SYMPOSIUM S
S: Thermoelectric Materials 2003-Research and Applications

December 1 - 3, 2003

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*Invited paper
10:30 AM *S1.1

The thermoelectric power of bismuth nanowires is theoretically calculated to be greatly enhanced, on the basis of the size quantization of the electron wavefunction in nanowires with diameters below 5 nm. This is expected to lead to the development of high figure of merit thermoelectric materials. We review here the experimental observation of such enhancement in composites containing nanowires with diameters down to 9 nm. When the wire diameter is further decreased, localization effect takes over and limits the thermopower. The theory further predicts the appearance of an energy gap in bismuth nanowires with diameters below 50 nm. We observe such a gap both in the temperature dependence of the resistivity and in optical reflectivity measurements, with a dependence on nanowire diameter consistent with theory.

11:00 AM S1.2
Phonon Thermal Conductivity of Superlattice Nanowires for Thermoelectric Applications. Chris Dumes and Geng Chen; Mechanical Engineering, MIT, Cambridge, Massachusetts.

An incoherent particle model has been developed to calculate the phonon thermal conductivity of nanowires and superlattice nanowires. It is argued that the surface roughness and geometric variations of most real nanowires prevent the formation of idealized confined dispersion relations. Instead, the 3D bulk dispersion is used, thus capturing only the classical size effects. The implications for thermoelectric applications are discussed using a model SiGe superlattice nanowire: the room temperature thermal conductivity may be reduced below the alloy limit (7.0 W/mK) when the diameter is less than 15 nm and/or the segment length is less than 20 nm.

Acknowledgement: This work was funded by the NSF (CTS0129688) and DOE (DE-FG02-02ER45 977).

11:15 AM S1.3

We present an experimental study of the thermoelectric transport properties of nanocomposites conducting polymer/bismuth sulfide, nanocomposite system. Successful growth of bismuth chalcopyrites in nanorod form of 18-15 nm diameter has allowed the formation of a core/shell particle, which utilizes the bismuth compound as a quantum-confined core and the conducting polyaniline as the outer shell of 2-3 nm thickness. True three dimensional quantum confinement of the carriers within the bismuth compound is obtained through the higher polyaniline bandgap energy as well as complete nanorod surface coverage. A bulk form of the core/shell material has been studied with x-ray diffraction and sintering techniques which resulted in a unique nanocomposite of nanorod core particles within a polyaniline matrix. The heterogeneous composite is found to exhibit decreased thermal conductivity due to increased phonon scattering which is desirable in thermoelectric materials. Additionally, the electrical conductivity and Seebeck coefficient is found to be responsive to doping levels of the outer polyaniline shell. This provides a convenient mechanism to control thermoelectric properties and subsequently allow another degree of freedom to be added to thermoelectric engineering techniques. We conclude by summarizing our main results and discuss future work with bismuth telluride and bismuth antimony nanocomposites.

11:30 AM S1.4
Solventothermal Preparations of Nanocrystalline Bi2Te3 Powders and The Study on Their Characterizations. Xiaoyu Jin, Xinbing Zhao, WeiChun Zheng and Bohui Liu; Department of Materials Science, Zhejiang University, Hangzhou, Zhejiang, China.

Bi2Te3 are best-known and technological important thermoelectric materials currently available near room temperature with highest figure of merit 27%1. In this paper, Bi2Te3 nanocrystals of 15-25nm were prepared via hydrothermal processes in which pyridine, absolute ethanol and distilled water were used as main medium respectively. The products were characterized by XRD and TEM, and the grain size has also been calculated by Scherrer Equation. A possible formation mechanism has been proposed. The results showed that the reaction products’ purity, crystallization degree and grain sizes were all increased with the increase of the dielectric constant and polarity of the solvent. A novel Bi2Te3 nanowires with several tens nanometers diameter and up to more than ten microns lengths have been prepared when distilled water was used as reaction medium.

1:15 PM S2.1
The Low Temperature Synthesis of [Bi2Te3]*3/[Ti(Te2)2]*2 Superlattices using a Modulated Elemental Reactant Technique. Fred R. Harris, Robert Schneemiller, Stacey D. Staudridge and David C. Johnson; Chemistry, The University of Oregon, Eugene, Oregon.

A family of metastable [Bi2Te3]*3/[Ti(Te2)2]*2 superlattices (where x and y denote the number of layers of each of the two components) was prepared by annealing modulated elemental reactant precursors at temperatures below 280 C. Above 300 C, the metastable superlattices disproportionate into a mixture of Bi2Te3 and TiTe2. Through the design of the structure of the initial precursor, precise control of the superlattice unit cell composition is obtained. This allows for a modulation mechanism for these superlattices, and we discuss how the electrical properties correlate with changes in their nano-architecture.

2:00 PM *S2.3

Thin-film structures on substrates offer the potential to enhance the performance of thermoelectrics, offering new capabilities such as small-footprint coolers for lasers and microprocessors to high-performance thermoelectric power conversion. High performance and efficient refrigeration in low-power applications is of great interest. Our recent focus has been to transition the enhanced figure of merit (ZT) in p-type Bi2Te3/Sb2Te3 and n-type Bi2Te3/Bi2Te3-xSex superlattices to performance at the module level with several device demonstrations. We have been able...
to obtain a best ZT of ~2 in p-n couple, the fundamental cooling or power conversion unit in an operational module. In addition, we have been able to demonstrate p-n couple ZT of as much as 1.6 from heat-to-power efficiency data. The thermal interface resistances between the active device and the external heat source have been optimized. A power level of 38 mW per couple for a DT of about 10K, with 4-micron-thick element, was obtained. This translates to an active power density of ~54 W/cm^2 and a mini-module power density of ~10.5 W/cm^2. In short, power devices with thin-film superlattices are a real possibility. In the cooling arena, we have been able to obtain active cooling with thin-film modules, usable in several laser and microprocessor cooling needs. This is in spite of severe thermal management issues that had to be overcome noting that the "true" superlattice thickness, hence the "true" ZT, and across the device are much higher. Characteristics unique to thin-film cooling modules such as sensitivity to atmosphere would be presented from a phenomenological point. The concept of High-Active-Flex, Low-Input-Output-Flux device, common to both power and cooling modules, and the application of the fundamental issues in thin-films, of thermoelectric devices with experimental data on elements, numerical modeling, and device data will be presented. The challenges that remain to be addressed in the full development of this technology and thoughts on further progress in microstructured materials will be presented.

2:30 PM S2.4
Influence of Doping Concentration and Ambient Temperature on the Cross-Plane Seebeck Coefficient of InGaAs/InAlAs superlattices. Yan Zhang1, Rajeev Singh2, Ali Shikouri3, Gehong Zeng4, Yi-Okin Liu5, and Yi-Jen Chu2. Electrical Engineering, UC Santa Cruz, Santa Cruz, California; 2ECE, Univ. of California, Santa Barbara; 3Santa Barbara, Santa Barbara.

Seebeck coefficient is one of the key parameters to characterize the thermoelectric figure of merit (ZT). Its measurement performs better to thin film superlattice layers of 1-3 micron thick is complicated due to the difficulty in measuring temperature accurately on both sides of the film. We have developed thin film heaters/sensors that could be integrated on top of superlattice devices ranging in size from 40 to 100 micron in diameter. By characterizing temperature distribution on top of the device for various device sizes and different superlattice thickness, we can obtain an accurate estimate for the cross-plane Seebeck coefficient. Measurements were performed on molecular beam epitaxy grown InGaAs/InAlAs superlattice structures lattice matched to InP substrate n-type doped with 0.3uInGaAs up to 1e18cm-3. Superlattice contained 25 periods of 5nm thick InGaAs n-doped with doping concentration varied from 2e18 to 4e18 cm-3. 2-3micron thick undoped InAlAs. Devices with various sizes were fabricated using conventional lithography, dry etching and metallization techniques. It was interesting to note that contrary to the behavior in bulk material, Seebeck coefficient did not decrease monotonically with doping. This is attributed to large potential barriers between InAlAs and InGaAs layers (on the order of 50meV) and the formation of minibands in the structure. A preliminary theory of thermoelectric transport is shown, and in the regime of small bandgap, few materials have been developed and calculations are compared with experimental results. It is anticipated that this regime of transport could enhance the thermoelectric power factor [Seebeck coefficient square times electrical conductivity] beyond what has been achieved with bulk materials. This enhancement can be combined with the reduction of thermal conductivity in multi layer structures and improve the ZT of the material.

2:45 PM S2.5
Thermal Stalility of p-type Bi2Te3/Sb2Te3 and n-type Bi2Te3/Bi1–xSbxSe Thin-Film Devices. Kip D. Cooksey, Brooks O’Quinn, Pratima Adgevali, Edward Silvahn, Michael Puchan and Roman Venkateswararaman. Center for Thermoelectrics Research, Research Triangle Institute, Research Triangle Park, North Carolina.

Thermoelectric devices have been constructed using thin-film Bi2Te3/Sb2Te3 and Bi2Te3/Bi1–xSbxSe superlattice thin films. Since these devices are intended for use in systems that will operate at elevated temperatures over their lifetime as in many power conversion devices, the thermal stability of the thermoelectric couple’s figure-of-merit is an important consideration. The ZT of p-type and n-type superlattice thin-film elements was evaluated at specific intervals during irradiation to elevated temperatures of 1200°C for up to 60 hrs. Results indicate that the figure-of-merit for p-type superlattice films is not compromised over time when exposed to these operating temperatures. In contrast, the figure-of-merit for n-type superlattice films is not compromised over time when exposed to elevated temperatures. Evaluation of these thin-film thermoelectric elements is reported and implications of the results are considered for thin-film thermoelectric modules. In addition, we will report on performance of these devices after exposure to short cycles of much higher temperatures that are relevant in many opto-electronic packages.

SESSION S3: Oxides
Chair: Lidong Chen
Monday December 1, 2003
Room 313 (Hynes)

3:30 PM S3.1

Density functional calculations are used to elucidate the electronic structure and reduced properties of materials in the Na0.5Co2O4 layered system, in the range 0.3<x<0.7. These materials display remarkably high thermopowers for metals, and with modifications become useful thermoelectrics. Here it is found that density functional electronic structures are able to reproduce the experimentally measured thermopowers. However, at this level of theory, weak ferromagnetic instabilities are found. Comparison with experiment indicates that there are substantial spin fluctuations in these materials associated with proximity to a ferromagnetic critical point, which is approached with decreasing x. The recent observation of superconductivity in water intercalated samples may be a manifestation of these quantum fluctuations, in which case, the superconducting at x would most likely have triple pairing. In any case, these quantum fluctuations are key to stabilizing the high mass, high carrier density, paramagnetic ground state of the thermoelectric material, which underlies their favorable thermoelectric properties.

3:45 PM S3.2
Thermoelectric Properties of B2-substituted Ca2Co3O6 Single Crystal, Masashi Mikami1, Kenji Chong2 and Ryoji Funahashi2,3

1CREST, Japan Science and Technology Corporation, Osaka, Japan; 2Osaka Electric-Communication Univ., Osaka, Japan; 3National Institute of Advanced Industrial Science and Technology, Osaka, Japan.

The recent discovery of large thermopower coexistent with low electric resistivity in Na0.5Co2O4 and Ca0.5Co2O4 has made layered-structured cobalt oxides recognized as promising candidates for thermoelectric materials. In these two-dimensional cobalt-containing oxides, it is proposed that the high thermoelectric performance is caused by unique structural and transport properties, such as a strong electron-electron correlation and a modulated structure. For Ca2Co3O6 in particular, it is reported that the B2-substitution for a part of Ca site enhances its thermoelectric properties in sintered polycrystalline material. In order to investigate accurately the origin of the superior thermoelectric properties in B2-substituted Ca2Co3O6, large single crystals are indispensable. Thus, we grew single crystals of B2-substituted Ca2Co3O6 by a solvothermal method. The average size of the plate-like crystals was 3x3x0.05mm3. The cation ratio (Ca, Bi)/Co of the grown crystals measured by an energy dispersive X-ray spectrometer tended to the phase of the starting ratio (Ca, Bi)/Co=3/4. For instance, the average cationic composition of the grown crystals was CaBi2Co3O6=3.93:4, while that of the starting material was CaBi:Co=2.70:3.4. So, the crystalline structure of the obtained crystals may correspond to the CaBi2Co3O6 phase rather than the Ca2Co3O6 phase. Thermoelectric properties in the direction of ab-axis were measured at various temperature ranges. Seebeck coefficient of Ca0.5Bi0.5Co3O6 is positive and 30 μV/K at room temperature. The electrical resistivity is about 3 mΩcm at temperature range of 300-1800K. The relation between the Bi content and thermoelectric properties will be presented.

