InTe_{1-\delta}$ Polycrystalline Compounds |
| P.5 | Bae Sang Hyun | khansh@koreatech.ac.kr | Study on the structural and thermoelectric properties of Cu-doped $Bi_2Te_3$ thin films |
| P.6 | Ballikaya Sedat | ballikaya@istanbul.edu.tr | Thermoelectric Properties and Thermal Stability of Nano $Cu_2Se$ Included $Ag_2Se$ |
| P.7 | Bohra Anil K. | anilbohra786@gmail.com | Thermoelectric power generation through single-leg of p-type $Bi_{1.95}Pb_{0.05}Te_3$ |
| P.8 | Branco Lopes Elsa | eblopes@ctn.tecnico.ulisboa.pt | Effect of the composition in the thermoelectric properties of $Cu_{12-x}M_xSb_4S_{13-y}Se_y$ (M = Mn, Fe) |
| P.9 | Byeon Dogyun | dogun04@gmail.com | Self-tuning carrier concentration effect of noble metal chalcogenides |
| P.10 | Chen Lei | lc648@uowmail.edu.au | Ultrolow Thermal Conductivity and High ZT in Graphene Doped p-type Polycrystalline SnSe |
| P.11 | Cho Hyunyong | gprhf1@naver.com | Localization effect and chemical potential tuning by CuI doping in $(Cu^I)_y(Bi_2Te_3)_{0.95-x}(Bi_2Se_3)_x(Bi_2S_3)_{0.05}$ quaternary system |
| P.12 | Choi Jin Sik | jinsik8365@naver.com | Thermoelectric transport properties of Sb-doped $SnSe_2$ compounds |

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| P.13 | Failamani Fainan | failamani.fainan@nims.go.jp | Thermoelectric Properties of YbTe-SnTe-based Solid Solutions |
| P.14 | Fanciulli Carlo | carlo.fanciulli@cnr.it | Thermomechanical properties of fast sintered polycrystalline SnSe composites |
| P.15 | Guo Quansheng | GUO.Quansheng@nims.go.jp | Thermoelectric Properties of excess Cu- and Ga-added $Cu_4Mn_2Te_4$ |
| P.16 | Hamawandi Bejan | | Rapid Synthesis, Processing and Characterisation of $Cu_{2-x}Se$ and its Solid Solutions |
| P.17 | Han Mi-Kyung | mikihan@ewha.ac.kr | Synergistically optimizing thermoelectric transport properties of n-type $Bi_2Te_3$ via $Cu^I$ and Sn co-doping |
| P.18 | Hashikuni Katsuaki | k-hashikuni@hiroshima-u.ac.jp | Thermoelectric Properties of Cu-deficient Thiospinel $Cu_{2-x}Ti_4S_8$ and the derivative $Cu_{2-x}Ti_{4.5}S_8$ |
| P.19 | Ulises Acevedo Salas | ulises.acevedo-salas@ensicaen.fr | Investigation of the thermoelectric properties of pyrites: interplay between magnetism and transport |
| P.20 | Heo Seung Hwae | hsh0104@unist.ac.kr | High performance textured SnSe thermoelectric thin films with controlled doping fabricated by a solution process |
| P.21 | Huang Mei-Jiau | mjhuang@ntu.edu.tw | An Investigation of the Thermal boundary resistance associated with the Twin Boundary in Bismuth Telluride |
| P.22 | Huang Ruomeng | R.Huang@soton.ac.uk | Thin film thermoelectric micro-generator by selective chemical vapour deposition |
| P.23 | Hwang Junphil | tainm7@naver.com | Model for reduction of phonon transport through coated grain structure and proposed mechanism |
| P.24 | Hwang Ui Gyeong | ghkddmlrud23@gmail.com | Charge transport properties of p-type $Bi_{0.3}Sb_{1.7}Te_3$-graphene oxide composites |
| P.25 | Jinfeng Dong | dongjf15@mails.tsinghua.edu.cn | Enhanced Thermoelectric Properties of Fine-Grained and Carrier Concentration Optimized GeTe |
| P.26 | Jood Priyanka | joodpriyanka@gmail.com | Engineered doping and nanostructuring leads to high efficiency PbTe materials and modules |
| P.27 | Kawamoto Naoyuki | KAWAMOTO.Naoyuki@nims.go.jp | Nanoscale thermal conductivity analysis of chalcopyrite thin films by STEM-based thermal analytical microscopy |
| P.28 | | | |

| P.29 | Khairul Fadzli Samat | khairul.fadzli@utem.edu.my | Thermoelectric properties enhancement of $Bi_2Te_3$ through Pt nanoparticles inclusion prepared by electrochemical deposition |
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| P.30 | Kim Fredrick | fredrick@unist.ac.kr | 3D printing of shape-conformable thermoelectric materials using all-inorganic $Bi_2Te_3$-based inks |
| P.31 | Kim Jin-Sang | jskim@kist.re.kr | N-type $Bi_2Te_{2.7}Se_{0.3}$/ZnO core-shell nanostructure for colossal improvement in the thermoelectric performance |
| P.32 | Kim Kwang-Chon | kwang@kist.re.kr | Enhanced thermoelectric properties of nano structured Bi-Sb-Te/MXene bulk nano composite |
| P.33 | Kim Min Ji | mgkim830@gmail.com | Effects of Cl-doping on Thermoelectric Transport Properties of $Cu_2Se$ |
| P.34 | Kim Sang-Il | sang1.kim@uos.ac.kr | Design of multi-defect structures in polycrystalline $(Bi,Sb)_2Te_3$ Alloys for low thermal conductivity |
| P.35 | Knizek Karel | knizek@fzu.cz | LDA+U calculation of electronic and thermoelectric properties of doped tetrahedrite $Cu_{12}Sb_4S_{13}$ |
| P.36 | Kumar Sunil | skbgudha@gmail.com | A Study on the effect of Conducting Interface on Electron and Phonon Transport in $Sb_2Te_3$-Graphene Nanocomposite for Thermoelectric Properties |
| P.37 | Lan Tianwey | lantw@gate.sinica.edu.tw | Enhancing the Figure of Merit in Nano-composite Thermoelectric Materials with Aerogel Addition |
| P.38 | Lee Go-Eun | leege0205@ut.ac.kr | Tetrahedrite $Cu_{12}Sb_4S_{13}$ Prepared by Using Mechanical Alloying and Hot Pressing |
| P.39 | Lee Ho Seong | hoseong2532@gmail.com | Microstructural characteristics and thermoelectric properties of Cu and Sb codoped GeTe thermoelectric materials |
| P.40 | Levinský Petr | levinsky@fzu.cz | Thermoelectric properties of magnesium doped tetrahedrite |
| P.41 | Luo Jun | junluo@shu.edu.cn | Boosting the Thermoelectric Performances of Lead Chalcogenides through Dynamic Doping and Hierarchical Phonon Scattering |
| P.42 | Mars Krzysztof | kmars@agh.edu.pl | Thermoelectric properties of Sn-Se layers prepared by pulsed magnetron sputtering |
| P.43 | Miku?a Andrzej | amikula@agh.edu.pl | First principle studies of Fe doped $Cu_2S$. Synthesis and computational investigations |

| P.44 | Mori Hitoshi | h-mori@presto.phys.sci.osaka-u.ac.jp | First-principles study on the thermoelectric properties of ternary chalcogenides |
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| P.45 | Mukherjee Shriparna | shriparnamuk@iisc.ac.in | Effect of Cu deficiency on the structural and thermoelectric properties of $Cu_2Te$ |
| P.46 | Nguyen Thi Huong | nguyenhuong2710@gmail.com | Huge anisotropy transport properties in $\alpha$-$In_2Se_3$ single crystal |
| P.47 | Nguyen Van Quang | nvquangphysics@gmail.com | Effects of Se/Sn Flux Ratio on Growth and Thermoelectric Transport Properties of SnSe Thin Films |
| P.48 | Novikov Sergei | S.Novikov@mail.ioffe.ru | Evolution of thermoelectric properties of melt-spun ribbons during crystallization |
| P.49 | Ochi Masayuki | ochi@phys.sci.osaka-u.ac.jp | Prediction of the high thermoelectric performance of pnictogen-dichalcogenide layered compounds with quasi-one-dimensional gapped-Dirac-like band dispersion |
| P.50 | Ohno Fumiya | s_f.ohno@p.s.osakafu-u.ac.jp | Crystal structure and thermoelectric properties of $Ge_2Sb_2Te_5$ prepared by spark plasma sintering |
| P.51 | Pham Anh Tuan | tuanpham405@gmail.com | Anisotropic thermoelectric properties of $SnSe_2$ single crystal |
| P.52 | Pi Ji-Hee | piji0627@naver.com | Thermal Stability and Mechanical Properties of Thermoelectric Tetrahedrite $Cu_{12}Sb_4S_{13}$ |
| P.53 | Pires Ana | pires.analuci@gmail.com | New Generation of Micro-Flexible Thermoelectric Devices to be Applied in Electronic Printing |
| P.54 | Popuri Srinivasarao | s.r.popuri@hw.ac.uk | Probing the Link between Structure and Thermoelectric Properties in SnSe |
| P.55 | Qiu Pengfei | qiupf@mail.sic.ac.cn | Improved thermoelectric performance in $Cu_2Se$-based liquid-like materials |
| P.56 | Ranganayakulu V.k. | ranga99@gate.sinica.edu.tw | Realizing Thermoelectric Performance in High Quality Crystalline GeTe by Sb Doping |
| P.57 | Rieger Felix | frieger@gwdg.de | Thermal conductivity measurements and HRTEM analysis of epitaxially grown $(Sb_{1-x}Bi_x)_2Te_3$ PVD thin films |
| P.58 | Romanenko Anatoly | anatoly.roman@gmail.com | Effect of jointly replacement in the anion and cation subsystem on conductivity and thermoelectric power of thermoelectrics based on layered transition metal dichalcogenides |

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| P.59 | Savic Ivana | ivana.savic@tyndall.ie | Temperature variation of electronic structure of n-type PbTe and its impact on thermoelectric transport |
| P.60 | Shin Ji Eun | gguri95@naver.com | Thermoelectric Properties of Bi-Te-M (M: Sb, Se) Poly Crystal Compounds Fabricated by an Oxide-reduction and Spark Plasma Sintering |
| P.61 | Song Jaemin | love8767@kicet.re.kr | Thermoelectric Properties of P-type $Cu_2Te$/Bi-Sb-Te Composite for Mid-Temperature Energy Harvesting |
| P.62 | Tak Jang-Yeul | takjangyeul@gmail.com | Promising thermoelectric performances of Cu-excess a-$Cu_{2+x}$Se for near-room-temperature applications |
| P.63 | Takaki Hirokazu | hrtakaki@bk.tsukuba.ac.jp | Thermoelectric properties of a magnetic semiconductor $CuFeS_2$ |
| P.64 | Tanaka Koki | syc04056@edu.osakafu-u.ac.jp | Relationship among crystal structure, band structure, and thermoelectric properties of defect-containing Ag-In-Te chalcopyrite structure compounds |
| P.65 | Tang Huai-Chao | thc13@mails.tsinghua.edu.cn | Enhanced Thermoelectric Properties and Thermal Stability of Copper Sulfide with Graphene Heterointerface |
| P.66 | Tatsuya Hirano | 2ES17047P@s.kyushu-u.ac.jp | Effects of Se substitution on the thermoelectric properties of $(SnS)_{1.2}(TiS_2)_n$ (n = 1, 2) |
| P.67 | Tippireddy Sahil | sahil@iisc.ac.in | Electronic and Thermoelectric Properties of Zn and Se Double Substituted Tetrahedrite |
| P.68 | Varghese Tony | tonyvalayilvarghese@u.boisestate.edu | Ultrafast Additive Manufacturing of Flexible Thermoelectric Films by Aerosol Jet Printing and Photonic Curing |
| P.69 | Voronin Andrei | voronin@misis.ru | Theoretical explanation of surface cracking in $Bi_2Te_3$ and $Sb_2Te1$ thermoelectric materials |
| P.70 | Wang Chenyang | cywang@shu.edu.cn | Enhancement in thermoelectric performance of Cu-dopped bismuth antimony telluride by the aqueous solution synthesis |
| P.71 | Wang Xinke | Xinke.Wang@cpfs.mpg.de | Thermoelectric stability of Eu- and Na-substituted PbTe |
| P.72 | Weon Ho Shin | weonho@gmail.com | Enhanced Thermoelectric Performance of Doped $Bi_{0.5}Sb_{1.5}Te_3$ by Melt Spinning Process |
| P.73 | Wy?ga Pawe? | pawel.wyzga@physik.tu-freiberg.de | Thermoelectric properties of indium thiospinel |

| P.74 | Xing Tong | txing@student.sic.ac.cn | Enhanced thermoelectric performance for n-type bismuth telluride based materials via microstructural modulation and tuning carrier concentration |
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| P.75 | Yoo Joonyeon | srw321@uos.ac.kr | Enhancement of Thermoelectric Figure of Merit for $Cu_{0.008}Bi_2Te_{2.7}Se_{0.3}$ by Metal Nanoparticle Decoration |
| P.76 | Zhang Jiye | jychang@shu.edu.cn | Fast Screening of Optimal Compositions for Thermoelectric Lead Chalcogenides Based on Gradient Materials and High Throughput Characterization |
| P.77 | Zuñiga Esteban | zuniga@physik.tu-freiberg.de | Thermoelectric Properties of Natural and Synthetic Pyrites. |
| P.78 | Huguenot Arthur | arthur.huguenot@ensc-rennes.fr | TRANSPORT PROPERTIES OF MOLYBDENUM SULFIDE CLUSTERS: EXPERIMENTAL & THEORETICAL RESULTS |
| P.79 | Miller Samuel | miller.sam.13@gmail.com | Polycrystalline $ZrTe_5$ Parametrized as a Narrow-Band-Gap Semiconductor for Thermoelectric Performance |
| P.80 | Shin Ji Eun | gguri95@naver.com | Thermoelectric Properties of $Cu_{2-x}Se$ Poly Crystal Compounds Fabricated by an Oxide-Reduction and Hot Press Process |
| P.81 | Varghese Tony | tonyvalayilvarghese@u.boisestate.edu | Ultrafast Additive Manufacturing of Flexible Thermoelectric Films by Aerosol Jet Printing and Photonic Curing |

## Modelling

| P.82 | Chakraborty Dhritiman | D.Chakraborty@warwick.ac.uk | Prediction of thermal conductivity in highly disordered nanocomposite structures: From large-scale Monte Carlo simulations to simple analytical models. |
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| P.83 | Chu Jing | pcj19@student.sic.ac.cn | Study on the interfacial stability of n-type $Yb_{0.3}Co_4Sb_{12}$/Zr/Ni thermoelectric joints at high temperature |
| P.84 | Feng Lei | feng@photon.t.u-tokyo.ac.jp | ZT enhancement of silicon thermoelectrics by germanium nanoinclusions using phonon-interference resonance |
| P.85 | Fomin Vladislav | vladdisslav.fomin@yandex.ru | The study of an influence of sample shape on the measurements error using laser flash method |
| P.86 | Foster Samuel | S.Foster@warwick.ac.uk | Quantum transport simulations for the thermoelectric properties of bipolar materials |

| P.87 | Imasato Kazuki | kazuki49@u.northwestern.edu | Grain boundary charge transport with an inhomogeneous description for polycrystalline thermoelectric materials |
|---|---|---|---|
| P.88 | Korotaev Pavel | korotaev@vniia.ru | Lattice dynamics and electronic structure in $CoSb_3$ skutterudites |
| P.89 | Lee Gyu Soup | mrlees2003@kaist.ac.kr | Two step simulation to optimize thermoelectric material for self-powered wearable applications |
| P.90 | Lee Heonjoong | leehnj@vt.edu | Modeling and analysis of segmented thermoelectric generator performance using effective properties |
| P.91 | Mukherjee Swarnadip | swarna.official@gmail.com | Design of Optimal Electronic Band-Pass Transmission for Improved Thermoelectric Performance |
| P.92 | Okawa Kenjiro | okawa.k@aist.go.jp | Heat Transfer Analysis on the Measurement of Thermoelectric Performances using a Harman Method |
| P.93 | Priyadarshi Pankaj | priyadarshi56@gmail.com | Superlattice design for maximal thermoelectric efficiency at finite power |
| P.94 | Savic Ivana | ivana.savic@tyndall.ie | Electron-phonon scattering in n-type PbTe from first principles calculations |
| P.95 | Sempels Eric | seme01@uqo.ca | Optimal thermal conductance for thermoelectric generators under various thermal boundary conditions |
| P.96 | Tukmakova Anastasiia | astukmakova@corp.ifmo.ru | Possible ways of temperature field inhomogeneity elimination during spark plasma sintering of thermoelectrics |
| P.97 | Vlachos Nikolaos | alterecosolutions@gmail.com | Power output design of a Thermoelectric Generator module using heat-transfer modelling and simulation: An application for the cement industry |
| P.98 | Yang Hailong | yhl1023@163.com | Structure and thermoelectric properties in substituted tetrahedrite |
| P.99 | Zhang Xiaolian | xiaolianzhang@whut.edu.cn | Pressure induced convergence of conduction bands in Al doped $Mg_2Si$ |
| P.100 | Tuley Richard | richard.tuley@etdyn.com | Hybrid Thermoelectric-Concentrated Photovoltaic System: Thermal Control and Monitoring |
| P.101 | Placha Katarzyna | katarzyna@etdyn.com | Assessing the Performance of Skutterudite Modules |

## Organic and Hybrid Materials

| P.102 | Araki Nayu | 4314002@ed.tus.ac.jp | Thermoelectric properties of diazonium salt modified carbon nanotubes: first principles simulations |
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| P.103 | Bahk Je-Hyeong | bahkjg@uc.edu | Flexible and scalable thermoelectric elastomers based on carbon nanotube-polydimethylsiloxane (CNT:PDMS) composites |
| P.104 | Horii Hikaru | 4317664@ed.tus.ac.jp | Ab Initio Simulation on Thermoelectric Properties of Carrier-Doped Graphene by Ferroelectrics |
| P.105 | Ichiro Imae | imae@hiroshima-u.ac.jp | Seebeck coefficients of conducting polymers correlated with doping levels |
| P.106 | Maeda Ryota | a120357w@st.u-gakugei.ac.jp | A New Synthesis Route of a Gel Film Formation Process and the thermoelectric properties of synthesized PEDOT/PSS films |
| P.107 | Mazzio Katherine | katherine.mazzio@helmholtz-berlin.de | Hybrid Polymer/Nanoparticle Composites for High-Performance Thermoelectrics |
| P.108 | Nam Woo Hyun | woohnam@gmail.com | Thermoelectric transport properties of interface-controlled Si composite using reduced graphene oxide |
| P.109 | Rueff Jean-Michel | jean-michel.rueff@ensicaen.fr | Search for new hybrid materials with thermoelectric properties |
| P.110 | Sato Naoki | m19b009@akita-pu.ac.jp | Enhancement of thermoelectric properties of PEDOT:PSS films by applying an alternating electric field during preparation |
| P.111 | Toshima Naoki | toshima@rs.tus.ac.jp | Buckypapers of Palladium Nanoparticle-Decorated Carbon Nanotubes as Effective Thermoelectric Materials |
| P.112 | Upadhyaya Meenakshi | mupadhyaya@umass.edu | Thermoelectric Properties of Disordered Semiconducting Polymers |

## Oxides

| P.113 | Alvarez Ruiz Diana Talia | Dianatalia.alvarezruiz@manchester.ac.uk | Enhanced electronic conduction and phonon scattering in the $Ga_2O1(ZnO)_m$ - $In_2O_3(ZnO)_m$ (m=9 and 15) solid solution by designing interfaces at the nanoscale level. |
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| P.114 | Andrei Virgil | andrei.virgil1@outlook.com | Understanding the links between percolation and thermoelectric performance: from polycrystalline materials to amorphous polymers |
| P.115 | Berardan David | david.berardan@u-psud.fr | Nanoscale microstructural and chemical analysis of Al-doped ZnO |
| P.116 | Das Sayan | sayandas.physics@gmail.com | Thermoelectric properties of Zn doped BiCuSeO |

| P.117 | Ekström Erik | Erik.ekstrom@liu.se | Growth and characterization of thin film $CaMnO_3$ and $CaMn_{1-x}Nb_xO_3$ for thermoelectrics. |
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| P.118 | Felizco Jenichi Clairvaux | jenichi.felizco.jz1@ms.naist.jp | Single Crystalline InGaZnO Nanowires for Potential Thermoelectric Applications |
| P.119 | Hira Uzma | 14130002@lums.edu.pk | High Temperature Thermoelectric Properties of Dual Doped $Ca_3Co_4O_9$ Ceramics |
| P.120 | Hirata Shinji | 3es17006w@s.kyushu-u.ac.jp | Synthesis and thermoelectric properties of oxide nanocomposites containing metal nanoparticles formed by exsolution reaction |
| P.121 | Kaiser Felix | felix.kaiser@cpfs.mpg.de | Synthesis, Structure and Thermoelectric Properties of Molybdenum Oxides |
| P.122 | Khan Tamal | tamalche15@gamail.com | Improvement of the Thermoelectric Properties of the Perovskite $SrTiO_3$ by Cr-Doping |
| P.123 | Kuei-Kuan Wu | langunaa@hotmail.com | Thermoelectric Properties of Al-doped Silver Antimonate |
| P.124 | Kumar Ashutosh | science.ashutosh@gmail.com | Enhancement of Thermoelectric Properties in co-substituted and Composite Oxide Systems |
| P.125 | Madathil Reshma Krishnan | reshma.madathil@smn.uio.no | Self-assembled $Ni_{0.98}Li_{0.02}O$ and $Zn_{0.98}Al_{0.02}O$ composite interface for thermoelectrics |
| P.126 | Madre Maria | amadre@unizar.es | High temperature stability of hot pressed Sr-doped $Ca_3Co_4O_9$ samples |
| P.127 | Novitskii Andrei | novitskiy@misis.ru | Influence of Bi to Sm ions isovalent substitution on thermoelectric properties of BiCuSeO oxyselenides |
| P.128 | Preaud Sébastien | sebastien.preaud@gmail.com | Thermoelectric properties of $InGaO_3(ZnO)m$, a layered oxyde with complex crystal structure |
| P.129 | Son Hyoung-Won | SON.Hyoungwon@nims.go.jp | Thermoelectric Properties $MgTi_2O_5$-Based Conductive Composite Materials Prepared by Spark Plasma Sintering |
| P.130 | Sotelo Andres | asotelo@unizar.es | Application of powder engineering to achieve high performances in textured Sr-doped $Ca_3Co_4O_9$ with very short processing times |
| P.131 | Veremchuk Igor | Igor.Veremchuk@cpfs.mpg.de | "Structural imperfections" in the transition metal oxides and thermoelectricity |

| P.132 | Yokota Yuui | yokota@imr.tohoku.ac.jp | Development of SrTiO3/TiO2 thermoelectric oxide with eutectic morphology |
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| P.133 | Lehner Tim | timothy.lehner.2011@live.rhul.ac.uk | Phonons in ZnO |
| P.134 | Vehus Tore | tore.vehus@uia.no | Hot side electrical contacts for oxide thermoelectric modules |

## Zintl Phases

| P.135 | Anno Hiroaki | anno@rs.tusy.ac.jp | Thermoelectric Properties of Si-Based Clathrates Prepared by Spark Plasma Sintering of Planetary-Ball-Milled Powders |
|-------|-------------|--------------------------|--------------------------|
| P.136 | Cerretti Giacomo | giacomo.cerretti@jpl.nasa.gov | Study of the effects of Cobalt metal inclusions in an $Yb_{14}MnSb_{11}$ matrix |
| P.137 | Ciesielski Kamil | k.ciesielski@int.pan.wroc.pl | High-pressure high-temperature synthesis and thermoelectric properties of half-Heusler antimonide TmNiSb |
| P.138 | Kihou Kunihiro | k.kihou@aist.go.jp | Thermoelectric properties of $Mg_3Sb_2$ single crystals grown by self-flux method |

## Additional Posters

| P.139 | Xiaoming Tan | | Chalcogenides: High thermoelectric performance in $Bi_{0.46}Sb_{1.54}Te_3$ nanostructured with ZnTe |
|-------|-------------|--------------------------|--------------------------|
| P.140 | Tingting Zhang | | Chalcogenides: Facile Room Temperature Solventless Synthesis of High Thermoelectric Performance $Ag_2Q$ (Q= S, Se, Te) via Dissociative Adsorption Reaction |

# Investigation of stability of doped SnS

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### Abstract

Recently, high thermoelectric performance has been reported in single crystalline SnSe [1]. SnS is an eco-friendly analog of SnSe [2]. However, a stable and effective doping of this compound is still questionable [3]. According to our observation, the main obstacles here are very low solubility of dopants and destabilization of SnS structure due to foreign species. Regarding a reasonable 60 % doping efficiency of Tl in SnSe [4], we started with Tl doping of SnS into cation sublattice. Hot-pressed polycrystalline samples were prepared along with single-crystalline samples by various growing technics. Further, we investigated a range of various substitutions in both cation and anion sublattice. Samples were examined for impurity phases by X-ray diffraction. X-ray fluorescence and Energy-dispersive X-ray for chemical analysis. Transport measurements of Seebeck and Hall coefficient, electrical and thermal conductivity were carried out in temperature range 300-700 K. The experiments suggest very low solubility of doping, e.g. less than 0.1 % for Tl. Higher concentration of dopants induces decomposition towards $Sn_2S_3$ phase.

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**Keywords:** tin monosufide, SnS, stability, solubility, doping

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# Effect of Charge Carrier Optimization on Thermoelectric Properties of Mn and Yb Doped SnTe

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## Abstract

Efficiency of any thermoelectric (TE) material has been constrained to a limited range of carrier concentration due to interdependency of three physical parameters.1 Recently, tin telluride (SnTe) based alloys are promising thermoelectric material analogous to lead chalcogenides due to identical crystal structure and complex band structure.2 Optimization of carrier concentration is a major challenge for SnTe which can be achieved by careful addition of extra 'Sn' and extrinsic isovalent doping at Sn sites.3, 4 We will discuss on the results of thermoelectric performance of Mn and Yb doped SnTe. With doping, the observed poor thermal conductivity is analyzed based on point defect and appearance of impurity driven soft phonon mode with anharmonicity in the lattice.5, 6

Acknowledgement

References

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5. S. Acharya, J. Pandey and A. Soni, Applied Physics Letters **109** (13), 133904 (2016).
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**Keywords:** SnTe, Band convergence, Soft phonon modes

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# Defect engineering and dopability of PbTe using phase boundary mapping

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## Abstract

A lack of control over the dopability of thermoelectric materials continues to limit the efficiency of potentially good material systems. Phase boundary mapping has recently been shown to be an effective means of defect engineering in materials such as $Mg_3Sb_2$, where Mg-rich conditions are required to achieve n-type behavior. However, defect engineering for dopability has been overlooked in many classic thermoelectric materials. This study highlights the necessity of defect engineering for dopability in a PbTe model system. We find that the principles of phase boundary mapping apply to material systems that do not have a history of difficult dopability. A simple defect model suggests Pb-rich and Te-rich conditions are required for n-type and p-type PbTe material, respectively. Ingots of iodine doped PbTe were annealed at 700 C under Pb-rich and Te-rich partial pressures and quenched. Drastic differences observed in the thermoelectric performance of the materials annealed under each condition agrees with the expectations from the defect model and demonstrates the effectiveness of phase boundary mapping to engineer dopability in PbTe. Lastly, the volatility of Te at relatively low temperatures is suggested as a possible reason why n-type PbTe is (apparently) obtained irrespective of the nominal composition. Thus, cognizance of the non-equilibrium conditions during material processing and measurement is also important.

