The Abdus Salam International Centre for Theoretical Physics

CONFERENCE ON

MODERN CONCEPTS AND NEW MATERIALS FOR THERMOELECTRICITY

11 - 15 March 2019

ICTP, Trieste, Italy

ABSTRACTS OF POSTER PRESENTATIONS

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MAGENTA project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 731976.

Investigation of Physical Properties of Bulk Metal Chalcogenide Materials for Thermoelectric Applications

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Metal chalcogenides are naturally rich in phase and structural variety, which offers an assured degree of freedom for tailoring its properties. Recently, tin telluride (SnTe) have gained enormous interest as a non-toxic substitute to lead telluride because of analogous crystal and band structure. For SnTe, the temperature dependent transport studies demonstrated the enhanced Seebeck coefficient and poor thermal conductivity in Mn doped self-compensated $Sn_{1.03}Te$ [1]. The poor thermal conductivity has been understood and explained based on the point defect scattering, appearance of soft phonon and impurity localized modes [1]. In addition, Mn doping results in modification of electronic band structure, via a systematic increment of magnetic moments, increase in effective thermal mass of charge carriers and overall enhancements in power factor [2]. Further, temperature dependent transport data and first-principles calculations on rare earth element (Yb) doping showed that with heavy atomic mass and strong spin-orbit coupling, the mild doping in SnTe can converge the two valence bands more effectively over Mn [3, 4].

Additionally, the investigations have also been done on large unit cell Argyrodite with intrinsic low lattice thermal conductivity. Here, Ag_8SnSe_6 has been demonstrated as an efficient thermoelectric material over Ag_8GeSe_6 due to high carrier concentration, large electronegativity difference between Ge and Sn, and high mobility in high temperature cubic phase [5]. Further, the extremely low thermal conductivity for both the samples has been explained with weakly bonded Ag ions to rigid anion sub lattice and presence of low frequency Einstein optic modes. Thus, Ag_8SnSe_6 has been demonstrated as an efficient thermoelectric material with $ZT \sim 0.62$ at 623 K, even at a very low carrier concentration ($\sim 10^{16}$ cm^{-3}).

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Analysis Of The Experimental Temperature-Baric Dependences Of The Thermoelectric Properties Of Semiconductors

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Research on the thermophysical and thermoelectric properties of semiconductors and their solid solutions has both fundamental and applied aspects related to the search for highly efficient thermoelectric materials. In semiconductor solid solutions, phonon scattering on lattice defects is more significant than for current carriers. Therefore, it is possible to achieve a significant decrease in thermal conductivity at relatively high values of electrical conductivity and thermal electromotive force. Here we present some results of a comparative analysis of the experimental temperature-baric dependences of the thermal conductivity, electrical conductivity and thermal electromotive force of polycrystalline and single-crystal semiconductors in the pressure range from 0.1 to 320 MPa and temperatures from 273 to 423 K. The results for single-crystal and polycrystalline tellurium, selected as a reference material, are discussed, as well as a number of compounds.

This work was partially supported by the RFBR grant 18-08-00059a.

Conductivity And Thermoelectric Effect In Electron Gas With Fractal Structure

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Systems with a fractal structure attract the attention of many researchers. Here we present the results of studies of the conductivity and thermoelectric effect in an electron gas with a fractal structure. The Kubo formula for conductivity is obtained. The dependences of the conductivity and thermopower on the chemical potential and temperature are studied for various values of the fractal dimension.

The static conductivity at zero temperature is shown as a function of the Fermi energy for various values of the fractal dimension. We have shown that the dependence of the thermopower on the fractal dimension is rather weak. The decrease in the thermopower with a decrease in the dimensionality is apparently due to a decrease in the number of charge carriers. The decrease in the fractal dimension leads to a significant decrease in the reflection coefficient. It is also shown that in a wide frequency range, the standing wave ratio turns out to be quite low, which means that the fractal antenna is able to work effectively in a wide frequency range.

This work was supported by the RFBR grant No. 18-08-00092a.