4:00 PM S3.3
Exploration of Thermoelectric Oxides and Development of Modules Consisting of the Oxide Devices. Ryoji Funahashi1,2,3, Stori Urama4, Masashi Mikami4, Katsuhisa Mizuno4, Takumi Kouchi2 and Kuni Chong2,3

1National Institute of Advanced Industrial Science and Technology, Tokyo, Osaka, Japan; 2Japan Science and Technology Corporation, Osaka, Osaka, Japan; 3Osaka Electra-Communication Univ., Osaka, Japan.

In order to accelerate exploration of new thermoelectric materials, a high-throughput screening (HTS) technique has been developed. Using this technique, 1000 samples can be prepared and evaluated their Seebeck coefficient (S) at room temperature in a day. It is clarified that Na2NiO and Na2NiO systems show n-type properties, LnNiO3 and LnNiO4 (Ln: La or Nd) are mainly formed in the samples possessing n-type property. Seebeck coefficient of LnNiO3 and LnNiO4 is ~20–10 μV/K at 973 K. While electrical
resistivity ($\rho$) of LaNiO$_3$ is as low as 5 mΩ cm, both NiNiO$_2$ and Nd$_2$NiO$_4$ show high resistivity of 25-50 mΩ cm at 77 K in air. Substitution of La with other cations seems to be effective to enhance power factor ($S^2/\rho$). Optimizing substituted cations and compositions has been tried by HTS. It is found out that Bi-substitution is effective to improve both Seebeck coefficient and resistivity of the LaNiO$_3$ system. At the present highest power factor is about 35.5 mW/m K$^2$ for La$_{0.9}$Bi$_{0.1}$NiO$_3$ at 273 K. Thermoelectric devices are prepared using hot pressed p-type $\mathrm{Cu_2ZnSnSe_4}$ and n-type $\mathrm{Cu_2ZnSnS_4}$ bulks. Thermal durability of the devices does not seem to be a problem. Presently, propeller type thermoelectric modules consisting of the oxide devices will be presented.

4:30 PM S.3.4
Thermoelectric Properties of Textured $\text{InGaO}_3(\text{ZnO})_{1-x}$ Ceramics, Ryoji Asahi, Chongtao Xin, Hisashi Kaga, Shingo Hirano, and Yoshikazu Tani. Frontier Research Department, Toyota Central R&D Labs., Inc., Nagakute, Aichi, Japan; Department of Materials Engineering, University of Tokyo, Tokyo, Japan.

Materials design and syntheses of the homologous compound $\text{InGaO}_3(\text{ZnO})_{1-x}$ are presented for the thermoelectric application. First principles calculations of doping energies, thermopowers, and thermal conductivities were performed to understand and optimize the thermoelectric properties. Ceramic samples were synthesized by a solid-state reaction at 1400 K for 24 h in air, followed by sintering at 1823 K for 24 h in air. Aluminum doping for a zinc site effectively enhanced an electrical conductivity and a power factor, as predicted by the calculations. A lower thermal conductivity, mainly due to a smaller elastic constant along the c-axis, was utilized a templated grain growth (TGG) technique to obtain highly textured ceramics. Planelet micro-crystallite of $\text{InGaO}_3(\text{ZnO})_{1-x}$, and $\text{In}_2\text{O}_3(\text{ZnO})_{1-x}$, which can facilitate the TGG process, were synthesized by flux method. The latter templates mixed with $\text{Ga}_2\text{O}_3$ powder, however, tended to form the spiral structure, $\text{Ga}_2\text{ZnO}_4$, during the reactive TGG process, resulting in the random orientation of $\text{InGaO}_3(\text{ZnO})_{1-x}$. We report thermoelectric properties of the textured ceramics and compare with the random ones.

SESSION 5: Skutterudites
Chair: Terry Tritt
Tuesday Morning, December 2, 2003
Room 313 (Hynes)

8:30 AM S.4.1
Effect of Ni in new skutterudite compounds $\text{Ca}_x\text{Co}_{2-x}\text{Ni}_x$. M Phuyet, B Lenoir, A Bruchon, M Delmotte, J Hejtmancik. C. Science, E Muller and H Scheurer. 1Laboratoire de Physique des Matériaux, UMR 7656, Ecole des Mines, Nancy, France; 2Laboratoire de Science et Genie des Matériaux et de Metallurgie, UMR 7584, Ecole des Mines, Nancy, France; 3Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic; 4Institute of Materials Research, German Aerospace Center (DLR), Cologne, Germany.

During the last ten years, skutterudite materials have been widely studied due to their unique physical properties. Antimonide skutterudites received particular attention from an engineering point of view since these materials exhibit better thermoelectric performance than state of the art thermoelectric materials when working at elevated temperatures. One of the most interesting properties is that their crystalline structure can be formed by guest atoms R. Actually, a phenomenon of hosting can appear for these fillers and reduce substantially the lattice thermal conductivity. It was remarked in different issues that the effecting rate in $\text{R}_x\text{Co}_2\text{S}_2$ compounds coupled with a substitution of cobalt by nickel may improve the thermoelectric performance. In this communication, we present and discuss results concerning the influence on the transport properties of nickel substitution in a new class of skutterudite compounds, with the alkaline earth calcium as the filler atom. All the compounds were synthesized by traditional metallurgical technique. The Seebeck coefficient, the electrical resistivity and the thermal conductivity have been measured in a wide range of temperature. It is shown that similarly to the case of $\text{Ba}_x\text{Co}_2\text{S}_2$, the substitution of Ni on the Co sites has a beneficial effect.

8:45 AM S.4.2
Synthesis and Thermoelectric Properties of $\text{CeFe}_{2-y}\text{Zn}_{y}\text{Co}_{2}\text{S}_2$ 12 Skutterudite Alloys. Thierry Callene, Jeff Schrimpf and Luan Lunn. Jet Propulsion Laboratory, Pasadena, California.

Advanced unipolar materials, in particular $\text{Co}_{2-5}\text{Se}_{3}$ and $\text{p-type CeO}_{4-5}\text{Fe}_{2-5}\text{S}_{12}$ are currently being developed at the Jet Propulsion Laboratory. These unipolar materials have the potential to achieve conversion efficiencies on the order of 15%, when operated at a hot-side temperature of 973 K and a cold-side temperature of 373 K. They could be integrated in a variety of thermoelectric power generation devices including Advanced Radiotrap Power Systems for future NASA deep space missions. Current skutterudite materials being used are limited to a hot-side temperature operation of about 775 K. Expanding this limit by a factor of four is one of the most promising strategies for the development of high temperature skutterudite materials. The synthesis of these materials can be obtained using a modified two-step process. The first step is the preparation of the oxide precursors and the second step is the solid state reaction to form the skutterudite material. The Seebeck coefficient, electrical resistivity, and thermal conductivity measurement results are presented and discussed as well the potential use of these materials into future generations of advanced unipolar devices.

9:00 AM S.4.3
Synthesis and thermoelectric properties of $\text{CeCu}_{2-6}\text{Rh}_{1-6}\text{Bi}_{2.12}$, Geoff D. Smith, Pool D. Asinovic and Thierry Callene. 1Materials Science, California Institute of Technology, Pasadena, California; 2Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, California; 3Jet Propulsion Laboratory, Pasadena, California.

Exotic filled skutterudite compositions were explored to determine their suitability for thermoelectric applications. While skutterudite occurs naturally as Ce$_2$Cu$_7$As$_3$, this work was undertaken with a nominal composition of Ce$_{0.75}$Rh$_{0.25}$Bi$_{2.12}$ after the theoretical work of Fonrasi and Sing (Appl Phys Lett, 1999). Study in this skutterudite system was undertaken to experimentally verify its potential in n-type thermoelectric applications. Both filled and unfilled samples from this system were synthesized and studied, with Cerium as the filling ion. Standard synthesis routes were quickly exhausted without much success, though as a result of our initial work the nominal composition was adjusted to $\text{CeRu}_{2.67}\text{Bi}_{1.33}$ to reflect a naturally stable ratio in RuBi skutterudites. Due to this dominant composition electroneutrality was expected to be achieved at 0.89 cerium filling and fully filled materials were expected to be strongly n-type. Unfilled $\text{CeRu}_{2.67}\text{Bi}_{1.33}$ was synthesized using a straightforward quench synthesis technique. The filled thermoelectric $\text{CeRu}_{2.67}\text{Bi}_{1.33}$ was synthesized using a combination of solid state reaction of elemental constituents and high pressure hot pressing. A 6.8 mV/nW device was used to provide the synthesized conditions of 6 GPa and dwell temperatures of 650C and 550C. Due to decreasing stability of filled skutterudites with increasing synthesis pressure high pressure synthesis requires low temperature hot pressing. As a consequence of this the filled thermoelectric is no longer stable phase at synthesis conditions of 12 GPa. The resulting material, a new fully filled skutterudite, exhibited p-type conductivity and an electrical resistivity of 1.75m$m^2$/m that decreases with increasing temperature. Thermoelectric Seebeck coefficients were measured on both pure samples. The crystal structure of these Rhodium-Ruthenium skutterudites were refined using Rietveld analysis of the X-ray diffraction data. Particularities of this synthesis route, details of the thermoelectric properties, as well as implications for other filled skutterudite systems will be discussed.

9:15 AM S.4.4

In materials with low carrier concentration, low frequency lattice phonons can be the limiting factor toward reducing thermal conductivity. We study optical phonon vibrations and correlate them with thermal conductivity for empty and filled skutterudite designed for thermoelectric applications, where low thermal conductivity is critical. Polarized Raman scattering spectra of crystallite and polycrystalline samples are compared with theoretical predictions and analysis in comparison to the thermal conductivity properties. Our equipment is on the $\text{Co}_{2-5}\text{S}_2$ skutterudite, and we determine Hall coefficients including materials with Ge, Sn, and La in the cages. We observe a strong correlation between aspects of the phonon spectrum and low thermal conductivity. This presents optical spectroscopy as a characteristic screening tool for potential thermoelectric applications and is a crucial step toward predicting lattice thermal conductivities.
9:30 AM S4.5
Spin dynamics of the skutterudites (Na,Ba,Ca)Fe$_4$Sb$_2$ probed by thermal and electrical transport. Michael Brandt, Narayani Senthilkumar, Andreas Leithe-Jasper, Jörg Miodo, Frank Steglich and Yuri Grim; Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

Spin fluctuations play a major role in determining the nature of electrical and heat transport in superconductors and iron-based magnets. In this paper we would be presenting the results of our rigorous experimental search in trying to understand the nature of spin dynamics in the novel thermoelectric materials called the skutterudites. We have probed the spin dynamics of the weak intertext ferromagnet NaFe$_4$Sb$_2$ and the non-magnetic compounds (Ba,Ca)Fe$_4$Sb$_2$ using electrical resistivity, specific heat, thermopower, and thermal conductivity in magnetic fields and Hall effect and compared with spin fluctuation temperature from $^{29}$Na NMR investigations. The allotropic melt were chosen to facilitate understanding the magnetic properties attributed to iron in the antimony framework without the complicating influence of the Fe in the RE based skutterudites. From the electrical transport, these materials can be classified as bad metal ($k_B T$) displaying an S-shaped $\rho(T)$ typical of spin fluctuating systems. The ratio of the effective paramagnetic moment $\mu_{pp}$ to the saturation moment $\mu_s$ is $\approx 6.5$ which fits qualitatively into the Rhodes-Wohlfarth plot. This points towards an electronic state that is intermediate between a ferromagnetic insulator and a paramagnetic metal according to the Stoner model. The Sommerfeld coefficient $\gamma$ is 145, 115, 135 $\mathrm{mJ/molK^2}$ for the Na, Ba and the Cs samples respectively which is rather high for a non f electron system. At low temperatures, the Hall resistivity of all the samples shows a linear dependence of the form $\rho_H \propto T$. The temperature dependence of spin fluctuations for NaFe$_4$Sb$_2$. The charge carrier concentration at 5 K is $6 \times 10^{17}$ $\mathrm{m^{-3}}$ corresponding roughly to 4 holes per formula unit which is comparable to the of Fe$_4$Sb$_2$. 1. T. Mory, Spin fluctuations in intermetallic electron magnets, Springer Verlag, 2. C. Uher, Semiconductors and Semimet. 68, 139, (2001). 3. A. Leithe-Jasper et al., (accepted). 4. A. Rahman et al., to be published in the proceedings of the ICM 2003. DRAWN THE LINE PER CONTINUOUS REFERENCE TO THE ICTP 1/9/03 PER AUTHOR'S REQUEST, Dr. Narayani Senthilkumar.