**Keywords:** PbTe, Lead Telluride, Chalcogenides, Lead Chalcogenides, Defect Chemistry, Defect Engineering, Phase Boundary Mapping, Thermoelectrics

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# Enhancement of Thermoelectric Performance in InTe$_{1-\delta}$ Polycrystalline Compounds

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## Abstract

The InTe has intrinsically low lattice thermal conductivity originating from the anharmonic bonding of In1+ ion in the lattice which scatters the phonons. Here we report the enhancement of thermoelectric properties in Te-deficient InTe$_{1-\delta}$ ($\delta$=0, 0.01, 0.1, 0.2) polycrystalline compounds. From the X-ray diffraction, the lattice volume is increased with increasing Te-deficiency concentration, implying that the chemical bond strengths in Te-deficient compounds are weaker than those of stoichiometric InTe. We suggest that the weakening of chemical bonding may cause more loose ionic bonding between In1+ atoms and In$^{3+}$Te$^{2-}$ clusters, resulting in the reduction of . Therefore, the lowest of 0.53 W/mK is achieved at 300K for InTe0.99, which is about 25 % lower than that of InTe. The resistivity and Seebeck coefficient are increased with increasing the Te deficiency due to the decrease of carrier concentration, resulting in enhancement power factor over a wide temperature range. The Te deficiency in InTe$_{1-\delta}$ increases the power factor by the increase of Seebeck coefficient and decreases the lattice thermal conductivity owing to the weak ionic bonding in the lattices induce the improvement of thermoelectric performance.

**Keywords:** InTe, Te deficiency, chemical bonding strength, low thermal conductivity

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# Study on the structural and thermoelectric properties of Cu-doped Bi$_2$Te$_3$ thin films

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## Abstract

Thermoelectric Cu-doped Bi$_2$Te$_3$ thin films were prepared by co-sputtering method with Cu and Bi$_2$Te$_3$ targets. The low quantities ( ˜ 5.4 at. %) of Cu dopant were controlled by the different RF power on Cu target, while the applied DC power on Bi$_2$Te$_3$ target was fixed. Cu-doped Bi$_2$Te$_3$ thin films were deposited at room temperature, and immediately annealed at 300 ◦C under an Ar gas atmosphere. When Cu contents were increased, both Cu$_x$Te and Te-deficient Bi$_x$Te$_y$ phases were formed and the lattice parameters of the $c$-axis were also increased. The thermoelectric properties of Cu-doped Bi$_2$Te$_3$ thin films were measured at near room temperature under an Ar gas atmosphere. We investigated the influence of low Cu doping on Bi$_2$Te$_3$ phase by comparing both the structural and thermoelectric properties.

**Keywords:** Bi$_2$Te$_3$, thin films, sputter, thermoelectric properties

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# Thermoelectric Properties and Thermal Stability of Nano Cu$_2$Se Included Ag$_2$Se

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## Abstract

Recently, silver chalgonedies have attracted great attention due to their potential application for room temperature power generation and local cooling. In this work, we report the thermoelectric and thermal stability properties of nano Cu$_2$Se included bulk Ag$_2$Se compounds. All samples were prepared melting + annealing + ball milling followed by spark plasma sintering. High temperature transport properties were assessed by Seebeck coefficient, electrical conductivity and thermal conductivity measurements. Structural properties were performed by PXRD and SEM-EDX analysis. The thermal expansion coefficient measurement show that thermal stability of Ag$_2$Se enhance with increasing nano Cu$_2$Se inclusion. The Seebeck coefficient sign indicates that electrons are dominant carriers in all samples. The electrical conductivity of all samples decreases with temperature likely shows a typical behavior of highly doped semiconductor. Room temperature PXRD and SEM pattern indicated that there are two phases of Ag$_2$Se and CuAgSe in nano Cu$_2$Se included compounds. The thermal conductivity is suppressed with nano Cu$_2$Se inclusions. The maximum ZT value reached ˜0.3 at both 300 K and 800 K for %5 Ag$_2$Se included samples that indicates nano Cu$_2$Se included bulk Ag$_2$Se compounds may have potential application in both room and mid-temperatures.

**Keywords:** Nano Cu$_2$Se, bulk Ag$_2$Se, thermal stability, Seebeck effect

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# Thermoelectric power generation through single-leg of p-type $Bi_{1.95}Pb_{0.05}Te_3$

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## Abstract

Now-a-days thermoelectric power generation is gaining much attention to recover waste heat. Since most of this heat exists in low temperature range, efficient thermoelectric materials operating in this range are highly needed. Till now conventional thermoelectric materials for low temperature power application ($< 300°C$) are Bismuth telluride ($Bi_2Te_3$) based al-loys. In the present work we have observed that doping of Lead (Pb) can change the n-type conduction of $Bi_2Te_3$ to p-type. Bulk $Bi_{2-X}Pb_XTe_3$ (x=0 to 0.5) samples were prepared by vacuum melt route followed by hot pressing. Optimized p-type $Bi_{1.95}Pb_{0.05}Te_3$ exhibited thermoelectric figure of merit (ZT) of ˜ 0.63 (at 386 K) in comparison to ZT of ˜0.47 (at 386 K) obtained in case of n-type $Bi_2Te_3$. The electrical contacts were fabricated on p-type $Bi_{1.95}Pb_{0.05}Te_3$ single leg with Ni as buffer layer and Ag strips were used as electrodes. In the fabricated single-leg efficiency of ˜4.9±0.4% has been achieved for a temperature difference ($\Delta T$) of 200 K. This work is an effort to reveal the prospect of Pb doped $Bi_2Te_3$ in the development of efficient thermoelectric power generators.

**Keywords:** chalcogenides, Thermoelectricity, Singleleg, Power generation, Bismuth telluride

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# Effect of the composition in the thermoelectric properties of $Cu_{12-x}M_xSb_4S_{13-y}Se_y$ (M = Mn, Fe)

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## Abstract

Tetrahedrites are copper sulfosalt minerals with general formula $Cu_{10}M_2Sb_4S_{13}$ (M = Cu, Mn, Fe, Co, Ni, Zn), where Sb can be partially replaced by Bi, As or Te and S by Se. They are earth-abundant and non-toxic materials that have intrinsically low thermal conductivities between 0.5-1 Wm-1K-1 and recently they have been shown to have good performance as p-type thermoelectric materials, presenting zT values with the order of one at around 700 K. Starting with the well studied composition $Cu_{12}Sb_4S_{13}$ through appropriate doping is possible to change the carrier concentration or the valence band configuration in order to maximize the power factor. Materials with $Cu1_{2-x-y}M_xSb_4S_{13-y}Se_y$ (M = Mn, Fe, $0 \leq x \leq 2$, $0 \leq y \leq 1$) compositions were prepared by melting the elements under vacuum, all samples were studied in the as-cast form. Powder X-ray diffraction show that all materials studied are mainly constituted by tetrahedrite. Aiming at a better understanding of the influence of composition on the power factor, we present the study of electrical transport properties between room temperature and 20 K, where we have simultaneously partially replaced copper by manganese or iron up to 2 and sulfur by selenium up to 1.

**Keywords:** tetrahedrite, thermoelectric materials, power factor

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# Self-tuning carrier concentration effect of noble metal chalcogenides

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## Abstract

We found new phenomena named as self-tuning carrier concentration in noble metal chalcogenides, which are characterized by the order-disorder transition in 350 ~ 400 K. Notably, the phase transition requires a rather wide temperature range of , where two phases coexist together. We applied a temperature gradient that produced along the vertical direction in the rectangular shape samples. The temperature range near the phase transition, this rather large temperature difference naturally produced three layers consisting solely of high-temperature phase at the hot side, low-temperature phase at the cold side, and the mixed-phase between them. With keeping the temperature difference along the vertical direction, we also applied temperature gradient producing in the horizontal direction so as to measure Seebeck coefficient. Surprisingly, the Seebeck coefficient, measured at the topmost surface, showed two sign reversals with an increasing temperature. The first principles calculations suggested that the sign reversal was brought about by the variation of carrier concentration in the topmost layer. We speculated that the coexistence of two phases in the sample made an alternation of carrier concentration due to the difference of chemical potential between the two phases, and the amount of the carrier concentration varied with a temperature because of the variation in the volume fraction of low- and high-temperature phases. In the presentation, we will show the detailed information about the thermoelectric properties together with the composition of materials, power factor, and dimensionless figure of merit.

**Keywords:** Thermoelectric materials, Self tuning carrier concentration

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# Ultrolow Thermal Conductivity and High ZT in Graphene Doped p-type Polycrystalline SnSe

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## Abstract

SnSe is one of the promising thermoelectric materials with high ZT along certain crystal direction. For pratical applications, it is desirable to achieve high ZT in polycrystalline bulks. Here, we report a significant enhancement of thermoelectric performance in graphene doped SnSe. The doping effects of graphene on the structures, electrical and thermal properties as well as hardness were systematically investigated for different doping levels. We found that a very low thermal conductivity of 0.15 W m-1 K -1 at 750 K was realised in 0.5 wt% graphene doped polycrystalline $p$-type SnSe, and a relatively high ZT of 0.8 was obtained at the same temperature. Also, a maximum Seebeck value of 580 $\mu$V/K was obtained at 423 K in 0.3 wt% doped sample, which is the same level with other reported SnSe systems. In addition, there is no obvious difference of S among different samples, which means the graphene contributes little to the Seebeck value. Electrical conductivity, meanwhile, increased by 50% with the increscent of doping concentration. The XRD results show that our samples are pure SnSe without any impurity. However, no peaks of graphene are found, therefore SEM and TEM are required for further structure study.

**Keywords:** p, type SnSe, ultrolow thermal conductivity, graphene

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# Localization effect and chemical potential tuning by CuI doping in $(CuI)_y(Bi_2Te_3)_{0.95}$-x$(Bi_2Se_3)_x(Bi_2S_3)_{0.05}$ quaternary system

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## Abstract

Bi2Te3-based compounds have long been studied as thermoelectric materials for room temperature cooling and waste heat recovery applications. Recent investigation showed that the quaternary compounds of $Bi_2Te_3$-$Bi_2Se_3$-$Bi_2S_3$ composite can be used to mid-temperature power generation under 500 ℃.[1] Here, we investigated thermoelectric proper-ties of $(CuI)_y(Bi_2Te_3)_{0.95-x}(Bi_2Se_3)_x(Bi_2S_3)_{0.05}$ (x= 0.05, 0.2 / y = 0.0, 0.003) compounds. From the x-ray diffraction and transmission electron microscopy, we confirmed lattice disor-der in $(Bi_2Te_3)_{0.95-x}(Bi_2Se_3)_x(Bi_2S_3)_{0.05}$ (x = 0.2) compound by multiple elements substi-tutions. The disorder carrier scattering induces the localized nature of electrical resistivity confirmed by the variable range hopping at low temperature. The temperature-dependent Seebeck coefficient of $(Bi_2Te_3)_{0.95-x}(Bi_2Se_3)x(Bi_2S_3)_{0.05}$ shows carrier type change from p- to n-type behavior at the intermediate temperature range (525 K for x = 0.05 and 360 K for x = 0.2). Strong carrier localization increases electrical resistivity, resulting in the degradation of power factor and thermoelectric performance. When we increase chemical potential to the conduction band minimum by CuI co-doping on the $(CuI)_{0.003}(Bi_2Te_3)_{0.95-x}(Bi_2Se_3)_x(Bi_2S_3)_{0.05}$ (x=0.05, 0.2) compounds, the carriers are delocalized and showed n-type behavior in Seebeck coefficient. The temperature-dependent thermal conductivity presents the suppression of bipolar conduction behavior. The simultaneous effect on the carrier optimization by chemical potential tuning and lattice disorder causes a high value of ZT 0.85 at 523K for CuI-doped $(Bi_2Te_3)_{0.75}(Bi_2Se_3)_{0.2}(Bi_2S_3)_{0.05}$, which is about 9 times enhancement of thermoelectric figure-of-merit than those of undoped ones.

**Keywords:** Carrier localization, variable range hopping, thermoelectric properties, induced disorder

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# Thermoelectric transport properties of Sb-doped SnSe₂ compounds

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## Abstract

We report thermoelectric transport properties of Sb-doped $SnSe_2$ compounds. Two types of Sb doping, cation-exchanged $(Sn_{0.96}Sb_{0.04})Se_2$ and anion-exchanged $Sn(Se_{0.96}Sb_{0.04})_2$, were performed in this experiment. All the compounds were prepared by conventional melt-ing and annealing process, followed by the consolidation using spark plasma sintering. The resulting compounds were characterized to be a homogeneous phase of layered hexagonal structure (JCPDS # 89-3197) without any secondary phase. Since Sb is a group-V element, it must serve as a donor when occupying the Sn site and should act as an acceptor when occupying the Se site. However, the cation-exchanged compound exhibited decreased $n$-type electrical conductivity as compared with undoped $SnSe_2$ compound, while the anion ex-changed compound exhibited increased $n$-type electrical conductivity. These contradictory doping effects were also observed in Seebeck coefficients. The mechanism is under investiga-tion based on density functional theory calculations, and detailed thermoelectric transport properties of the compounds will be presented.

**Keywords:** $SnSe_2$, Thermoelectric, charge transport, spark plasma sintering, doping

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# Thermoelectric Properties of YbTe-SnTe-based Solid Solutions

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## Abstract

SnTe-based thermoelectrics have been widely investigated as alternatives for PbTe mainly due to less toxicity of Sn. The thermoelectric performance of SnTe, however, is inferior to that of PbTe due to several factors: (i) excessive hole concentration due to intrinsic Sn vacancy, (ii) large valence band offset, and (iii) lower mass of Sn compared to Pb. Factors (i) and (ii) lead to lower Seebeck coefficient while (iii) contributes to the high lattice thermal conductivity, and together they result in low ZT of pristine SnTe of ~0.4. Improvements of the TE properties of SnTe have been realized by various methods such as carrier tuning, band convergence, resonant states, nanostructuring, etc [1]. Recently magnetic doping has been found to improve the power factor due to enhanced carrier effective mass [2]. In this study, the effect of magnetic doping by Yb on SnTe is investigated. A complete solid solution exists between YbTe and SnTe above ~950 K [3], which allows wide doping range. Preliminary results show that 5% Yb doping increase the Seebeck coefficient up to 170 $\mu$V/K, and shifts the maximum power factor towards the lower temperature. Yb doping also significantly reduces the thermal conductivity down to ~2 W/mK at 773 K, which is comparable to that of high ZT SnTe-based materials.1 Overall, a maximum ZT of 0.7 at 773 K is obtained. References

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**Keywords:** SnTe, magnetic doping, tellurides, solid solution

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# Thermomechanical properties of fast sintered polycrystalline SnSe composites

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## Abstract

Tin selenide recently came to the research community interest due to the high performances observed in single crystals. Despite the high ZT of the material, the need to improve the mechanical behavior of the material suggested to move to the polycrystalline form trying to achieve a material easily workable preserving the thermoelectric characteristics of the material. However, the results reported for the polycrystalline SnSe compound are generally far from the expected ones. The characteristic mainly affected by passing to polycrystalline phase, considering the data reported in literature, seems to be the electrical conductivity. In fact, it not only scales due to the new microstructure, but it also changes in temperature behavior. At the same time the ultra-low thermal conductivity is not improved by the presence of phonon scattering introduced by the polycrystalline microstructure. In this work, composites have been produced starting from SnSe powders sintered using open die pressing technique. Metallic particles have been added to improve the carrier mobility into the system trying to achieve a conductivity behavior closer to the best one reported in literature. On the other side, insulating particles have been introduced to improve the phonon scattering. In both cases the effects of the composite phase on mechanical stability of the sintered material has been investigated.

**Keywords:** Tin Selenide, Thermoelectric composites, mechanical properties

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# Thermoelectric Properties of excess Cu- and Ga-added $Cu_4Mn_2Te_4$

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## Abstract

Magnetic semiconductors, such as $CuFeS_2$ and Mn-doped $CuGaTe_2$ with chalcopyrite structure, could be considered as promising power-generation materials due to their excellent transport properties [1, 2, 3]. Here we report the preparation and thermoelectric properties of $Cu_4Mn_2Te_4$, which is antiferromagnetic with $T_N = 50$ K. [4]
$Cu_4Mn_2Te_4$ adopts a spinel-related structure. Each unit cell contains eight formula units ($Z = 8$). The Te ions form a cubic closest-packing ($ccp$) with Cu occupying half of the tetrahedral sites and Mn half of the octahedral sites. When temperature is over 723 K, Cu and Mn will statistically occupy half of the tetrahedral sites and half of the octahedral sites, respectively. Thermoelectric properties measurements show that Cu4Mn2Te4 displays an electrical conductivity 2500 W–1cm–1 and Seebeck coefficient 20 $m$V K–1 at 325 K .[5] Its thermoelectric performance might be improved through electron doping.

In this work, we have prepared Cu4Mn2Te4 with excessive Cu and Ga-doped modifications by reacting the elements in sealed quartz tubes followed by spark plasma sintering (SPS) technique. And then investigated the effects of the contents of extra Cu and Ga on thermoelectric properties. All samples are mainly composed by the Cu4Mn2Te4 phase, as observed from the powder X-ray diffraction (XRD) pattern. According to the thermoelectric transport properties measured, we demonstrate that the thermoelectric figure-of–merit for Cu4Mn2Te4 could be enhanced by 100 ~ 130% through adding excessive Cu or Ga doping.[6]

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**Keywords:** spinel, thermoelectric

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# Rapid Synthesis, Processing and Characterisation of Cu2-xSe and its Solid Solutions

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## Abstract

A rapid synthesis route was used for the fabrication of bulk nanostructured Cu2-xSe. Starting from readily available materials and by means of energy-efficient microwave (MW)-assisted thermolysis, nanostructured Cu2Se and Cu1.8Se were synthesized. The synthetic scheme was shown to be very sensitive to the reaction conditions and the final product composition is easily determined by controlling the reaction temperature. The process yields nanostructured Cu2Se at the reaction temperature of 250 oC, while the product is Cu1.8Se at 200 oC, within a reaction duration of 5 minutes. We have utilized the solid-solution concept with inclusions of one TE material into a matrix of another aiming to improve power factor, which in turn may lead to high ZT values. In this respect our chosen materials compositions were Cu2Se, Cu1.8Se and their mixture with different proportions; specifically, 5wt% and 10wt% Cu1.8Se introduced into Cu2Se. SPS sintering process has been used to consolidate pellets. Powder samples and compacted pellets have been characterized in detail. Scanning electron microscopy (SEM) revealed the presence of secondary globular nanostructures in the order of 200 nm consisting < 50nm primary particles. HR-TEM confirmed crystalline nature of primary particles with irregular truncated morphology. The phase purity of the as-synthesized materials is high, as identified by the XRD analysis. Inclusion of Cu1.8Se in Cu2Se has caused reduction in electronic resistivity, which gradually decreased from pure Cu2Se towards the direction of pure Cu1.8Se. Power factor of the sample 10 wt% Cu1.8Se inclusion has reached much higher values than the rest of the samples. Our synthetic scheme and detailed results are presented. The developed rapid synthesis may lead to production of large scale TE nanopowders and TE elements/legs for niche device applications.

**Keywords:** Chalcogenides, Colloidal Synthesis, Copper selenide, Solid, solution, Power factor, Nanocrystal, SPS

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# Synergistically optimizing thermoelectric transport properties of n-type Bi2Te3 via CuI and Sn co-doping

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## Abstract

A series of (CuI-Sn)-substituted and (CuI-Sn)-added Bi2Te3 samples have been prepared by high temperature solid state reaction and consolidated using spark plasma sintering technique and their thermoelectric properties were investigated from room temperature to 525 K. In order to better assess the effects of codoping of Sn and CuI in the Bi2Te3 thermoelectric properties we also prepared single doped SnxBi2-xTe3 and SnxBi2Te3 samples for comparison.

We report n-type Bi2Te3 with a maximum ZT ˷1.2 at 425 K and an average ZTave ˷ 1.02 at 300-525 K, which was achieved through a Sn and CuI co-alloying approach. We find that the lattice thermal conductivity can be largely reduced through introducing CuI, and the Seebeck coefficient can be enhanced through introducing Sn in Bi2Te3 system. Combining two strategies via Sn and CuI co-alloying in Bi2Te3, results show that the power factor can be enhanced and thermal conductivity can be reduced simultaneously through alloying small amount of Sn with CuI.

Through synergistically optimizing electrical and thermal transport properties of n-type Bi2Te3 via Sn and CuI co-alloying, the ZT value is distinctly enhanced to 1.2 at 425 K, and the average ZTave value over the entire work temperature is evidently higher than that of ZTave ˷0.54 in Sn-doped Bi2Te3 and ZTave ˷0.83 in CuI-doped Bi2Te3. This work indicates that one can improve the average ZT over a broad temperature range using a co-alloying approach.

**Keywords:** n, type, Bi2Te3, co, doping

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# Thermoelectric Properties of Cu-deficient Thiospinel Cu2–xTi4S8 and the derivative Cu2–xTi4.5S8

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## Abstract

Ti-S based compounds with the edge-shared TiS6 octahedron network are attracting much attention as n-type thermoelectric (TE) materials due to the high power factor (PF). We reported that the PF and $ZT$ for the Cu2Ti4S8 thiospinel is enhanced by reducing the electron carrier concentration $n$ with the substitution of Co for Ti [1]. In this work, we have adopted another method to reduce $n$ by introducing defects into Cu sites. We report here the stability of Cu-deficient samples and carrier tuning effects on the TE properties.

The samples were prepared by the direct reaction of elements followed by a pulsed-electric-current sintering. Powder XRD analysis and EPMA showed that the thiospinel phase Cu2–$x$Ti4S8 is stable for $x$ less than 1.0, and a Ti-rich phase Cu2–$x$Ti4.5S8 is formed for $x$ between 1.0 and 1.25. Excessive Ti atoms occupy the octahedral voids in the TiS6 octahedron network. With increasing $x$ from 0 to 0.75 in Cu2–$x$Ti4S8, the value of $n$ decreases from 12 to $8.6 \times 10^{21}$ cm–3, resulting in the enhancement of PF from 0.2 to 0.4 mWK–2m–1 at 670 K. The additional Ti4+ in Cu2–$x$Ti4.5S8 with $x = 1$ gives rise to the large $n$ value of $6.7 \times 10^{22}$ cm–3. Both the electrical resistivity and Seebeck coefficient in the Ti-rich phase are weakly temperature dependent, and the PF stays at 0.2 mWK–2m–1 from 300 to 670 K. Unexpectedly, the lattice thermal conductivity does not depend on $x$. The maximum $ZT$ value of 0.07 is realized at $x = 0.75$ in Cu2–$x$Ti4S8 for the lowest electronic thermal conductivity and highest PF. We will discuss the relation between the TE properties, electron effective mass, and the electronic structure.

K. Hashikuni *et al.*, Appl. Phys. Lett. **109**, 182110 (2016).

**Keywords:** thiospinel, defect, carrier concentration tuning

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# Investigation of the thermoelectric properties of pyrites : interplay between magnetism and transport

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## Abstract

The pyrite $CoS_2$ exhibits remarkable electronic properties, with a large power factor of ˜ 1mWm-1K-2 at high T, which is constant from 100K up to high temperature. A strong interplay between magnetism and transport properties has also been observed at low T, with the evidence for magnonic contribution to the thermopower. Here, we will show how the transport properties can be tuned in this pyrite by doping, and the interplay between doping, magnetism and thermoelectric properties will be discussed. A detailed analysis of the magnetic properties will be presented.

**Keywords:** Sulfides, pyrites, magnetism

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# High performance textured SnSe thermoelectric thin films with controlled doping fabricated by a solution process

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## Abstract

The thermoelectric (TE) effect has drawn great interest from various discipline due to its capability to direct energy conversion between heat and electricity and vice versa. Recently, tin selenide(SnSe), attracted huge attention in thermoelectric society because of its intrinsically ultralow thermal conductivity, while showing reasonable electric conductivity. This property is highly dependent to its unique layered structure, that inhibit the thermal conduction by reducing lattice vibration drastically. However, layered structure of tin selenide also scatters the electrons in a-axis, so only few researches that achieve high thermoelectric performance with polycrystalline structure has been reported. On the other hand, even though the single crystalline tin selenide shows exceptionally high efficiency, its layered structure makes single crystalline tin selenide to be easily cleaved along b-c plane. Also, it has poor thermoelectric properties in low to mid-range temperature. Here, we report solution based SnSe thin film fabrication technique with highly textured crystal structure using amine-thiol cosolvent approach and phase transition between Sn2Se64- complex, SnSe2 and SnSe crystal.

**Keywords:** tin selenid, cosolvent, thin film, spin coating

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# An Investigation of the Thermal boundary resistance associated with the Twin Boundary in Bismuth Telluride

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## Abstract

In use of the molecular dynamics (MD) simulations, we investigate the thermal boundary resistances (TBRs) associated with different types of twin boundaries in the bismuth telluride (Bi2Te3) and the effective thermal conductivities when twin boundaries appear periodically. The simulation results show that the Te1-type has a lowest interfacial energy, which explains why it is often observed in the laboratory, and the Te2-type has a largest interfacial energy and therefore a largest thermal boundary resistance. The TBR associated with a pair of twin boundaries separated by 4UC is found about twice as large as that of a single twin boundary of the same type. It implies one can count the effect of twin boundaries individually and ignore their coupling effect on heat transfer as long as they are separated more than 4UC. Finally reductions in both the in-plane and cross-plane effective thermal conductivities of the Bi2Te3 systems embedded periodically with twin boundaries are observed; the reduction associated with the Te1-type is the least and that associated with the Te2-type is the most.

**Keywords:** Bismuth Telluride, Twin boundary, Thermal boundary resistance, Molecular Dynamics Simulation

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# Thin film thermoelectric micro-generator by selective chemical vapour deposition

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## Abstract

Here we report the chemical vapour deposition of both n-type Bi2Te3 and p-type Sb2Te3 thermoelectric materials using our novel single-source reagents. Not only do these reagents produce high quality thin films with competitive thermoelectric properties but, furthermore, they permit very highly selective deposition of the thin film semiconductor materials specifically onto the conductive TiN surfaces on lithographically patterned TiN/SiO2 substrates [1-2]. Aside from the positional control, this system offers great orientational control over the crystal structures through both pattern size and deposition temperature, which offers a convenient method to deliver key structural requirements necessary to improve the thermoelectric efficiency. This highly and well-controlled selective deposition behaviour has enabled a novel processing method for the fabrication of integrated, material-efficient thin film thermoelectric micro-generator.

The selective chemical vapour deposition of Bi2Te3 and Sb2Te3 thermoelectric materials in both micro and nano-meter structures will be presented. The prototype thin film thermoelectric micro-generators will be fabricated based on selective deposition and tested to demonstrate their capability in serving as a power solution for "internet of things" applications.

S. L. Benjamin, C. H. de Groot, C. Gurnani, A. L. Hector, R. Huang, E. Koukharenko, W. Levason and G. Reid (2014) Controlling the nanostructure of bismuth telluride by selective chemical vapour deposition from a single source precursor. *Journal of Materials Chemistry A*, 2, 4865-4869.

R. Huang, S. L. Benjamin, C. Gurnani, Y. Wang, A. L. Hector, W. Levason, G. Reid and C. H. de Groot (2016) Nanoscale arrays of antimony telluride single crystals by selective chemical vapour deposition. *Nature Scientific Report*, 6, 27593.