Investigation of the Theoretical Exergy Efficiency of Solar Thermoelectric Generators

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Abstract

The optimal configurations for obtaining the maximum exergy efficiency from solar thermoelectric generators (STEGs) were determined in this study. The STEG properties investigated included the optimal hot-side temperature, the length-weighted current density, the thermoelement area ratio, the length of the thermoelectric (TE) legs and the thermal concentration ratio. It was observed that optimal hot-side temperatures existed which correspond to maximum exergy efficiencies of the STEG systems. In the absence of optical concentration, these exergy efficiencies were as much as 6 – 8% for a hot-side temperature range of 1750C – 2770C though with thermal concentration ratio as large as 600 – 700. These optimal hot-side temperatures were found to be independent of both the TE device geometry and the thermal concentration ratio but varied with the dimensionless figure- of-merit of the device as well as the properties of the optical component and the solar absorber used. With the optimised design configuration, complicated optical systems (which usually include tracking mechanism) may be eliminated, and the required amounts of TE material minimised. This would ultimately result in substantial reductions in material, manufacturing and system costs.

Shannon entropy and self-organization process of microtubules

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Abstract: We investigate the Shannon entropy as a function of temperature and dipole moment in microtubule's systems. The results show that the Shannon entropy is an increasing function of dipole moment but can be an increasing or decreasing function of temperature. At certain points, the transmission process occurs; this phenomenon is justified by the oscillation behavior observed on the graphs. This observation is the first characterization of chimera's states where the disorder and the order coexist: This fact can be interpreted as the self-organization process occurring in microtubules.

Thermoelectric Properties of Nanowires

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Abstract

Nanostructured thermoelectric devices have gained great interest owing to their tunable properties due to quantum confinement effect and large surface to volume ratio. The present study is focused on the computation of the thermoelectric profiles of semiconductor nanowires (NWs) under first principles density functional theory approach. The computed shape and diameter dependent electronic and thermoelectric properties of the nanowires replicate the anisotropic behavior of the NWs. Our results show that the properties of the NWs are significantly modified from their bulk counterparts due to size and shape dependent strong quantum confinement effects.

Keywords

DFT, Nanowire

Automation of thermal conductivity measurement by 3- omega method using Arduino

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We present an ongoing development of a method for automating thermal conductivity measurement in the frequency domain. A thin metal strip is sputtered on top of the measured sample and AC current is passed through the strip at frequency ω. This causes joule heating at DC and 2ω frequency and a linear thermal response causes thermal fluctuations at 2ω, that leads to resistance changes in the strip at the same frequency. By Ohm's law the ω current and 2ω resistance when multiplied produce a small voltage at 3ω where the phase and amplitude depend on the thermal properties of the material. The 3ω method for thermal conductivity measurement can be applied to bulk amorphous solids and crystals as well as amorphous films tens of microns thick [1]. In the Wheatstone bridge of the 3-omega experimental setup, a fine potentiometer is replaced by a light dependent resistor controlled by Arduino, enabling full, easy and cheap automation of measurement. Further development will involve high-temperature measurement by integration with tube furnace including "proof of concept measurement" of silicon, borosilicate glass and Kapton.

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Electronic Structure, Elastic and Thermoelectric properties of Fe2Tage Alloy: An *ab-intio* Study

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Abstract

In search for novel magnetic materials, we discuss the computer estimation of structural, electronic, mechanical, thermodynamic and magnetic properties of yet-to-be synthesized but stable Fe_2TaAl alloy. We make use of density functional theory and mechanical/dynamical aspects for this resolution. The scrutiny of structural and mechanical stability outlines the $L2_1$ structure as the stable phase. Interestingly, while the Fe_2TaX (X=Al,Ga,In) compounds are reported to be nonmagnetic semiconductors, the Fe-Ge compound comes out to be a ferromagnetic half-metal. The computed electronic structure reveals a half-metallic gap E_{HM} = 0.05 eV for the PBE functional; while as for the mBJ potential, E_{HM} = 0.21 eV in spin-down channel. From the elastic studies, the present material falls out to be a ductile one along with a Debye temperature of 279.06 K. The magnetic evolution predicted from Slater-Pauling rule (Mt-24) manifests the total integral magnetic moment to be one Bohr magneton, and the same is reflected from *ab intio* simulations. Possible d-d hybridization is observed to present the origin of energy gap in spin down channel.

The calculated thermoelectric coefficients like S, present a room temperature value of power factor

~4.5 mW/K^2m. This material could possibly have application in spintronics as well as thermoelectrics.