9:45 AM S4.6
Thermoelectric Properties of Filled Skutterudite Y$_{x}$Ce$_{1-x}$Fe$_4$P$_{12}$ (T=Fe, Ru or Os) (0 $\leq x \leq 0.3$). Ram Girir, C. Sekine$^1$, Y. Sirono$^1$, I. Inagawa$^1$, C. H. Lee$^2$ and A. Yamamoto$^1$.

Filled skutterudite compounds Y$_{x}$Ce$_{1-x}$Fe$_4$P$_{12}$ (T=Fe, Ru or Os) (0 $\leq x \leq 0.3$) have been prepared at high temperature and high pressure. The samples were characterized by x-ray diffraction. Electrical resistivity, Seebeck coefficient and thermal conductivity were measured. Dramatic suppression in thermal conductivity (K) has been found in Ce$_{1-x}$Fe$_4$P$_{12}$ with 10% Y doping. Thermal conductivity of Y$_{x}$Ce$_{1-x}$Fe$_4$P$_{12}$ (T=Fe, Ru or Os) gradually decreases with increase of Y concentration. Mixing more than one rattler (Y and Os), considered raising randomization, caused to decrease the significant values of thermal conductivity.

SESSION S5: Low Dimensional Systems and Nanostructures
Chair: Mary Anne White
Tuesday, December 2, 2003
Room 513 (Hynes)

10:00 AM S5.1

Materials Science and Engineering, Kyoto University, Kyoto, Japan; 2Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai, China.

Thermal conductivity and other thermoelectric properties were investigated on beta-Zn$_2$Sb$_3$ and CoSb$_3$ thin films. They are prepared by co-deposition of the specific sets of Zn, Sb and Co targets by RF magnetron sputter deposition. A deposition thickness of thin films were annealed for crystallization at temperatures 603 and 473 K, respectively for beta-Zn$_2$Sb$_3$ and CoSb$_3$. Thermal conductivity measurement was performed based on an AC calorimetry method using a commercial thermal diffusivity meter (LinerPIT, Ulsan-Riko, Inc.). For this measurement, a thin film was deposited on one half of a pico-Bolometer homogenously of films 30µm thick. The Zn$_2$Sb$_3$ thin films investigated are Zn-rich with respect to the stoichiometric composition. Their thermal conductivity decreases with decreasing film thickness and the grain size of thin films strongly depends on their thickness. A nanoscale grain size in a ~30µm thick film specimen gives rise to an almost 50% reduction in its thermal conductivity (100 K). The temperature dependence of thermal conductivity of ~30µm thick film specimen seems to be weak and the thermal conductivity of the thin film is seen to be significantly lower than that of the bulk specimen. Low electrical resistivity and high Seebeck coefficient can be achieved simultaneously in the film specimen with properly controlled thickness and microstructure. A ZT of 1.2 at ~40K has been obtained for ~30µm thick Zn$_2$Sb$_3$ film specimen. In contrast, the thermal conductivity of ~200µm thick film specimen was found to be about 1.1 W/mK at room temperature, which is almost one tenth smaller that of the bulk specimen, although its power factor is much smaller than that of bulk specimens.

10:45 AM S5.2
Theoretical Prediction of Thermal Conductivity of Nano-composites, Ronggui Yang and Gang Chen; Mechanical Engineering Department, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Nano-composites have tailed mechanical, electrical and optical properties. In one hand, many experiments have been tried to obtain high thermal conductivity material using carbon nanotube based nano-composites for thermal management of electronics, especially the thermal interface materials. The other hand, the research is due to the interface scattering between the nano-particles and the host material, and the phonon rarefaction effect might be explored for lower thermal conductivity, which can be very useful for improving the performance of thermoelectric devices. In this paper, we study theoretically the thermal conductivity of nano-composites with nanodot (nano-fiber) embedded in the host semiconductor material. We predict the thermal conductivity dependence on the interface condition, the size of nanodots, the volume fraction, and the bulk properties of the constituent materials. Acknowledgments: This work is supported by NSF (CTS012988).

11:00 AM S5.3

Alloying PbSn$_{0.98}$Tc$_{0.02}$ with SnTe provides an important variable in controlling the band structure of PbTe$_{1-x}$Sn$_x$Te$_x$. By changing the Sn concentration, we can tailor the total bandgap offset energy between the alloy nanodots and the PbTe spacer layer. The SnTe quantum dot superlattices (QDSL) structures show an increase of 1300$\mu$V/K for PbTe$_{1-x}$Sn$_x$Te$_x$ QDSL materials grown by molecular beam epitaxy and investigated for applications in thermoelectric devices. This paper describes the growth and characteristics of n-type and p-type QDSL materials. The typical unicouple device consists of a substrate-free, bulk-like (typically 0.1 mm in thickness, 10 mm in width, and 5 mm in length) slab of nanocrystalline PbSn$_{0.98}$Te$_{0.02}$ as the n-type leg and a metal wire as the p-type leg. Results on arrays of unicouple TE devices will be presented. Projections of future thermoelectric performance expectations for PbTe based QDSL materials will be presented.

11:30 AM S5.4
Crystalllographically-Oriented Electrochemically-Deposited Blenneth Nanowires, Oded Rabin$^1$, Gong Chen$^2$ and Mildred S Dresselhaus$^2$.

1Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts; 2Mechanical Engineering, Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; 3Physics, Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Nanowires of thermoelectric materials have been predicted to have superior thermoelectric characteristics over the bulk material. Both the deviation of the electron effective mass and the enhancement of surface scattering are expected to increase the value.
of the Seebeck coefficient and decrease the value of the thermal conductivity in low-dimensional systems. In this paper, recent advances in the preparation of bismuth nanowires by electrochemical deposition into porous anodic alumina templates are presented. Previously, bismuth nanowires have been synthesized via electrochemical deposition, pressure injection of the melt, and vapor phase condensation in the pores of porous anodic alumina templates. While electrochemical deposition is advantageous for the preparation of large quantities of small diameter nanowires, in terms of their crystal quality nanowires obtained by this method thus far are inferior to samples prepared by other methods: they are polycrystalline and show no preferred crystallographic orientation along the main nanowire axis. These materials properties are highly relevant to the thermoelectric performance, particularly for materials such as bismuth, since low effective carrier masses, long mean free paths and phase coherence lengths are desirable. We have found synthetic conditions that lead to improvements in the crystallinity and orientation of 200μm nanowire arrays. Comparison of the structural and transport properties of these samples to those of samples prepared by other methods will be functional for verifying and improving theoretical predictions over the influence of structural factors on thermoelectric performance. We gratefully acknowledge the support from DOE (DE-FG02-02ER45597) and ONR (contract N00014-02-1-0865).

11:45 AM S5.5
A Variational Solution of the Thermoelectric Transport Properties of Two-Component NanoComposite Systems.
Patrick L. Gieriec and Kevin L. Stokes, Advanced Materials Research Institute, University of New Orleans, New Orleans, Louisiana.

The successful fabrication of a nanocomposite in bulk form consisting of an anisotropic assembly of nanoscale sized particles has required an increased understanding of the thermoelectric properties of these materials and their thermoelectric transport properties. Our particular nanocomposite consists of nanorods that are within the quantum confined regime of one dimensional carrier transport. Upon fabrication of the bulk composite, these nanorods are embedded with a three dimensional conducting matrix that exhibits altered transport properties. We address the nanorod component by assuming a single parabolic band within the one dimension density of states to accommodate the single dimensional transport of the quantum confined carriers. Both elastic and inelastic scattering of electrons or holes is accounted for by solving the variational form of the Boltzmann transport equation. Inelastic interactions include the three dimensional bath of longitudinal and transverse phonons and the phonon drag potential scattering term with the one dimensional confined electrons of the quantum well. An altered lattice thermal conductivity of both the confined and surrounding conducting matrix is calculated separately to account for umklapp and boundary scattering of the acoustic phonons which undergoes considerable interface scattering with the embedded nanorod system. Exact expressions for the bulk effective electrical resistivity, thermal conductivity, Seebeck coefficient and figure of merit are then obtained through the field decoupling transformation, which is a special case of two component composites. Our method is easily generalized to any two component composite and is independent of the components geometry as well as applications of one or two dimensional transport, and any transport regime within quantum confinement. Application to the emerging field of nanocomposites is discussed and comparison to available experimental data is presented.

SESSION S6: Complex Bulk Materials and Measurement Systems
Chair: Kevin Stokes
Room S13 (Hynes)
Tuesday Afternoon, December 2, 2003
1:00 PM S6.1
Anisotropy in Thermoelectric Properties of CsBi2Te5,
Duck-Young Chung1, S D Minhas1, Jeffrey Dyck2, Citrad Uher2 and Mercouri G Kanatzidis1,1, Chemistry, Michigan State University, East Lansing, Michigan; 1Physics and Astronomy, Michigan State University, East Lansing, Michigan; 1Physics, University of Michigan, Ann Arbor, Michigan.

CsBi2Te5 has been reported as a promising thermoelectric material (ZT ~ 0.8 at 255 K), which could efficiently function as low temperature for cooling applications. The compound crystallizes in a needle-type morphology reflecting monoclinic unit cell parameters of a = 5.9305(8) Å, b = 4.4025(1) Å, c = 14.5188(3) Å, β = 101.480(1) deg. The structure features NaCl-type [Bi2Te4] slabs that are infinitely extended along the needle axis (a-axis) and Bi-Te bonds interconnecting slabs along c-axis which build up layers separated by Cs layers with high atomic displacement parameters. These morphology and structural characteristics imply highly anisotropic features in its thermoelectric properties. TE properties previously reported on CsBi2Te5 have been performed along the needle (b-) axis since effective charge transport is generally expected to be along the needle axis. Electronic structure calculations, however, indicate that the layers in which the charges are confined to move are almost perpendicular to the interconnected [Bi2Te4] layers and this phenomenon is in presence of the Bi2Te4 layers which is unique for the systems consisting of Bi-Te network. Also, a large ZT value of the hole-doped CsBi2Te5 reflects a large anisotropy in the carrier effective masses associated with the Bi-Te bonds (σ-axis) in the valence band. Theoretical investigation of the electronic and thermoelectric properties is necessary to fully understand this material. Here, TE properties of CsBi2Te5 measured along all primary directions will be discussed and compared with the prediction from band structure calculations.

1:45 PM S6.2
Electronic structure and thermoelectric properties of A3Mo4Sb12Te30, Naim Scheinlin and Holger Kleinkne, Chemistry, University of Waterloo, Waterloo, Ontario, Canada.

The binary antimonide Mo3Sb2 is metallic, but its band structure exhibits a gap of ca. 0.6 eV located above the Fermi level. We proved that Mo3Sb2 can be chemically modified to become semiconducting by replacing 2 Sb atoms with 2 Te atoms (per formula unit) [1]. This material could be an attractive candidate for the thermoelectric energy conversion, as its thermal conductivity may be lowered by creating the rattling effect upon intercalation of small cations [2], and its band structure may be tailored, i.e. the band gap size modified. Simply put, the higher the Te content and the higher the cation amount, the smaller is the band gap, which can virtually reach any value below 0.5 eV [3]. Cations such as A = Mn, Fe, Co, Ni, Cu, and Mg can be added into the cubic void formed by Sb and Te atoms. With such small cations A (~ 0.2-0.3 Å) which may lead to a rattling effect depending on the size of the cation. E.g., the Ni-Sb contacts in NiSb2 are as short as 2.4 Å, while the Mg-Sb bonds in MgSb2 are 2.82 Å. Physical property measurements of Seebeck coefficients, electrical and thermal conductivity are in progress. E.g., thus far we have attained Seebeck coefficients of up to 200 μV/K. We will present both the experimental and the theoretical results of this ongoing study. [1] E. Dressel, A. Szepenkovskie, H. Kleinkne. J. Mater. Chem. 2009, 19, 2969-2974; [2] G. Dressel, H. Kleinkne, Mat. Res. Soc. Symp. Proc. 730, 131 - 136 (2002). [3] N. Scheinlin, E. Dasdik, H. Kleinkne, Can. J. Chem., in press.

2:00 PM S6.3
Thermoelectric Properties of Cubic AgPb2SrTe4S2.3,
Mercouri G Kanatzidis1,2, Koei-Fong Hiu3, Jongwhan Do3, Tim P Hogen4, Fu Guo5 and Sim Loo5, 1Chemistry, Michigan State University, East Lansing, Michigan; 2Electrical and Computer Engineering, Michigan State University, East Lansing, Michigan.