**Keywords:** selective deposition, thin film thermoelectric generator

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*Speaker

# Model for reduction of phonon transport through coated grain structure and proposed mechanism

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## Abstract

We developed an expression for phonon scattering through the coated grain. The model assumed the coated grained media as closed-packed core-shell particulate media. To consider correlated scattering effect between multiple coated grains, we used dependent scattering model. In this study, we propose optimum shell thickness, the ratio of material properties such as Young's modulus, the mass of constituent atoms between core and shell, etc, to enhance phonon scattering in the coated grain structure. We have found that our model adequately explains thermal conductivity of RGO (reduced graphene oxide) coated TiO2 (Nanoscale **9**, 7830 (2017)). We also present experimental validation for reduction of thermal conductivity of SnTe/CdTe core-shell system. The lattice thermal conductivity of SnTe/CdTe coated grained system is reduced by 30%. Overall, we believe that our finding could be useful for designing efficient thermoelectric material based on the coated grain structure.

**Keywords:** Thermal conductivity, Phonon scattering, Coated grains

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# Charge transport properties of p-type Bi0.3Sb1.7Te3-graphene oxide composites

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## Abstract

We present charge transport properties of $p$-type Bi0.3Sb1.7Te3-graphene oxide composites. Bi0.3Sb1.7Te3 ingots were prepared by conventional melting and annealing process, and they were pulverized into powders using spex-mill. The spex-milled powders were coated with controlled amount of graphene oxide (GO, 0 ˷ 0.2 wt%), followed by the consolidation using spark plasma sintering. With increasing the GO content, electrical conductivity of the Bi0.3Sb1.7Te3-GO composite decreased and Seebeck coefficient increased. Strong anisotropy in the electrical conductivity was observed depending on the measurement directions, and it became much stronger as the GO content increased. On the other hand, there was no anisotropic effect in the Seebeck coefficient. Detailed effect of the GO on the charge transport properties were discussed based on Hall measurements, and the results will be presented.

**Keywords:** Thermoelectric, Bi2Te3, Graphene oxide, ZT, spark plasma sintering

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# Enhanced Thermoelectric Properties of Fine-Grained and Carrier Concentration Optimized GeTe

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## Abstract

As a lead free material, GeTe-based alloys have been intensively studied as p-type thermoelectric materials. Although a high $ZT$ close to unity could be obtained in GeTe, the high carrier concentration make the further $ZT$ enhancement difficult due to a low power factor and a high thermal conductivity. In this work, a fine grained GeTe was fabricated by mechanical alloying (MA) and spark plasma sintering (SPS), which successfully suppressed the formation of Ge vacancy and hence achieved a low carrier concentration about cm-3 and a high mobility over 120 cm2V-1s-1. As a result, a high $ZT$ of 1.2 was obtained in pristine GeTe. Subsequently, Bi was doped to further suppress the carrier concentration to cm-3. The Seebeck coefficient was enhanced both by a reduction of carrier concentration and the band convergence effects induced by Bi doping. Simultaneously, the thermal conductivity was extensively decreased and a $ZT$ value up to 1.9 was attained. This work demonstrates the potential of GeTe as a state-of-the-art thermoelectric material and further possible $ZT$ enhancement when additional strategies like nanostructuring are introduced.

**Keywords:** germanium telluride, vacancy, machanical alloying, spark plasma sintering

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# Engineered doping and nanostructuring leads to high efficiency PbTe materials and modules

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## Abstract

PbTe is the best performing thermoelectric material in mid to high temperature range with reported $ZT$ close to 2 in nanostructured form. This talk describes our recent efforts to fabricate high-efficiency modules using newly-developed thermoelectric materials based on nanostructured PbTe.

High purity Te, Pb, Na, Ge and PbI2 were annealed at 1323 K for 10 h to obtain ingots which were then crushed into powders and compacted using pulsed electric current sintering at 773 K/1h under uniaxial pressure of 30 MPa. Na was used as an acceptor and PbI2 as a donor, whereas Ge was employed for nanostructuring. The samples were sintered with and without the diffusion barrier to fabricate the module and investigate the thermoelectric properties, respectively. Nanostructured PbTe and cascaded Bi2Te3/nanostructured PbTe module with 8 p/n couples were developed in order to evaluate power generation characteristics, which were also investigated using COMSOL Multiphysics with measured thermoelectric properties of the p and n legs.

Excess Na (4%) was used as p-type dopant to greatly enhance the power factor by generating extra charge carriers through increased solubility at high temperatures. Minute amounts of Ge ($\leq 1\%$) addition provided nanostructures which greatly reduced the lattice thermal conductivity. Several nanoscale homogeneities were observed, such as disk-shaped nanostructures, pseudo-spherical nanoprecipitates, and Ge-Na impurity clusters of various sizes. Temperature induced doping and nanostructuring provided an optimized $ZT$ close to 2 for PbTe-Ge-Na p-type leg. Exceptionally high efficiency was obtained in cascade Bi2Te3/nanostructured PbTe-Ge module.

**Keywords:** Thermoelectrics, PbTe, nanostructuring, doping, power generation

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# Nanoscale thermal conductivity analysis of chalcopyrite thin films by STEM-based thermal analytical microscopy

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## Abstract

It is important to be able to measure thermal properties and to observe thermo-induced phenomena in nanoscale materials, e.g. heat-sink composites, thermal diodes, thermoelectric materials, etc. [1]. In particular, it is highly desirable to develop an advanced technique for simultaneous observation of a given structure, e.g. its lattice defects, grain boundaries, and impurities which induce phonon scattering, and measuring its thermal transport properties. In this study we developed scanning transmission electron microscopy (STEM)-based thermal analytical microscopy (STAM) by combining the world-smallest thermocouple with a scanning heat input from a focused electron beam in a 300 keV JEM-3100FEF STEM. Constantan and chromel nanoprobes [2,3] for assembling a thermocouple were prepared by electrochemical etching. The diameter of the thermocouple was below 10 nm. We prepared a TEM specimen made of CuFeS2 (Chalcopyrite) for nanoscale thermal transport analysis as a model material by using a focused ion beam.

A nanoscale thermocouple was attached to the corner of a TEM specimen for the local temperature measurements. A STAM image could be obtained by using an electron beam-induced heat scanning with a constant current. The STAM image shows a two-dimensional temperature distribution constructed by using generated thermoelectromotive force acquired by the attached thermocouple. The STAM image revealed temperature gradient within CuFeS2 layer; the temperature gradually decreases with increasing the distance from M point, thus following the Fourier's law. In the presentation, we will analyze the thermal transport under high spatial and temperature resolutions.

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N. Kawamoto et al., Nanotechnology 26 (2015) 465705.

**Keywords:** thermal conductivity, STEM, TEM, thermocouple, chalcopyrite

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# Thermoelectric properties enhancement of Bi2Te3 through Pt nanoparticles inclusion prepared by electrochemical deposition

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## Abstract

Excellent properties of thermoelectric materials contribute critical breakthrough to develop a high performance thermoelectric device. Nowadays, a lot of researches are performed with various strategies to enhance the thermoelectric properties of certain materials such as using nanocomposites approach. In this paper, the study of the thermoelectric performance of electrodeposited platinum-bismuth telluride nanocomposites (Pt/Bi2Te3) is presented. An electrolyte solution containing nitric acid and bismuth-telluride ions was mixed with various concentrations of Pt nanoparticles (Pt-Nps). 1.0 wt.% to 1.9 wt.% of Pt-Nps in the composites have been successfully synthesized to investigate the thermoelectric material performance. It is found that at 1.9% of Pt-Nps weight percentage in the Bi2Te3 matrix, the power factor increased to 1.8 x 10-3 W/mK2 which is almost 20% higher than the pure Bi2Te3. Meanwhile, the evaluation on thermal conductivity of the composite shows promising improvement which is more than 40% reduction as compared to the Bi2Te3. As a result, higher ZT is obtained for the Pt (1.9wt.%)/Bi2Te3, about more than twice of ZT of the electrodeposited Bi2Te3 film at room temperature.

**Keywords:** Bismuth Telluride, Platinum nanoparticles, Nanocomposites, Electrodeposition, Nano, inclusion

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# 3D printing of shape-conformable thermoelectric materials using all-inorganic Bi2Te3-based inks

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**Abstract**

Thermoelectric energy conversion offers a unique solution for generating electricity from waste heat. However, despite recent improvements in the efficiency of thermoelectric materials, the widespread application of thermoelectric generators has been hampered by challenges in fabricating thermoelectric materials with appropriate dimensions to perfectly fit heat sources. Herein, we report an extrusion-based 3D printing method to produce thermoelectric materials with geometries suitable for heat sources. All-inorganic viscoelastic inks were synthesised using Sb2Te3 chalcogenidometallate ions as inorganic binders for Bi2Te3-based particles. 3D-printed materials with various geometries showed homogenous thermoelectric properties, and their ZT of 0.9 (p-type) and 0.6 (n-type) were comparable to the bulk values. Conformal cylindrical thermoelectric generators made of 3D-printed half rings mounted on an alumina pipe were studied both experimentally and computationally. Simulations show that the power output of the conformal, shape-optimized generator is higher than that of conventional planar generators.

**Keywords:** 3D Printing, Chalcogenide, Shape, conformable thermoelectric material

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# N-type Bi2Te2.7Se0.3/ZnO core-shell nanostructure for colossal improvement in the thermoelectric performance

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## Abstract

Thermoelectric materials are necessary to have a high electrical conductivity and a low thermal conductivity simultaneously to realize high thermoelectric figure-of-merit ($Z=\alpha2\sigma/$). However, the intimate coupling between electronic conductivity and thermal conductivity renders the enhancement of thermoelectric performance difficult. Nanostructuring of thermoelectric materials has been a major strategy to improve the thermoelectric performance because frequent phonon scattering at nano-grain boundaries effectively reduces the thermal conductivity without significant loss of electronic carrier. However, easy grain growth of Bi2Te3 during the sintering process diminishes the reduction of thermal conductivity. Here, we propose a novel way to form a nanostructured Bi2Te2.7Se0.3 thermoelectric element to achieve a low thermal conductivity. Bi2Te2.7Se0.3 fine powders are coated by atomic layer deposition (ALD) of very thin ZnO films (< 3 nm). The ALD technique is known to achieve a precise thickness control at a sub-nm scale and have excellent conformality even on complex shaped substrate. The Bi2Te2.7Se0.3/ZnO core-shell structured powders are sintered by using a spark plasma sintering process. ZnO-coated Bi2Te2.7Se0.3 thermoelectric element shows small grains compared to the uncoated Bi2Te2.7Se0.3. The thermal conductivity is significantly decreased by the small grains and the thin ZnO layers at the grain boundaries. Consequently, the figure-of-merit of the n-type Bi2Te2.7Se0.3 is drastically improved. We believe that the utilization of ALD technique for nanostructuring crucially contributes to enhance thermoelectric performance of Bi2Te3-related materials.

**Keywords:** Core – Shell Structure, Bi2Te2.7Se0.3, ZnO, Atomic Layer Deposition

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# Enhanced thermoelectric properties of nano structured Bi-Sb-Te/MXene bulk nano composite

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## Abstract

Recently, thermoelectric materials combined with nanotechnology exhibits the possibility of greatly enhancing the thermoelectric performance based on nanoscale phenomena such as grain boundary decoration and phonon scattering at interfaces. MXenes are 2D materials exfoliated from ternary carbide and nitride ceramics. Metallic conductivity and good mechanical properties make MXenes a good candidate for use in thermoelectric composites. In this study, we develop novel $Bi_{0.4}Sb_{1.6}Te_3$/MXene composites made of BST powders coated with nanoscale MXene layers via spark plasma sintering. In bulk $Bi_{0.4}Sb_{1.6}Te_3$/MXene composites, grain boundaries are engineered with decorated MXene layers. The composite exhibits the maximum ZT value of 1.43 at 345K, when measured over the temperature range of 300-500 K. In the composite, MXene layers serve to reduce thermal conductivity without the decrease of electrical conductivity, leading to the enhancement of ZT. Thin MXene layers are expected to scatter short-wavelength phonons while allowing the electrical transport without the loss of electrical conductivity. The detailed thermal and electrical properties of the $Bi_{0.4}Sb_{1.6}Te_3$/MXene composites will be discussed with respect to the enhanced thermoelectric performance.

**Keywords:** Nano composite, (BiSb)2Te3, MXene

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[*]Speaker

# Effects of Cl-doping on Thermoelectric Transport Properties of Cu2Se

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## Abstract

Cu2Se, comprising of low-price, abundant, and non-toxic constituent elements, has been gaining much attention recently due to its high $ZT$ at high temperatures. Since the first report on its excellent $ZT$ of $b$-Cu2Se (1.5 at 1000K) arising from liquid-like phonon behavior, there have been many approaches to enhance its thermoelectric performance through doping in Cu-site with aliovalent elements (In, Ni, Zn, Mn, ...) and allying in Se-site with isovalent elements (S and Te). Although there has been a report on the exceptional thermoelectric properties of $a$-Cu2Se1-$x$I$x$ in the vicinity of its transition temperature from $a$ - to $b$-phase, to the best of our knowledge, doping effects in Se-site with aliovalent element has not yet been reported in $b$-Cu2Se.

Here, we report thermoelectric transport properties of Cl-doped Cu2Se compounds. The Cu2Se1-$x$Cl$x$ compounds ($x = 0$ ~ 0.08) were prepared by solid state reaction followed by the consolidation using spark plasma sintering. The substitution of Se with Cl led to the decrease in the hole concentration, enabling both the optimization of power factor and the reduction of electronic thermal conductivity in $b$-Cu2Se. Meanwhile, the electrical conductivities in Cl-doped compounds decreased drastically as the temperature reached ~ 700K, and it was due to the melting of secondary phase of CuCl ($Tmelt$ ~ 696K). As a result, the power factor enhancement could only be achieved up to 623K. However, we could achieve considerably enhanced $ZT$ in the Cl-doped compounds within the temperature range, and detailed results will be presented.

**Keywords:** Thermoelectric, ZT, Cu2Se, spark plasma sintering

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# Design of multi-defect structures in polycrystalline (Bi,Sb)2Te3 Alloys for low thermal conductivity

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## Abstract

Bismuth antimony telluride (Bi,Sb)2Te3 alloys are the most widely used bulk thermo-electric materials near room temperature developed in 1950s. Nevertheless, widespread use of commercial applications using (Bi,Sb)2Te3 alloys are yet constrained because of low thermoelectric conversion efficiency $zT$. In order to enhance the $zT$, total thermal conductivity of the alloy must be reduced. Many studies have showed that defect structure in (Bi,Sb)2Te3 alloys can reduced lattice thermal conductivity $k_{latt}$ effectively, including point defects (0 dimension, 0D), dislocations (1D), grain boundaries (2D), or nano-sized inclusions (3D). However, there is little report on estimating $k_{latt}$ quantitatively at designed defect density or on providing comprehensive prospective of multiple defect structures in minimizing $k_{latt}$ of (Bi,Sb)2Te3 alloys. Here, we analyzed the experimental $k_{latt}$ of (Bi,Sb)2Te3 alloys with the aforementioned defect structures by using Debye-Callaway model, and estimated the $k_{latt}$ at different defect densities providing design rule for each defect structure in reducing $k_{latt}$. Furthermore, the influence of multiple defect structure was evaluated based on the analysis on individual defect structure, providing comprehensive prospective in minimizing $k_{latt}$ based on different frequency-dependency of phonon scattering by different defects. Therefore, this work provides the optimal design of multi-defect structure for high-performance (Bi,Sb)2Te3 alloys. With the suggested optimal multiple defect structure with grain boundaries, dislocations and nanoinclusions, the very low $k_{latt}$ of ~0.24 W/mK is anticipated, and $zT$ as high as ~2.5 can be achievable near room temperature with a typical power factor of (Bi,Sb)2Te3 alloys.

**Keywords:** thermal conductivity, (Bi, Sb)2Te3 materials, Callaway model, phonon engineering, defect structure

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# LDA+U calculation of electronic and thermoelectric properties of doped tetrahedrite Cu12Sb4S13

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## Abstract

Tetrahedrite-based thermoelectric materials have received much attention in the recent years due to their good thermoelectric performance and earth-abundance. The parent compound Cu12Sb4S13 exhibits high power factor, which is mainly derived from its low electrical resistivity. Further enhancement of ZT by lowering thermal conductivity is achieved in substituted compounds, primarily at the Cu site Cu(12-x)M(x)Sb4S13 [1]. In this work we have studied the impact of substitution effects on thermoelectric power factor using density-functional theory (DFT) electronic structure calculations in combination with calculation of thermoelectric properties by BoltzTrap program [2].

The bands crossing the Fermi level are mainly composed by Cu d-orbitals. In order to assess the substitution effect for similar level of doping, we have calculated electronic structure of Zn, Mg and vacancy substituted tetrahedrites, which have similar level of d-band filling i.e. $\sim$ 9.91. Seebeck and Hall coefficients are positive for all the studied compounds. The highest Seebeck coefficient was calculated for Cu9Zn2Sb4S13, which has also the lowest electrical conductivity. The thermoelectric properties of Cu11ZnSb4S13 and Cu11MgSb4S13 are similar. Within the approximation of equal relaxation time the power factor is the highest for Cu11ZnSb4S13, but for all the studied doped compounds is lower than for the parent Cu12Sb4S13. On the other hand the substitutions create charge and chemical disorder which is expected to decrease the thermal conductivity.

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**Keywords:** Tetrahedrite, LDA+U calculation, BoltzTrap

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# A Study on the effect of Conducting Interface on Electron and Phonon Transport in Sb2Te3–Graphene Nanocomposite for Thermoelectric Properties

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## Abstract

Nanocomposites are of great interest for thermoelectric application as presence of the large phonon scattering and increase in electrical conductivity would result in the enhancement of figure of merit (ZT) [1]. Antimony telluride (Sb2Te3) is best suited p-type semiconducting material for the room temperature thermoelectric applications due to good electrical performance and low value of thermal conductivity, and has superior heat to electrical energy conversion efficiency.

In the present work, Sb2Te3 nanocomposite using conducting filler (Graphene) have been synthesized by simple chemical route and its thermoelectric properties are investigated. The obtained temperature dependent figure of merit (ZT) of the Sb2Te3–Graphene nanocomposites exhibit the positive effect of conducting filler at interfaces in thermal conductivity and electrical conductivity. The positive sign of Seebeck coefficient for Sb2Te3–Graphene nanocomposite confirms p-type semiconducting behavior. The electrical conductivity of Sb2Te3–Graphene nanocomposite increases whereas the Seebeck coefficient and thermal conductivity decreases as compared to Sb2Te3 nanosheets sample resulting in overall enhancement of the figure of merit for the nanocomposite. The enhanced ZT of Sb2Te3–Graphene nanocomposite has been attributed to increase in charge carrier mobility through the intimate contact of graphene sheet with the surface of Sb2Te3 nanosheets. The decrease in the thermal conductivity of nanocomposite sample was observed without much affecting the Seebeck coefficient. In addition, surface potential study of nanocomposite also has been carried out to study the nature of different phases present in Sb2Te3–Graphene.

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**Keywords:** Seebeck Coefficient, Electrical Conductivity, Sb2Te3 Nanocomposite

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# Enhancing the Figure of Merit in Nano-composite Thermoelectric Materials with Aerogel Addition

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## Abstract

Reducing the thermal conductivity while preserving the power factor is an effective way to enhance the $zT$ of materials.[1-3] Here we discovered that Bi0.5Sb1.5Te3 composites incorporated with _˜3.3wt % (30 vol. %) aerogel follow this unique characteristic and reach a high $zT$ value of _˜1.44 at 350 K. The aerogel is a fantastic material having extremely high porosity and low thermal conductivity due to its mesoporous nanostructure. Mixing the Bi0.5Sb1.5Te3 matrix with appropriate silica aerogels only slightly decreases the Seebeck coefficient, but doesn't deteriorate the electrical conductivity. The power factor of the composites can be maintained as high as the pristine one. Most importantly, the thermal conductivity of aerogel composites is significantly reduced by enhancing phonon scattering. The gains in $zT$ for samples with aerogel come primarily from a reduced lattice thermal conductivity (lat), as well as enhanced power factor for material. As a consequence, the combination of high $\sigma/$ ratio and not deteriorated Seebeck coefficient leads to the highe $zT$ values.

**Keywords:** thermal conductivity, nanocomposite

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# Tetrahedrite Cu12Sb4S13 Prepared by Using Mechanical Alloying and Hot Pressing

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## Abstract

Tetrahedrite, Cu12Sb4S13, has attracted much attention as a thermoelectric material because of its abundant raw materials and very low thermal conductivity due to complicated crystal structure. The Cu atoms vibrate with large amplitudes due to lone-pair electrons of Sb atoms, which lead to the low lattice thermal conductivity. Tetrahedrites are generally synthesized by using melting process, which needs careful reaction due to low boiling point of S and requires a long period of annealing for phase transformation and homogenization. In this study, Cu12Sb4S13 was successfully prepared by using mechanical alloying as a solid-state route and consolidated by using hot pressing. Single phase of Cu12Sb4S13 was synthesized by mechanical alloying at 350 rpm for 24 h, and sound compact was obtained by hot pressing at 723 K for 2 h under 70 MPa. A maximum ZT of 0.87 was achieved at 723 K for undoped Cu12Sb4S13.

**Keywords:** thermoelectric, tetrahedrite, mechanical alloying, hot pressing

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# Microstructural characteristics and thermoelectric properties of Cu and Sb codoped GeTe thermoelectric materials

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## Abstract

Energy harvesting using thermoelectricity has been very attractive because thermoelectric generators can directly convert heat into electricity. The thermoelectric performance is evaluated by the figure-of-merit, $ZT = S2sT/k$, where S, s, T and k are the Seebeck coefficient, electrical conductivity, absolute temperature, and thermal conductivity, respectively. To improve a ZT value, it is required to increase the Seebeck coefficient and electrical conductivity and to reduce the thermal conductivity. However, this is very challenging because the electrical conductivity and thermal conductivity are coupled together with Wiedeman-Franz law, $k = sTL$, where L is the Lorenz number.

GeTe thermoelectric material has a high carrier concentration due to a Ge vacancy, leading to the high electrical conductivity and low Seebeck coefficient. Therefore, to increase Seebeck coefficient, it is necessary to suppress the carrier concentration by doping element with three valence electrons. GeTe-based thermoelectric materials have a characteristic herringbone structure with an alternating bright and dark contrast, resulting from domains with different polarities caused by cubic-to-rhombohedral phase transformation. A herringbone structure is beneficial to increasing a phonon scattering, leading to reduction of thermal conductivity. High ZT values about 750 K have been achieved by simple solid-state substitution of Ge in GeTe by Sb, Bi, Mi, Sn+Pb, and In. However, studies on pair substitution in GeTe-based thermoelectric materials have not been performed in detail.

In this work, we investigated the microstructure and thermoelectric properties of GeTe-based materials codoped with Sb and Cu atoms. Especially, the effects of doping elements on the herringbone structure were examined in detail. In this presentation, we will discuss them.

**Keywords:** GeTe, TEM, Herringbone structure

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# Thermoelectric properties of magnesium doped tetrahedrite

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## Abstract

Tetrahedrite, a naturally occurring sulfosalt mineral, can be described by the general composition Cu10(Zn,Fe,Cu,...)2(Sb,As)4S13. Recently, synthetic tetrahedrites have been shown to posses favourable thermoelectric properties at moderate temperatures. Their high thermoelectric potential lies within their extremely low lattice thermal conductivity which, despite the moderate positive Seebeck coefficient, gives rise to peak ZT values close to unity. A wide range of elements can be substituted into tetrahedrite and many of these substitutions have been studied with respect to thermoelectric or other properties. Nevertheless, all tetrahedrites reported to date contained exclusively d- and p-block elements of the periodic table.

In this contribution we demonstrate that magnesium, an s-block element, can also be substituted into tetrahedrite on the Cu site. We successfully prepared a series with the nominal composition Cu12-xMgxSb4S13, where x = 0.5, 1, 1.5. The increase of unit cell size and chemical mapping performed with XRD and EDX confirmed that approximately half of the magnesium atoms were incorporated in the tetrahedrite structure, while the other half exist in electrically insulating MgS precipitates. Thermoelectric data, measured both above and below room temperature, have shown that the effect of Mg2+ is similar to that of other polyvalent substituents. That is, the filling of valence band holes leads to an increase of the Seebeck coefficient, increase of electrical resistivity and decrease of the electronic part of thermal conductivity.

This work was supported by the Czech Science Foundation, grant No. 18-12761S.

**Keywords:** Tetrahedrite, magnesium substitution, measurement, TE properties, Cu12–xMgxSb4S13

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# Boosting the Thermoelectric Performances of Lead Chalcogenides through Dynamic Doping and Hierarchical Phonon Scattering

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**Abstract**

Here we report the peculiar behavior of Cu ions in the Cu-doped lead chalcogenides which increases their thermoelectric performances. For the electrical transport, a dynamic doping effect is achieved because more Cu ions enter into the crystal lattice of lead chalcogenides and provide extra charge carriers as the temperature increases, which guarantees optimized carrier concentration in a wide temperature range. For the thermal transport, the presence of Cu-rich nanoprecipitates and dislocations at low temperature range as well as the vibration of Cu atoms around the interstitial sites of lead chalcogenides at high temperatures result in hierarchical phonon scattering and significantly reduced lattice thermal conductivity in the whole temperature range. As a result, a peak thermoelectric materials figure of merit $zT$ up to 1.45 and thermoelectric device figure of merit $ZT$ close to unity are attained in the PbSe sample with 0.375 at% Cu. Enhanced thermoelectric properties are also realized in the Cu-intercalated PbTe and PbS systems, implying that the temperature-driven dynamic behavior of Cu ions in a rigid lattice can serve as a general strategy to optimize the thermoelectric performance of IV-VI compounds.

**Keywords:** Lead Chalcogenides, Dynamic Doping, Carrier Concentration, Hierarchical Phonon Scattering, Interstitial Atom

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# Thermoelectric properties of Sn-Se layers prepared by pulsed magnetron sputtering

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## Abstract

SnSe thin films were obtained on glass substrates by pulsed magnetron sputtering. The target material was synthesized in quartz ampoules by melting elemental powders mixed in equimolar proportions. The ingot was crushed and the resulting powder was consolidated in a graphite die by hot pressing. The polycrystalline sinter, 50 mm in diameter and thickness of 4 mm, was used as a target. Experimental deposition conditions were optimized to obtain stoichiometric SnSe layers. The layers were analyzed for microstructure and phase composition by SEM/EDS and XRD. The Seebeck coefficient, resistivity, thermal conductivity, carrier concentrations and mobility measurements were performed in the temperature range 300 – 600 K using Thin Film Analyzer (TFA, Linseis). Thermoelectric properties of the Sn-Se layers are discussed with reference to the deposition parameters and related structural features.

**Keywords:** SnSe layers, magnetron sputtering

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# First principle studies of Fe doped Cu2S. Synthesis and computational investigations

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## Abstract

Copper sulfide ($Cu_2S$) belongs to Cu-based superionic conductors characterized by excellent thermoelectric properties particularly in high-temperature range (700–1000 K). In recent years, the figure of merit (ZT parameter) of 1.5 – 2.0 has been recorded for these materials which makes them extremely attractive from the application point of view. The problem is relatively low durability of $Cu_2S$ based materials caused by excessive migration of copper ions. One of the possible solutions may be the introduction of ions (e.g. Fe) into $Cu_2S$ structure, which could stop this excessive migration. Such approach seems appropriate, because of the good stability of another Cu-based thermoelectric material, namely $CuFeS_2$ (tetrahedral structure) which, however, is characterized by much worse thermoelectric properties (ZT about 0.2–0.3).

The aim of this studies was to check whether it is possible to introduce a small amounts of iron ions into bulk $Cu_2S$ structure in such a way that the system maintains initial $P2_1/c$ monoclinic structure, without precipitation of other phases (including $CuFeS_2$ or FeS) and to investigate the influence of such doping on thermoelectric properties.

