Deutscher Akademischer Austauschdienst
German Academic Exchange Service

Study of Structural and Electronic Properties of Low-Dimensional Systems of Technological Importance

Name of all Researchers from LUH and IIT Indore and their designations/institutes including coordinating persons from LUH and IIT Indore:

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Project Description

The confinement of electrons in two or even one dimensions leads to well-known quantum confinement effects, but also, even more important, to an increase of electron correlation and to a wealth of instabilities such as Peierls transitions, spin and charge density waves or triplet superconductivity. With progressive miniaturization, these processes will become more and more relevant when considering potential applications such as nanoelectronics/molecular electronics, energy storage, solar cell research etc. The understanding of basic physics behind the effect of miniaturization is a crucial first step in order to achieve the desired properties in their respective application. Within this broad field, dealing both with fundamental properties and aspects of applications, we will focus on two subjects that exploit the complementary expertise of groups in Hannover and Indore.

a. In this part we want to concentrate on graphene as an expitaxial conducting material grown on silicon carbide (SiC) [1]: both groups have experience with this material that can be formed in controlled way (through high temperature thermal decomposition method, by varying different growth parameters), providing a pathway for bandgap engineering through an appropriate quality and quantity of epitaxial graphene and heterojunction interface layer between EG and SiC for the suitable application, e.g., designing solar cell, for enhancing the solar energy conversion efficiency in hydrogen production from water splitting, for environment friendly fuel cell application. and environmental remediation. While the Indore group has used this material in a variety of applications [2], the Hannover group has concentrated on more fundamental aspects such as plasmon excitations [3] and on nanopatterning graphene, which leads to conducting edge channels [4] with new special properties.
   We take this complementary expertise to start detailed investigations on the influence of nanopatterning, i.e. of the explicit properties of such edge states for photocatalytic activity and reactivity in context with metallic interdiffusion, e.g. of Li ions.
b. Nanostructuring is a good approach towards reaching an appropriate balance of electrical and thermal conduction via the phonon – glass – electron – crystal strategy. With progressing advances in Nanoscience, protocols for control of appropriate carrier concentrations and morphology have been established for a variety of materials. We intend to use this knowledge in designing thermoelectric materials of our choice and study the correlation between crystal structure and thermopower. The candidate of our choice is a highly promising thermoelectric material, Tin selenide [5] and the best TE material known so far, Bismuth telluride (Bi2Te3), and its variants [6].

The main focus of this part is to identify perfect dopant and/or structure for SnSe with which its thermoelectric properties are enhanced and determine the correlation of electrical & thermal properties with corresponding local crystal structure. Extended X-ray Absorption Fine Structure spectroscopy (EXAFS) provides a relatively simple way to determine the local crystal structure around the atom of interest contained in a solid. This information is not accessible by the common X-ray diffraction technique which relies entirely on the long range crystalline order of the samples under study. Photoemission spectroscopy of the other hand provides a picture of electronic band structure. This proposal presents a four-year programme of carrying out a systematic investigation into the thin-film and nanoparticles of thermoelectric Tin Selenide (SnSe) and its substitutional variants.

This part involves the follwing steps:

i. Generation of thin films and superlattices: The particularly challenging step is the growth of stacks, since spontaneous wetting of material A on B normally prevents the opposite so that one cannot work close to equilibrium.
ii. Nanostructures: Preparation of morphology-controlled nanocrystalline samples of SnSe, decoration of SnSe2 on the preferred morphologies of SnSe nanostructures. Hannover: Exploration how to select specific growth modes in order to single out one or the other type of nanostructure. Use of vicinal substrates or substrates that are prestructured by e-beam lithography.
iii. X-Ray Diffraction (XRD) measurements followed by Rietveld analysis, Energy Dispersive X-ray (EDX) spectroscopy. FE-SEM and TEM images will also be recorded to clarify the morphologies of the obtained nanocrystalline samples. Hannover: AFM, STM and LEED.
iv. Tests of crystal quality during growth: Methods: LEED (Hannover), RHEED and HRXRD. Temperature dependent transport properties and room temperature optical properties by four-probe electrical resistivity measurement, XPS and UV-Vis spectroscopy.
v. EXAFS: correlation of structure with electrical and thermal properties.
vi. Electrochemical analysis by cyclic voltammetry and thermoelectric properties.

References

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[2] *In Situ X-ray Study of the Solid Electrolyte Interphase (SEI) Formation on Graphene as a Model Li-ion Battery Anode*. Sudeshna Chattopadhyay, Albert L. Lipson§, Hunter J. Karmel, Jonathan D. Emery, Timothy T. Fister, Paul A. Fenter, Mark C. Hersam, and Michael J. Bedzyk, Chem. Materials 24 (15), 3038 (2012)
[3] *Multiple plasmon excitations in adsorbed two-dimensional systems*. H. Pfnür, T. Langer, J. Baringhaus, C. Tegenkamp, J. Phys.: Condens. Matter 23 (2011) 112204
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[5] *SnSe Nanocrystals: Synthesis, Structure, Optical Properties, and Surface Chemistry*. Baumgardner W. J, Choi J. J, Lim Y, and Hanrath T, J. Am. Chem. Soc., (2010), 132, 9519
[6] *Thin Film thermoelectric devices with high room-temperature figures of merit*. R. Venkatasubramanian et al. Nature, (2001) 413

Planned activities

1st year	a. Preparation of SnSe samples by MBE technique, identification of optimal growth conditions for single layers on various substrates (Hannover) b. Interface characterization by XPS/UPS LEED (Hannover) bulk characterization by XRD, EDX/FESEM and TEM (Indore) c) stripe patterning of graphene on SiC (Hannover)
2nd year	a. Detailed measurement of temperature dependent electrical stivity and thermopower using in-house facility built by the Investigator (Indore) MBE growth of SnSe/Si stacks (Hannover) b. Discussion over the obtained results and planning for communicating the research findings to established scientific journals for publication (both) c. Measurements of catalytic activities of nanopatterned graphened (Indore) d. Rrefinement of nanopatterning of graphene (Hannover)
3rd year	a. Preparation of nanostructured SnSe decorated with SnSe2 samples (IIT Indore) Growth of SnSe on vicinal Si surfaces (Hannover) b. Characterization by XRD, EDX/FESEM and TEM. c. Band gap engineering by edge states on graphene (Hannover) d. Test of solar cell efficiency (Indore)
4th year	a. Detailed study of optical and electrochemical measurements Raman, UV-Vis spectroscopy and cyclic voltammetry (Indore) b. Discussion over the obtained results and planning for communicating the research findings to established scientific journals for publication (Hannover)

Establishing fellowships for student exchange on the master level

Apart from encouraging students to go abroad to study for one semester or longer to study at IIT Indore, we will actively stimulate exchange of physics students on the master level by allocation of two fellowships per year both for outgoing students from LUH and for incomings from Indore. The selection will be done locally by the faculties.

Teaching cooperations

Mutual exchange on

- most important subjects with respect to basic research and potential applications,
- teaching methods in physics,
- primary aims of student training and ways to achieve these goals.

Sustainability Factors

1. Common publications on the scientific outcomes of this proposal are planned.
2. Mutual exchange on the docent level is planned to lead to
    - discussions on goals of student education and ways how to achieve them
    - improvement of coordination of study programs so that exchange of students on the master level and mutual recognition of parts of the study programs can be guaranteed