Thermoelectric heat to electricity converters could play a key role in future energy conservation and management utilizing materials whose phonon drag and effective thermoelectric materials need to be identified that are suitable for high temperature applications. The material system AgPb2SrTe4S2 has been synthesized and its properties determined. With 0.2 ≤ n ≤ 18 and when n ~ 11, the AgPb2SrTe4S2 exhibits a thermoelectric figure of merit at high temperature. At this temperature range the AgPb2SrTe4S2 surpasses in performance other bulk thermoelectric materials. The new series of compositions AgPb2SrTe4S2 exhibits a family of materials with cubic crystal structure. The various members of the series are designed to exhibit maximum mass fluctuation generated by Ag-Pb-Sr disorder and they also show interesting microscopic inhomogeneities that may be responsible for the observed high power factors of these materials. Several members were investigated extensively through doping and crystal processing variations. The maximum ZT is achieved at high temperatures (700-800 K) making these materials suitable for possible power generation applications. If time permits we will also present data for the corresponding selenide analogs.
of the transport properties, and has been useful for measuring electrical conductivity, sample uniformity, and contact resistance. A second measurement presented in the paper is a computer-controlled drift measurement system with the vacuum chamber partially submerged in a liquid nitrogen flask. This drift system has the capability of simultaneous measurements of electrical conductivity, thermoelectric power, and thermal conductivity over a temperature range of 80-400 K. Various reference materials, such as Ni, stainless steel, Mo, Bi2Te3, etc., were used to evaluate the above systems. The design and implementation of these measurement systems along with data from the reference materials, and new thermoelectric materials will be presented in this paper.

2:45 PM S6.5 Effect of K/Bi Ordering on the Electronic Structure of K
\(_{2}\)BiSb\(_{3}\) by Daniel Bilic, Paul Larson, S. D. Mahanthi, and M. G. Kanatzidis. 

K
\(_{2}\)BiSb\(_{3}\) belongs to a class of complex Bi-Te-Se systems which show great potential for thermoelectric performance. The compound forms in two distinct phases: (i) K
\(_{2}\)BiSb\(_{3}\) (tridymite with space group P-1) and (ii) K
\(_{2}\)BiSb\(_{3}\) (monoclinic with space group P 2\(_{1}\)/m). In the \(\beta\)-phase, there are four sites with mixed K/Bi occupancy. To understand the electronic properties of these two phases, we have carried out electronic structure calculations within the \textit{ab initio} density functional theory (DFT) using full potential linearized augmented plane wave (LAPW) method. The generalized gradient approximation (GGA) was used to treat the exchange and correlation potential. Spin-orbit interaction (SOI) was incorporated using a second variational procedure. The \(\alpha\)-phase is found to be a semiconductor with an indirect band gap of 0.4 eV. For the \(\beta\)-phase, we have chosen two different ordered structures with extreme OCCs of K and Bi atoms at the “mixed sites.” Both systems are semi-metal\(^{1}\). To incorporate the effect of mixed occupancy we have chosen a supercell with an alternative K/Bi occupancy at the “mixed sites.” This system is found to be a semiconductor with an indirect gap of 0.38 eV. We have shown that the mixed occupancy is crucial for the system to be a semiconductor because the Bi atoms at the “mixed sites” stabilize the Se-Se bonds of the nearest neighbor Se bonds by lowering their energy. We find a strong anisotropy in the effective mass near the conduction band minimum, with the smallest effective mass along the mixed K/Bi chains. This large anisotropy suggests that \(\beta\)-K
\(_{2}\)BiSb\(_{3}\) can be an excellent n-type thermoelectric material.

\(^{1}\)Supported by the Office of Naval Research.

the film samples with microscale electrodes and temperature sensors. The work also explores thermoelectric characterization of nanowires using an electrically conductive AFM tip.

4:45 PM S7.6
Structural analysis and thermoelectric properties of TiO-1 clathrate compounds in the Ba-Ge-Ga system.
Norihiko Liashok Okamoto, Takumi Nishii and Haruyuki Inui, Materials Science and Engineering, Kyoto University, Kyoto, Japan.

There has been great interest in TiO-1 clathrate compounds of a stoichiometric composition of $M_{24}X_{48}$ (M=alkali or alkaline earth metals, X=Si, Ge, Ga) because of their good thermoelectric properties. These clathrate compounds have been known to possess a cubic crystal structure belonging to the space group of Pm-3n with two kinds of cage structures consisting of X atoms, $X_{24}+tetrakaidecahedron and X_{20}$dodecahedron. Recently, the binary-type TiO-1 clathrate compound of the BaGeGa$_4$ is expected to have a stoichiometric composition of Ba$_4$Ge$_{24}$ with half the 6c sites for Ge being randomly occupied by vacancies. However, our recent transmission electron microscopy (TEM) observations have indicated that Ba$_4$Ge$_{24}$ possesses a superlattice structure with the lattice constant twice large as that for other TiO-1 clathrate compounds due to an ordered arrangement of Ge vacancies at 6c sites. Our tentative assignment indicates that the space group is changed to Ia3d; 6c sites of the space group of Pm-3n are converted to 24c and 36d sites of the space group of Ia3d and either of these two sites is occupied by vacancies. Upon alloying with Ga, Ga atoms preferentially occupy these sites corresponding to 6c sites in the space group of Pm-3n for a small level of Ga additions and the electrical conductivity mechanism changes from that of semiconducting for binary to that of metallic for Ga-doped alloys. Therefore, the occupancy behavior for Ge sites may play an important rule in controlling its transport properties. We will present the results of crystal structural and microstructure analysis by TEM as well as thermoelectric property measurements for TiO-1 clathrate compounds in the Ba-Ge-Ga system and discuss the occupancy behavior for Ge sites in relation to the observed thermoelectric properties.

SESSION S8: Poster Session: Thermoelectric Materials and Technology
Chair: Joseph Heremans, Tim Hogan, Dave Johnson, George Nolte, Jeff Snyder and Jihai Yang
Tuesday, December 2, 2013
8:00 PM
Exhibition Hall D (Hynes)

S8.1 A Step-like Structure of the Electrical Conductivity of the p-type Cd$_{2}$Ga$_{5}$Se$_{8}$ Spinel Semiconductors. Tadashi Hiron1, Andrzei Krzywinski2, Eva Malicka3, Jacek Kusiak1, and Alicja Waskowska1, 2, 3 Instituto de Fisica, University of Silesia, Katowice, Poland; 1Institute of Chemistry, University of Silesia, Katowice, Poland; 2Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland.

Single crystals of the Cd$_{2}$Ga$_{5}$Se$_{8}$ system were grown by vapor transport in closed quartz ampoules with anhydrous chromium chloride, CrCl$_3$. The crystallographic data for CdSe$_{2}$ and Cd$_{2}$Ga$_{5}$Se$_{8}$ as solid phases. Single crystals of octahedral shape with well-formed regular [111] faces had the edge length of 3 mm [1]. The magnetic studies revealed that in the composition range of 0 < x < 0.06 the single crystals under study were ferromagnets [2]. The structure refinements of the Cd$_{2}$Ga$_{5}$Se$_{8}$ spinel single crystals were done using a KM4 4-circle diffractometer and a SHFLEX RD computer program [3]. The composition has been confirmed by microprobe analysis with a Cambridge electron microprobe operating at 20 kV (accelerating voltage), a beam current of 5 x 10$^{-7}$ A and a counting time of 10,000 ms. Standards were used GaAs for Gao. The electrical conductivity of the spinel single crystals under study has been measured in a (001) direction using the four-point dc method and in the temperature range from 8 to 310 K. The thermoelectric measurements were carried out at room temperature. The above investigations showed that all compounds under study are p-type semiconductors. For the sample with x=0.015 a step-like structure of the electrical conductivity (SLS EC) has been discovered in the magnetic regions in which the short and long range magnetic interactions took place, respectively. A presence of a few per cent of the Ga ions in the octahedral sites makes the easier dissolution of the ferromagnetic clusters finally leads to a rapid increase of the electrical conductivity with temperature increasing giving so-called the step-like structure. The remaining single crystals with larger Ga concentration x showed a type two temperature dependence of the electrical conductivity similarly as it was reported for the pure Cd$_{2}$Ga$_{5}$Se$_{8}$ spinel [4]. It means that the non-magnetic gallium ions play a sensitive role in the electronic transport. For the first time the SLS EC phenomenon in the Zn$_{0.65}$Ga$_{0.35}$Cr$_{0.15}$Se$_{8}$ spinel was observed also for a small concentration of Ga ions located in the octahedral sites of the unit cell [5]. The SLS EC phenomenon observed in the spinel single crystals above mentioned, could be attractive because of the intriguing physical properties of materials and possible for technological applications. References: [1] S. Okazawa, K. Nishio, and H. T. L. Lui, J. Alloys Compd. 292, 90 (1999); [2] I. Okazawa, J. Phys. Soc. Jpn. 43, 34 (2001); [3] B. H. S. PALS Program for the Determination of Crystal Structures, University of Gentingen, 1986; [4] H. L. T. Lui, J. Appl. Phys. 37, 1398 (1966); [5] T. C. Gree, E. Malicka, I. Okazawa, J. Phys. Chem. Solids, 2013.

S8.2 Thermoelectric Properties of High Symmetry Quaternary System Ag-Pb-Sb-Te. Juewong Do1, Mercour G. Kamasa2, Pu Guo2, Sun Lee2 and Tim Homes3, 4 Department of Chemistry, Michigan State University, East Lansing, Michigan; 3Department of Electrical and Computer Engineering, Michigan State University, East Lansing, Michigan.

The thermoelectric (TE) properties of high symmetry quaternary tellurides, Ag$_x$Pb$_{1-x}$Sb$_{1-y}$Te$_{2+y}$ were investigated. These materials crystallize in the space group, Pm-3n and have the NaCl crystal structure type with Ag, Pb, Sb and Te dispersed on the Na$^+$ cationic sites. Such complex compositions cause the transformation of two cubic phases, Ag$_4$Sb$_2$Te$_6$ + Pb$_4$Te$_6$ may give rise to complex electronic band structures and tunable thermoelectric properties. Materials with high symmetry crystal structures and disorder in the heavy element sublattice, Ag-Pb-Sb-Te could be attractive for TE investigations due to their likelihood to produce high ZT. Heavy elements and disorder are the main sources of phonon scattering, which have low phonon frequencies and therefore low thermal conductivity. Also, the high symmetry structure with possible high degeneracy of band extrema (i.e. large number of valleys in conduction band or peaks in the valence band) often results in high power factor. The charge transport and thermal conductivity of these materials were examined as a function of m and n. A p-type Ag$_x$Sb$_{1-y}$Te$_2$ phase with high ZT value (high thermopower and low thermal conductivity) is especially emphasized in this report.

S8.3 Thermoelectric Properties of Quenched Yb$_2$Cu$_{2}$O$_{6.1}$-d Samples. Julio E. Rodriguez and Alvaro Marino, Department of Physics, Universidad Nacional de Colombia, Bogota, Colombia.

We have performed a study of temperature dependence of thermal conductivity, k(T), Seebeck coefficient, S(T) and electrical resistivity, p(T) on oxygen deficient polycrystalline samples of Yb$_2$Cu$_{2}$O$_{6.1}$-d (0≤d≤1). Measurements of S(T), p(T) and k(T) were carried out as a function of the oxygen content at the temperature range between 77K and 300K. The influence of oxygen content on the transport properties and the dimensionless merit figure, ZT, was studied. With the reducing of oxygen content the Seebeck coefficient and the electrical resistivity show an systematic increase, while k(T) decreases. ZT(T) exhibit an enhancement up to comparable values to those of conventional semiconductors (0.1 < ZT < 0.5). This behavior suggests that the charge carrier density is decreasing while the oxygen level decreases and opens the possibility to use this kind of materials as active thermoelectric elements.

S8.4 Seebeck Coefficient and Thermal Conductivity of YBCO Ceramics. Julio E. Rodriguez and Alvaro Marino, Department of Physics, Universidad Nacional de Colombia, Bogota, Colombia.

Measurements of Seebeck coefficient, S(T) and thermal conductivity, k(T) on polycrystalline Yb$_2$Cu$_{2}$O$_{6.1}$-d ceramics were carried out in the temperature range between 77K and 300K. The samples were prepared by solid-state reaction method and subjected to different annealing time process at 500°C. The Seebeck coefficient was found to be very sensitive to the oxygen content and its ordering in the Cu-O chains. S(T) data changes from values of 5 μV/K at 200K, to values higher by one order of magnitude. The thermal conductivity showed a decreasing with the annealing time and its values was between 1.0W/mK and 5W/mK. By using the Wiedemann-Franz (WF) model and electrical resistivity measurements it was possible to determine the relative electronic and phonon contributions to the total thermal conductivity.