A two-stage synthesis of $Cu_{2-x}Fe_xS$ materials (where $0.01 \leq x \leq 0.1$) have been carried out. The resulting materials are characterized by XRD and SEM studies. Simultaneously, based on *ab initio* calculation (Wien2k package, DFT formalism) the geometry optimization for some model Fe doped $Cu_2S$ superstructures have been carried out. On the basis of obtained results, the most probable location site of Fe ions in $Cu_2S$ structure was determined, the analysis of electron density topology (Critic2 package) and electronic structure was performed.

### Acknowledgements

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# First-principles study on the thermoelectric properties of ternary chalcogenides

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## Abstract

Multi-valley band structure, which is realized in PbTe and Bi2Te3, is one of the favorable band structure for enhancing thermoelectric efficiency. $P$-type AgBiSe2 in the low-$T$ phase has also multi-valley character, so that it has been regarded as promising and expected to exhibit high thermoelectric efficiency [1]. In the high-$T$ phase, a recent study has already shown that $p$-type AgBiSe2 has a high $ZT$ of 1.5 at around 700K [2]. $P$-type AgBiSe2 in the low-$T$ phase has not been reported yet, but it has been pointed out that it may have the potential to achieve $ZT$ value of 0.4-0.7 at room temperature [1]. TlBiSe2, which has the same crystal structure as AgBiSe2 in the low-$T$ phase and has been focused from the viewpoint of topological insulator, has already been studied by first principles calculation. Those studies have revealed that the band structure of TlBiSe2 and its analogous substances possess also multi-valley band structure [3]. Thermoelectric properties of some of them have already been reported, which show that their thermal conductivities are very low.

In the present study, we analyze the thermoelectric properties of about 20 chalcogenide compounds represented as ABCh2, which has the same crystal structure mentioned above, using first-principles calculation and Boltzmann equation. From the calculation results, we will select promising candidates for the composition. and discuss similarities and differences in their electronic structure in detail.

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Ref. [3] B. Singh *et al.*, Phys. Rev. B **86**, 115208 (2012).

**Keywords:** first principles calculation, chalcogenide, oxide, Boltzmann equation

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# Effect of Cu deficiency on the structural and thermoelectric properties of Cu2Te

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## Abstract

Cu2Te is a superionic conductor belonging to the Phonon Liquid Electron Crystal class of thermoelectric (TE) materials. A systematic study of its structural investigation in correlation with TE properties is interesting. The effect of copper deficiency on the structural and thermoelectric properties of Cu2Te has been investigated herein. Samples with chemical formula Cu2-xTe (where x=0, 0.4, 0.75) are synthesized via solid state method. Powder X-ray Diffraction analyses reveals that the samples have different crystal structures and various polymorphic forms depending upon Cu:Te stoichiometry. Electron Probe Microanalysis equipped with Wavelength Dispersive Spectrometry shows that all the samples are copper deficient, which is probably due to ease of formation of Cu vacancies. Transport properties are measured in the temperature between 300 and 600 K. Electrical conductivity ($\sigma$) decreases with increase in temperature indicating a metallic like behavior for all the samples. Positive Seebeck coefficients ($S$) for all the samples indicates that majority carriers are holes. The pristine sample has higher $S$ (29.5 $\mu$V K-1 at 573 K) and lower $\sigma$ (2513 S cm-1 at 573 K) compared to the other two samples. This is possibly due to a lower carrier concentration in the pristine compound in comparison to the Cu-deficit samples. The deficiency of Cu results in formation of Cu vacancies leading to the increase of carrier concentration and higher electronic thermal conductivity. The maximum thermoelectric figure of merit of 0.05 at 573 K is achieved for the pristine sample owing to its higher power factor (0.22 mW m-1 K-2) and lower thermal conductivity (2.5 W m-1 K-1). This study therefore emphasizes that Cu vacancies should be controlled in Cu2Te to enhance its thermoelectric performance.

**Keywords:** Copper telluride, vacancies, phase transitions, polymorphism, thermoelectricity

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# Huge anisotropy transport properties in $\alpha$-In2Se3 single crystal

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## Abstract

Using the temperature gradient method, we have successfully grown the $\alpha$-In2Se3 single crystal. The optical and transport measurements revealed that our samples made by this process show a good crystalline with the band gap of 1.375 eV and strong anisotropy properties of both electrical resistivity and Seebeck coefficient. The electrical resistivity anisotropic ratio finds to be approximately 43300 at 300 K and drops to roundly 3650 at 400 K. The Seebeck coefficient values are 252 $\mu$V.K-1, and 397 $\mu$V.K-1 at 400 K belong to the in-plane and out-of-plane of layers, respectively.

**Keywords:** In2Se3 single crystal, anisotropy, transport properties

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# Effects of Se/Sn Flux Ratio on Growth and Thermoelectric Transport Properties of SnSe Thin Films

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## Abstract

We have investigated the effects of Se/Sn flux ratio on the growth and thermoelectric transport properties of (h00) oriented SnSe thin films on MgO (100) substrate using MBE. All films were epitaxially grown at 294 oC with various Se/Sn flux ratios of 0.8, 0.9, 1, 3, 5, and 7. The crystal structure of the obtained SnSe thin films was orthorhombic ($Pnma$ space group) with $a$-axis (h00) orientation. A 90o rotated bi-layer structure was observed in sample with Se/Sn ratios of 0.8, 0.9, and 1, while the third layer's orientation rotated 45o was simultaneously observed in samples with higher Se/Sn ratio of 3, 5 and 7. One more layer's orientation rotated 135o was observed in sample with Se/Sn ratio of 7. Interestingly, the best crystalline film was obtained at the Se/Sn ratio of 1. Thermoelectric and transport properties of films were also strongly affected by the Se/Sn flux ratio. The highest power factor; 8.51 $\mu$W cm-1 K-2 was obtained at 650 K in sample at flux ratio of 0.8. TEM images showed very good crystallinity of our samples in consistent with their high resistivity. Our results suggest a possibility to reduce thermal conductivity of SnSe thin film along $a$-axis by controlling layer's orientation.

**Keywords:** 2D materials, SnSe, MBE, thin film, layered, thermoelectric

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# Evolution of thermoelectric properties of melt-spun ribbons during crystallization

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## Abstract

Properties of as-prepared melt-spun thermoelectrics are almost unknown. Due to very high cooling rate in the melt-spinning process, the resulting material samples immediately after the preparation are in highly non equilibrium structural state, close to amorphous. Usually the samples have shape of thin ribbons with typical thickness of about 5 – 10 microns, and width of order of 1 mm. The thermoelectric properties of such ribbon samples, which in most case are extremely fragile, is very difficult to measure, especially at elevated temperatures. On the other hand, the material, prepared by melt-spinning is usually further processed by applying high temperatures and pressure to obtain bulk thermoelectrics. The information about the evolution of the ribbon properties during high-temperature heat treatment can help to optimize the technological parameters such as time and temperature of pressing, used in preparation of bulk samples. In this work we study the Seebeck coefficient and electrical resistivity of melt-spun ribbons of skutterudites In0.2Ce0.1Co4Sb12.3, Co4Sb11.6Te0.4,and of Bi0.5Sb1.5Te3 alloy in the course of high-temperature heat treatment. The properties were measured during in-situ annealing at temperatures from 100 K to 750 K, using homemade equipment. It was found that initial state of the ribbons is stable up to about 600 K. Power factor of the Bi0.5Sb1.5Te3 alloy decreases in the course of isothermal annealing. The dependence of power factor of the skutterudites on the annealing time is non-monotonic, having a maximum at comparatively short annealing time.

**Keywords:** meltspinning, ribbons, crystallization

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# Prediction of the high thermoelectric performance of pnictogen-dichalcogenide layered compounds with quasi-one-dimensional gapped-Dirac-like band dispersion

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## Abstract

Theoretical design of high-performance thermoelectric materials has been a central and challenging problem in the field of thermoelectrics. One of the difficulties for it is the fact that an ideal electronic structure is hard to realize in real materials with many complexities. In this study [1], we theoretically demonstrate that pnictogen-dichalcogenide layered compounds, which originally attracted attention as a family of superconductors and have recently been investigated as thermoelectric materials [2], can exhibit very high thermoelectric performance by realizing one of the ideal electronic band structures: a quasi-one-dimensional gapped-Dirac-like band dispersion (cf. [3]). This special band dispersion allows the co-existence of the high density of states and group velocity near the band edge. In these compounds, the $px,y$-orbitals of pnictogens and chalcogens form a square-lattice network, which guarantees the qusai-one-dimensional band dispersion with respect to two directions. We clarify that such a one-dimensionality can be enhanced by using light and heavy elements for pnictogen and chalcogen, respectively, because of a change of the ionic radii and the strength of the spin-orbit coupling. In particular, we find that LaOAsSe2, a material that has yet to be synthesized, has a powerfactor that is six times as large as that of the known compound LaOBiS2, and can exhibit a very large $ZT$, which amounts to around two in high temperatures, under some plausible assumptions. Because our target materials have high controllability of constituent elements and feasibility of carrier doping, experimental studies along this line are strongly awaited. [1] M. Ochi, H. Usui, and K. Kuroki, Phys. Rev. Applied **8**, 064020 (2017). [2] Y. Mizuguchi *et al.*, Cog. Phys. **3**, 1156281 (2016). [3] T. Inohara *et al.*, Appl. Phys. Lett. **110**, 183901 (2017).

**Keywords:** low dimensionality, Dirac dispersion, materials design, first principles calculation, bismuth dichalcogenides

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# Crystal structure and thermoelectric properties of Ge2Sb2Te5 prepared by spark plasma sintering

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## Abstract

Ge-Sb-Te materials have gained renewed interest as potential thermoelectric (TE) materials, because of superior electronic structures for the cubic and hexagonal phases, and low lattice thermal conductivity originating from intrinsically complex structures for the hexagonal phase and resonant bonding for the cubic phase. An extraordinary high $ZT$ value over 2 was reported for Ge-Sb-Te materials by adjusting of carrier concentrations and controlling of microstructures. In particular, TE properties of Ge2Sb2Te5 (GST) have been investigated to explore the possibility of their TE applications. The GST compounds have two types of crystal structures: one is metastable cubic structure (GST-c) and the other is stable hexagonal structure (GST-h). The GST-c changes into the GST-h at about 500 K. In our previous study, we prepared the cubic GST in the bulk form by using a combination of melt spinning technique and room-temperature high-pressure pressing and evaluated its low temperature TE properties. In this study, the cubic GST were sintered at around phase transition temperature in a short time by spark plasma sintering (SPS) apparatus. By using such a method, we predicted the GST-c was not able to completely change into the GST-h, and rather contained some kinds of disorders. Disorder in Ge-Sb-Te materials was well studied theoretically and experimentally for application of phase-change materials, and known to significantly affect their electronic structure. Therefore, the TE properties of Ge-Sb-Te materials would be significantly affected by disorders. The purpose of this study is to clarify how disorders of crystal structure induced by SPS affected the TE properties of GST. We will discuss the relationship among SPS processing parameters, introduced defects, and TE properties of the obtained samples of GST.

**Keywords:** crystal structure, metastable phase, spark plasma sintering, Ge2Sb2Te5

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# Anisotropic thermoelectric properties of SnSe2 single crystal

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**Abstract**

We have synthesized bulk SnSe2 single crystal to investigate the thermoelectric properties. The Seebeck coefficient of SnSe2 is negative in the whole temperature range, indicating n-type semiconducting behavior. Highest power factor (PF) reached at 673 K along ab-plane directions. The thermoelectric performance along c-axis, however, reached the even highest value of ZT = 0.15 at same temperature due to extremely low thermal conductivity. The measurement sound velocities show that the ultra-low thermal conductivity mainly contributed from weak interlayer bonding.

**Keywords:** tin diselenide, single crystal, low thermal conductivity

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# Thermal Stability and Mechanical Properties of Thermoelectric Tetrahedrite Cu12Sb4S13

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## Abstract

Tetrahedrites have been focused as environmentally-friendly materials with high thermoelectric performance. They consist of complex structures containing Cu, Sb and S elements, which are useful for low thermal conductivity due to lone-pair electrons of Sb. Synthetic tetrahedrites have been studied on the phase relations and stability regions in the Cu-Sb-S ternary compound. Undoped tetrahedrite is stable up to around 600 K but the thermal stability may be changed by incorporating doping elements. However, different transformation temperatures on the tetrahedrite have been reported according to synthesis processes. In this study, intrinsic and doped Cu12Sb4S13 powders were synthesized by using mechanical alloying, and then the synthesized powders were hot pressed. The thermal stability and mechanical properties were examined with different conditions: atmosphere (air and vacuum), aging temperature and aging time.

**Keywords:** tetrahedrite, thermoelectric, thermal stability, mechanical

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# New Generation of Micro-Flexible Thermoelectric Devices to be Applied in Electronic Printing

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## Abstract

Thin and flexible micro thermoelectric generators (TEGs) are being envisaged in the last decade as alternative power sources, constituting a new business opportunity for the packaging industry such self-powered wearable electronics and/or to be used on remote places for low power consumption devices. The main strategies to obtain this goal are by depositing high performance thermoelectric materials onto the top of flexible substrate, organic polymeric materia or by combining both resulting in a composite. This last strategy unveil better achievements in the last years and the more promising due to low cost production and scalability to the market. Although a thorough search is being under pursuit, the results unveil to be always smaller than the direct inorganic material thin films. Thus, the main goal of this work is to conceive a flexible and easy printed TEG prototype for energy harvesting. Towards this goal, Bi2Te3 thermoelectric material was synthetized by solid-state reaction using a close quartz-tube in a N2 atmosphere. The achieved material was submitted to a ball milling process to reduce the mean particle size down to 50 $\mu$

**Keywords:** Thermoelectric Materials, Organic polymers, Bi2Te3, Power Output

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# Probing the Link between Structure and Thermoelectric Properties in SnSe

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## Abstract

SnSe has recently attracted attention due its large peak thermoelectric figure of merit, ZT $\sim$ 2.5 at 923 K in single crystals [1]. The high ZT values are intimately linked to the structural phase transition from Pnma to Cmcm symmetry at 800 K.

We have revisited the temperature dependence of the crystal structure of SnSe using variable temperature neutron powder diffraction (4-1000 K). Distortion mode analysis reveals previously unobserved Sn motions perpendicular to the SnSe layers. These displacements, combined with the primary motion of Sn within the layers, broaden the phase transition by +/- 200 K [2]. In addition, heat capacity data were collected over the same wide temperature interval to gain insight into the lattice dynamics of SnSe. The heat capacity was fitted satisfactorily using two Debye modes with Debye temperatures $\Theta_{D1}$ = 345(9) K and $\Theta_{D2}$ = 154(2) K [3]. The energies of these modes scale with the bond strengths of the short and long bonds in the crystal structure, and correspond to the upper energies of the two bands present in phonon density of states calculations. The presence of two lattice energy scales demonstrates that SnSe incorporates some of the key traits of classical phonon glass electron crystal materials, and suggests that searching for materials with widely diverging bond distances may be a possible route to uncover high ZT materials.

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**Keywords:** SnSe, high ZT, Distortion mode analysis, Neutron Diffraction, Thermoelectric

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# Improved thermoelectric performance in Cu2Se-based liquid-like materials

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## Abstract

Thermoelectric materials require an optimum carrier concentration to maximize electrical transport and thus thermoelectric performance. Element-doping and composition off-stoichiometry are the two general and effective approaches to optimize carrier concentrations, which have been successfully applied in almost all semiconductors. In this study, we propose a new strategy coined as bonding energy variation to tune the carrier concentrations in Cu2Se-based liquid-like thermoelectric compounds. By utilizing the different bond features in Cu2Se and Cu2S, alloying S at the Se-sites successfully increases the bonding energy to fix Cu atoms in the crystal lattice to suppress the formation of Cu vacancies, leading to much lowered carrier concentrations toward the optimum value. Combing the lowered electrical and lattice thermal conductivities, and the relatively good carrier mobility caused by the weak alloy scattering potential, ultrahigh $zTs$ are achieved in slightly S doped Cu2Se with a maximum value of 2.0 at 1000 K, 30% higher than that in nominally- stoichiometric Cu2Se.

**Keywords:** Cu2Se, bonding energy, alloying

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# Realizing Thermoelectric Performance in High Quality Crystalline GeTe by Sb Doping

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## Abstract

GeTe is not only a classical thermoelectric material but also the well-known leading material due to its exclusive structural, electrical and thermal properties. Pristine GeTe shows high electrical and thermal conductivity due to the intrinsic defect, such as the Ge vacancy. In our work through the Bridgman method, we are able to synthesize high quality crystalline Ge1-xSbxT ingots and measure their thermoelectric properties. The remarkable $zT$ value was achieved above 2 as T = 700 $\tilde{\ }$ 740 K when 8% Ge is placed by Sb. We also demonstrated that the thermoelectric performance of $p$-type solid ternary Ge1-$x$Sb$x$Te is largely enhanced compared to pristine GeTe alloys. The substitution of Sb on Ge offers the excess carriers that shift the Fermi energy to where the thermoelectric power factor is optimized which enables us a precise control of the carrier concentration. Meantime, spontaneous reduce the thermal conductivity arisen from enhancing phonon scattering by doping effect. In summary, the combination of optimal power factor and highly crystalline leads to the higher $zT$ values.

**Keywords:** germanium telluride, antimony, crystal

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# Thermal conductivity measurements and HRTEM analysis of epitaxially grown (Sb1-xBix)2Te3 PVD thin films

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## Abstract

For high ZT values in thermoelectric materials like the Chalkogenite-type (Sb1-xBix)2Te3, high Seebeck coefficients, high electrical and low thermal conductivities are needed at once. For the systematic improvement of ZT values, precise measurements of those quantities are of highest importance. These layered materials have distinct anisotropic properties which are relevant for possible thin film devices. Since the heat flows parallel to the c-axis, mainly the electrical and thermal conductivities in c-direction have to be measured. In this work we present the c-axis thermal conductivity of epitaxially grown Sb2Te3 and (Sb1-xBix)2Te3 (x ≤ 0,15) PVD thin films in the temperature range of 100 to 300 K as obtained by 3omega measurement. By studying thickness series, we were able to identify precisely the impact of the insulation layer as well as the thermal boundary resistances and subtract them. HRTEM and EELS investigations done with an image $C$S corrected Titan 80-300 (FEI) confirmed regularly grown films with very low concentrations of defects such as stacking faults. The analysis of the substrate/film interface structure and the distribution of doping sheds light on the peculiarities of film growth.

**Keywords:** 3omega method, thermal conductivity, epitaxial thin film, Sb2Te3, HRTEM, EELS, Kapitza resistance

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# Effect of jointly replacement in the anion and cation subsystem on conductivity and thermoelectric power of thermoelectrics based on layered transition metal dichalcogenides

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## Abstract

According to the experimental data and preliminary theoretical calculations, $WS_2$ and $WSe_2$ as a representative of layered transition metal dichalcogenides is a perfect candidate for efficient thermoelectric energy converters. Another representative of layered transition metal dichalcogenides, $TiS_2$ and $TiSe_2$ is also considered promising. Jointly replacement in the anion and cation subsystem allows breaking the rigid relationship between the electrical conductivity and the thermoelectric power. As a result, it is possible to increase the power factor and quality factor of thermoelectric materials. Temperature dependences of the electrical conductivity and Seebeck coefficient of bulk samples of transition metal dichalcogenide polycrystals with niobium substitutions for transition metal and selenium substitutions for sulfur - $(W, Ti)_{1-x}Nbx(S_{1-y}Se_y)_2$ have been studied at low temperatures. To create effective thermoelectric converters, materials with a positive and negative thermoelectric power are needed. $W_{1-x}Nb_x(S_{1-y}Se_y)_2$ have a positive Seebeck coefficient and $Ti_{1-x}Nb_x(S_{1-y}Se_y)_2$ – negative Seebeck coefficient. The two-dimensionalization of electron transport properties is detected at niobium concentrations $x > 0.1$ for $W_{1-x}Nb_x(S_{1-y}Se_y)_2$ and for all samples $Ti_{1-x}Nb_x(S_{1-y}Se_y)_2$. At room temperature Seebeck coefficient (at equal electrical conductivities) is several times higher in the samples with quasi-two- dimensional transport than in the samples with three-dimensional transport. This take place because in two-dimensional systems the Fermi Energy is less than in three-dimensional systems at identical values of the charged carrier concentration. The calculation of the power factor at room temperature shows its nine times increase.

**Keywords:** Transition metal dichalcogenide, electrical conductivity, Seebeck coefficient, quasi, two, dimensional transport, power factor

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# Temperature variation of electronic structure of n-type PbTe and its impact on thermoelectric transport

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## Abstract

Some of the most efficient thermoelectric materials are semiconductors with narrow band gaps, such as lead chalcogenides PbX (X=Te, S, Se) [1,2]. However, the small band gaps of these materials make their thermoelectric transport properties very sensitive to the gap variations. Remarkably, PbTe exhibits a large band gap change with temperature, ranging from 0.19 eV at 30 K to 0.38 eV at 500 K [2,3]. An accurate description of the electronic structure as a function of temperature is thus essential for the modelling and design of efficient thermoelectric materials with narrow gaps. In this work, we report a fully ab initio calculation of the temperature dependence of the electronic structure of PbTe, using density functional perturbation theory [4] and electron-phonon Wannier [5] approach. We obtain the temperature variation of the direct band gap in PbTe in a very good agreement with experiments [2,3]. Furthermore, we find that the temperature dependence of PbTe's band gap considerably increases the electron-phonon scattering above room temperature. Consequently, the temperature variations of the energy gap reduce the electronic conductivity and the thermoelectric figure of merit of PbTe at high temperatures, resulting in a possible limitation for thermoelectric applications.

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**Keywords:** abinitio simulations, energy conversion, electron transport

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# Thermoelectric Properties of Bi-Te-M (M: Sb, Se) Poly Crystal Compounds Fabricated by an Oxide-reduction and Spark Plasma Sintering

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## Abstract

The Bi-Te-M (M: Sb, Se) compound has been highly treated as important thermoelectric material due to higher thermoelectric performance than other materials near room temperature. The conventional thermoelectric compound has been fabricated based on the melting and solidification process for single crystal growth technique. Lately, with the development of nanostructuring technology, many studies have used rapid solidification-grinding technique and high energy milling technique. However, these process technologies are difficult to commercialize at low cost because it requires long time and high energy as well as using expensive pure metal or alloy as an initial raw material. Thus, new attempts have been made to apply powder metallurgy process to the research and development of poly crystal Bi-Te-M (M: Sb, Se) thermoelectric material. Previously, the authors proposed oxide-reduction process using a low-cost oxides as a starting material that can be used to synthesize Bi-Se-Te-based and Bi-Sb-Te-based thermoelectric powders. In the present study, the focus is the characterization of the thermoelectric properties of Bi-Te-M (M: Sb, Se) compound powders synthesized by the oxide reduction process. The Bi-Te-M (M: Sb, Se) compound powders were sintered by means of the spark plasma sintering process. The thermoelectric properties of the sintered bodies were evaluated by measuring the Seebeck coefficient, electric resistivity and thermal conductivity. The change in the thermoelectric property of the sintered body discussed with the chemical composition and microstructure of the sintered body.

**Keywords:** thermoelectric, bismuth telluride, oxide reduction, powder synthesis

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# Thermoelectric Properties of P-type Cu2Te/Bi-Sb-Te Composite for Mid-Temperature Energy Harvesting

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## Abstract

In this study, we investigated the thermoelectric properties of Bi-Sb-Te by incorporating chemically synthesized Cu2Te nano-inclusions. Cu2Te nano particles were prepared via simple chemical reaction, and then certain amount of Cu2Te were blended with Bi-Sb-Te powders by chemical mixing and drying method to secure the homogeneity. SEM and EPMA analysis were carried out to confirm the microstructures of composite powder and SPSed pellet. It is verified that adding Cu2Te nano-inclusions resulted in more hole carriers, which contributed to great enhancement of the electrical conductivity. As a result, varying the amount of Cu2Te nanoparticles can be a promising technique to effectively modulate the temperature dependence of ZT value, applicable for mid-temperature thermoelectric power generation.

**Keywords:** Bismuth Telluride, thermal conductivity, temperature dependence, thermoelectric properties

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# Promising thermoelectric performances of Cu-excess a-Cu2+xSe for near-room-temperature applications

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## Abstract

Finding the alternatives for Bi2Te3, the only thermoelectric material for near-room temperature (RT) applications, is of great importance in thermoelectrics. Here, we report very promising near-RT thermoelectric figure of merit ($ZTmax = 0.9$ at 390 K, $ZTave = 0.68$ within RT ~ 390 K) of Cu-excess $\alpha$-Cu2+$x$Se, comprising of low-price, abundant, and non-toxic constituent elements. The addition of excess Cu led to the decrease in the hole concentration by suppressing the formation of Cu vacancy, resulting in the power factor optimization in the Cu-excess compounds. These effects of the Cu-addition were also elucidated by the calculations based on density functional theory and Boltzmann transport equation. Furthermore, we measured directly the Lorentz number (2.12$10^{-8}$ V2 K-2 at RT) of $\alpha$-Cu2Se for the first time, and also unveiled the origin of its very low lattice thermal conductivity (0.27 W m-1 K-1 at RT). Based on phonon calculation, it was suggested that its ultra-low lattice thermal conductivity is associated with structural instability of $\alpha$-Cu2Se arising from interaction between Cu+ ions. Our results propose that Cu-excess $\alpha$-Cu2Se is a very promising thermoelectric material to replace Bi2Te3 for near-RT applications.

**Keywords:** $\alpha$, Cu2Se, Thermoelectric, Power factor optimization, Lorentz number, Thermal conductivity

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# Thermoelectric properties of a magnetic semiconductor CuFeS2

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## Abstract

As a high performance thermoelectric material, a magnetic semiconductor CuFeS2 is attracting much attention because of its high power factor. CuFeS2,which is known as chalcopyrite, is a natural magnetic semiconductor, has a large Seebeck coefficient of approximately 500 $\mu$V/K, is expected to be a key candidate to establish a new route to achieve a high power factor with a magnetic material. In addition to potentially large Seebeck coefficient in CuFeS2, the power factor is tunable by its carrier concentration, then it is possible to obtain high power factor.

We present theoretical calculations of the thermoelectric properties of a magnetic semiconductor CuFeS2. The electrical contributions, namely the Seebeck coefficients, electrical conductances, and electronic thermal conductances, are investigated using first-principles calculation techniques based on density functional theory and the nonequilibrium Green's function formalism. The lattice thermal transport properties are analyzed using the nonequilibirium molecular dynamics simulation method. Using a combination of the calculated electronic contributions and the lattice thermal contribution, the thermoelectric figures of merit are calculated and analyzed in doped configurations for the theoretical prediction of the highest thermoelectic energy conversion efficiency. It is shown that dilute doping enhances the figure of merit by 2.5 times compared to 3% doping which was previously experimentally obtained to give the best thermoelectric performance among samples studied.