Keywords: Electronic Structure; half-metallic materials; chemical bonding and mechanical properties; Debye Temperature; Thermodynamic properties

Defect Assisted Current Transport Mechanism in III-V Semiconductors for Thermoelectric Applications

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Thermoelectric materials provide green energy source. Presently practical thermoelectric technology comprises mainly of Bi_2Te_3 and SiGe based materials. Bi_2Te_3 is however not only scarce and toxic, but also have a low maximum operating temperature of approximately 150°C. For SiGe, small efficiencies and narrow room for enhancement necessitate the search for a better high temperature thermoelectric material. Wide band-gap GaN and its clan of alloys are promising contenders to fill this role because they are very stable at high temperatures and non-toxic. GaN's bulk thermal conductivity ($\sim 200\ Wm^{-1}K^{-1}$) at room temperature is roughly two orders of magnitude higher than the SiGe[2]. Therefore it is critical to diminish the thermal conductivity of GaN so as to raise the ZT value to a suitable level. Two strategies have been put forward to increase the ZT value: first, decrease lattice thermal conductivity by increasing the phonon scattering, by alloying, selective implantation. Secondly, spatially isolate the donors (or acceptors) from electrons by means of modulation-doping technique and band-gap engineering. Tong et al[3] estimated using the alloying strategy that the enhanced thermoelectric performances of ternary over binary alloys are largely caused by reduced lattice thermal conductivity. However, there is currently no report of using defect engineering by selective implantation to tune GaN thermoelectric properties. In the present work, we have studied the effect of irradiation on the thermoelectric properties of GaN. An un-intestinally doped n-type GaN was irradiated by 100 MeV oxygen and 200 MeV silver ion beams accelerated by Pelletron, a tandem accelerator in Inter University Accelerator center, New Delhi. Thermopower of all the samples are measured. Negative thermopower is observed which confirms the formation of n-type sample. On irradiation, thermopower increased with increase in fluence and energy of the ion beam. The exact reason for such behavior is still unknown. However formation of defects and vacancies on irradiation could be a cause for such an increase. Scattering factor is calculated for all the samples using Boltzmann equation. Value of scattering factor greater than 4 is observed for oxygen irradiated sample which cannot be accounted by energy relaxation time approximation. Activation Energy due to thermopower and conductivity is also measured which suggests a second transport mechanism of the carriers due to hopping in the defect levels. Proposed study aims at designing novel devices based on understanding of defects. This study also presents future scope for hybrid devices for photovoltaic and thermoelectric energy harvesting.

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Improving the thermoelectric properties of P3HT with lithium salt as a dopant

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The interest in organic thermoelectrics is rapidly increasing because they have benefits such as light weight, low thermal conductivity, and high flexibility. Poly(3-hexylthiophene) (P3HT) is one the polymer which recently has been used extensively for thermoelectric application. P3HT has large Seebeck coefficient compared to other conducting polymer like PEDOT, however, it suffers from its low conductivity. So it is important to decrease the resistance in P3HT layers. There were a lot effort to increase the conductivity of P3HT, like using different molecular configurations[1], using different solvents [2] or tuning the additive [3].

Here, we have investigated the effect of Lithium salt as a dopant on the electrical conductivity of P3HT. In this study, thermoelectric devices were prepared by simple spin coating. Then the films were annealed at 150 °C for 15 min under N_2 environment. Silver electrical contacts (90 nm thick) for thermoelectric measurement were deposited onto the P3HT films via controlled thermal evaporation. The distance between two silver contact was 6 mm. Seebeck coefficients, resistance and output power of thermoelectric devices were measured by homemade system under vacuum condition. The seebeck coefficient and resistance of device at room temperature were 176 μV/K and 290 kΩ. Besides, the output power at 43 degree temperature difference was 87.1 pW.