S8.5 Effects of Sb-doping on electric transport properties of Co-based half-Heusler compound. Yasuhisa Ono1, Slavko
Electric transport properties of half-Heusler compound NbCoSn and lightly doped NbCoSn have been studied in the range from 80 K to 850 K. As-prepared samples exhibit metallic behavior of the electric resistivity $\rho (T)$ in the temperature range from 80 K to 850 K. The electric resistivity appreciably increases during the annealing process at 1123 K for 6 days. Unusual increase in $\rho$ at about 200 K and a local minimum around 400 K is observed for annealed NbCoSn. Small enhancement of $\rho$ is also found in this sample. The $S$-doped samples are metallic over the whole temperature range. Relative large positive Seebeck coefficient $S = (320 \pm 100)$ $\mu$V/K is obtained for NbCoSn:Sn 0.01 at 850 K (28 $\times$ 10$^{-5}$ $\mu$V/K for sample without Sn and 3 $\times$ 10$^{-2}$ $\mu$V/K for Sn-doped sample). The band structure is calculated based on the crystal structure determination of NbCoSn, indicating that the NbCoSn is an indirect semiconductor with a band gap of approximately 1 eV. This result is contrary to the metallic behavior of $\rho$ in the present samples. Since ion radii of Nb and Co are similar, 0.78 A for Nb and 0.79 A for Co, mixing of Nb and Co at their sites may close the band gap, i.e., semimetal band structure. This assumption is supported by the marked annealing effect on $\rho$ and much higher $\rho$ value in the annealed samples than in metallic half-Heusler compounds, TGO:Sn and TiNiSn.

S8.6 Synthesis and Thermoelectric Properties of AgBi$_2$S$_3$
Jun Ho Kim$^1$, Pu Guo$^2$, Tim Hegman$^2$ and Mercouri Kanatzidis$^3$
$^1$Department of Chemistry and Center for Fundamental Materials Research, University of Strathclyde, Glasgow, Scotland; $^2$Department of Electrical and Computer Engineering, Michigan State University, East Lansing, Michigan.

Recent investigations of new perspective thermoelectric materials have been devoted to compounds based on alkali metal, bismuth, and chalcogenics such as Cd$_{x}$Sn$_{(1-x)}$ and Bi$_{x}$Se$_{(1-x)}$. In order to yield a high figure of merit (ZT) promising thermoelectric materials are fundamentally required to have high electrical conductivity, high thermoelectric materials have focused on the optimization of ZT by virtue of creating composites with complex structure and composition that affect an increase in thermopower and a decrease in thermal conductivity. In comparison with alkali metal bismuth chalcogenides, the silver analogues yield lower band gap energies due to the more covalent bonding contribution in their structures that can lead to higher electrical conductivity. Among minerals of bismuth chalcogenides, the silver compounds exhibit a variety of structures and compositions such as AgBi$_2$S$_3$, Ag$_2$Bi$_2$S$_4$, Ag$_2$Bi$_3$S$_5$, and Ag$_2$S$_5$, all of which exhibit unique thermoelectric properties of high electrical conductivity and low thermal conductivity.

S8.7 Calculating Seebeck Coefficients for Arbitrary Temperature Gradients.
Peter P.F. Rodgers$^4$ and Timothy D. Sands$^5$
$^4$Applied Science and Technology, University of California, Berkeley, California; $^5$School of Materials Engineering and School of Electrical & Computer Engineering, Purdue University, West Lafayette, Indiana.

A novel computational scheme has been used to predict the electric potential generated by arbitrary temperature gradients in semiconductor materials. Written in object-oriented code, the Discrete State Simulation (DSS) is a coupled cellular automata simulation that builds upon the objects and rules of quantum mechanics. The DSS models both the discrete non-equilibrium processes in systems that emerge through an ensemble of scattering events that are localized in vibronic modes. By tracking the energy-momentum-position coordinates of the individual particles that define the vibronic state at a node, the DSS models the equilibrium concepts such as temperature. Consequently, the DSS can represent physical systems that are described by more than one temperature and that contain physical features that defy definitions of temperature. Using modified bootstrap sampling algorithms, the local distribution functions induced by external fields and temperature gradients, (2) field-dependent transitions from linear mobility to non-linear mobility, (3) saturation of the electronic density of states, are generated by multiple phonon scattering modes, and (4) charge separation and electric potentials generated by temperature gradients. Ensemble averages were sensitive to the structure of the physical properties of the system, and to quantum coupling strengths. Seebeck coefficients were sensitive to the features of the electronic and the vibrational band structures, and their associated coupling coefficients.

S8.8 Formation of Misfit Dislocations and the Thermoelectric Properties of PbTe/SnTe/PbTe Heterostructures.
Elena Ivanovna Gogotsi$^1$, Olga Nizhegorodskaya$^2$, Nataliya Verkhoturova$^2$, Yegor Vekov$^2$, Mildred S. Dresselhaus$^3$ and Gene Dresselhaus$^3$
$^1$Theoretical & Experimental Physics, NTU "Kharkov Polytechnic Institute", Kharkov, Ukraine; $^2$Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Theoretical predictions and subsequent experimental confirmations of the possibility of a significant enhancement in the thermoelectric figure of merit in the IV-VI based superlattices stimulate substantial interest in studying IV-VI low-dimensional structures. The fulfillment of the theoretical predictions depends on structural and kinetic factors, which determine the degree to which a real structure corresponds to a model. The main goal of the present work is to study the influence of the transition from a strained to a dislocation structure of the interface on the thermoelectric properties of PbTe/SnTe/PbTe heterostructures grown on KCl substrates by thermal evaporation in vacuum. The electron microscopy study of the growth mechanisms of PbTe and SnTe layers on another one another was carried out. The dependence of the thermoelectric properties on the SnTe layer thickness d (0.5-6.0 nm) at a fixed thickness of PbTe layers were investigated. In the thickness dependences of the Seebeck coefficient, the Hall coefficient, electrical conductivity, and charge carrier mobility, anomalies at d ~ 2.0-2.5 nm, corresponding to the transition from pseudomorphic growth to the formation of edge misfit dislocations at the interfaces, were detected. At d ~ 2.5 nm, we also observed maximum values of the thermoelectric figure of merit. It is suggested that the observed effect is a general occurrence and should be taken into account when optimizing growth technologies and when considering the change in the properties of superlattices resulting from a change in the mechanism of growth and from varying the thicknesses of the constituent layers.

S8.9 Fabrication and Testing of Advanced Thermoelectric Unicouple for Power Generation Applications.
Jeff S Nakamoto, Thierry Colbe, Jean Pierre Fleural and Jeff Snyder, JPL, Pasadena, California.

High-efficiency, segmented thermoelectric unicouples employing advanced thermoelectric materials with superior thermoelectric figures of merit are currently under development at the Jet Propulsion Laboratory (JPL). These segmented unicouples include a combination of state-of-the-art thermoelectric materials based on Bi$_2$Te$_3$ and novel p-type ZnTeS$_2$, p-type CoFe$_2$S$_4$-based alloys and n-type CoS$_3$-based alloys developed at JPL. The maximum predicted thermal to electrical efficiency is about 14% for a hot-side temperature of 975K and a cold-side temperature of about 300K. The project describes the design and fabrication of the segmented unicouples and tested them under various conditions for thermal and electrical performance. Some testing results are presented and compared to model predictions. In addition, various techniques for fabricating unicouple are presented. The thermal and electrical testing procedure is briefly described and discussed.

S8.10 Transport properties of quasi-one-dimensional nanostructures.
Miuu Viktorovich Vodernko, O. N. Uryupin, Yu. V. Ivanov and Yu. A. Kuznetso, Tifl Fizicheskoi Technicalniy Institute, St. Petersburg, 194021, Russia.

Quantum-dimensional semiconductors (quantum wires) are perspective materials for thermoelectric applications. Unfortunately, it is difficult to produce sufficiently thin and long nanowires. Therefore, thermoelectric properties of short quantum wires (such as carbon nanotubes) or thick wires (bismuth injected into the pores of an anodized aluminum template) are studied now. We produce nanowires using the natural mineral chrysotile asbestos. It consists of thin asbestos tubes. The internal diameter of the tubes depends on the mineral deposit and varies from 2 to 15 nm. The length can reach 1 cm. The pressure injection of melted semiconductor into asbestos tubes leads to a formation of long wire bundle. Temperature dependences of thermoelectric power, thermal resistance, and current-voltage characteristics of such InSb and Bi wires were investigated experimentally. Theoretical and experimental results of materials obtained are discussed.

S8.11 Synthesis And High Temperature Thermoelectric Properties Of Tin-based Earth Metal Hexaborides MB$_6$ (M=Mg, Ca, Sr, Ba).
Masato Takeda, Yoosuke Kuriya, Keisuke Yokoyama and Takahiro Miura, Department of Mechanical Engineering, Nagasaki University of
Technology, Nagoya, Japan.

Boron-rich semiconductors such as boron carbide are candidate materials for high-temperature thermoelectric (TE) conversion, because they exhibit relatively high performance as a p-type material at high temperatures. Despite a number of studies searching for n-type materials in boron-rich environments, only a few n-type ones but with insufficient TE performance were reported. We found that CaSb and SrSb are n-type materials with high TE performance; in particular, dimensionless figure-of-merit $ZT$ of SrSb reached approximately 0.3 at 1200 K [1, 2]. To discuss the possibilities of further improvement in their TE performance, we synthesized alkali-earth metal hexaborides (CaSb$_6$, SrSb$_6$, BaSb$_6$) and examined the relationship between carrier concentration and TE performance. The experiments (Hall coefficient, Seebeck coefficient, and electrical conductivity) revealed that the TE properties of the hexaborides depend only on carrier concentration, and optimum carrier concentration achieves maximum power factor was estimated to be approximately $2 \times 10^{19} \text{cm}^{-3}$. The results suggest that the substitution of metal atoms while maintaining the optimum carrier concentration will be effective to improve overall TE performance, namely figure-of-merit, because such substitution will reduce lattice thermal conductivity and not significantly affect electrical properties. We also fabricated a TE device using SrSb$_6$ and boron carbide as n-type and p-type elements, respectively. To the best of our knowledge, this is the first demonstration of the TE device composed of only boron-rich solids. [1] Mutsushi Takeda et al., Mater. Res. Soc. Symp. Proc. 691 (2002) 209. [2] Mutsushi Takeda et al., Proc. 21st Int. Conf. Thermoelectrics (2002) 173.

S8.12 Abstract Withdrawn


The electronic and thermal properties of bulk materials are altered when they are incorporated into quantum wells. Two-dimensional quantum wells have been synthesized by alternating layers of B4C and B6C in one system and alternating layers of Si and SiO2Ge0.2 in another system. These structures are being investigated as candidate thermoelectric materials for high figures of merit (ZT). The predicted enhancement is attributed to the confined motion of charge carriers and phonons in the two dimensions and separating them from the ion scattering centers. Sputtering techniques have been used to prepare these multilayer films with thickness $> 10$ micrometers. Films have been deposited on single-crystal Si micrometer thick silicon substrates. The Seebeck coefficient ($S$) and resistivity ($\rho$) properties of these films have been determined over a broad range of temperatures from 4.2 K to 1200 K and were previously reported. The $S/\rho$ values for these P type B-C and N type SiGe films were more than a factor of 10 to 20 times higher than bulk P type B-C and N type SiGe. This couple reported between 300 and 2500 C and was fabricated on a 5 micrometer thick Si substrate with $\sim 11$ micrometers QW film thickness. The 14% efficiency was calculated by dividing the power out of the couple by the power in. The 14% efficiency was obtained with no exception for any expected power losses, such as through the Si substrate and the heater wires. The experimental setup was known as a measured efficiency of $\sim 5.5\%$ for B2Fe5 bulk alloys, assuring the data's accuracy. The experimental point and the predicted values agree quite well. A confirmation that these quantum well materials exhibit a much higher figure of merit than bulk alloys is that the maximum efficiency was achieved at a ratio of load resistance to QW couple resistance of 3 yielding a $ZT$ of $4.1 \text{ at T=150 degree C}$. This P type couple alloy met their maximum efficiency at a resistance ratio of $\sim 1.2$ when their VT value is close to 1. In another separate experiment, the B4C/B6C film was used as a cooler creating a maximum temperature difference of $\sim 45$ degree C. This temperature difference gives $ZT = 3$ for T=250 degree C. For this experiment, the P type B4C/B6C was joined to small Cu wires. The QW film was the same material and thickness as used in the couple mention above for the power generation.