**Keywords:** Magnetic semiconductor, Chalcopyrite, Density functional theory, Nonequilibrium Green's function, Molecular dynamics

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# Relationship among crystal structure, band structure, and thermoelectric properties of defect-containing Ag-In-Te chalcopyrite structure compounds

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## Abstract

Chalcopyrite structure compounds ABX2 (A=Cu, Ag: B=Al, In, Ga; X=S, Se, Te) are attractive high performance thermoelectric materials because they have superior electrical properties [1, 2]. They form a large group of compounds due to a flexibility of choice of doping elements. Therefore much efforts to improve the thermoelectric performance of chalcopyrite compounds have been conducted mainly by elemental doping [3-5]. There also exist ordered defect compounds whose structure is derived from that of chalcopyrite compounds. However, a comparative study of the chalcopyrite and ordered defect chalcopyrite compounds in terms of crystal structure, band structure, and thermoelectric properties are still few [6-7]. In this study, we focused on the ordered defect chalcopyrite compounds of AgIn3Te5 and AgIn5Te8, and chalcopyrite compounds of AgInTe2 in the (Ag2Te)1-$x$(In2Te3)x system. We prepared these compounds by direct reaction of Ag, In, and Te elements in sealed tubes. The obtained ingots were crushed into fine powders, followed by spark plasma sintering (SPS) at various condition. The thermoelectric properties' measurements and ab-initio calculations based on the crystal structure reported previously [6] were conducted. We will discuss the relationship among crystal structure, band structure, and thermoelectric properties of Ag-In-Te systems.

**Keywords:** chalcopyrite, defect, electrical properties, thermal conductivity, crystal structure, band structure

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# Enhanced Thermoelectric Properties and Thermal Stability of Copper Sulfide with Graphene Heterointerface

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## Abstract

Copper sulfide has received wide attention as a potential thermoelectric material with abundant resource. While the liquid-like Cu ions play an important role for the low L and high $ZT$ values, grain-boundary engineering is needed to further enhance the phonon scattering and the thermal stability of Cu2-$x$S. Here, we introduced the 3D graphene heterointerface into the Cu2-$x$S matrix by a facile technique. A significant $ZT$ enhancement was realized with the highest $ZT$ up to 1.56 with a high $PF$ of 1197 $\mu$W m-1K-2 achieved for the sample with 0.75wt% graphene at 873 K. Additionally, the composite showed excellent reproducibility of $PF$ after five cycles testing from room temperature to 873 K, which confirmed the practical application potentiality of this composite.

**Keywords:** copper sulfide, graphene, grain, boundary engineering, thermoelectric

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# Effects of Se substitution on the thermoelectric properties of (SnS)1.2(TiS2)n (n = 1, 2)

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## Abstract

A layered compound $Ti_{1+x}S_2$ is a promising $n$-type thermoelectric (TE) material due to the high power factor (PF). By intercalating one SnS layer into the van der Waals gap between TiS2 layers as (SnS)1.2(TiS2)2, the PF is maintained while the lattice thermal conductivity is suppressed, leading to the enhancement of $ZT$ to 0.4 at 780 K. In this work, we aimed to enhance $ZT$ of (SnS)1.2(TiS2)$n$ with $n = 1$ as well as $n = 2$ by further reducing the thermal conductivity. For this purpose, we substituted Se for S as $Sn_{1.2}Ti_nS_{1.2+2n-x}Se_x$ ($x = 0, 1.2, 3.2, 5.2$).

The samples were synthesized by the direct reaction of the elements at 1100 K, and then sintered at 973 K under a uniaxial pressure of 50 MPa. The powder x-ray diffraction patterns indicated that the crystal structures of the samples except for $x = 3.2$ with $n = 1$ are isomorphic with the reported structures of (SnS)1.2(TiS2)$n$. Furthermore, preferential orientation of the out-of-plane [001] direction parallel to the pressing axis was observed. The TE properties were therefore investigated along the in-plane direction. The PF's for the $x = 0$ samples with $n = 1$ and $n = 2$ were 0.4 and 0.7 mW K–2 m–1, respectively, at temperatures between 300 K and 670 K. By the substitution of Se at $x = 1.2$, the PF increased at around 300 K due to the modification of electronic structure, and the lattice thermal conductivity was reduced in the entire temperature range. For the $n = 2$ system, further Se substitution at $x = 5.2$ decreased the PF. Consequently, the $ZT$ values at 670 K for the $x = 0$ samples with $n = 1$ and $n = 2$ were 0.15 and 0.25, respectively, which decreased by the Se substitution. Whereas, for the $n = 2$ system, the $ZT$ value was enhanced from 0.07 for $x = 0$ to 0.11 for $x = 1.2$ at 300 K.

**Keywords:** TiS2, (SnS)1.2(TiS2)2, misfit layer compound

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# Electronic and Thermoelectric Properties of Zn and Se Double Substituted Tetrahedrite

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## Abstract

Tetrahedrites are promising thermoelectric materials due to their complex crystal structure, which is responsible for the existence of intrinsic low thermal conductivity. In this study, influence of Zn and Se double substitution on electronic and thermoelectric properties of tetrahedrite is investigated. The samples $Cu11Zn1Sb4S13-xSex$ ($x = 0$, 0.25, 0.5, 0.75, 1, 2) are prepared via solid state synthesis followed by field assisted sintering. The X-ray diffraction patterns confirm tetrahedrite as the major phase. Electron probe micro analysis shows slight off-stoichiometry of Se content in all samples with minute secondary phase of $CuSbS2-ySey$. X-ray Photoelectron Spectroscopy of the sample $Cu11Zn1Sb4S12.5Se0.5$ reveal Zn and Se to be in +2 and -2 oxidation states respectively. Density functional theory (DFT) results show that Se substitution introduces additional bands at Fermi level (EF), which are more dispersive as compared to the parent compound $Cu11Zn1Sb4S13$. The electrical resistivity decreases with increase in Se content upto $x = 1$ which could be due to the enhanced mobility caused by Se states as indicated by DFT results. But Seebeck coefficient is invariant with x, due to enhancement of DOS at EF. The overall effect leads to an increase in power factor of the $Cu11Zn1Sb4S13-xSex$ samples as compared to the parent compound. The Zn+2 substitution at Cu+1 tetrahedral site results in decrease of carrier thermal conductivity due to decrease in the charge carrier contribution. The double substitution of Zn and Se results in the decrease of lattice thermal conductivity due to additional phonon scattering caused by Cu-Zn and S-Se mass difference. A maximum zT of 0.86 at 673 K is exhibited by $Cu12Zn1Sb4S12.75Se0.25$ due to relatively high power factor among the samples (0.9 mW/mK2 at 673 K) coupled with very low total thermal conductivity (0.67 W/m-K at 673 K).

**Keywords:** Tetrahedrite, X, ray diffraction(XRD), Density functional theory(DFT), X, Ray Photoelectron spectroscopy(XPS), Transport properties

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# Ultrafast Additive Manufacturing of Flexible Thermoelectric Films by Aerosol Jet Printing and Photonic Curing

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## Abstract

Wearable devices and Internet of things are rapidly growing market in this time, one of the main barrier to the growth of this field is the requirement for a long lasting power sources for these device. Low temperature thermoelectric materials are highly efficient in powering this low power electronic devices using temperature difference between hot object and ambient temperature. But conventional thermoelectric are rigid, bulk and manufactured using expensive and time consuming techniques. The objective of this project is to obtain miniaturized In-plane flexible thermoelectric with legs dimensions of $1\mu$mX $50\mu$mX5mm using an Aerosol Jet printer and sinter these films using an ultrafast photonic sintering techniques to get high power output per unit area. Conventional sintering takes minimum of 6 to 7 hours to finish whereas our new photonic sintering techniques only take 2 to 3 seconds to sinter films on low temperature flexible substrates. The N type films printed shows an electrical conductivity of 16500 S/m and Seebeck coefficient of 109 $\mu$V/K and a power factor of $196\mu$W/mK$^2$. This is a highly scalable and low cost process to fabricate flexible thermoelectric devices on different low temperature substrates and the devices demonstrated here opens up many opportunity to transform thermoelectric energy harvesting and cooling applications.

**Keywords:** Aerosol Jet printing, Photonic sintering, Flexible thermoelectric generator, Additive manufacturing

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# Theoretical explanation of surface cracking in Bi2Te3 and Sb2Te3 thermoelectric materials

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## Abstract

Texture of Bi2Se0.3Te2.7 alloy is an important factor forming the property anisotropy and technological applicability of an ingot for fabricating modules. The maximum level of thermoelectric parameters may be achieved only for grains with the orientation at which the (0001) basal planes are parallel to the ingot axis because of favourable anisotropy. The objects for the study were samples of thermoelectric materials with n-type conductivity based on triple solid solutions of Bi2Te2.7Se0.3 obtained by crystallisation by modified Bridgman method. Such an approach makes it possible to get a structure in which the cleavage planes are oriented parallel to one another and growth axis. During the operation of the studied materials in generator modules, several cases of modules failures at the temperature of 170 ∘C were detected. These failures were caused by irreversible changes in the structure of the contact layer. Deformations occur only in n-type materials. We performed first-principles DFT-calculations for modelling relaxation and substitution processes in Bi2Te3 and Sb2Te3 crystals. Calculations were implemented by Vienna ab-initio Simulation Package, which is based on plane waves and the projector augmented wave method. The Perdew–Burke–Ernzerhof approximation of the exchange correlation functional was used. Crystal constants obtained in these calculations are well consistent with experimental data. We added vacancy and Sn atom in each structure. It is found that potential barrier for Bi to Sn substitution in Bi2Te3 is 0.11 eV while for the case of Sb to Sn substitution in Sb2Te3 it is 0.47 eV for. Relaxation of the added bismuth atom in Bi2Te3 showed that location between tellurium atoms bound van der Waals interaction is energetically favorable. All these results theoretically explain experimental data obtained earlier.

**Keywords:** bismuth telluride, anisotropy, DFT, calculation, Bridgeman method, solid solutions, thermoelectric material

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# Enhancement in thermoelectric performance of Cu-dopped bismuth antimony telluride by the aqueous solution synthesis

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## Abstract

Bismuth telluride based materials are the best-commercialized thermoelectric materials for electric power generation and refrigeration in the near room-temperature region. In our work, Cu-doped p-type Bi0.5Sb1.5Te3 compounds have been prepared by a facile hydrothermal method. In Bi0.5Sb1.5Te3 compound, Cu+ ions are distributed on the crystal site of Bi/Sb, introducing additional holes. With Cu doping, the hole carrier concentration significantly increases without compromising the carrier mobility, leading to the enhancement of electrical conductivity and the suppression of bipolar effect. Meanwhile, the lattice thermal conductivity can be effectively reduced because of the stronger anharmonicity caused by Cu dopants. Finally, the $zT$ values of ˷1.2 at room temperature and ˷1.5 at 150ºC have been achieved for the sample with 0.6 wt% Cu.

**Keywords:** bismuth antimony telluride, thermoelectric, hydrothermal method, microstructures

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# Thermoelectric stability of Eu- and Na-substituted PbTe

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## Abstract

Pristine PbTe shows a metal–semiconductor transition around 500 K going in parallel to the $p$–$n$ transition in the electrical conductivity [1]. Na is widely used as substituting element in $p$-type PbTe-based thermoelectric materials. Even small concentration of Na (0.5 ~ 2 mol %) improves the metallic behavior in comparison to the binary PbTe. With two local atomic arrangements of Na in PbTe, different Pb-by-Na substitution mechanisms have different influence on the thermoelectric activity of the ternary materials [2]. Recently, through band convergence to increase power factor, together with all-scale hierarchical architectures (atomic/nano/mesostructures) to decrease lattice thermal conductivity, high $ZT$ values in Na-doped PbTe-based bulk materials were achieved using various substitutions of Pb by M (M = Mg, Sr, Mn, Eu) [3-6]. However, the chemical reasons for increased $ZT$ of those materials are worth discussing. Our previous study revealed that the isovalent substitution of Pb2+ by Eu2+ in PbTe have no influence on the thermoelectric figure-of-merit of bulk materials [1]. The Na incorporation into the PbTe lattice drastically changes the thermoelectric properties. The presence of the dual-substitutions by Eu and Na can increase $ZT$ to 2 at 760 K. Here we present systematic investigations of structural and chemical features, carrier transports, and thermoelectric properties of the Pb-Na-Eu-Te quaternary system. In addition, we provide thermal stability studies of these materials related to thermoelectric applications.

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**Keywords:** PbTe, substitution, stability, ZT

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# Enhanced Thermoelectric Performance of Doped Bi0.5Sb1.5Te3 by Melt Spinning Process

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**Abstract**

In this study, we have investigated the thermoelectric properties of Bi0.5Sb1.5Te3 by Cu doping and employing the melt-spinning (MS) process. By varying the doping amount, we could modulate the temperature-dependence of thermoelectric properties, where the maximum ZT temperature could be readily shifted to the elevated temperature. The power factor could be enhanced by incorporation of Cu, and especially big increase for high temperature. The lattice thermal conductivity is reduced by MS process, which gives the reduction of grain size of the materials. Our materials show the boost-up in average ZT value more than 40% compared to Bi0.5Sb1.5Te3, which could be utilized as the application of Bi-Te based thermoelectric materials for mid-temperature power generation.

**Keywords:** Thermoelectric, Carrier optimization, Melt spinning, Power generation

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# Thermoelectric properties of indium thiospinel

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## Abstract

The mineral-like sulfides, *e.g.* thiospinels, are constantly attractive for energy harvesting studies [1]. One member of that group, indium sulfide $In_2S_3$, is widely investigated for photovoltaic and catalytic applications [2,3]. It crystallizes with spinel-type structure (space group [SG]: *Fd-3m*, $a = 10.8321(2)$ Å at 750 K) and is stable in the temperature range of 687 – 1023 K [4,5]. One third of tetrahedra are vacant *i.e.* ([Vac1/3In2/3]tetr.[In2]oct.S4) [4,5]. The cubic phase transforms to tetragonal (SG: $I41/amd$, $a = 7.6227(2)$ Å, $c = 32.357(2)$ Å at 310 K) below 687 K due to the ordering of vacancies [4,5]. Structural disorder in $In_2S_3$ results in low lattice thermal conductivity.

To understand the influence of the crystal structure on the thermoelectric performance, thorough investigation of the samples from the compositional region between $In_{2.67}S_4$ and $In_3S_4$ was performed. The homogeneity range of thiospinel phase was established and its crystal structure was refined. The transport properties are affected by the degree of structural disorder *i.e.* concentration of In-vacancies and the change of the structure with the temperature. In particular, these compounds exhibit low thermal conductivity ($<$ 1 W·m-1K-1) in the whole studied temperature range (300 - 770K). Consequently, obtained $ZT$max equals 0.2 for all compositions.

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**Keywords:** indium sulfide, structural disorder, thermoelectric properties

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# Enhanced thermoelectric performance for n-type bismuth telluride based materials via microstructural modulation and tuning carrier concentration

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## Abstract

Recently, high $zT$s around 300 K have been witnessed in polycrystalline Bi2Te3-based alloys, which greatly accelerate the development of TE refrigeration. However, at elevated temperatures, the $zT$s for most of the Bi2Te3-based alloys are quickly degraded. Thus, so far, the applications of Bi2Te3-based alloys in TE power generation are still limited. In our previous work, we successfully suppressed the intrinsic excitation by introducing tiny amount of electron acceptors (Cd, Cu, and Ag) in p-type Bi2Te3-based alloys. However, so far, the related investigation in n-type Bi2Te3-based alloys is still lack. In this study, tiny amount of excessive Te and I dopant are used as the electron donors to optimize the TE performance in n-type Bi2Te2.4Se0.6 alloys at elevated temperatures. The electron donors significantly reduce the minority carrier partial electrical conductivity $\sigma m$, and thereby lessen the negative effect of intrinsic excitation on the electrical and thermal transports. Likewise, it is found that the bipolar thermal transports in these n-type Bi2Te2.4Se0.6 alloys also obey the "conductivity-limiting" mechanism. Due to the suppressed intrinsic excitation, the peak $zT$ in these n-type Bi2Te2.4Se0.6 alloys is successfully shifted up to the higher temperatures. A maximum $zT$ of 1.0 at 400 K and average $zT$ of 0.8 at 300-600 K have been realized in Bi2Te2.41Se0.6. Such $ZT$ value is attractive for both thermoelectric cooling and low-temperature waste-heat recovery application.

**Keywords:** bismuth telluride, intrinsic excitation, power generation

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# Enhancement of Thermoelectric Figure of Merit for Cu0.008Bi2Te2.7Se0.3 by Metal Nanoparticle Decoration

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## Abstract

Introducing nanoinclusion in thermoelectric materials is expected to lower the lattice thermal conductivity by intensifying the phonon scattering effect, thus enhancing their thermoelectric figure of merit zT. We fabricated Cu0.008Bi2Te2.7Se0.3-based nanocomposite with metal nanoparticles by using metal acetate precursors. Metal nanoparticles of ~ 40 nm were successffully dispersed at grain boundaries of Cu0.008Bi2Te2.7Se0.3 matrix. The analysis on the reduction of the lattice thermal conductivity by the nanoparticles and the enhanced zT of n-type Cu0.008Bi2Te2.7Se0.3 will be reported

**Keywords:** nanoparticle, Bi2Te2.7Se0.3 materials, thermal conductivity, Callaway model

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# Fast Screening of Optimal Compositions for Thermoelectric Lead Chalcogenides Based on Gradient Materials and High Throughput Characterization

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## Abstract

Developing high-performance thermoelectric materials is one of the most important issues in the field of thermoelectrics. However, it is inefficient to prepare and characterize the samples by the traditional "serial" strategies, which hampers the development of new thermoelectric materials. In this work, we demonstrated a strategy for the rapid preparation and characterization of bulk thermoelectric materials with compositional gradient. Compositional gradient materials of PbSe-SrSe and PbSe-PbS systems were fabricated as composition spread libraries. Then the spatial distribution of compositions, resistivities, Seebeck coefficients and thermal conductivities of the materials were characterized using the high throughput methods including energy-dispersive X-ray analysis (EDX), potential and Seebeck microprobe (PSM), and the combined uniform plate heating and infrared thermography techniques. Based on these high throughput characterizations, the composition-structure-property relationships of the PbSe-SrSe and PbSe-PbS can be rapidly constructed, and the optimal composition ranges for these thermoelectric lead chalcogenides were determined. It can be expected that the developed strategy and techniques can also be used to speed up the process of optimizing the performance of other thermoelectric systems.

**Keywords:** Gradient materialsHigh throughputLead Chalcogenides

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# Thermoelectric Properties of Natural and Synthetic Pyrites.

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## Abstract

Natural pyrites became an object of numerous investigations due to their promising thermoelectric and photovoltaic properties [a,b,c]. As it is known these properties depend strongly on the impurities, which appear in the minerals in accordance with type of their geological setting. In this study we try to understand the thermoelectric properties of natural single crystalline pyrite from Sch´onbrunn in Saxony (Germany).

The mineral was characterized by XRD and EDX studies as well as by chemical ICP-EOS analysis. They reveal $FeS_2$ stoichiometrical formula and minor silicate impurity. The $FeS_2$ composition of the crystal from Sch´onnbrun is nicely confirmed by the comparison of its unit cell parameter with the Vegard-plot for the synthetically prepared by us $FeS_2$-$x$ ($0 < x < 0.2$) series. Also a small improvement of the thermoelectric performance (by a factor of 1.5) is observed for the studied pyrite. The further studies on the natural pyrites from different hydrothermal ores from Saxony, Germany are planned.

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**Keywords:** Pyrite, FeS2, Natural crystal, germany, synthetic, impurities

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# TRANSPORT PROPERTIES OF MOLYBDENUM SULFIDE CLUSTERS: EXPERIMENTAL & THEORETICAL RESULTS

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## Abstract

In molybdenum cluster chemistry, the Chevrel phases have been extensively studied mainly because of their superconducting properties. Theses phases consist of a stacking of $Mo_6Q_8$ (Q = S, Se, Te) units and contain channels where additional metal atoms can be inserted. Investigations of their transport properties have shown that they are interesting candidates at high temperature (1000K).[1]

Molybdenum clusters with a nuclearity higher than six can also be obtained and derive from the one-dimensional trans-face sharing of Mo6 octahedra. Among them the ternary $Ag_xMo_9Se_{11}$ (with x ~ 3.6 – 3.8) show outstanding low lattice thermal conductivities that give rise to a rather high value of the dimensionless thermoelectric figure of merit ZT of 0.65 at 800 K for x = 3.8 – 3.9.[2,3] Several additional molybdenum cluster selenides such as $Ag_3In_2Mo_{15}Se_{19}$ [4], $Ag_2Tl_2Mo_9Se_{11}$ [5] and $Cu_{1.3}Cs_2Mo_{12}Se_{14}$ [6] have been synthesized and their crystal structures have been studied by single crystal X-ray diffractions techniques.

Since this family of materials seems to be promising for thermoelectric power generation applications, sulfide molybdenum analogs containing vaious cluster have been synthesized and characterized. In some cases, transport properties were measured to assess their thermoelectric potential. Band structure calculations were carried out for a better understanding of their structural and physical properties.

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**Keywords:** sulfide, molybdenum, cluster, modeling

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# Polycrystalline ZrTe5 Parametrized as a Narrow-Band-Gap Semiconductor for Thermoelectric Performance

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## Abstract

The transition-metal pentatellurides HfTe5 and ZrTe5 have been studied for their exotic transport properties with much debate over the transport mechanism, band gap, and cause of the resistivity behavior, including a large low-temperature resistivity peak. This has previously been attributed to charge density waves, polaronic conduction, and other phenomena. Single crystals grown by the chemical-vapor-transport method have shown an $n$-$p$ transition of the Seebeck coefficient at the same temperature as a peak in the resistivity. We show that behavior similar to that of single crystals can be observed in iodine-doped polycrystalline samples but that undoped polycrystalline samples exhibit drastically different properties: they are $p$ type over the entire temperature range. Additionally, the thermal conductivity for polycrystalline samples is much lower, 1.5 W/mK, than previously reported for single crystals. It is found that the polycrystalline ZrTe5 system can be modeled as a simple semiconductor with conduction and valence bands both contributing to transport, separated by a band gap of 20 meV. This model demonstrates to first order that a simple two-band model can explain the transition from $n$- to $p$-type behavior and the cause of the anomalous resistivity peak. Combined with the experimental data, the two-band model shows that carrier concentration variation is responsible for differences in behavior between samples. Using the two-band model, the thermoelectric performance at different doping levels is predicted, finding zT = 0.2 and 0.1 for $p$ and $n$ type, respectively, at 300 K, and zT = 0.23 and 0.32 for $p$ and $n$ type at 600 K. Given the reasonably high zT that is comparable in magnitude for both n and p type, a thermoelectric device with a single compound used for both legs is feasible.

**Keywords:** Effective mass model, pentatelluride, two, band model, processing

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# Thermoelectric Properties of Cu2-xSe Poly Crystal Compounds Fabricated by an Oxide-Reduction and Hot Press Process

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## Abstract

Recently, the development of thermoelectric materials which do not use tellurium has become active due to the resource problems such as the scarcity of resources and the instability of the price of tellurium. Therefore, thermoelectric research have focused on the development of earth-abundant, environmentally friendly and low-cost elements, such as Cu2-xSe compounds. By the way, the conventional thermoelectric compound has been fabricated based on the melting and solidification process for single crystal growth technique. Lately, with the development of nanostructuring technology, the characteristics of poly crystal thermoelectric material are better than single crystal. For the production of poly crystal thermoelectric material through nanostructuring technology, many studies have used rapid solidification-grinding technique and high energy milling technique. However, these process technologies are difficult to commercialize at low cost because it requires long time and high energy as well as using expensive pure metal or alloy as an initial raw material. Thus, the author proposed an oxide-reduction process capable of producing a compound powder at low temperature and in a short time using a low-cost oxides as a starting material. In the present study, the focus is the synthesis of Cu2-xSe compound powders using oxides and the characterization of the thermoelectric properties according to the composition of Cu2-xSe compounds fabricated by combination of the oxide-reduction and hot press process. The Cu2-xSe compound powders synthesized using copper-oxide and selenium-oxide as starting materials. The thermoelectric properties of the sintered bodies were evaluated by measuring the Seebeck coefficient, electric resistivity and thermal conductivity.

**Keywords:** thermoelectric, copper selenide, oxide reduction, powder synthesis

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# Ultrafast Additive Manufacturing of Flexible Thermoelectric Films by Aerosol Jet Printing and Photonic Curing

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## Abstract

Wearable devices and Internet of things are rapidly growing market in this time, one of the main barrier to the growth of this field is the requirement for a long lasting power sources for these device. Low temperature thermoelectric materials are highly efficient in powering this low power electronic devices using temperature difference between hot object and ambient temperature. But conventional thermoelectric are rigid, bulk and manufactured using expensive and time consuming techniques. The objective of this project is to obtain miniaturized In-plane flexible thermoelectric with legs dimensions of $1\mu$mX $50\mu$mX5mm using an Aerosol Jet printer and sinter these films using an ultrafast photonic sintering techniques to get high power output per unit area. Conventional sintering takes minimum of 6 to 7 hours to finish whereas our new photonic sintering techniques only take 2 to 3 seconds to sinter films on low temperature flexible substrates. The N type films printed shows an electrical conductivity of 16500 S/m and Seebeck coefficient of 109 $\mu$V/K and a power factor of $196\mu$W/mK$^2$. This is a highly scalable and low cost process to fabricate flexible thermoelectric devices on different low temperature substrates and the devices demonstrated here opens up many opportunity to transform thermoelectric energy harvesting and cooling applications.

**Keywords:** Flexible thermoelectric, Aerosol Jet printing, Photonic sintering, Additive manufacturing

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[*]Speaker

# Prediction of thermal conductivity in highly disordered nanocomposite structures: From large-scale Monte Carlo simulations to simple analytical models.

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## Abstract

Nanostructuring is a promising approach for next generation thermoelectric materials yielding ultra-low thermal conductivities and enhanced thermoelectric performance. Some of the lower thermal conductivities in nanocrystalline materials have been achieved in materials that include hierarchically sized features, at the atomic size, the nanoscale, and the mesoscale. These can scatter phonons of various wavelengths and reduce phonon transport throughout the spectrum. However, understanding qualitatively, but more importantly quantitatively how hierarchical disorder reduces thermal conductivity in nanostructured materials, is still far from clear.

In this work, we solve the Boltzmann transport equation for phonons using the Monte Carlo method in Si-based nanostructures with a large degree of disorder. We examine thermal conductivity in structures with nanocrystalline grain boundaries, in addition to nanopores in both an ordered and highly randomized fashion. Such materials have recently demonstrated experimentally ultra-low thermal conductivities, even below the amorphous limit [1, 2]. We find that the influence of nanocrystallinity by itself on the thermal conductivity becomes dominant when the grain sizes become smaller than the average mean free path of phonons. We also show that the reduction in thermal conductivity in porous structures is significantly higher when the pores are randomized in terms of size and position, compared to when they are placed in an orderly fashion. Finally, we extract simple, analytical models that accurately captures the thermal conductivity in nanostructures which include a combination of nanograins and nanopores, either in ordered, or randomized fashions.

Taborda *et* al. *Nat. Sci. Rep.,* 6, 32778, 2016.
Tang *et* al. *Nano Let.* 10(10), 4279-4283. 2010.

**Keywords:** Modelling and simulations, Monte Carlo simulations, Thermal conductivity, disordered silicon nanomaterials, porous silicon material, nanocrystalline silicon material.

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# Study on the interfacial stability of n-type Yb0.3Co4Sb12/Zr/Ni thermoelectric joints at high temperature

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## Abstract

For skutterudite(SKD) based TEGs, which have outstanding efficiency in the medium temperature range with low generating cost, the main challenge is the major element, Sb, diffuses and reacts with almost every common electrode material such as Ni, Cu, Al. Consequently, the barrier is added between the TE material and the electrode comprising the typical structure of the TE joint. Here we fabricated n-type Yb0.3Co4Sb12/Zr/Ni thermoelectric joint to study the block effect of Zr as a diffusion barrier and the mechanism of the formation of the diffusion layer. We find that the bonding between the Yb0.3Co4Sb12 and Zr with diffusion layer was formed without cracks and holes after sintering and the contact resistivity at the joint was 1.02 $\mu\Omega\cdot$cm2. By EDS analysis, the diffusion layer was conformed as ZrSb2 and the thickness of that was 1.64 $\mu$m. After being aged at 600 ∘C for 3 days, the thickness of the diffusion layer reached 15.3 $\mu$m and the contact resistivity reached 10.63 $\mu\Omega\cdot$cm2. The block effect of Zr almost equals to that of Ti. But the mechanism is different, because the diffusion layer at the Yb0.3Co4Sb12/Zr/Ni thermoelectric joints is only one constituent. The relationship between the thickness of the diffusion layer and the square root of aging time is linear. It means the mechanism of the formation of the diffusion layer is controlled by the diffusion step.