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Seebeck coefficient and the electronic structures of Fe ion Implanted $CoSb_3$ Thin Films

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In the present study, single phase CoSb3 films were deposited on Si (100) substrates by pulsed laser deposition (PLD) using a CoSb3 polycrystalline target. The optical reflectance of the pristine film is found to be ~ 70% with estimated direct band gap of 0.73 eV. These films were implanted by 120 keV Fe-ion beam with three different fluences: 1×1015, 2.5×1015 and 5×1015 ions/cm2 in CoSb3 films. All the films were characterised by X-ray diffraction (XRD), Raman spectroscopy, Atomic force microscopy (AFM), Rutherford Back Scattering (RBS) and X-ray absorption spectroscopy (XAS). XRD data revealed that the ion implantation decreased the crystalline nature of films which was recovered after the rapid thermal annealing process. AFM shows that the roughness of the films increases with ion fluence for the first two ion fluences and then it decreases for 5×1015 ions/cm2. The thermopower S is varied with the fluences for a temperature range of 300 K to 420 K and found to be highest, i.e., 254 mV/K at 420 K for the film implanted with 1×1015 ions/cm2. The resistivity r for all the implanted sample is found to be low when compared with pristine sample which may be attributed due to the creation of large number of vacancies (2213.8 per Fe ion) leading to the increase of hole concentration. The changing of sign of S from negative for pristine sample to positive for Fe implanted samples confirms that Fe ions were electrically active and acted as electron acceptor by replacing the Co atoms. XAS measurement confirm that Fe ion has occupied the Co site in the cubic frame of the Skutterudite and exist in 3+ oxidation state in the CoSb3 structure.

Electronic states of pseudospin-1 fermions in α − T3 lattice ribbons in a magnetic field

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Abstract

The electronic states on a finite width α−T3 ribbon in a magnetic field are studied in the framework of low-energy effective theory. Both zigzag and armchair types of boundary conditions are analyzed. The analytical solutions are compared with the results of numerical tight-binding calcu- lations. It is found that the flat band of zero energy survives for all types of boundary conditions. The analytical estimates for the spectral gap in a weak magnetic field are discussed. For zigzag type boundary conditions the approximate expressions for the edge and bulk electron states in the strong magnetic field are found.

High-temperature hysteresis loops in electrical resistivity of SU8 – graphene composites

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SU8 is a polymer photoresist particularly suitable in production of micro-electromechanical (MEMS) systems, as it enables definition of microstructures with large depth- to lateral-dimension ratio. It is electrical and thermal insulator; otherwise, it would be an excellent candidate for manufacturing microelectronic components on a chip. By creating different composites, the aim is to increase the electrical and heat conductivity of SU8 while retaining its photolithographic properties. An example of such composites are SU8 – silver nanoparticles, used for fabrication of passive electronic elements and circuit interconnects on flexible substrate[1]. However, light absorption on metallic nanoparticles limits microstructures aspect-ratio patterned on the composite. Graphene with its favorable electrical, thermal, mechanical and chemical properties is an excellent candidate for SU8-matrix filler.[2]

In this work, we present the electrical resistivities of the SU8-graphene composite with graphene weight percentage (wt.) spanning from 0.3% to 4%. Room temperature electrical resistivities show high concentration dependence: they vary from 50,000 Wm for concentration of 0.3% to 10 Wm for wt. 4%. Temperature dependence of the electrical resistivity shows universal behavior for all samples: up to approximately 500 K resistivity is activated, $r(T) \sim \exp(T_0/T)$, followed by a faster temperature drop at higher temperatures. At high-temperature regime, resistivity shows hysteresis loops with peculiar time-evaluation at constant temperature.

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Electronic transport and magnetic studies of Fe intercalated Bi_2Se_3

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Abstract

Topological insulators (TI) are a class of quantum materials that has attracted a lot of attention in recent past because of the robust surface states that are protected by time reversal symmetry. Among the most studied 3D TIs, Bi_2Se_3 is the well-studied compound because of the large bulk band gap ~300meV [1]. Bi_2Se_3 has layered crystal structure that allows the incorporation of dopants in the van der Waals gap between layers. To study the effect of intercalation of magnetic transition element, single crystals of $Fe_xBi_2Se_3$ ($0 \leq x \leq 0.15$) were prepared using self-flux melt grown method. Phase purity and structural analysis of the samples were done using powder X-ray diffractometer. The length of unit cell increases along c-axis with intercalating Fe atoms. The electrical resistivity measurements show metallic behaviour. The electrical resistivity decreases with decreasing temperature and approaches a constant value below 30 K for both the compounds. Doping of Bi_2Se_3 with Fe induces the ferromagnetism in an otherwise diamagnetic compound which has been confirmed through temperature and field dependent magnetization measurements. The calculated magnetic moment is much smaller (0.014 μ_B/Fe) than the moment of 2.2 μ_B/Fe atom expected for a free Fe^{3+3+} [2][3][4].

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