Due to its large thermopower and low resistivity, the ceramic oxide NaCo$_2$Cu$_4$O$_{24}$, is a promising and attractive candidate for potential thermoelectric applications. This is especially the case for NaCo$_2$Cu$_4$O$_{24}$, which is a ceramic compound with high decomposition temperature and chemical stability in air and without toxic elements involved. A review of previous work on the ceramic oxide system will be presented. Electrical and thermal transport properties of NaCo$_2$Cu$_4$O$_{24}$ single crystal made by NaCl flux method have been previously measured and reported. A conventional mixed oxide method was used to prepare polycrystalline NaCo$_2$Cu$_4$O$_{24}$ samples. In order to reduce the loss of sodium during the heating rate, atmosphere sintering with specific crucible arrangement and using calcined NaCo$_2$Cu$_4$O$_{24}$ as atmosphere powder was employed in our study. The effects of oxide structure, microstructure size, and Na concentration, which are substantially influenced by the heating rate, sintering temperature and holding time on the thermoelectric properties, such as Seebeck coefficient, electrical and thermal conductivity were investigated and will be reported. As well, the influence of oxygen flow during calcination and sintering processing on the thermoelectric properties was studied.

S8.15 Transport Properties of CoGe$_4$, Se$_5$, R. E. Ertzkenr; Matt Beckman1, Joshua Martin1, G. Nolte1 and J. Yung2.

1Department of Physics, University of South Florida, Tampa, Florida; 2Materials Processes Laboratory, GM R&D and Planning, Warren, Michigan.

S8.16 Order-Disorder Transition in the Crystalline CaCo$_6$Vb Material. Nicola Zinn Zincken1, Amy Pope2, Donny Winkler3, Terry Tritt4, Verlee Kepness5, Davide Mandra6 and Brian Sales7.

1Physics, Clemson University, Clemson, South Carolina; 2Physics, University of Mississippi, Oxford, Mississippi; 3Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

We performed the electronic and thermal transport measurements of single-phase polycrystalline CaCo$_6$Vb. The resistivity, thermopower, thermal conductivity and heat capacity have been measured between 10 K and 300 K. From the electrical transport data we observed evidence of some type of a phase change in CaCo$_6$Vb with distinct changes in the temperature dependence of the resistivity, thermopower, thermal conductivity and heat capacity around T = 11 K. In addition, the elastic properties measured resonant ultrasound (RUS) techniques investigated over a similar temperature range indicate a large "resonance dip" at T = equal to 11 K. The cubic CaCo$_6$Vb crystal, which is 1/1 cubic approximating force of the recently discovered hexagonal icosahedral Co$_6$Vb, undergoes a reversible order-disorder transition at about 11 K. This makes the system very interesting compared to the quasi-crystal phase Gd$_5$Vb.

S8.17 Electronic Structure Calculations for PrFe$_{12}$P$_{12}$ Filled Skutterudite Using Extended Hückel Tight-Binding Method, Donald H. Galvan, Fisico Quimica, Centro de Ciencias de la Materia Condensadas UNAM, Ensenada, Baja California Norte, Mexico.

To get insight into the electronic properties of PrFe$_{12}$P$_{12}$ filled skutterudite, band electronic structure calculations, Total and Projected Density of States (PDOS), and Mulliken Population Analysis were performed. The energy bands yield a semi metallic behavior with a direct gap (at gamma) of 0.10 eV. Total and Projected DOS provides information of the contribution from each orbital of each atom to the total DOS. Mulliken Population analysis suggest ionic behavior for this filled skutterudite.

S8.18 Performance of Integrated Thin-Film Thermoelectric in Cooling Hot-Spots on Microprocessors-Experimental Setup and Results, Jai K Chaudhary1,4, Randall Alley1,4 and Bronwyn M. Vaffnau1,4,1 Center for Thermoelectrics, Research Triangle Institute, RTP, North Carolina; 2Electrical and Computer Engineering, North Carolina State University, Raleigh, North Carolina.
The increasing performance of microprocessors results in increased thermal density and local power density equal to or greater than the power density of 2W/cm². In comparison, thin-film thermoelectrics [TFT] have measured ZT values of ~2 at 300K, 1.15 response time and potential to pump heat fluxes of several watts/cm². TFTs can ensure that junction temperatures do not exceed the rated 85°C - 95°C range at such hot spots, to guarantee device performance and reliability. We have performed tests by thermally stressing a Pentium Processor and identifying significant drops (~5°C) across the heat sink, which enabled more efficient heat transfer to the copper heat spreader. This extends the performance of air cooling, integrated with TFT, as a cost effective solution with minimal impact on system design. A secondary test setup was built for a 16mm2 TFT to be placed on the HotSpot (~4mm2) of the processor, identified by infrared images. The TEC was powered by a custom-built OPA388 Amplifier circuitry. A SHW Polier module assembly, with liquid cooling for accurate calorimetric measurements of the COP of the system was included. Initial characterization was performed, by simulating the processor load with an aluminum block encasing a 50W resistive load. We will present the effect of cooling on the direct power dissipation of the processor with the standard SPEC CPU2000 benchmarks. The ability of TFT for reliable processor overclocking will also be discussed.

**S8.19**
Thermoelectric properties of perovskite type titanate.
Hiroaki Mutai, Ken Kurasaki and Shinshuke Yamanaka; Nuclear engineering, Osaka university, Suita, Osaka, Japan.

The polycrystalline perovskite type titanate, La doped CaTiO3-SrTiO3-BaTiO3 solid solutions were prepared by the solid state reaction. The electrical conductivity, the Seebeck coefficient, and the thermal conductivities of the samples were measured from room temperature to 873 K. All the samples showed metallic type conduction. The electrical conductivity decreased with increasing temperature, according to about T-1.5. This behavior indicates that the carriers are scattered mainly by lattice in the temperature range. The Seebeck coefficient value increased with temperature almost linearly. In the SrTiO3-BaTiO3 solid solution, the electrical conductivity decreased and Seebeck coefficient slightly increased with the lattice parameter. The result indicates that the shorter Ti-Ti distance is desirable for the enhancement of the power factor. The highest thermal conductivity was seen in the La doped SrTiO3, and decreased by Ca and Ba substitution. The figure of merit had a peak around 400-800 K and the value was above 3.5 at 4 K.

**S8.20**
Thermoelectric properties of β-β′-Bi2Cu2S2 related compounds.
Hironori Ueda, Hiroaki Mutai, Ken Kurasaki and Shinshuke Yamanaka; Nuclear Engineering, Osaka University, 2-1, Yamadaoka, Suita, Japan.

Polycrystalline-sintered samples of β-Bi2Cu2S2 based compounds have been synthesized by melting in sealed quartz ampoules. β′ phase is obtained by quenching from 973K to room temperature. The crystal structure of the samples has been determined by a powder X-ray diffraction (XRD) method. The electrical resistivity and Seebeck coefficient of β-Bi2Cu2S2 increase with increasing temperature. β-Bi2Cu2S2 shows extremely low thermal conductivity, about 0.6 W/mK at room temperature. The dimensionless figure of merit ZT of β-Bi2Cu2S2 shows relatively high value, 0.37 at 800K. The effect of element substitutions on ZT of β-Bi2Cu2S2 has been studied. The temperature dependence of the electrical resistivity of β-Bi2Cu2S2 changes to metallic behavior by substituting elements, indicating the generation of holes in the valence band.

**S8.21**
Li Zhihan and Zhang Duming; Physical Department, Hun Zhong University of Science and Technology, Wuhan, Hubei, China.

We modify the Sedov theory to describe plasma shock waves generated in a pulsed laser ablation process. Under the reasonable asymptotic behavior and boundary conditions, the propagating rules in the global space free (including close areas and mid far areas) of pulsed-laser-induced shock waves are established for the first time. In particular, the temporal behavior of energy causing the difference of the propagation characteristics between the practical plasma shock wave and the ideal shock wave in point explosion model is delicately discussed. The theoretical result is in good agreement with the corresponding experimental data. In addition, some important free parameters which could not directly be obtained from other previous works are determined naturally on the basis of our model.

**S8.22**
Substitution effect on the thermoelectric properties of CoTiSn based Half-Heusler compounds.
Yoshiki Kawai, Hiroshi Ito, Mutai, Ken Kurasaki and Shinshuke Yamanaka; Nuclear Engineering, Osaka University, Suita, Osaka, Japan.

Half-Heusler compounds are known to be intermetallic compounds with relatively large Seebeck coefficients and semimetallic to semiconductor like transport properties. This makes them attractive for study as potential candidates for thermoelectric materials. In the present study, we focus on the substitution effect on the thermoelectric properties of CoTiSn based Half-Heusler compounds. The thermoelectric transport properties of the Half-Heusler compounds were measured in the temperature range between 300 K and 900 K. The high temperature electrical resistivity and thermoelectric power (TEP) were measured simultaneously by a standard four-probe d.c. method using ULVAC ZEM-1. The high temperature thermal diffusivity were measured by a laser flash method using ULVAC T-7000 and the heat capacity were measured by a differential scanning calorimeter using ULVAC Triple DSC. The thermal conductivity was estimated from the density, thermal diffusivity, and heat capacity. The TEP and resistivity show strong substitution dependence. The substitution dependence of the thermoelectric properties were discussed by using the results of the first-principle electronic band calculation.

**S8.23**
Thermoelectric Properties of NaZn13 type Intermetallic Compounds.
Yasutaka Akagi, Atsushi Yamamoto, Chul-Ho Lee, Hiroaki Takuma, Teru Noguchi, Haruhiko Obara, Tsutomu Iida and Yoshihumi Takahashi; Materials Science, Tokyo University of Science, Noda, Japan; *Energy Electronics Institute, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan.

Good thermoelectric performance is usually found in a semiconducting material with extremely low thermal conductivity. Recently semiconducting chalcogenide compounds, i.e. SrGe4Ge30, have attracted a great attention due to their glass-like low thermal conductivity. The origin of the low thermal conductivity has been discussed in connection with their special crystal structure, periodic IV group element cages of large coordinated polyhedra with alkane or rare earth metal residing inside. Intermetallic compounds such as NaZn13, BaCd11, and Tl2Sn17-prototype are known to have a similar ‘cage’ crystal structure. This paper describes experimental results of syntheses and evaluations of polycrystalline samples of SrZn13, BaZn13, LaZn13, LaSn13, SrSn13, BaSn13, and LaSn13 were prepared on the route of melting the metals at a molar ratio of 1:12 in an evacuated quartz tube above their melting points. The samples were ground thoroughly, then hot-pressed into pellets. The polycrystalline sample of LaGe13 was prepared by arc-melting under argon atmosphere with subsequent annealing at 1273K for 1 week. The powder X-ray diffraction and energy dispersive X-ray spectroscopy (EDX) revealed that BaSn13 and LaGe13 samples were single phase, while the SrSn13 and LaSn13 samples contained small amount of the impurity phase of metal zinc. The electrical resistivity and the Seebeck coefficient measurements were performed from 39K to 673K for SrSn13, BaSn13, and LaSn13, from 39K to 873K for LaGe13. The thermal conductivity was determined at room temperature. Through the electrical resistivity and Seebeck coefficient measurements, SrSn13, BaSn13, LaSn13, and LaGe13 were found to be a good metallic conductor. Among them the Seebeck coefficient of LaGe13 was actually higher than a metal 30µV/K at 400K. The lattice components of the thermal conductivity calculated for SrSn13, BaSn13, LaSn13, and LaGe13 assuming Wiedemann-Franz law were 1.1W/mK, 8.6W/mK, 7.3W/mK, and 9.8W/mK, respectively.

**S8.24**
Thermoelectric Properties of Hot-Pressed GaN and InN.
Atsushi Yamamoto1, Yasuo Iwamura2,3 and Shigeo Yamaguchi1,3; 
1Energy Electronics Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan; 2Department of Electronic, Electrical and Information Engineering, Kanagawa University, Yokohama, Kanagawa, Japan.

We made an attempt to obtain bulk III-Nitride semiconductors such as InN, GaN and InGa1-xN alloy using hot-press method in order to determine the high temperature thermoelectric properties. In general,
bulk synthesis of III-nitride compounds requires high-pressure nitrogen to suppress decomposition of nitriles. In this study, we successfully obtained high-purity bulk samples by pyrolyzing the nitride powder prepared by pyrolysis reaction of a complex salt. The hot-pressed samples were confirmed to be single phase by X-ray diffraction, and showed relative density of 50% for GaN and 70% for InN. The samples had good mechanical strength, which was enough to handle in subsequent electrical and thermal measurement. The hot-pressed nitride samples showed negative Seebeck coefficient at room temperature and high temperature, the Seebeck coefficient and the resistivity were -1.8x10^-8 V/K and 1.9x10^-4 Ω·m for GaN and 1.5x10^-3 Ω·cm for 300 K, respectively. The room temperature thermal conductivity determined by laser flash method with porosity correction were 1.7 W/mK for InN and 2.0 W/mK for GaN. For InN the Seebeck coefficient and the resistivity increased monotonously with increasing temperature, which indicates that InN is metal or degenerated semiconductor. The maximum power factor and figure of merit in InN within the measured temperature range were 2x10^-7 W/mK and 1.5x10^-5 W/K·K at 650 K, respectively.