**Keywords:** Skutterudite, Thermoelectric joint, Interfacial diffusion

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# ZT enhancement of silicon thermoelectrics by germanium nanoinclusions using phonon-interference resonance

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## Abstract

We report an unambiguous phonon-interference resonance effect originating from germanium nanoparticles (GeNPs) embedded in silicon (Si) matrix and its resulting ZT enhancement. A combination of phonon wave-packet method with atomistic dynamics and finite element method in continuum theory is used to characterize the resonance effect. We find multimodal phonon resonances, caused by destructive interference of coherent lattice waves propagating through and around the nanoparticle, give rise to sharp phonon transmittance dips, blocking phonon transport in the lower-end frequency range (from sub- to a few THz) that is hardly diminished by other nanostructures. The finiteness of wave packet width broadens and shallows the transmittance dip, i.e., deterioration of the phonon-interference resonance effect, unless it is two-orders-of-magnitude larger than the particle size, which bears universal significance in other coherent phonon wave related phenomena that utilize local resonance. Atomistic Green's function is employed to evaluate phonon transport reduction including such resonance effects. The electron transport calculation is conducted using non-equilibrium Green's function with tight-binding model and it finds a modest degradation of electrical properties due to similarly conductive property of Ge and Si. The ballistic transport calculations of phonon and electron are extended to diffusive regime by incorporating other diffusive scattering events with effective mean free paths in Landauer formula, for evaluating ZT which is realistic and comparable directly to experiments. The five-fold ZT enhancement of GeNPs embedded structure compared to bare Si demonstrates the effective decoupled phonon and electron transport, and similar scenarios with other materials and configurations are beneficial for silicon thermoelectrics.

**Keywords:** phonon interference resonance, nanoparticle, electron and phonon transport, ZT, silicon thermoelectrics

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# The study of an influence of sample shape on the measurements error using laser flash method

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### Abstract

Laser flash method is a common way to evaluate thermophysical properties of thermo-electric materials. A significant disadvantage of method is very strict sample size and shape requirements that limit measurement accuracy and reproducibility. The main goal of this study is to evaluate how sample size and shape deviation affects the accuracy of measurments during the laser flash method. Comsol multiphysics software was utilized to model measurement process based on actual unit parameters. The ideal sample had a cylindrical shape with diameter of 12.7 mm and height of 2.1 mm. The sample was made of graphite. Different values of upper surface slope were set by the surface angle variation. It was considered that there were no other factors that may cause any additional deviation. As a result, the relation between potential measurment error and angle of the slope was revealed. The dependence of error value on the slope angle has been obtained and analyzed. The curve has a form similar to a parabolic one. It is shown that amount of error value of 4 % was observed with a slope of not more than 0.5 degree [1]. The study shows that surface slope has a significant impact on laser flash measurements accuracy. It may help to improve laser flash method due to more comprehensive picture of the process. [1] Jan Zajas, Per Heiselberg. DCE Technical Report No. 144. "Measurements of thermal diffusivity, specific heat capacity and thermal conductivity with LFA 447 apparatus". ISSN 1901-726X, Aalborg University. 2013.

**Keywords:** laser flash method, thermoelectric materials, finite elements method, error estimation, thermal conductivity measurement

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# Quantum transport simulations for the thermoelectric properties of bipolar materials

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## Abstract

Low bandgap thermoelectric materials (e.g. BiTe, PbTe and their alloys) suffer from degraded performance at high temperature due to an increase in the bipolar thermal conductivity [1, 2]. Efforts to reduce the bipolar effect have included alloying to increase the band gap [3], while theoretical studies have shown that superlattice barriers can filter minority carriers and consequently maintain ZT at high temperatures [4]. In addition, a large number of studies are currently devoted to nanostructuring such materials to reduce their overall thermal conductivity.

In this work we theoretically address the issue of reducing bipolar conduction effects in low bandgap nanostructured materials by employing the quantum mechanical Non-Equilibrium Green's Function (NEGF) method. We consider materials with embedded nanoinclusions, a typical deliberately included feature in experimentally realised materials. The NEGF method is most suitable for such studies as it is geometry flexible and can include electron phonon interactions, as well as all quantum mechanical effects at the nanoscale.

We show that nanoinclusions themselves (even up to the 15% densities that we examine), can provide some reduction in the bipolar thermal conductivity in certain cases, although the effect is small. Importantly, however, we show that suppressing bipolar conduction is accompanied by an improvement in the overall power factor of the order of 10%. Given the importance of nanoinclusions in reducing lattice thermal conductivity, this power factor improvement in the bipolar regime shows that additional benefits in the ZT of nanostructured materials can be achieved under proper optimisation.

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J. Bahk *et.* al. Phys. Rev. B, **93**, 165209, 2016

**Keywords:** modelling, nonequilibrium Green's function, bipolar thermal conductivity, nanoinclusions

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# Grain boundary charge transport with an inhomogeneous description for polycrystalline thermoelectric materials

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## Abstract

It's well-known that grain boundaries can significantly affect figure of merit $zT$ of thermoelectric (TE) materials, due to the enhanced carrier scattering from grain boundary poten-tial barriers. Conventional grain boundary transport models for TE materials (*e.g.* SiGe[1], Mg2Si[2], NbFeSb[3]) typically treat their contribution to resistance using Matthiessen's rule on the carrier scattering rate. However, in some TE materials like Mg3Sb2[4], SnSe[5], or Na1–xPbmSbySem+2, the width of the space-charge region (*e.g.* ˜10 nm) can be compa-rable or even longer than the carrier mean free path, which violates the basic assumption of Matthiessen's rule. We propose that, by treating the grain boundary region as a secondary phase, we can model the conductivity and thermopower of, for example, n-type Mg3Sb2-based materials with various doping levels and different average grain sizes at temperatures between 300-600K. Our model can also explain the thermally activated mobility observed below 500K, which can not be fully explained by conventional trasnport model using ionized-impurity scattering (see [6] for more details). The results can be further applied to other TE materials with strong grain boundary effect, providing a potential direction of improving the $zT$ of polycrystalline thermoelectric materials.

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Kuo, J. J., Kang, S. D., Imasato, K., Tamaki, H., Ohno, S., Kanno, T., & Snyder, G. J., Energy & Environmental Science (2018).

**Keywords:** grain boundary, charge transport model, thermally activated mobility

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# Lattice dynamics and electronic structure in CoSb3 skutterudites

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## Abstract

By means of *ab-initio* Born-Oppenheimer molecular dynamic simulation we investigate the influence of thermal motion of ions on the electronic structure of CoSb3 skutterudite. The average electronic structure at finite temperature was obtained by averaging electronic structure along molecular dynamics trajectory. As a result of thermal motion of ions, electronic bands shift and broaden. The obtained temperature behavior of electronic structure is in a qualitative and quantitative agreement with the results of optical absorption experiments. Such a renormalization of electronic energy levels should affect electronic transport properties, and therefore to be considered while developing thermoelectric modules. [1] P.Korotaev and A.Yanilkin, Jour. Mat. Chem. C 5, 10185 (2017)

**Keywords:** skutterudites, molecular dynamics, electronic strucure

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# Two step simulation to optimize thermoelectric material for self-powered wearable applications

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## Abstract

Wearable devices have great potential to pioneer new market areas. Since the wearable device is attached to the body, it is possible to generate electricity from the body heat instead of relying on the battery. Although there are various methods to increase thermoelectric power generation using the body heat such as structural optimization, and heat management of the thermoelectric generator(TEG), the performance of the TEG is still highly dependent on the TE material. If the heat flux through the device is constant, the output is greater for the TE material with high figure of merits (ZT). However, the heat flux through a TEG attached to the body changes depending on the properties of a TE material. The high material ZT does not guarantee the maximum performance of the TEG in wearable applications. In this study, two-step simulation was conducted to find the optimal composition of material properties for the maximum power generation. The material properties of p-type BiSbTe3 according to the carrier concentration were calculated by using the first principles. From the material properties, the power density of the TEG *vs.* the carrier concentration was calculated with a thermoelectric resistance model of the wearable TEG system. The result shows that optimum carrier concentration for the highest material ZT is different from that for the maximum power density. The material with the maximum ZT did not generate the highest power density. As the thermal conductivity of the TE material decreases, the gap is reduced because the temperature difference across the TEG increases as the effect of the parasitic thermal resistance of entire system decreases. The result shows that engineering for TE material should be performed with considering the entire thermal system, not only considering the improvement of material ZT.

**Keywords:** Thermoelectric Generator, Human Body Heat, Device Simulation, First, Principles Calculation, Material Engineering

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# Modeling and analysis of segmented thermoelectric generator performance using effective properties

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## Abstract

Development of new architectures for thermoelectric generators (TEGs) is crucial for optimal and efficient operation over a wide temperature range, from 200∘C to 700∘C. In addition, a comprehensive mathematical model that considers heat transfer and thermal losses needs to be developed to model and analyze the geometrical effects on the characteristics of TEG. The model should also account for the thermal and electrical contact resistances. In this study, an analytical and numerical model for a segmented TEG was developed which was validated using single couple devices. The model of the TEG was used to investigate steady state behavior as a function of geometric parameters as well as operating conditions. The performances under different geometric parameters was analyzed where the thickness of layers and area ratio of TEG's legs were varied. The analyses also quantify the effect of thermal losses such as conductive and radiative heat losses on performance of TEG using effective properties. Comparative studies revealed that the thermal losses of TEG predominantly increases heat transfer at the hot substrate and subsequently increases the power output, while the increase in heat input directly affects the efficiency of TEG. The results of parametric study showed that the efficiency increased as P-type and N-type leg area approaches a certain optimal ratio and each layer of the segmented TEG operates within optimal temperature range. In addition, the effective properties and compatibility factor of the device accounted for the improvement of performance with optimized geometric architectures.

**Keywords:** Modeling, effective methods, segmented thermoelectric generator, thermal loss, heat transfer

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# Design of Optimal Electronic Band-Pass Transmission for Improved Thermoelectric Performance

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## Abstract

A perfect electronic band-pass (BP) transmission having a certain width is theoretically demonstrated to be ideal for nanoscale thermoelectric (TE) generators in terms of generating maximum power-efficiency trade-off. In a recent work, we have shown that a resonant tunneling double barrier heterostructure when embedded in a typical electronic anti-reflection cavity (ARC), produces an almost perfect BP transmission which is also strongly immune to the disastrous charging effect. While being extremely effective in terms of delivering an excellent trade-off between output TE power and heat conversion efficiency, this device proposal, on the other hand, is practical, robust, viable and easily realizable within the current fabrication capabilities as well. Given the main focus on realizing a perfect BP transmission, we have also explored various design possibilities of ARC to achieve an optimal design manifesto instead of relying on the standard one. In this process, we have found that the ground state transmissivity (area under transmission) for various combinations of ARC barrier height and width exhibits a hyperbolic nature at its maximum values. This result prompts us to explore the TE performance of other viable design proposals. To illustrate the supremacy, we propose two other proposals alongside our previous one and it is theoretically shown using the Non-Equilibrium Green's Function (NEGF) technique within the self-consistent charging effects that the new structures strongly enhance the output power at a given efficiency or vice-versa and therefore offer an excellent trade-off between them. This study suggests the optimal device design for an improved TE generator and would therefore give rise to a lot of interest in pursuing realistic TE designs via lineshape engineering.

**Keywords:** Thermoelectric, power, efficiency, NEGF, anti reflection, bandpass, transmission

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# Heat Transfer Analysis on the Measurement of Thermoelectric Performances using a Harman Method

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## Abstract

To estimate the dimensionless figure of merit $zT$ of thermoelectric materials, the measurement of three parameters, namely the Seebeck coefficient, the electrical resistivity, and the thermal conductivity, is required. In general, these measurements are performed using different setups, which can influence the accuracy of $zT$. An alternative method to obtain the $zT$ is the Harman method, which can directly estimate $zT$ through AC and DC voltage measurements using $zT = (V\mathrm{DC} \text{-} V\mathrm{AC} / V\mathrm{AC})$, where $V\mathrm{DC}$ and $V\mathrm{AC}$ are the voltage across the sample by applying the DC and AC, respectively [1,2]. However, in the actual experiment, the estimated value of $zT$ deviates from the ideal value because this formula is based on the assumption of an adiabatic condition. There have been only a few studies on the quantitative correction [3,4]. In recent studies, the analysis of the several sources of heat losses was limited to the macroscopic system derived from the heat balance equation [5,6]. Here, in order to accurately determine $zT$ using the Harman method, we performed thermal analysis using the heat conduction equation, which is based on the Fourier law. We developed the thermal correction using the one-dimensional heat conduction model, considered as heat losses of convection, Joule heating, Thomson heating, and conduction through lead wires. From this analysis, the temperature distribution in the sample was investigated. Our results indicate that a correction factor for each heat loss should be added to the original formula for highly accurate Harman measurement.

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M. S. Kang *et al.*, *Sci. Rep.* **6**, 26507 (2016).

**Keywords:** Material measurement, Harman method, Thermal analysis

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# Superlattice design for maximal thermoelectric efficiency at finite power

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## Abstract

Thermoelectrics (TE) convert heat energy from a temperature gradient to electrical energy and vice-versa. Bulk TE materials, however, offer a very low conversion efficiency. It was mathematically shown that a Dirac-delta transport function could enhance the thermoelectric figure of merit, to reach a conversion-efficiency approaching the Carnot efficiency, but vanishing zero output power. Thus, this trade-off between output power and efficiency can be further explored using nanostructures by tailoring the lineshape of the transmission function . This leads to the idea of using superlattices (SL) in TE, to achieve the rectangular boxcar transmission function that produces a unity transmission coefficient over a band-pass energy range. We study extensively the thermoelectric performance in terms of efficiency at maximum power output, of various SL structures such as anti-reflective SL and Gaussian distributed SL. Suitable designs that can favorably influence the electron transmission through the SL for maximum transmissivity, immune to the charging effect are presented using the non-equilibrium Green's function (NEGF)-Poisson formalism. Out of all configurations, we demonstrate that the SL with a Gaussian distributed barrier thickness offers the highest achievable efficiency at maximum power output. We also analyze our device designs with the conventional figure of merit approach to counter support the results so obtained, and note a high $zTel = 6$ value in the case of Gaussian distribution of the barrier thickness. With the existing advanced thin-film growth technology, the suggested SL structures can be certainly achieved.

**Keywords:** Nanostructured thermoelectrics, Boxcar transmission, Gaussian superlattice

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# Electron-phonon scattering in n-type PbTe from first principles calculations

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## Abstract

In PbTe, one of the most efficient thermoelectric materials, the main scattering mechanism for electrons has been attributed to acoustic phonons to explain the temperature dependence of the mobility [1]. However, a recent study suggested that longitudinal optical (LO) phonon scattering is important in PbTe [2]. In order to determine the dominant scattering mechanism, we build accurate models of electronic and phonon bands, and electron-phonon scattering solely from first principles. We show that it is necessary to go beyond standard density functional theory to accurately describe the electronic states and deformation potentials of PbTe near the band gap. Our calculations show that acoustic phonon scattering in n-type PbTe is much weaker than previously thought [2]. We found that LO scattering dominates the electronic transport in PbTe over a large range of temperatures and carrier concentrations. At higher doping concentrations, screening weakens LO scattering, making acoustic and LO scattering comparable. We further calculate thermoelectric transport properties by solving the Boltzmann equation in the generalized transport relaxation time approximation. Our calculated values of the electronic mobility and power factor of PbTe are in very good agreement with experiment [3]. Our results may stimulate future search for new polar thermoelectric materials with weak acoustic phonon coupling.

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**Keywords:** lead telluride, electron phonon, first principles, transport

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# Optimal thermal conductance for thermoelectric generators under various thermal boundary conditions

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## Abstract

Power optimisation of a thermoelectric generator, through thermal analysis, is shown to depend on thermal boundary conditions. As such, optimal thermal conductance criteria for heat exchangers and thermoelectric modules are developed for several thermal boundary conditions, including in the presence of heat losses and fluid flows. An effective internal resistance and thermoelectric conductance are defined to consider their interconnected influence on thermal transport and generated power.

Modelling of the thermoelectric effect and co-optimisation of heat and electrical aspects demonstrates that the commonly used thermal impedance matching criterion is subject to several restrictions and limited in application. This criterion states that maximum power generation for a thermoelectric generator is achieved when the thermal resistance of the thermoelectric modules is equal to that of the heat exchangers. Under constant temperature difference, thermal impedance matching is shown to be optimal only if an effective thermoelectric conductance that includes the effect of the load resistance is considered and only after having maximised the conductance of the generator's heat exchangers. With constant heat flux, output power is maximal when the thermoelectric conductance is minimised, regardless of impedance matching.

When considering heat losses and fluid flows, the optimisation changes as a balance must be struck between the temperature difference and the heat flux. This demonstrates a completely different approach to designing a thermoelectric generator under realistic thermal conditions. Optimality criteria for load resistance and thermal conductance are developed for each thermal boundary condition to maximise power. Optimal design considerations are presented in accordance with these findings.

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[*]Speaker

# Possible ways of temperature field inhomogeneity elimination during spark plasma sintering of thermoelectrics

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## Abstract

Spark plasma sintering (SPS) is widely used for thermoelectrics fabrication. Sintering temperature plays a crucial role in nanostructure formed and thermoelectric properties obtained. However, temperature field in a sample during SPS is not easy to measure. Ordinary, such measurements are implemented using a pyrometer or thermocouples. These approaches can not provide a precious measurements or give a whole picture of temperature distribution in a sample volume. Numerical approach is a convenient way to analyze a sintering temperature. There are few works on SPS simulation taking into account a thermoelectric effect; however, it may be significant for materials with high Seebeck coefficient, especially, thermoelectrics. This fact may cause a gradient of sintering temperature field in a sample volume and structure inhomogeneity.A finite elements method was used to simulate SPS process of several types of thermoelectrics. The model considered as time-dependent, 2D-axisymmetric. The model presented in this study takes into consideration the impact of thermal expansion, contact resistances and thermoelectric effect. It is shown that sintering in ordinary symmetric SPS setup configuration (die is symmetrically located, punches have equaled height) cause gradient temperature field in a sample. Temperature gradients in both radial and vertical directions exist. Possible ways of temperature gradient elimination (in the volume of a sample) due to the change of setup configuration are proposed.

**Keywords:** spark plasma sintering, finite elements method, synthesis simulation, thermoelectric effect, temperature field management

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# Power output design of a Thermoelectric Generator module using heat-transfer modelling and simulation: An application for the cement industry

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## Abstract

Growing awareness of global warming, energy shortages and increasing prices of fossil fuels, along with stringent emission regulations, give the impetus for research on new technologies for more efficient, environmentally friendly and cost-effective energy production. An initiative towards achieving this goal is large-scale application of Thermoelectric Generators (TEG) in industries using gas and steam turbines or other power systems with considerable energy losses. If large energy losses through the exhaust gases can be converted in part into electricity by the noiseless, pollution-free, reliable and easy-to-use TEG, obvious benefits will be obtained. TEGs are devices that convert temperature differences into usable electricity. The current paper focuses on analysing the power output of a TEG module that can be used in a cement production plant through a waste-heat-recovery system. A detailed three-dimensional heat-transfer and fluid dynamics model is used to identify critical geometrical parameters through the COMSOL Multiphysics software. The model is used to calculate temperature differences between cold and hot side of thermoelectric modules (TEMs) and thus study the effect on power output of the TEG. In other words, the larger the temperature differences between the hot and the cold and hot side of TEM, the better the power performance of the TEG. The optimization analysis of the geometric parameters of the TEG was carried out using standard orthogonal array of Taguchi method. An L16 orthogonal array with five controlling factors at four levels was employed in the design of experiments method. The identified design through this systematic analysis leads to a significant increase of peak and average output power of the TEG module.

**Keywords:** Thermoelectric Generator, heat transfer modelling, cement industry, COMSOL, Taguchi

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# Structure and thermoelectric properties in substituted tetrahedrite

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### Abstract

Tetrahedrites ($Cu_{10+x}Tr_{2-x}Sb_4S_{13}$, Tr=Mn, Fe, Co, Ni, Zn) are a new class of materials suitable for thermoelectric applications [1]. They are mineral compounds, which compete with p-type state-of-the-art thermoelectric materials. In recent studies, isovalent substitution has been shown to be an effective method to enhance the power factor through increased band degeneracy near the Fermi level and independent of charge carrier concentration modifications [2,3]. Isovalent doping would also lead to local structural perturbations in the crystal, which cause thermal conductivity reduction [4,5].

An experimental investigation of $Cu_{12}Sb_4S_{13-x}Se_x$ shows that these compounds exhibit power factor enhancements via reduced electrical resistivity and unaltered Seebeck coefficient [6]. Both in synthetic and natural tetrahedrites, As, Bi and Te were found to substitute for Sb. Unlike As and Bi substitutions which are not expected to affect the transport properties, the Te atom has an extra electron with respect to Sb and thus can change the Fermi level in the electronic structure. Whereas Te and S are isovalent, Te substitution for S in tetrahedrite has never been reported in literature.

The aim of our work was to understand why in tetrahedrite Te atoms prefer to substitute for Sb instead of S. This work was performed by means of first-principle density functional theory approaches [7-9] coupled with a topological analysis of the electron density using Bader's QTAIM method [10-12].

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**Keywords:** tetrahedrites, DFT

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# Pressure induced convergence of conduction bands in Al doped Mg2Si

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## Abstract

Aluminum doped Mg2Si is a type of nontoxic and economical thermoelectric material. High-Pressure High-Temperature technology provides a fast and low-cost way to synthesize this material. It is found that the impurity Al could split the triply degenerate conduction band bottom of Mg2Si, according to DFT calculations. Thereupon we have simulated the system under external pressures ranging from 0 to 4GPa. As a result, the lowest conduction band is shifted upward as the pressure increases and particularly, degenerates with the upper 2-fold degenerate band near 2GPa. The convergence of the conduction band bottom results in a larger density-of-states effective mass and thus produces a larger Seebeck Coefficient. Present calculations have been validated by experiments.

**Keywords:** Mg2Si, Density Functional Theory, High Pressure, Convergence of Conduction Bands

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# Hybrid Thermoelectric-Concentrated Photovoltaic System: Thermal Control and Monitoring

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**Abstract**

Concentrating photovoltaic systems use lenses or mirrors to concentrate the incident light onto a small area, high efficiency photovoltaic cell. To minimise the photovoltaic (PV) cell costs, typical concentration ratios used are around 300-1000, resulting in incident irradiances 30-100 W/cm2. These concentration ratios are well suited to the use of high efficiency III-V semiconductor, triple junction PV cells, as used in this work. These high power densities can lead to thermal issues with the PV cell, as the PV cell efficiency declines with increasing temperature, and may even reduce its lifetime, especially if the PV cell temperature rises above 85 ∘C.

We discuss a Bismuth Telluride based thermoelectric module applied to a hybrid PV-TE system, with the PV cell bonded to the top surface of the thermoelectric module. The thermoelectric module can be used to sensitively monitor the PV cell's temperature via its open circuit voltage as well as to provide active, rapid and controllable cooling of the PV cell. The thermoelectric module and thermal system were modelled using the finite element analysis software COMSOL Multiphysics. The modelled results are compared to the experimentally realised system, which demonstrated the importance of good thermal interfaces and a high thermal conductance of the thermoelectric module to improve passive cooling. This feedback has led to a second generation thermoelectric module design with improved performance.

**Keywords:** Photovoltaic, Cooling, Thermal control

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# Assessing the Performance of Skutterudite Modules

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## Abstract

Hundreds of scientific papers have been published on skutterudite materials in recent years, but only a few thermoelectric modules have been demonstrated due to the challenges associated with thermoelectric module assembly such as integration of multiple different elements, scalable manufacture, and device design. The major limitation to fully realizing the potential of high temperature thermoelectric materials is the lack of cost effective and reliable Ohmic contact technology which is essential for achieving the performance promised from materials measurement. This includes mechanical strength, high thermal and electrical conductivity of interconnections and crucially their long-term thermal stability.

Here, we demonstrate realization of a high-temperature, 7-couple skutterudite-based thermoelectric module with a maximum power output of PMAX = 416 mW at $\Delta$T = 42 degC and power density of ~475 mW/cm2 per pellet area. Experimental data of module performance has been related to simulation results from finite element analysis using COMSOL Multiphysics® software. Different manufacturing parameters have also been investigated and their influence on electrical, mechanical and microstructural features of bonded components are reported here. The long-term reliability has been evaluated through isothermal annealing at hot-leg working temperatures to investigate the stability and evolution of the joint, including an estimation of the lifetime.

**Keywords:** Skutterudites, modules, modelling

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# Thermoelectric properties of diazonium salt modified carbon nanotubes: first principles simulations

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## Abstract

Carbon nanotubes (CNTs) are expected to be potential candidates for flexible thermoelectric materials with high power factor. In contrast to high PF, the figure of merit ZT of a CNT is not so high because of its high thermal conductivity. Recently, several techniques to reduce the thermal conductivity of CNTs have been proposed. The diazonium salt modification of CNTs is known as one of such techniques because chemical modification of diazonium salts introduces the sp3 hybridizations, which play a role of phonon scatterers, to the sp2-hybridized hexagonal network in a CNT. However, the details of influence the diazonium salt modification on thermoelectric properties of CNTs have not clarified yet.

In this talk, we present first-principles simulation results on thermoelectric properties of CNTs modified by diazonium salts. We show the dependence of the coverage of diazonium salts on the electrical conductivity, the Seebeck coefficient and the power factor of a semiconducting CNT with diameter 0.794nm. The electrical conductivity decreases rapidly with increasing the coverage of diazonium salts, whereas the Seebeck coefficient increases due to a charge transfer from the diazonium salts to the CNT. The power factor decreases due to the rapid reduction of electrical conductivity, but ZT is known to be increased by the diazonium-salt modification because of the rapid reduction of thermal conductivity. In addition, we clarify the optimal carrier density of CNTs for a fixed coverage of diazonium salts.

**Keywords:** carbon nanotube, diazonium salt, power factor, first principles simulation

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[*]Speaker

# Flexible and scalable thermoelectric elastomers based on carbon nanotube-polydimethylsiloxane (CNT:PDMS) composites

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## Abstract

State-of-the-art thermoelectric (TE) materials are mostly inorganic that are rigid, toxic, and expensive. There is an increasing interest in development of flexible thermoelectric materials based on organic materials and carbon nanotubes due to their advantages such as low cost, non-toxicity, lightweight and mechanical flexibility. However, they suffer from low carrier mobility, difficulties in doping, and poor scalability to large thicknesses. Therefore, polymer composites comprising a low-cost elastomer matrix with embedded conducting media can be promising candidates for cost-effective flexible thermoelectric materials. In this work, we report scalable solution synthesis and thermoelectric properties of single walled carbon nanotube (SWCNT)-polydimethylsiloxane (PDMS) composites. PDMS is a silicone-based non-conducting elastomer that is highly flexible, solution-processable, scalable in production, and biocompatible, suited for wearable energy harvesting. Randomly distributed SWCNT networks embedded in PDMS matrix provide electrical conduction paths based on percolation transport to achieve high electrical conductivity in the composites. Our composites with varying weight percentages of SWCNTs made of mixed metallic and semiconducting (s-) CNTs in PDMS show a steady increase in thermopower up to 40% CNT before saturation of thermopower. The maximum thermopower is obtained to be ~60 $\mu$V/K, approaching that of pure SWCNTs, ~70 $\mu$V/K without doping. This value is expected to further increase to ~150 $\mu$V/K by selectively embedding s-CNTs only or even higher with appropriate doping. The electrical conductivity also increases in the range of 10 ~ 80 S/cm with CNT content in the range of 10 ~ 40%. The composites are highly flexible and can be molded into the desired thickness on the order of several millimeters.