**SB.25**


Boron-rich cluster compounds are attractive materials for their stability under high temperature and in unfriendly (e.g. acidic) environments. Magnetic properties of some new rare earth boron cluster compounds have recently attracted increasing interest, being magnetically dilute materials but displaying a variety of properties. Short range magnetic transitions in REB12 and structurally-related RE4B12 clusters, long range order in GeB12, and 2-dimensional spin glass behavior in the homologous series REB12CN, REB12F2CN, REB12Se2CN [1]. Interestingly, it has been indicated that the clusters of boron in chalcogenide glass, play an important role in mediating the magnetic interaction which is a novel phenomenon. Boride compounds such as the well known metal-doped boron cluster compounds have recently been investigated as possible thermoelectric materials [2], because the structure of the boron cluster is a potential thermoelectric material [3].

The boron cluster compounds investigated up to high temperatures reaching over 1000 K. Relatively large Seebeck coefficients are observed and the electrical conductivity increases rapidly with temperature, which is typical for chalcogenide glasses. The resistivity and Seebeck coefficient do not show a significant decrease in value. Possibility of using or modifying these novel boron cluster compounds for high temperature thermoelectric application will be discussed. This work is supported in part by a PRESTO fund project from the Japan Science and Technology Corporation JST [1] for example, T. Mori, A. Leithe-Jasper, Phys. Rev. B 66 (2002) 214419, T. Nakajima, T. Shimizu, K. Kimura, J. Solid State Chem. 154 (2001) 13, D. G. Cahill, E. H. Sargent, R. C. Watson, R. O. Pohl, A. G. Sack, Phys. Rev. B 40 (1989) 3254.

**SB.26**

**Materials of the thermoelectric conversion unit system within radiation heat transfer and the analysis**, Toshinori Ota and Junichi Ochimi, Research Laboratory, Ishikawajima-Harima Heavy Industries Co., Ltd, Yokohama, Kanagawa, Japan.

We propose development of the thermoelectric conversion system which is responsible for efficient waste heat recovery. In order to recover waste heat, this system is used in the industrial processes. The amount of waste heat is converted into a usable electrical energy, and can be utilized directly by the processes. The waste heat recovery system is used in the industrial processes. The waste heat is converted into a usable electrical energy, and can be utilized directly by the processes. The module efficiency is an important parameter for the system. The temperature range of the module is limited due to the material properties. The module efficiency is an important parameter for the system. The temperature range of the module is limited due to the material properties. The module efficiency is an important parameter for the system. The temperature range of the module is limited due to the material properties.
0 from 300 K to 10 K. Thus, these compounds exhibit relatively large power factors, $PF = a'p$, with a $PF > 10^4 \text{W/m}^2 \text{K}^2$ at $T = 300$ K. This power factor is comparable to that of the n-type Bi$_2$Te$_3$ type materials. Plate-like crystals of TiSe$_2$ can be grown by the iodine vapor transport method to sizes of over 1 cm. In this synthetic approach some dopants can be integrated into the parent compound, effectively providing a means to tune electronic properties. We will present results of element doping on the electronic properties in these materials.

S8.31
Crystallographic Features of Rhenum Disilicide.
Katsushi Tanaka 1, Haruyuki Inui 1, Takuya Ohsaka 1, Satoshi Tsuda 4 and Manakicho Mizumaki 5
3. National Research and Development Centre, Saitama.
5. Tokyo Institute of Technology, Yokohama, Japan.

We propose a method of convenient measurements of thermoelectric properties including thermal decay time constants ($\tau$) and thermal diffusivity constants ($D$) for a thermoelectric material. A composition-spread method is utilized for fabricating a film whose doping concentration varies from 0 to 0.125 continuously. An improved transient gratig method that is a new version including higher spatial resolution and much more precise fitting function compared with the past conventional method is employed for characterization of the physical properties of the film. A demonstration is given for our reference material, (Ca$_{1-x}$ Sr$_x$)$_2$CoO$_4$.

S8.32
Thermo Physical Property Measurements of (Ca$_{1-x}$Sr$_x$)$_2$CoO$_4$ Films Using an Improved Transient
Grating Method.
Yoshiki Takata 1, Hajime Hamed 2, Yutaka Adachi 1, Yoshiki Wada 1, Takanori Miyata 4, Kenji Inaka 5 and Noriyoshi Kinoshita 5
1. Tokyo Institute of Technology, Yokohama, Japan.
2. The University of Tokyo, Tokyo, Japan.
3. National Research and Development Centre, Saitama.
4. Tokyo Institute of Technology, Yokohama, Japan.
5. Tokyo Institute of Technology, Yokohama, Japan.

We propose a method of convenient measurements of thermoelectric properties including thermal decay time constants ($\tau$) and thermal diffusivity constants ($D$) for a thermoelectric material. A composition-spread method is utilized for fabricating a film whose doping concentration varies from 0 to 0.125 continuously. An improved transient gratig method that is a new version including higher spatial resolution and much more precise fitting function compared with the past conventional method is employed for characterization of the physical properties of the film. A demonstration is given for our reference material, (Ca$_{1-x}$Sr$_x$)$_2$CoO$_4$.

S8.33
Investigation of the Properties of Electrochemically
Deposited Semiconductor Materials for Thermoelectric
Applications.
Cheol-Koo Hong 1, J A Herman 1, N Myung 1, J R Lim 1 and J-P Fleury 2
1. Jaguar Jet Propulsion Laboratory, Pasadena, California.
2. Jet Propulsion Laboratory, California Institute of Technology, La Cañada Flintridge, California.

At JPL, it is our desire to fabricate thermoelectric micro-devices for power generation and cooling applications using an electrochemical deposition (ECD) technique. We believe that the performance of our current micro-device developed is limited by the properties of the ECD materials. Therefore, the objective of this study is to develop ECD methods for obtaining n-type Bi$_2$Te$_3$ and p-type Bi$_{2-x}$Sb$_x$Te$_3$ thermoelectric materials with new bulk properties, as well as optimizing film morphology and transport properties, which makes use of ECD are Si$_2$O$_5$/Si wafers with either 1 $\mu$m Bi$_2$Te$_3$ or 1 $\mu$m Bi$_{2-x}$Sb$_x$Te$_3$, sputtered on top. From our experimental observations, ECD at higher temperatures typically leads to higher deposition rates but also increases film porosity. In general, the ECD films change their morphology from porous to smooth when the ECD potentials change from very negative to less negative vs. saturated calomel electrode (SCE) reference. The films of Bi$_2$Te$_3$ and Bi$_{2-x}$Sb$_x$Te$_3$ were initially obtained under various deposition conditions. See 2 for a compilation of the results. The Seebeck coefficients and transport properties were then measured along the direction parallel to the substrates before and after annealing at 250°C for 2h. From the data obtained, ECD n-Bi$_2$Te$_3$ material can achieve a high Seebeck coefficient (189 $\mu$V/K) when it is deposited at $-110$ mV vs. SCE. The in-plane resistivity, in-plane mobility, and carrier concentration are $5.9 \text{m}\Omega\text{-cm}, 42 $ cm$^2$ V$^{-1}$ s$^{-1}$ and $2.5 \times 10^{15}$ cm$^{-3}$, respectively. From the results, we have found the best conditions for depositing high quality Bi$_2$Te$_3$ and Bi$_{2-x}$Sb$_x$Te$_3$ materials with thermoelectric properties comparable to those of their state-of-the-art bulk samples.

S8.34
Effect of High Valence Metal Doping on Thermoelectric
Properties of [Ca$_2$CoO$_3$]-[0.62Co$_2$O$_3$]. Kanusuke Ijima 1, Shigeru
Horii 2, Yuchi Ishinomori 3, Wataru Sato 4, Koichi Kusunose 1
1. Department of Applied Chemistry, University of Tokyo, Tokyo, Japan.
2. PRESTO, Japan Science and Technology Corporation (JST), Kanagawa, Saitama, Japan.
4. [Ca$_2$CoO$_3$]-[0.62Co$_2$O$_3$] has been attracted as an excellent thermoelectric material for power generation at high temperatures because its single crystal was reported to show a practical figure of merit (ZT) over 1 [1]. Recently, our group reported that the thermoelectric properties of Ca$_2$CoO$_3$ polycrystalline bulk were dramatically improved by combination of magnetic-axis alignment and demagnetization processes [2]. However, the Ca$_2$CoO$_3$ bulk was found to show large oxygen nonstoichiometry (0.68-0.14) at high temperatures through the thermogravimetric measurements [3], resulting in oxygen content dependent thermoelectric properties [2]. On the other hand, it is theoretically predicted that Seebeck coefficients $S$ of layered calcium ferrites can be enhanced by lowering magnetic CoO$_2$ layers [4]. Therefore, the enhancement of Seebeck coefficient is expected by the doping of high valence metals to the Ca site in the Ca$_2$CoO$_3$ layer. In the present study, we attempted to synthesize high valence metal-doped Ca$_2$CoO$_3$ compounds [Ca$_2$Co$_{1-x}$M$_x$O$_3$]-[0.62Co$_2$O$_3$, $M$ = Re, Mo, or Nb] and evaluated their thermoelectric properties and oxygen nonstoichiometry. Moreover, $\alpha$-axis aligned and for dense polycrystals of these compounds were prepared. The single-phase compounds could be obtained up to $x = 0.135$ for $M = \text{Re}, \text{Mo}$ and $x = 0.11$ for $M = \text{Mo}$ by the solid state reactions in air. High valence metal-doped Ca$_2$CoO$_3$ compounds exhibited dramatically suppressed oxygen nonstoichiometry. Moreover, Seebeck coefficients of the doped compounds increased with doping concentration ($\alpha$) and the electrical resistivity ($\rho$) systematically increased with doping level as compared with the conventional sintered bulk samples, however, it was remarkably improved by applying intermediate cold pressing processes down to almost comparable values with that of undoped Ca$_2$CoO$_3$. Consequently, excellent power factors ($S^2\rho$) were also obtained for the high valence metal-doped Ca$_2$CoO$_3$. Thermoelectric properties of these doped Ca$_2$CoO$_3$ at high temperatures, where oxygen composition is stable, will be compared with oxygen nonstoichiometric pure Ca$_2$CoO$_3$ [1] Hishinuma et al., Jpn. J. Appl. Phys. 39 (2000) L1127, [2] Iwamori et al., Jpn. J. Appl. Phys. 2 (2003) L1198, [3] Shimizu et al., Jpn. J. Appl. Phys. 42 (2003) L1194, [4] Kishida et al., Phys. Rev. B 63 (2000) 085216.

S8.35
Jarrod Short 1, Sim Lee 1, Saneetea Lai 1, Theodore Kyriss 2, Kwei Fung Hsu 2, Mercouri Kanatzidis 2, and Tim Hogen 2
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2. Materials Research Institute, University of New Orleans, New Orleans, Louisiana.

In the field of thermoelectrics, the figure of merit of new materials is based on the electrical conductivity, thermoelectric power, and thermal conductivity of the sample, however additional insight is gained through knowledge of the carrier concentrations and mobility in the materials. The figure of merit is commonly related to the material properties through the $B$ factor which is directly dependent on the mobility of the carriers and the electrical resistivity. To gain additional insight on the new materials of interest for thermoelectrical applications, a Hall Effect system has been developed for measuring the temperature dependent carrier concentrations and mobilities. In this paper, the measurement system will be described, and recent results for several new materials will be presented.

S8.36
Synthesis and Polyaniline-Coating of Bismuth Chalogenides.
Ven B Reddy 1, Patrick L Garrity 2, and Kevin L Stokes 2
1. Advanced Materials Research Institute, University of New Orleans, New Orleans, Louisiana.
2. Department of Chemistry, University of New Orleans, New Orleans, Louisiana.

$\rho$ style="text-align: justify;" Our interest in the synthesis of bismuth chalogenides stems from their possible enhancement of the thermoelectric properties in nanophase. One of the authors earlier
reported in efficient high-temperature synthesis of bismuth sulfide nanobelts [1]. Kevin Stokes et al. [2] also reported the high-temperature synthesis of bismuth sulfide nanobelts as follows: a solution of thiocarbamide in phenyl ether and a small amount of diethylene glycol at about 60 °C under 500 °C was added to a solution of bismuth oleate in phenyl ether and excess oleic acid. The resulting mixture was cooled to room temperature using a water bath. Phenyl bis(oleyl) thiocarbamate was precipitated by centrifugation and washed with ethanol and acetone. Synthesis of highly crystalline bismuth telluride nanosheets involved the reaction of bismuth triol on phenyl ether and excess oleic acid with triethylene glycol in toluene at 110 °C for 4-5 h. The resulting mixture was centrifuged and washed with ethanol and acetone. Longer reaction times adversely affect the monodispersity of nanorod populations and give a large proportion of larger particles. From the viewpoint of environmental and energy-saving issues, there has recently been a great increase in the research and development of thermoelectric power generation systems. However, since binary compounds lower their coefficient of thermal conductivity, Bi$_2$Te$_3$ and PbTe have been found for room-temperature applications and since Te is scarce, volatile, and toxic, the application of Bi$_2$Te$_3$ and PbTe has been limited in commercial use. In terms of the reduction in the electrical conductivity, we have focused on the properties of III-nitrides and III-nitrides and have recently studied their thermoelectric properties. The nanorods studied here were III-nitride doped and III-nitride-doped films such as Al$_{1-x}$In$_x$N and Al$_{1-x}$In$_x$O$_y$N$_z$ prepared by the reactive radio-frequency sputtering method. They were grown on SiO$_2$ glass substrates at 100 °C using N$_2$ and Ar gases. First, the in-plane thermal diffusivity $D$ of the semiconductor films (1100 nm) was measured using an ac calorimetric method in the temperature range of 300-730K. The results showed that at intermediate temperature the thermal diffusivity has a minimum value of 1.6-1.7 x 10$^{-7}$ m$^2$/s for AlN, 7.6-8.2 x 10$^{-7}$ m$^2$/s for Al$_{0.8}$Ga$_{0.2}$N, and 7.0 x 10$^{-7}$ m$^2$/s for Al$_{0.9}$In$_{0.1}$N. Furthermore, in addition to the values of $D$ and $c$, we measured the mass density of the samples. The thermal conductivity was determined to be 1.1 K/W-mK. However, the thermal conductivity of the nitride films was not reported. This study will be a milestone for the development of a thermoelectric device. The n-type doped ZnO-based thermoelectric materials were fabricated by a spark plasma sintering (SPS) process. Three bath compositions, pure and M-doped ZnO (M=Al, Ni), were prepared from the nanosized powders which were synthesized by a polymerization complex method. The SPS process was performed at the temperature range of 850 - 900°C under an applied pressure of 40MPa for 5 minutes in vacuum atmosphere. The Seebeck coefficient, electrical and thermal conductivities of the specimens were measured with the variation of the temperature. SEM and TEM observation showed that the nano-sized pure and M-doped ZnO powders with the range of 20-50nm were successfully synthesized. PL and XRD analysis confirmed that Al and Ni were successfully doped in ZnO structure. The M-doped specimens showed higher electrical conductivity than pure ZnO and showed metallic conductivity behavior. In case of Ni-doped ZnO, the electrical conductivity increased with increasing the amount of doping, but in case of Al-doped ZnO, the electrical conductivity reduced with increasing the amount of doping because of the native oxide, which has poor electrical conductivity and acts as an electron conduction scattering center. The thermal conductivity of M-doped specimens remarkably decreased because the defects which are introduced form doping and oxygen vacancies and nano sized secondary phases in grain boundaries reduced thermal conduction by the phonon scattering, which is very useful for improving the thermoelectric performance of the specimens.
Microstructure Design Approach to Thermoelectric Materials. Licheng Chen, Xin Shi, Xiangyang Huang and Jun Jia. State Key Lab of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, 200050, China.

Thermoelectric performance of polycrystalline materials is greatly influenced by their microstructures including grain sizes, grain boundaries, grain orientation, and distribution of the secondary phase in composites, etc. The material microstructures are sensitive to the preparation processes and the starting materials. These make the understanding of the microstructure influence on thermoelectric transport properties very complicated. In present study, we synthesized half Heusler-based and skutterudite-based composites using CVD, mechanical milling and γ-A12O3 particles as the dispersion phases, and BZT3-based sintered materials with textured surfaces. For ZnNi2Sb-based half-Heuslers and CuSbS2-based skutterudites, when dispersion particles are randomly and uniformly dispersed in the matrix, ZT values are not enhanced because of power factor reduction even though thermal conductivity is also reduced. When the dispersion particles are dispersed homogeneously on the grain boundaries coating the matrix grains, an enhancement in ZT values is observed due to a reduction in lattice thermal conductivity and an increase in thermopower in spite of a somewhat decrease of electrical conductivity. In these samples, the carrier scattering mechanisms are much different than those of the matrix materials. This is considered to be due to the special grain boundary structures. The BZT3-based sintered materials with preferred orientations have successfully been fabricated through a spark plasma sintering (SPS) technique by controlling the particle size and the sintering process. The half-Heusler textured BZT3-based materials show high mechanical strength and significant anisotropy in thermoelectric transport properties. Thermoelectric performance perpendicular to the pressing direction (with c-axis preferred orientation) is comparable to that of single crystal materials in the same crystallographic orientation. Details of the microstructure effect on thermoelectric transport properties will be reported in this paper.

9:45 AM S9.5 Effects of Alloying Elements on Thermoelectric Properties of ReSi2. Min Won, Okuno, Shunji, and Hiyuuki Inoue; Materials Science and Engineering, Kyoto University, Kyoto, Japan.

Binary rhodium dinitride is of interest owing to potentials as a promising candidate material for thermoelectric applications. The stoichiometry of the alloy is determined to be ReSi2.75 instead of ReSi2 and the crystal structure belongs to the monoclinic system with an ordered arrangement of Si vacancies in the parent C15 lattice. Binary ReSi2.75 exhibits a significantly anisotropic thermoelectric properties such that the value of Seebeck coefficient along [110][111] is positive (320μV/K at 330 K) while it is negative (-380μV/K at 600 K) along [110][111]. This may result from the highly anisotropic electronic structure of ReSi2.75. The dimensionless figure of merit (ZT) for binary ReSi2.75 is as high as 0.7 at 1073 K when measured along [100] while the ZT value along [100] is moderate (0.15 at 900 K). We have attempted to improve the electrical properties of the measured samples. This is achieved by alloying with Al, Ge, Mo and some other transition metals. Al and Ge substitution for Si in ReSi2.75 improve the ZT value along [100] in the whole temperature range (325-1073 K). The temperature dependence of electrical resistivity measured along [100] indicates that the conduction mechanism changes from semiconducting to metallic upon alloying with Al and the value of electrical resistivity at room temperature for Al-added alloys is significantly reduced by two orders of magnitude when compared to the binary compound. Deut substitution for Si in ReSi2.75 reduce the value of electrical resistivity along [100] in the whole temperature range by an order of magnitude. Magnetic substitution for He in ReSi2.75 increase the ZT value along [100] in the whole temperature range. Improvement of thermoelectric properties along [100] and [100] occurs in different ways depending on alloying elements. Nice ZT values can be achieved for both orientations when alloyed with Ge. Then p- and n-type legs can be fabricated from a single crystal providing contact loss of conversion efficiency. The effects of microstructural
changes caused by alloying with these ternary elements on the thermoelectric properties will also be presented.

10:30 AM #S10.1
Antimony Telluride Under Pressure. Gerald Denis Mahan, Physics, Penn State University, University Park, Pennsylvania.

John Boddin's group has reported large increases under pressure in the figure of merit of commercial laserunnified antimony single crystal alloys [1]. Since the major component of the alloy is antimony telluride, we have sought an explanation of this phenomena by performing electronic structure calculations of antimony telluride under pressure [2,3]. These calculations provide a transport density of states, which is used to calculate the pressure-temperature dependence of the electrical resistivity and Seebeck coefficient. We find antimony telluride is an indirect gap material, and the indirect gap closes under uniaxial pressure of 5.6 GPa. At T=300 K both the electrical conductivity and Seebeck increase under pressure as the band gap closes, in agreement with the experimental findings. The calculations also show that the band gap does not close, and not much happens, when biaxial stress is used instead of uniaxial pressure. This result also agrees with the experiments. 1) D.A. Polvani, J.F. Meng, N.V.C. Stakke, J. Sharp, and J.V. Boddin, Chemistry of Materials, 15 (6), 2006-2071 (2001) 2) M. Baranski and G.D. Mahan, in: Proc. Conf. on Thermoelectrics (1996). [IEEE Cat. No. 96TH8307] pp. 713-714] 3) Thonhauer, T.J., Scheidegger J.O., Sofo J.V. Boddin and G.D. Mahan (submitted to Phys. Rev. B)
electron emission by real time microscopic acquisition methods. Sulfur
doped nanocrystalline and CNT films exhibit a strong temperature
dependence in emission at temperatures considerably lower than
1000°C with emission originating from singular sites. These materials
are presented as the electron emitter for thermionic energy converters.
Extensive studies on electron emission from nanocrystalline carbon,
I.e. CNT and nanocrystalline diamond films have shown that these
materials exhibit electron emission from sites with a reported
size smaller than 10 nm and an emission site density in the order of
10^5 cm^-2. Although the exact origin of this emission behavior is still
unknown it is evident that electronic and topographic field
enhancement are in part responsible for the observed emission
behavior. High field enhancement exhibiting surface regions
Corresponding to an increase in the local electric field which causes
electrons to be removed from these surface areas in a highly efficient
way. This effect could play an important role in a new generation of
thermionic energy converters by eliminating space charge effects that
occur at films surface emitters in addition to manufacturing advantages
by increasing the micro-spot emission mode distance. This research is
supported by the ONR.

260 PM S11.3
SiGeC Cantilever Micro Cooler, Gheorghe Zeng1, Edward Croke2,3,
Yan Zhang2, James Christofferson2, Ali Shokouhi2 and John E.
Bowers1;1, University of California, Santa Barbara, California; 2,
University of California, Santa Cruz, California; 3HRL Laboratories,
Malibu, California.

Fabrication and characterization of SiGe-based cantilever micro
cooler is described. Silicon on insulator (SOI) was used in the
substrate, and the two layers of 3 um thick p-SiGe0.07/Ge0.075
and 1.14 um thick n-SiGe0.07/Ge0.075 were directly grown on the SOI using
molecular beam epitaxy. All layers were lattice matched to the silicon
substrate. Subsequently a unique micro cooler was fabricated using
conventional integrated circuit processing and the cantilever structure
was formed by removing the backside silicon layer of SOI substrate
using deep reactive ion etching. Devices with different sizes were
fabricated and characterized. By etching the top n-doped layer in one of
the legs and by depositing metal electrode at the junction between
the two legs, a unique cooler was fabricated without a need for regrowth.
This could simplify substantially large scale integration and
array fabrication of these devices. In these micro refrigerators, heat is
transferred laterally from the junction between legs to the two
contacts. Cooling by 1.2 K at room temperature has been measured.
Calculations show that heat conduction through the 0.2 micron thick
silicon buffer layer on top of the SOI substrate is the main limitation
to the device cooling performance.

2:15 PM S11.4
Experimental characterization and modeling of InP-based
micro coolers R. Singh, D. Vashisth, Y. Zhang, M. Negues, A.
Shokouhi, UCSI Y. Okuno, Y-J. Chiu, Gelhong Zeng, John
Bowers UCSB, Rajeev Singh, Duryodhan Vashisth, Yan Zhang,
Millon Negues, Ali Shokouhi, Y Okuno, Y-J Chiu, Gelhong Zeng and
John Bowers; Electrical Engineering, University of California, Santa
Cruz, Santa Cruz, California.

In this paper we present experimental and theoretical characterization of
InP-based heterostructure integrated thermionic coolers. In
particular, we characterize the effect of doping on overall device
performance. Several thin-film cooler devices have been fabricated and
analyzed. They contain a one-micron thick superlattice structure
composed of 25 periods of InGaAs wells and InGaAsP barriers
(bandgap ~1.3 microns) with a thickness of 10 and 30 nm,
respectively. All the layers are lattice-matched to the InP substrate.
Highly doped InGaAs layers are used on the top and bottom of the
superlattice for contact doping purposes. N-type doping in the InGaAs
quantum well was varied from 1.5x10^18 to 8x10^18 cm^-3, while the
quaternary barrier layer was undoped. Device cooling performance
was measured at room-temperature. Device current vs. voltage
relation was characterized in a wide temperature range from 10K to
room-temperature. Detailed models of electron transport in
superlattice structures were used to simulate device characteristics
and performance. Experimental results show that low-temperature
electron transport is a strong function of well layer doping and that
device maximum cooling decreases as doping increases. Theoretical
models for both LV curves and maximum cooling agree well with
experimental results. The results indicate that low-temperature
electron transport is a strong function of the potential barriers and
energy filtering in heterostructure thermionic coolers.

3:30 PM S11.5
System Constraints on Materials for Thermoelectric/
Thermionic Power Generation, Peter Meger and Rajeev Ram;
Research Laboratory of Electronics, MIT, Cambridge, Massachusetts.

The traditional metric quantifying a material’s effectiveness in a