**Keywords:** hybrid thermoelectric, flexible material, carbon nanotube, PDMS

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# Ab Initio Simulation on Thermoelectric Properties of Carrier-Doped Graphene by Ferroelectrics

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## Abstract

It is required that both the electrical conductivity and the Seebeck coefficient are high for developing high thermoelectric power factor (PF). Currently, graphene has attracted attention as a potential material with high PF. It is, however, necessary to dope proper carriers into graphene because the thermoelectric performance has an optimum value for a carrier density due to the trade-off relation between the conductivity and the Seebeck coefficient. As carrier injection methods, the chemical doping is difficult to finely control the carrier density and also reduces the conductivity of graphene. On the other hand, the electric field doping uses an external power source, which is not suitable for the application to the energy harvesting. We thus propose a new carrier injection method using the spontaneous polarization of ferroelectric materials, which does not need an external power source. To validate this new method, we have investigated the carrier injection to graphene by the spontaneous polarization of Polyvinylidene Fluoride (PVDF) using the first-principles calculation based on the density functional theory. We found that electrons (holes) are injected into up to the third layer of multilayer graphene from the interface when multilayer graphene contacts a surface of positive (negative) polarization of PVDF. This means that the thermoelectric properties of graphene can be controlled by injecting carriers using the polarization of PVDF. It is then necessary to optimize a carrier density to improve thermoelectric performance of graphene. The optimum value of the carrier density in graphene is known as approximately $10^{12}$ cm$^{-2}$. Because a carrier density of $7 \times 10^{13}$ cm$^{-2}$ was injected in our calculation, it is possible to optimize thermoelectric performance by reducing the polarization.

**Keywords:** Graphene, Ferroelectrics, PVDF, Carrier Injection, DFT

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# Seebeck coefficients of conducting polymers correlated with doping levels

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## Abstract

Thermoelectric properties of conducting polymers such as poly(3-hexylthiophene) and poly(3,4-ethylenedioxythiophene) were investigated in correlation with doping level measured by a potential-step chronocoulometry (PSC) method. It was found that the log–log plot of Seebeck coefficients against doping levels showed a good linearity.

**Keywords:** conducting polymers, potential, step chronocoulometry, doping level

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*Speaker

# A New Synthesis Route of a Gel Film Formation Process and the thermoelectric properties of synthesized PEDOT/PSS films

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## Abstract

Characteristics of organic thermoelectric materials such as flexibility, light weight, and printability are noteworthy advantages over inorganic materials. Poly(3,4-ethylenedioxythio phene)/poly(4-styrenesulfonate) (PEDOT/PSS) films have attracted attention as a promising candidate for thermoelectric modules as an energy harvester. We have developed an original PEDOT/PSS film formation process called as a gel film formation process. It is perfectly different from the direct film formation process such as a spin coating method and a drop casting method. Without common treatment processes such as a pre- or post-treatment [1,2], the gel film formation process can enhance the thermoelectric properties.

The dropped amount of PEDOT/PSS in polar solvents and the gel formation time in polar solvents were changed during our process. The less dropped amount of PEDT/PSS resulted in the thinner film. Power factor ($PF = S\hat{}2\sigma$) of the films increased with decreasing the film thickness or increasing the treatment time. The effect on PEDOT/PSS by solvents is reported to cause a reduction of surplus insulating PSS [3]. We have applied a fitting function given by a diffusion equation to the measured data of electrical conductivity for the purpose of understanding of the reduction behavior of PSS during our process.

In this presentation, we will report the possible enhancement of the thermoelectric properties of PEDOT/PSS films.

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**Keywords:** PEDOT/PSS, energy harvesting, original film formation process

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# Hybrid Polymer/Nanoparticle Composites for High-Performance Thermoelectrics

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### Abstract

Hybrid materials consisting of inorganic nanostructures surrounded by conducting polymers have been proposed for thermoelectric applications near room temperature. The performance of thermoelectric materials are typically discussed in terms of the dimensionless figure of merit ZT = S2$\sigma$-1T, where S is the Seebeck coefficient, $\sigma$ is the electrical conductivity, is the thermal conductivity, and T is the temperature. Improving ZT can be challenging due to the interrelation of these parameters with the carrier concentration. Hybrid composites are attractive because of the low intrinsic thermal conductivity of the polymer, utilizing nanostructuring as a route towards improved phonon scattering, application of energy filtering effects, and their solution processability which allows for use of high-throughput device manufacturing methods. In this contribution, we focus on our recent synthetic developments. We typically begin by synthesizing chalcogenide nanowires that are encapsulated in conducting polymers, which we later use as templates for the growth of a variety of compounds, such as Ag, Bi, and Pb-based chalcogenides, with tunable stoichiometry. Depending on the compounds of interest, this can result in improved properties, or allow us to tune our composites from p-type to n-type. We detail the development of the structural and morphological properties of our hybrids and then relate these properties to the thermoelectric performance. Ultimately, we aim to develop high-performance composites for low-cost room temperature thermoelectric applications.

**Keywords:** polymer, hybrid, chalcogenide, synthesis

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# Thermoelectric transport properties of interface-controlled Si composite using reduced graphene oxide

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## Abstract

We report the effects of interface control using reduced graphene oxide (RGO) on thermoelectric transport properties of polycrystalline Si composites. In this experiment, Si powders were prepared by the pulverization of As-doped Si wafer using high-energy ball milling. The Si powders were coated with RGO in dimethylformamide solution, followed by the consolidation using spark plasma sintering. The interface control using RGO exerted beneficial effects on thermoelectric transport properties of the Si composite. First, the interface-controlled Si composite exhibited significantly enhanced charge transport properties as compared with conventionally prepared Si composite, and the mechanism was discussed based on our high-temperature Hall measurement results. Second, we could suppress lattice thermal conductivity in the composite significantly thanks to the additional phonon scattering at the Si-RGO interfaces. Consequently, both the enhancement in electrical conductivity and the reduction in lattice thermal conductivity were simultaneously achieved through the interface control using RGO. These desirable features led to the enhancement of $ZT$ in the interface-controlled composite, and detailed results will be presented.

**Keywords:** Si, reduced graphene oxide, interface control, charge transport, thermoelectric

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# Search for new hybrid materials with thermoelectric properties

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## Abstract

Hybrid materials have been widely studied these last years for their great potential in the fields of magnetism, luminescence, catalysis, biology. These materials are composed of an organic subnetwork connected to an inorganic network that both possess their own property. The presence and in the best case the coupling of these two properties could be of great interest to design new materials for selected applications like energy generation. Hybrid materials could be obtained by direct reaction of an organic precursor with an inorganic salt leading to the formation of materials such as Metal Organic Framework's (MOF's) and Coordination Polymers or by intercalation of an organic guest in an inorganic host. For this study, we explored this second route to synthesize hybrid materials with thermoelectric properties by using a well-known inorganic layer materials in which will be inserted organic molecules. The first result concerning the synthesis, the structural characterisation and the thermoelectric properties (magnetism, resistivity and Seebeck coefficient ) will be presented.

**Keywords:** hybrid material intercalation host guest

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# Enhancement of thermoelectric properties of PEDOT:PSS films by applying an alternating electric field during preparation

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## Abstract

PEDOT:PSS is one of the most hopeful thermoelectric material for realizing energy harvesting system because of its flexibility and relatively high dimensionless figure of merit ZT. Ishida et al. drastically improved the electrical conductivity of PEDOT:PSS by adding a small amount of ethylene glycol (EG). Recently, our group reported that the electrical conductivity of PEDOT: PSS could be improved by applying a DC electric field during film formation. Meanwhile, Schwarz at al. reported that the an alternating (AC) electric field agglomeration is more efficient in formation of uniform carbon black network than a DC method. In this work, we synthesized PEDOT: PSS thin films under an AC field and evaluated their electrical conductivity and Seebeck coefficient S as a function of repetition frequency for field. PEDOT:PSS solution added 3% EG was dropped onto quartz substrate, and it was dried and solidified under an alternative rectangular or a sine wave electric field of 1.25 kV/cm with a repetition rate up to 4 kHz. The dry process was carried out at room temperature for 3 hours followed by annealing for crystallization at 130 for 30 min under the electric field. increases gradually with increase of repetition frequency for electric field. The highest values of 1370 S/cm and 1250 S/cm were attained for rectangular and sine wave application, respectively. Rectangular wave application seems to be more effective for enhancement than sine wave application, probably due to a high frequency component included in a rectangular wave. On the other hand, S was almost constant. This suggests that carrier density does not change and mobility increases with . It is plausible that crystallization would be promoted by an external electric field, which acts on the PEDOT:PSS solution more deeply when the frequency of electric field become higher.

**Keywords:** PEDOT:PSS, organic thermoelectric materials, electric field, electrical conductivity

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# Buckypapers of Palladium Nanoparticle-Decorated Carbon Nanotubes as Effective Thermoelectric Materials

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## Abstract

Since a single carbon nanotube (CNT) has a high thermal conductivity ($> 3000$ W/m K) with high electrical conductivity (10,000-100,000 S/cm), the CNTs were thought not to be useful as thermoelectric (TE) materials. However, when CNTs are randomly assembled to form sheets (buckypapers) or hybridized to form hybrid films, then their thermal conductivities decrease dramatically due to the phonon scattering at the interfaces of CNTs. Thus, many interesting CNT-containing hybrid materials with high TE performance have been reported (C. Yu et al. *ACS Nano* **2011**, *5*, 7885; Y. Nonoguchi et al. *Sci. Rep.* **2013**, *3*, 3344; N. Toshima et al. *Adv. Mat.* **2015**, *27*, 2246). TE properties of CNT-containing hybrid materials are depending upon those of CNTs themselves. But purified CNTs are very expensive. Recently super-growth CNT (SGCNT; K. Hara et al. *Sci.* **2004**, *306*, 1362), which is more defective but less expensive than the purified one, has been mass-produced by Nippon ZEON Corp. Here we present the preparation and TE performance of the bucky-paper composed of Pd nanoparticle (NP)-decorated SGCNTs as novel hybrid TE materials. The decoration of SGCNTs with Pd NPs was carried out by both a physical and a chemical method. In the physical method, separately prepared Pd NPs were mixed with SGCNTs, while, in the chemical method, the Pd NPs were prepared in the dispersion of SGCNTs in N-methylpyrrolidone. The 17.4wt% Pd NP-decorated SGCNT buckypaper, prepared by the chemical method, showed much higher electrical conductivity (160 S/cm) at 345K than that of the blank SGCNT one (90 S/cm), which resulted in the hybrid films with about 2 times higher power factor than the blank. We discuss the mechanism of this improvement in TE performance of the SGCNT buckypaper by decoration with Pd NPs. Acknowledgements: This work was supported by MEXT, NEDO and Nippon ZEON Corp., Japan.

**Keywords:**  CNT, Pd nanoparticles, Hybrid, Buckypaper

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# Thermoelectric Properties of Disordered Semiconducting Polymers

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## Abstract

Recently, improved thermoelectric (TE) properties have been reported in organic semiconductors based on the polymer PEDOT:PSS, reaching ZT~0.25 upon optimizing the carrier concentration. This, combined with advantages such as low cost, easy synthesis, and an inherently low thermal conductivity, makes polymers a very attractive choice for commercially viable TE applications. A long-standing problem in TE materials is the interdependence of transport coefficients, which makes it difficult to simultaneously increase the Seebeck coefficient and electrical conductivity. In this work, we investigate the TE properties of disordered organic semiconductors. Our charge transport model is based on electron hopping between localized sites with a Gaussian disorder model for their energies. We numerically solve Pauli's master equation to compute the time-averaged occupational probabilities of the sites from which relevant transport quantities are calculated. Our results show that larger overlap between localized electronic states can improve conductivity without adversely affecting the Seebeck coefficient. Positional disorder affects the overlap between neighboring states and aids in the formation of conduction paths with an increased probability of carriers in high energy sites, ultimately leading to simultaneous increase in conductivity and Seebeck. We introduce positional correlation to investigate the role of partial ordering and find that it negatively affects conductivity. On the other hand, energetic disorder widens the density of states and leads to increased energy gap between neighboring sites, thus hindering transport and adversely affecting both conductivity and Seebeck. We conclude that both positional and energetic disorder greatly impact TE properties, with positional generally increasing and energetic disorder decreasing them

**Keywords:** Thermoelectrics, Organic semiconductors, disorder

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# Enhanced electronic conduction and phonon scattering in the Ga2O3(ZnO)m - In2O3(ZnO)m (m=9 and 15) solid solution by designing interfaces at the nanoscale level.

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## Abstract

The Ga2O3(ZnO)9 and In2O3(ZnO)9 homologous phases have attracted attention as thermoelectric (TE) oxides due to their layered structures. Ga2O3(ZnO)9 exhibits low thermal conductivity, while In2O3(ZnO)9 possesses higher electrical conductivity. The crystal structure and thermoelectric properties of the solid solution of Ga2O3(ZnO)9 - In2O3(ZnO)9 were studied to tune their TE performance.

We prepared high quality $(1-x)$Ga2O3(ZnO)m - $x$In2O3(ZnO)m ($x$= 0.2, 0.4, 0.6, 0.8 and 1.0 with $m$=9 and 15) ceramics by the solid-state route using B2O3 and Nd2O3 as additives. The crystal structures were analysed by XRD, HRTEM and atomic resolution STEM-HAADF-EDS. A layered structure with compositional modulations was observed in all samples in the ZnO-Ga2O3-In2O3 system. All the compositions exhibited nanoscale structural features identified as Ga- and In-rich inversion boundaries (IB's). Small In additions in the Ga2O3(ZnO)m compounds triggered basal and pyramidal In IB's typically found in the In2O3(ZnO)m system. The (Ga0.8In0.2)2O3(ZnO)m compounds do not exhibit the structural features of the *Cmcm* Ga2O3(ZnO)m compound, which is formed by a stacking of Ga rich IB's along the pyramidal plane of the wurtzite ZnO, but features resemble the crystal structure exhibited by the *R-3m* In2O3(ZnO)m with basal and pyramidal In IB's.

The structural changes led to improved thermoelectric performance. (Ga0.8In0.2)2O3(ZnO)9 showed low thermal conductivity of 2 W/mK and high-power factor of 150 $\mu$W/mK2 giving a *ZT* of 0.07 at 900 K.

The processing conditions of selected compositions were optimised to increase the *ZT*. Fast cooling rates increased the electrical conductivity without increasing the thermal conductivity due to improved microstructure and crystal structure. By combining the low thermal conductivity of the Ga2O3(ZnO)9 and the high electrical conductivity of the In2O3(ZnO)m compounds led to a higher *ZT* in solid solution compounds.

**Keywords:** Oxides, homologous compounds, ZnO, thermoelectric

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# Understanding the links between percolation and thermoelectric performance: from polycrystalline materials to amorphous polymers

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## Abstract

The seminal works of Hicks and Dresselhaus created a shift in the thermoelectric and sustainable research, by highlighting the advantages of using complex nanostructures in favour of the crystalline counterparts.[1,2] While new promising classes of materials including polycrystalline compounds,[3] conductive polymers,[4-6] hybrid composites,[7-9] and aerogels[10] have since emerged, a strong belief still remained that only a dense material packing may lead to a high, theoretically predictable performance. Nevertheless, recent contributions made significant steps towards rationalising the apparently unusual behaviour of such disor-dered polymers,[11,12] whereas a corresponding model for other particulate systems is still required. Accordingly, this contribution aims to provide an overview on the differences and similarities between these seemingly distinct materials, focusing on the key role of percolation for the thermoelectric performance. To pinpoint the influence of grain size, conductivity and morphology on the percolation governing the Seebeck coefficient and electrical conductivity, a series of cases are discussed, involving $Cu_2O$, doped $ZnO$, polyaniline, graphite, CNTs and composites thereof. Results indicate that percolation may hold the key towards unifying these diverging directions in thermoelectric research.

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**Keywords:** percolation, polycrystalline, oxide particles, amorphous polymers

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# Nanoscale microstructural and chemical analysis of Al-doped ZnO

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## Abstract

Al-doped ZnO belongs to the most efficient n-type thermoelectric oxides, with best reported ZT values between 0.3 and 0.6 at high temperature. As this material crystallizes in a simple crystal structure and consists of light elements, its thermal conductivity is quite high, and the moderate ZT values mostly originate from large values of the power factor, which can be tuned by the doping or co-doping. However, the best performances are hard to reproduce, and seem to be very sensitive to the synthesis process and thermal treatments. Besides, although a solubility limit of Al close to 0.3% has been confidently observed using SIMS (with a resolution of about 100x100 nm$^2$), with the precipitation of ZnAl2O4 above this limit that contributed to the reduction of the lattice thermal conductivity, the concentration of carriers and the electrical properties (and thus the power factor) keep depending on the concentration of Al well above 0.3%, which seems contradictory. While trying to produce Al-doped ZnO/SiO2 nanocomposites, we have studied the microstructure and composition of Al-doped ZnO samples at the nanoscale using a combination of atom probe tomography and ultra-STEM observations. Surprisingly, we have seen that the local concentration of aluminum in the matrix can locally reach about 2% *without precipitation of ZnAl2O4* with a size of enriched clusters of the order of 10nm. This poster will summarize our observations, which may contribute to explain part of the discrepancies in the literature dealing with the (thermo)electric properties of Al-doped ZnO.

**Keywords:** oxides, ZnO

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# Thermoelectric properties of Zn doped BiCuSeO

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## Abstract

The layered BiCuSeO is a promising thermoelectric material due to its ultra-low thermal conductivity and moderate Seebeck coefficient. Doping of monovalent/divalent elements at the Bi site helps in reducing the electrical resistivity. In this report, $Bi_{1-x}Zn_xCuSeO$ (x=0.0, 0.02, 0.04, 0.06, 0.08, 0.1) has been prepared by solid-state synthesis method to elucidate the Zn doping effect at the Bi site. The density functional theory was used to predict the defect formation energy of Zn at both Bi and Cu site and found to be 0.189 eV and 0.194 eV respectively. The ZnO was used as a precursor to dope Zn at the Bi site preferably in the oxide layer. The X-ray diffraction patterns were matched with BiCuSeO (PDF#45-0296), which indicates that the phase purity of the samples. The sub-hundred nanometers of the particles were observed in the microstructure of $Bi_{0.9}Zn_{0.1}CuSeO$ may be due to the unreacted ZnO nanoparticles. The electrical resistivity and the Seebeck coefficient of the samples decreased with increase in the doping concentration. The electrical resistivity of all the doped samples showed a transition from metallic to semiconducting behavior around 473 K. The Seebeck coefficient of the samples x=0.06, 0.08, 0.1 showed a very weak temperature dependence above 523 K. The highest power-factor of 0.35 mW/m-K2 was obtained for x=0.02 at 773 K. The total and the lattice thermal conductivity increased with increasing x, which might be due to the strong covalent bonding between Zn and O atom. Highest zT of 0.48 at 773 K has been obtained for x=0.02 mainly due to increased power-factor.

**Keywords:** Zn doping, Electrical resistivity, Seebeck coefficient, Thermal conductivity

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# Growth and characterization of thin film CaMnO3 and CaMn1-xNbxO3 for thermoelectrics.

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## Abstract

Oxides are promising as thermoelectric materials as they are a stable, cheap and environmentally friendly alternative to tellurides which are both rare, expensive and toxic. Thin films are interesting to study because of the possibility to characterize the effect of nano-structuring, e.g. grain size and multilayers. Additionally, thin films have potential applications where small dimensions are important, for example on chip cooling. In this study, CaMnO3 thin films have been grown by two step sputtering-annealing method. First rock salt structured Ca0.5Mn0.5O films were deposited by radio frequency (RF) reactive magnetron cosputtering from elemental targets of calcium (Ca) and manganese (Mn), followed by annealing at 700 ◦C for 3 h in oxygen flow to form the final phase of perovskite CaMnO3. For niobium (Nb) doping in CaMn1-xNbxO3 thin films cosputtering was performed from elemental targets of Nb, Ca, and Mn, with varying target power at Nb-target, while keeping constant power at Ca, and Mn-targets. The crystal structures of the films were assessed by X-ray diffraction
*theta*-2
*theta*, and pole figure analyses, and plan-view scanning electron microscopic studies. The grown films are confirmed to be textured and phase pure. Four point probe measurements at room temperature show a decrease in electrical resistivity from 2 cm for pure CaMnO3 film to 0.1 cm for CaMn1-xNbxO3 film. The decrease in resistivity is an effect from increased carrier concentration due to Nb-doping.

**Keywords:** CaMnO3, thin film, thermoelectrics

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# Single Crystalline InGaZnO Nanowires for Potential Thermoelectric Applications

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## Abstract

InGaZnO nanowires are an interesting material for thermoelectric applications owing to the combination of single crystalline nanostructure, which promotes better charge transport properties, and natural superlattice structure, which reduces thermal conductivity caused by interface phonon scattering. However, only few investigations have been devoted to producing InGaZnO nanowires, and these few studies employed extremely high temperatures ($> 1400 \circ$C) or long processing time (12-96 h). In this study, high aspect ratio InGaZnO nanowires were grown for the first time at a low temperature of $700 \circ$C via a novel bimetal-catalyzed growth. Amorphous InGaZnO thin films (200 nm) were deposited on Si substrates (1cm x 1cm) via RF magnetron sputtering using sintered (In:Ga:Zn ˜2:2:1) targets at room temperature. Mo (100 nm) and Au (20 nm) thin films were then deposited using electron beam evaporation. Finally, annealing was performed at $700 \circ$C for 2h under N2 atmosphere. SEM analysis revealed high aspect ratio nanowires, with diamaters of ˜100-200 nm, and lengths of ˜10-30 $\mu$m. EDX line profile revealed the composition of the nanowire body to be composed of In, Ga, Zn and O, while Mo and Au were detected on a nanoparticle at the nanowire tip. This verifies their role as a bimetal catalyst. The single crystalline nature of the nanowires, as well as their superlattice structure, was also confirmed using TEM analysis. The nanowire growth is proposed to be caused by a synergistic effect of the catalytic activities of both Mo and Au. Mo is known to induce crystallization of amorphous semiconductors at a lower temperature than their crystallization temperature, while Au has been widely used as a nanowire growth catalyst. Electrical characterization was also performed on a single nanowire, which showed an ohmic behaviour. The measured conductivity is about 1.12 S/cm.

**Keywords:** IGZO, nanowire, thermoelectric nanowire, superlattice nanowire

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# High Temperature Thermoelectric Properties of Dual Doped Ca3Co4O9 Ceramics

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## Abstract

In this work, we have investigated the effect of Na and W dual doping on structural and thermoelectric properties of Ca3-$2x$Na$2x$Co4-$x$W$x$O9 ($0 \leq x \leq 0.075$) polycrystalline samples. Powder X-ray diffraction data show that all samples are phase pure, without any detectable secondary phase. The diffraction peaks shift to lower angle values with increase in doping content ($x$), which is consistent with the larger ionic radii of doped ions. The X-ray photoelectron spectroscopy data reveal that a mixture of Co2+, Co3+ and Co4+ valence states are present in these samples. The electrical resistivity, Seebeck coefficient and thermal conductivity are all improved with doping. The maximum thermoelectric power factor ($PF = S2/rho$) of 2.7 x 10-4 W/mK2 is obtained for $x = 0.025$ sample at 1000 K, which is 2.2 times higher than the undoped sample. The corresponding thermoelectric figure of merit ($ZT$) of 0.21 at 1000 K is also much higher than the pristine sample. These results indicate that Na and W dual doping is a promising approach for improving high temperature thermoelectric properties of Ca3Co4O9 system.

**Keywords:** X, ray diffraction, Dual doping, Thermoelectric power factor, Thermoelectric figure of merit

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# Synthesis and thermoelectric properties of oxide nanocomposites containing metal nanoparticles formed by exsolution reaction

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## Abstract

Whereas oxide materials generally have high phonon thermal conductivity due to their simple crystal structures and light constituent elements, some oxides such as strontium titanate show preferable electrical properties as thermoelectrics. One of common approaches to reduce the phonon thermal conductivity is introduction of nanocomposite structure. Nanocomposite structures such as nanoparticles are expected to selectively scatter phonons, and thereby reduce the phonon thermal conductivity without seriously decreasing the electrical conductivity. Moreover, if metallic nanoparticles are introduced into oxide matrix, an increase in the electrical conductivity and a decrease in the thermal conductivity can be realized at the same time. However, grain growth of the nanoparticles is likely to occur during sintering.

In this paper, we present a novel microstructural control using exsolution reaction of metallic nanoparticles from oxides under a reducing atmosphere. This reaction proceeds at relatively low temperature, suggesting a possibility of preservation of the nanostructure. Xiao *et al.* reported synthesis of Nb-doped strontium titanate containing Ni nanoparticles as catalysts [1]. The Ni nanoparticles are about 50 nm in diameter, and are expected to selectively reduce phonon thermal conductivity. Here we report synthesis and the thermoelectric properties of Nb-doped strontium titanate nanocomposites containing Ni nanoparticles, and discuss the relation between the structure and the properties in detail.

G. Xiao *et al., ACS Appl. Mater. Interfaces*, **6**, 19990 (2014).

**Keywords:** Nanocomposite, Oxides, Metal Nanoparticle, Selective Phonon Scattering

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# Synthesis, Structure and Thermoelectric Properties of Molybdenum Oxides

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## Abstract

Transition metal oxides (TMOs) gain increased interest in the thermoelectric community due to their vast availability, potential for high-temperature application and wide range of tunable transport properties [1]. Molybdenum oxides reflect the latter due to a variety of structures even in the binary system [2]. Spark-plasma sintering (SPS) is suitable to synthesize single-phase bulk material of these phases whose structures are refined from X-ray diffraction experiments. Transport measurements over a wide temperature range (1.8 K $\leq T$ $\leq$ 760 K) reveal relative low Seebeck coefficients as the major drawback for thermoelectric (TE) application yet, but allow insight into the dependence of the electrical transport on the crystal structure.

Besides metallic phases (MoO2, Mo4O11, Mo17O47), especially Mo18O52 with classical semi-conducting behaviour qualifies for further TE optimization due to its low lattice thermal conductivity (lat < 1 Wm-1K-1). Above 440 K a transition from $p$-type to $n$-type is found.

Detailed investigations on the pseudo-2D conductor $\gamma$-Mo4O11 illustrate that classical Wiedemann-Franz approximations can yield substantial errors even for oxides with metallic character. The SPS-synthesis of bulk material also allows an understanding of correlations between the electrical transport and the grain size in comparison to single-crystals from chemical vapour transport reactions.

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**Keywords:** molybdenum, oxides, spark plasma sintering, electrical transport, thermal transport, x ray diffraction

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# Improvement of the Thermoelectric Properties of the Perovskite SrTiO3 by Cr-Doping

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## Abstract

In recent years, among different thermoelectric (TE) materials, SrTiO3 have been receiving great attention due to their greater capacity and conversion between electrical energy and heat energy. The thermoelectric properties of the SrTiO3 can be improved by substitutional doping on different sites (A-site and B-site) in the lattice. In this study, the improvement of the thermoelectric performance of the perovskite SrTiO3 by Cr-doping has been investigated. The doped SrTiO3 with Cr were synthesized by the conventional solid-state reaction method. The electronic transport properties including Seebeck coefficient, electrical conductivity, and thermal transport properties in a moderate temperature regime from 300 K to 900 K have been investigated. The large absolute value of Seebeck coefficient with low thermal conductivity achieved by Cr-doping. The electrical conductivity quite low but increased with increasing doping level up to x=0.002 mole and hence the power factor increased with increasing doping level up to x=0.002 mole. The maximum $ZT$ value was observed for SrTi0.098Cr0.002O3 at 773 K by the combination of high value of Seebeck coefficient and low thermal conductivity.

**Keywords:** Perovskite oxide, doping, vacuum hot, pressing, electronic properties.

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# Thermoelectric Properties of Al-doped Silver Antimonate

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**Abstract**

The defect pyrochlore structure of silver antimonate was investigated in photocatalytic activities because of its narrow band-gap. The valence band edge of high thermopower $AgSbO3$ can be modified by substitution at Ag or Sb site. The thermoelectric samples of Ag1-xAlxSbO3 were prepared by a conventional solid-state method followed by consolidation using a hot-press process. A metallic $AlSbO3$ as a dopant with the same structure as $AgSbO3$ has shown to influence the electrical conductivity and Seebeck coefficient of parent material. In this work, we present a comparative study of Al-doped samples by evaluating the thermoelectric properties include electrical resistivity ($\rho$), Seebeck coefficient (S) and thermal conductivity () at the same operating temperature range.

**Keywords:** pyrochlore oxide, defect control, thermoelectric property

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# Enhancement of Thermoelectric Properties in co-substituted and Composite Oxide Systems

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## Abstract

Thermoelectric (TE) materials provide an opportunity to harvest waste heat to useful electrical power. The existing best TE materials like Bi2Te3 are not suitable for high temperature applications because of their chemical instability. Oxide thermoelectric materials are stable at high temperatures and hence are promising candidates to be used in TE generators. However, the difficulties in oxide systems are their low figure of merit (ZT). We explore methods for enhancing the value of ZT in oxide systems. Here, we will talk about two examples where we have been able to enhance the ZT of parent oxide compounds *via* (a) co-substitution and (b) compositing. We have shown that co-substitution in LaCoO3 system enhances the Seebeck coefficient and electrical conductivity at higher temperature and reduces the thermal conductivity via increased phonon scattering and hence shows high figure of merit (ZT=0.14 at 480 K). We have also explored TE properties of (1-x)LaCoO3.(x)La0.7Sr0.3MnO3 composite, where an enhanced ZT (0.09 at 620 *K* for x=0.05) is observed as compared to LaCoO3 system. Strategies for further enhancement of ZT will also be discussed.

**Keywords:** Seebeck coefficient, Figure of merit, composites

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# Self-assembled Ni0.98Li0.02O and Zn0.98Al0.02O composite interface for thermoelectrics

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## Abstract

Among the thermoelectric (TE) materials candidates, oxides have been rapidly developed in the last decade because of potential advantages over non-oxides in terms of chemical and thermal stability at high temperatures. One of the factors limiting the ideal performance of a conventional oxide TEG arises from the use of metal interconnects , which are vulnerable to inter-diffusion, cracking, evaporation, and oxidation. To overcome these challenges, Span and co-workers proposed the use of a direct p-n junction [1], despite the expected high electrical contact resistance. Using a composite interconnect from the desired p- and n-type oxide material at the interface (p-c-n) can increase the effective contact area and reduce the resistance.

p-type NiO and n-type ZnO are promising oxide materials for high-temperature thermo-electrics [2, 3]. In the present work, we investigate a composite consisting of Ni0.98Li0.02O and Zn0.98Al0.02O, prepared by a citric acid sol-gel method [4]. X-ray diffraction and scanning electron microscopy confirm the presence of both NiO and ZnO phases. Current-voltage characteristic curves of direct planar p-n and composite p-c-n junctions were investigated, with the latter showing less resistive behaviour, attributed to the increased effective contact area.

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**Keywords:** oxides, composite, p, n junction

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# High temperature stability of hot pressed Sr-doped Ca3Co4O9 samples

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## Abstract

Since 1997, with the discovery of large thermoelectric (TE) properties in NaxCoO2 great efforts have been carried out to explore new CoO families with high TE performances. Following this intense research work, some layered cobaltites, such as Ca3Co4O9 and Bi2AE2Co2Ox (AE = Sr, Ca and Ba) were also found to exhibit promising thermoelectric properties. As layered Co-oxides show strong crystallographic, electrical, and thermal anisotropy, a proper grain alignment is necessary to attain high TE properties in bulk samples. Moreover, adequate doping can further improve their electrical conductivity and reduce thermal conductivity. On the other hand, when intended to be used in practical applications, they have to maintain their properties practically unchanged during long time under working conditions, that is, high temperatures (˜1000 K) under air atmosphere. In this work, the effect of long thermal treatments under working conditions on the mechanical and thermoelectric properties of Sr-doped textured Ca3Co4O9 samples has been studied. Ca2.93Sr0.07Co4O9 has been prepared through the classical solid-state method and textured using the hot-uniaxial pressing technique (30 MPa and 1123K). The initial samples showed very attractive TE properties (PF ˜ 0.6-0.7 mW/K2m at 1000 K) as well as mechanical ones (flexural strength ˜ 300 MPa at room temperature). The samples were then maintained at 1023 K under air for different periods of time (0, 24, 96, 384 and 1536 hours). The evolution of their microstructure, as a function of aging time, has been studied and related with their TE and mechanical properties.

**Keywords:** Oxides, Ca3Co4O9, texture, thermal aging, mechanical properties

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# Influence of Bi to Sm ions isovalent substitution on thermoelectric properties of BiCuSeO oxyselenides

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## Abstract

BiCuSeO oxyselenides have become one of the most promising oxide thermoelectric materials due to their moderate electrical transport performance, extremely low thermal conductivity and potential high-temperature chemical stability. It has been reported that isovalent substitution of Bi ions by rare earth elements such as La could lead to the band gap changes resulting in the increase of the thermoelectric performance [1]. In this work, we examined the effect of isovalent Bi substitution by Sm on the thermoelectric properties of $p$-type Bi1-$x$Sm$x$CuSeO ($x$ = 0; 0.02; 0.04; 0.06; 0.08) synthesized by a facile method combining a solid-state reaction and spark plasma sintering. The band gap estimations pointed to the narrowing of the band gap with Sm-doping. This change in the band structure led to a dramatic decrease of the Seebeck coefficient and a sharp increase of the electrical conductivity, while the thermal conductivity demonstrated a slight increase with the respect to Sm-doping level. In addition, the result revealed that there is a moderate difference of ~15 % between the total thermal conductivity measured in perpendicular and parallel directions relative to the pressing direction, while the electrical transport properties exhibited isotropic behavior. Considering the trade-off between Seebeck coefficient and electrical conductivity the figure of merit $zT$ was not strongly affected by the Bi substitution. Nevertheless, the BiCuSeO band gap variation can be a useful tool for enhancing the thermoelectric properties of $p$-type BiCuSeO oxyselenides. Calculated from the measured data the $zT$ exceeds 0.65 at 973 K for the undoped sample, which is one of the highest values for pristine BiCuSeO among literature data.

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Y. Liu, J. Ding, B. Xu, J. Lan, Y. Zheng, B. Zhan, B. Zhang, Y. Lin, C. Nan, Appl. Phys. Lett. 106 (2015) 233903.

**Keywords:** BiCuSeO, band gap tuning, spark plasma sintering, Sm doping

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# Thermoelectric properties of InGaO3(ZnO)m, a layered oxyde with complex crystal structure

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## Abstract

Thermoelectricity is an efficient way to face the need for renewable energy over the world. However most of the efficient thermoelectric materials developed to date are sensible to oxidation at high temperature. Therefore, these materials are difficult to use in several industrials process, such as high temperature furnaces or thermal power plant. To solve this problematic, oxides are good candidates for their properties of thermal stability and resistance to oxidation. One of the most promising family of compounds for such applications are TCO's (Transparent conductive oxides) where ZT values of 0.5 and 0.3 were found in doped ZnO and In2O3 respectively.

The main issue preventing the ZT from rising in these compounds is the too large values of their thermal conductivity. In order to reduce these values there is a high interest in studying lamellar oxides with a complex structure such as the In2O3(ZnO)m. The large number of atoms in the lattice combined with the reduction of the symmetry increases significantly the number of optical phonon modes. Besides, phonons scattering at the interfaces decreases their mean free path. Previous works on these materials have led to a significant reduction of the thermal conductivity, with ZT values around 0.25.

In this work the family of compounds InGaO3(ZnO)m is studied in order to reduce the thermal conductivity further, through the increased distortion of the coordination polyhedrons and local disorder. Previous work on this material was done mainly with thin films or single crystals, very few with polycrystalline bulk materials. Besides, the influence of $m$ on the transport properties was hardly studied.

In this poster, I will discuss our recent results, focusing on the influence of the synthesis method on the quality of the material, and I will show that low thermal conductivity can be obtained for an optimal value of $m$.

**Keywords:** Transparent Conductive Oxide, layered oxide

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[*]Speaker

# Thermoelectric Properties MgTiO-Based Conductive Composite Materials Prepared by Spark Plasma Sintering

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## Abstract

Bulk polycrystalline MgTiO has low thermal conductivity and high thermal shock resistance, but its electrical conductivity is extremely low. On the other hand, TiN exhibits excellent electrical conductivity, but its thermal conductivity is quite high and Seebeck coefficient is extremely low. In this study, we aimed to develop a new type thermoelectric material which has low thermal conductivity of MgTiO and high electrical conductivity of TiN by preparation of MgTiO/TiN composite material.
The samples were prepared by spark plasma sintering (SPS) of commercially available MgO, TiO (rutile) and TiN powders at 1100 °C for 10 min under 80 MPa in vacuum. The TiN content was controlled from 0 to 30 vol.%. After sintering, all samples were characterized by XRD, SEM, Laser Flash and ZEM.

All the composites exhibit relatively low thermal conductivities (2.6-6.2 W/mK) at the room temperature compared to that of TiN (28.8 W/mK). It is considered that microcracks in the bulk, which were formed during sintering process, effectively suppressed the increase of thermal conductivity of composites. The electrical conductivities of composites were extremely improved compared to MgTiO with increasing TiN content although Seebeck coefficients decreased. While the maximum ZT is still not high, forming such composites [1] seems an effective strategy considering the unmeasurably low performance of MgTiO by itself, and analysis of interfaces will be discussed.

T. Mori and T. Hara, *Scripta Mater.*, **111**, 44-48 (2016).

**Keywords:** Spark Plasma Sintering, Composite material, Oxide, Reactive sintering

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# Application of powder engineering to achieve high performances in textured Sr-doped Ca3Co4O9 with very short processing times

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## Abstract

Thermoelectric (TE) materials can directly transform a temperature gradient into useful electric power without any moving part owing to the Seebeck effect. This characteristic makes them very promising to harvest the wasted heat released in the classical energy transforming systems, increasing their efficiency and helping to fight against global warming. In spite that oxides still have relatively low performances, when compared with intermetallic materials, their chemical composition is usually heavy metals-free. This is an important advantage, as it avoids scarce and expensive elements which can limit their massive applications. On the other hand, typical processing routes for these TE oxides include solid state reactions, which are characterized by long thermal treatments, leading to expensive procedures when considering their industrial production. The goal of this work is the drastic reduction of processing time, when compared with the optimal conventional route, to obtain high-density textured Sr-doped Ca3Co4O9 materials without losing TE and mechanical performances. The precursors evolution will be studied to establish the best milling and calcination conditions to reduce the number and time-length of these steps. With the optimal precursors, texturing will be performed through hot uniaxial pressing at different temperatures, pressures and time, to maximize the samples density, and their mechanical and thermoelectric performances, while minimizing the processing costs.

**Keywords:** Oxides, Ca3Co4O9, processing, mechanical properties

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# "Structural imperfections" in the transition metal oxides and thermoelectricity

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## Abstract

Oxides are considered as interesting candidates for high-temperature thermoelectrics due to their stability, lack of toxicity and low cost. Most complex metal oxides are electrical insulators. However, the presence of mixed valence states, due to a partial reduction of metal ions (e.g. W5+, Mo5+, Ti3+), and the accompanying "structural imperfections", such as crystallographic shear planes, pentagonal columns, etc., lead to the appearance of free carriers and therefore quasi-metallic electrical conductivity.
Binary and ternary oxides range from materials with large densities of planar crystallographic defects (Magnéli phases with a single type of shear plane, block structures with intersecting shear planes and phases with more defective block and channel structures). Crystallographic or microstructural features of these oxides are in 0.3–2 nm size range, so that oxide phonons can efficiently interact with them.

The known high-temperature synthesis methods reveal difficulties in controlling the reaction progress at elevated temperatures and the homogeneity and shaping of the final product. Our SPS studies of reaction mechanisms reveal that the formation of phases follows a diffusion-control reaction between the reaction components induced by dc current. While conventional sintering methods deliver equilibrium phases, the non-equilibrium conditions in SPS may allow the formation of metastable non-equilibrium compounds.

We report the SPS-assisted investigation of a part $M$ – O (M – Ti, V, Mo, W) binary systems in regions $TiO2$ – TiO and $M O3$ – $M O2$ ($M$ – Mo, W) phases, which were used as a starting components in the synthesis.

We will show how the formation of the different types of the "structural imperfections" in the non-conductive oxides influence on the crystal structure, electrical and transport properties of the synthesized sub-oxides.

**Keywords:** transtition metal oxides, planar crystallographic defects, SPS synthesis

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# Development of SrTiO3/TiO2 thermoelectric oxide with eutectic morphology

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## Abstract

Eutectic material with a phase-separated structure (eutectic structure) can be fabricated by a unidirectional solidification from the melt with the chemical composition at a eutectic point, and it has been investigated as a scintillator with an optical waveguide structure and high strength material. In many studies of thermoelectric materials including nanopowder, some improvements of thermoelectric properties were observed due to the phonon scattering at the boundaries. If the eutectic structure composed of scattering phases in the matrix phase of a thermoelectric material can be achieved, the eutectic structure can improve the thermoelectric properties. Therefore, we tried to develop a novel thermoelectric material with the eutectic structure and the thermoelectric properties were investigated. In this study, the eutectic material of the SrTiO3 [STO] and TiO2 [TO] was selected as a first try of thermoelectric eutectic material.

Starting materials, SrCO3 and TiO2 powders ($> 4N$), were mixed as the nominal composition at the eutectic point of STO and TO (SrO : TiO2 = 20 : 80) and the mixed powder was sintered at 1200∘C in air several times. Then, a STO/TO eutectic material was grown from the melt the sintered powder by a micro-pulling-down (m-PD) method using an iridium crucible. In addition, the Nd, La and Pr-doped STO/TO eutectic materials were grown by the same growth method. Grown eutectic materials were cut and polished for measurements of thermoelectric properties.

Grown STO/TO, and Nd, La and Pr-doped STO/TO eutectic materials were composed of the uniformly dispersed TO phase with a rod-shape in the STO matrix phase. The thermal conductivity of the Nd:STO/TO eutectic material was lower than half that of Nd:STO single crystal. Details of the fabrication by the m-PD method, the local structures, thermoelectric properties will be reported.

**Keywords:** eutectic material, SrTiO3, oxide, melt growth

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# Phonons in ZnO

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## Abstract

Zinc Oxide is an important semiconductor, widely used in piezoelectric transducers, optical waveguides, acoustooptic media, conductive gas sensors, transparent conductive electrodes and varistors. ZnO and related alloys have been proposed for thermoelectric applications due to high thermal stability, corrosion resistance, non-toxicity and low cost. A large thermal conductivity means there are currently limited thermoelectric applications, however it has been shown recently that a combination of Al-doping and nanostructuring reduce thermal conductivities by a factor 20 compared to bulk, whilst maintaining excellent electrical transport properties, to achieve a material with outstanding thermoelectric performance. The lattice contribution dominates the thermal conductivity of ZnO and, therefore, studying the lattice dynamics using neutron scattering techniques is the key to optimizing this important thermoelectric property. We report inelastic neutron scattering measurements that are in excellent agreement with our first-principles density-functional calculations. These data demonstrate the importance of anharmonicity and multi-phonon contributions in ZnO when modelling thermal transport properties.

**Keywords:** Phonons, Anharmonicity, Neutron Scattering, Multi, phonon, Ultra, low thermal conductivity, ZnO, Zinc Oxide, Nanostructured, Doped

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# Hot side electrical contacts for oxide thermoelectric modules

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## Abstract

*Oxide thermoelectric materials are good candidate materials for energy harvesting application at high temperature in harsh environments. However, to ensure high power output and stability over time, particularly the hot side electrical contacts needs to be chosen so that the contact resistance is low and remains low over time. Until now, mostly noble metals have been used. Since they have very high electrical conductivity and do not oxidize severly even at the high operating temperature they are a natural choice, but adds to the cost of the total system. In this work we present results of testing several different non-noble metals as alternative hot side contact. Through both isothermal and cycling tests we show that the formation of stable interfaces of many of these contact materials holds promise as a* way of contacting oxide thermoelectric modules.

**Keywords:** Metal contacts, Oxide modules, Long term Stability, Thermal cycling

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# Thermoelectric Properties of Si-Based Clathrates Prepared by Spark Plasma Sintering of Planetary-Ball-Milled Powders

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## Abstract

Recently, nanostructured bulk materials or nanocomposites have received much attention as practical materials, rather than thin films or superlattices, for use of thermoelectric applications because of their unique properties associated with the nano-interface effects. The potential barrier at grain boundary may contribute to enhance the Seebeck coefficient due to the energy filtering effect. In addition, the increase in density of interfaces would increase with decreasing grain size and may have a great influence on the scattering of phonons. Incorporating nanostructures into bulk materials will be a useful route to a further improvement of thermoelectric properties. $Ba_8Ga_{15}Si_{31}$ (BGS) clathrate particles ranging in size from several tens nanometers to submicron were prepared by a planetary ball milling technique, and their sintered materials (nano-BGS) with microstructures were prepared by a spark plasma sintering (SPS) technique, under the conditions of short sintering time, relatively high sintering pressure, and relatively low sintering temperature, preventing the grain growth. Nano-BGS samples were characterized by powder x-ray diffraction measurements, scanning electron microscope observation, and energy dispersive X-ray spectroscopy. In comparison with bulk-BGS prepared by SPS of micro powders, nano-BGS samples showed relatively large Seebeck coefficient, about –110 microV/K, at low temperature range. Relatively low thermal conductivity, as low as 0.8 W/(mK) at RT, was accomplished for nano-BGS. However, the electrical conductivity was extremely low, the orders of 0.001–0.1 S/cm at RT. These behaviors may be attributed to the increased scattering at the interfaces and pores in the microstructures. The design and control of interfaces is a significant issue to further improve the thermoelectric properties of Nano-BGS.

**Keywords:** Clathrate, planetary ball milling, nanoparticle, spark plasma sintering, interface, Seebeck coefficient, thermal conductivity, electrical conductivity

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# Study of the effects of Cobalt metal inclusions in an Yb14MnSb11 matrix

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## Abstract

Composites materials are made of two or more constituents with the intent of obtaining a final material that shows better characteristics than its components. In thermoelectrics, there are several cases in which the performances have been increased through the mixing of two different materials. The clearest examples are organic-inorganic composites where conducting materials are embedded in polymeric matrixes,[1,2] but due to the poor electric properties and thermal stability of polymers, their use remains limited. A different and more interesting case is when the composite is a mixture of an already promising TE material and a pure metal. Recent studies showed that a considerable increase in the zT can be obtained when nano-inclusions are blended in a material matrix.[3][4] In this work we studied the effect of Co metal inclusions in an Yb14MnSb11 matrix. The idea behind is to increase the thermoelectric properties of the 14-1-11 phase through the decoupling of the electrical transport properties ($\sigma$, S). By choosing metals characterized by high Seebeck coefficients, the inclusions are expected to provide a boost to the electrical conductivity, through the injection of free carriers, while affecting only marginally S. At the same time, the dispersed nano-agglomerate would create active phonon scattering centers that can further reduce the thermal conductivity. Moreover, an investigation of the chemical reactivity of the metal with the matrix has been analyzed, along with the evaluation of a possible percolation limit. References [1] B.T. McGrail, A. Sehirlioglu, E. Pentzer, Angew. Chemie - Int. Ed. 54 (2015) 1710–1723. [2] D. Portehault, V. Maneeratana, C. Candolfi, N. Oeschler, I. Veremchuk, Y. Grin, C. Sanchez, M. Antonietti, ACS Nano 5 (2011) 9052–9061. [3] Y. Liu, D. Cadavid, M. Ibáñez, S. Ortega, S. Martí-Sánchez, O. Dobrozhan, M. V. Kovalenko, J. Arbiol, A. Cabot, APL Mater. 4 (2016) 104813. [4] J.M. Ma, Improving the Mechanical Strength and Power Conversion Efficiency of High Temperature Thermoelectrics - PhD Thesis, University of California, 2014.

**Keywords:** thermoelectric, Zintl phases, doping

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# High-pressure high-temperature synthesis and thermoelectric properties of half-Heusler antimonide TmNiSb

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## Abstract

Half-Heusler (HH) compounds have been recognized as prospective candidates for thermoelectric applications. Recent exploratory reports indicated that $f$-electron bearing HH phases might possess better thermoelectric performance than their intensively studied counterparts based on $d$-electron transition metals due to smaller thermal conductivity. In this work, high-pressure high-temperature (HPHT) method was applied to synthesize polycrystalline samples of the HH alloy TmNiSb. The obtained materials were characterized by X-ray powder diffraction and scanning electron microscopy with energy-dispersive spectroscopy mapping. The results revealed that the ingots sintered at temperatures 20-750C consists of HH matrix and some Ni-rich precipitations. The most homogeneous specimen was obtained for the highest temperature from this range. Above 750C, the material was found to decompose into NiSb and pure thulium. Electrical resistivity ($r$) and Seebeck coefficient ($S$) measurements were carried out in the temperature interval 350-1000 K. The samples were found to exhibit semiconducting-like behavior with the values of $r$ ranging from 7 to 35 uOhmm, and no clear dependence on the synthesis temperature. All the specimens prepared showed positive S with the maximum magnitude increasing with increasing the sintering temperature from 70 up to 150 uV/K, observed at 550 K for the specimen synthesized at 750C. Accordingly, the power factor (PF) was found to rise from 3 up to 13 uW/(K^2cm). The obtained fairly large values of PF motivate further studies of the HPHT-prepared TmNiSb samples to determine their thermoelectric figure of merit. This work was partly supported by the National Science Centre (Poland) under research Grant no. 2015/18/A/ST3/00057.

**Keywords:** half, Heusler, rare earth compound, high, pressure high, temperature (HPHT) method

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# Thermoelectric properties of Mg3Sb2 single crystals grown by self-flux method

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## Abstract

Because waste heat recovery attracts great attention recently in environmental research area, attention to thermoelectric materials increases intensively. Several new thermoelectric materials with a figure-of-merit of ZT > 1 has been reported for the past decade. Mg3Sb2 is one of the promising thermoelectric materials that achieved ZT > 1.5 [1]. To clarify the origin of its high performance, intrinsic properties must be examined using Mg3Sb2 single crystals. Single crystal growth of Mg3Sb2 was already reported by S. Kim, et al. [2]. They grew single crystals with a slightly Mg rich composition of Mg : Sb = 3.5 : 2 in view of the high vapor pressure of Mg. In this work, we optimized the growth condition to obtain larger single crystals. Self-flux method was applied to grow single crystals with Mg or Sb as a flux. Thermoelectric properties of grown single crystals were, then, examined. Details of single crystal growth and results of measurements will be report in the conference.
H. Tamaki, H K. Sato, T. Kanno, *Adv. Mater.* 28, 10182 (2016).

S. Kim et al., *J. Mater. Chem. A*, 2, 12311 (2014).

**Keywords:** Mg3Sb2, single crystal growth, Zintl phase, pnictides

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# High thermoelectric performance in Bi0.46Sb1.54Te3 nanostructured with ZnTe

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## Abstract

Defect engineering and nano-structuring are the core stratagems for improving thermo-electric properties. In bismuth telluride alloys nanosizing individual crystallites has been extensively studied in efforts to reduce the thermal conductivity but nanostructuring with second phases has been more challenging. In this study, we demonstrate a thermoelectric figure of merit $ZT$ of 1.4 at 400 K, realized in Zn-containing BiSbTe alloys (specifically Bi0.46Sb1.54Te3) by integrating defect complexity with nanostructuring. We have succeeded in creating nanostructured BiSbTe alloys containing ZnTe nanoprecipitates. We present a melt-spinning-based synthesis that forms in-situ ZnTe nanoprecipitates to produce extremely low lattice thermal conductivity of ˷0.35 Wm-1K-1 at around 400 K, approaching the amorphous limit in the Bi1-xSbxTe3 system, while preserving the high power factor of Bi0.46Sb1.54Te3. These samples show excellent repeatability and thermal stability at temperatures up to 523 K. Theoretical calculations and experimental results show that Zn is inclined to form dual site defects, including two substitutional defects $Zn'Bi/Sb$ and a Te vacancy, to achieve full charge compensation, which was further explicitly corroborated by Positron annihilation measurement. The strong enhancement of thermoelectric properties was validated in a thermoelectric module fabricated with the melt-spun p-legs (ZnTe-nanostructured BiSbTe) and zone-melt n-legs (conventional BiTeSe) which achieved a thermoelectric conversion efficiency of 5.0% when subjected to a temperature gradient of 250 K, representing about 40% improvement compared with a commercial zone-melt-based module.

**Keywords:** BiSbTe, ZnTe, dual site defects, melt, spinning, band alignment, panoscopic approach, thermoelectric performance

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# Facile Room Temperature Solventless Synthesis of High Thermoelectric Performance Ag2Q (Q= S, Se, Te) via Dissociative Adsorption Reaction

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## Abstract

The very basic Ag2Q (Q=S, Se, Te) compounds constitute an important class of versatile materials with applications in thermoelectrics, optics, spintronics, magnetotransport, and solid-state ionics. Yet it is surprising that they are not fully understood partly because they present synthetic challenges in yielding high quality samples with repeatable properties. Simultaneous control of the stoichiometry, microstructure, and compositional homogeneity is a prerequisite for the fundamental and technological studies of Ag2Q, but is hard to attain by traditional methods (e.g., growth-from-the-melt, wet chemistry approaches) in view of the volatile nature of Q, and highly mobile Ag+ ions above the superionic phase transition at very low temperatures (e.g. 407 K for Ag2Se, 420 K for Ag2Te). In this work, we report a room-temperature self-sustaining synthesis method of Ag2Q that occurs at room temperature and requires no solvent. Technically, this method has minimum requirement of energy input, instrument and atmosphere control, yet creates rich microstructures, outstanding stoichiometry and compositional homogeneity. It is hard to find methods simpler than this. Scientifically the new procedure is based on the dissociative adsorption of Q by Ag and the reaction kineticsis in line with *Hard-Soft-Acid-Base* (HSAB) scheme (rate order Ag2Te > Ag2Se > Ag2S). For Ag2Se compound, the low carrier concentration achieved ₋˜1018 cm-3 and the optimized weighted majority-to-minority carrier mobility ratio observed in the samples as corroborated by the state-of-the-art thermoelectric performance of $ZT$ ₋˜1.2 at 390 K attest to the superiority of the synthesis route in yielding highly stoichiometric Ag2Se samples.

**Keywords:** Ag2Q (Q=S, Se, Te), dissociative adsorption reaction, HSAB scheme, thermoelectric performance

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