HL 40: Thermal, acoustic and transport properties

Time: Wednesday 9:30–12:30 Location: POT 151

HL 40.1 Wed 9:30 POT 151

Thermal stability of tellurium-hyperdoped silicon — •Mohd Saif Shaikh[1,2], Mao Wang[1], Zichao Li[1,3], Yufang Xie[1,3], Teresa Isabel Madeira[2], Dietrich R.T. Zahn[2], Slawomir Prucnal[1], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Semiconductor Physics, Chemnitz University of Technology, 09126 Chemnitz, Germany — [3]Dresden University of Technology, 01062 Dresden, Germany

Si doped with Te, a deep level impurity, at concentrations higher than the solid solubility limit (hyperdoping) was achieved by ion-implantation and nanosecond pulsed laser melting. The resulting material exhibit a strong sub-bandgap optical absorption, showing potential for room-temperature broadband infrared photodetectors. Te-hyperdoped Si is supposed to be meta-stable i.e. Te atoms tend to move out from the substitutional sites forming inactive clusters and precipitates. Here, we examine the thermal stability of Te-hyperdoped Si after furnace annealing. We conclude that the samples are stable up to 400°C for 60 minutes but at higher annealing temperatures Te-impurities tend to form clusters and the sub-bandgap optical absorption decreases. Rapid thermal annealing was also applied to Te-implanted Si and the results will be compared. Understanding the deactivation process upon thermal annealing is crucial during device fabrication steps, to maintain the satisfactory performance of devices utilizing such chalcogen hyperdoped Si structures.

HL 40.2 Wed 9:45 POT 151

Optimized internal-coordinates Gartstein potential for graphene, boron nitride and their nanotubes — •Francesco Libbi[1], Nicola Bonini[2], and Nicola Marzari[1,3] — [1]Theory and Simulation of Materials (THEOS), École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Physics Department, King's College, London, United Kingdom — [3]National Centre for Computational Design and Discovery of Novel Materials (MARVEL)

The lattice dynamics and, in particular, the quadratic behaviour of the flexural acoustic modes in low-dimensional materials play a fundamental role in their thermo-mechanical and thermal transport properties. A first-principles evaluation of these properties can be computationally very demanding and can be affected by numerical errors which break translational or rotational invariance. In order to overcome these problems in graphene-like materials, we develop an internal-coordinate potential with 13 parameters tuned on first-principles phonon calculations. We show that the potential not only reproduces very well the phonon dispersion of graphene, but that the same potential also describes correctly the vibrational properties of carbon nanotubes of arbitrary diameter and chirality. In addition, it is very easy to modify it adding a cubic term to reproduce the dominant anharmonic force constants. This allows a good estimate of lattice thermal conductivities. The potential form works well also for other 2D honeycomb lattice materials, including the case of hexagonal, polar, boron nitride.

HL 40.3 Wed 10:00 POT 151

Probing curling of current induced electric field in real space in graphene using KPFM — •Sayanti Samaddar[1], Kevin Janssen[1,2], Tjorven Johnsen[1], Zhengzhing Wang[3], Daniel Neumaier[3], Marcus Liebmann[1], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Otto-Blumenthal-Str., 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-6,9), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Advanced Microelectronic Center Aachen (AMICA), AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen

We conduct local transport measurements using Kelvin Probe Force Microscopy (KPFM) to investigate gated single layer graphene on SiN (150 nm)/Si substrate at room temperature. This allows us to image two quantities: (1) doping fluctuations and (2) local electric fields due to electric current. As charge neutrality is approached, the initially homogeneous and uniformly directed electric field lines start developing prominent curvature that ultimately lead to inversion at certain locations that are dominated by short range scattering. The inverted electric field implies a local back flow of current i.e. formation of current vortices. These current vortices systematically disappear at high source to drain current. Since vortex formation could be a manifestation of viscous flow of electrons [1], we investigate the plausibility of a hydrodynamic description by deducing the relevant transport length scales, from the gate dependent electric field maps at large gate voltages, taking different possible scattering mechanisms into account.

[1] D.A. Bandurin et al., Science 351, 1055-1057 (2016)

HL 40.4 Wed 10:15 POT 151

Transport properties of natural and synthetic $FeAs_xS_{2-x}$ ($0 \leq x \leq 0.01$) pyrites — •Esteban Zuñiga-Puelles[1,2], Raul Cardoso-Gil[2], Matej Bobnar[2], Igor Veremchuk[2], Cameliu Himcinschi[1], Jens Kortus[1], and Roman Gumeniuk[1] — [1]TU Bergakademie Freiberg, Freiberg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Synthetic polycrystalline and natural (Schönbrunn mine, Saxony, Germany) pyrites show comparable electrical resistivities (corresponding to the energy gaps ~ 0.7-0.9 eV) and Seebeck coefficients (-350 to -400 μV K^{-1} at 600 K). On the other hand, their thermal conductivities are similar (*i.e.* nearly temperature independent ~40-20 W m^{-1} K^{-1}) above 200 K. Below this temperature natural pyrite reveal a strong and well pronounced maximum, which became strongly reduced in synthetic samples. Such an effect is caused by much smaller grain size ($\leq$ 100 μm) in synthetic FeS_2, which results in additional scattering mechanisms (*i.e.* on point defect and/or grain boundaries). Therefore, mineral from Schönbrunn is further considered as a model system.

Interestingly, electrical transport properties of pyrites from other mines in Saxony varies from metallic (*n*-type conductivity) to semiconducting (*p*-type conductors). To shed light on such a behavior, $FeAs_xS_{2-x}$ ($0 \leq x \leq 0.01$) compounds were synthesized. The increase of As-content x in this system results in a decrease of the electrical resistivity as well as in the shift of the type of conducting mechanism towards hole-like one.

HL 40.5 Wed 10:30 POT 151

Magneto-transport properties via exact solution of the linearised Boltzmann equation — •Francesco Macheda[1] and Nicola Bonini[2] — [1]King's College London, Strand, London, UK — [2]King's College London, Strand, London, UK

Understanding and predicting the electrical and thermal transport in crystalline materials is crucial for the development of a new generation of electronic devices. In solids, transport coefficients can be conveniently calculated via the solution of the linearized Boltzmann transport equation (BTE), where the electronic and vibrational properties of the system, including electron-phonon interactions, are computed using density functional theory. Here we will present our recent developments to compute a wide range of transport coefficients in doped semiconductors and metals, such as Hall and drift mobilities, Seebeck and magneto-Seebeck coefficients and Lorenz number, also including the effects of phonon drag. We will show several examples of these calculations for semiconductors and metals that are of interest for technological applications. We will also discuss the application of this method to mono-layer graphene, whit a particular focus on magneto-transport effects.

HL 40.6 Wed 10:45 POT 151

Photo-induced metal-insulator transition in $Cu(d_6\text{-DCNQI})_2$ single crystals — •Lisa Schraut-May[1], Sebastian Hammer[1], Florian Hüwe[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Low dimensional organic metals based on radical anion salts offer a wide range of exciting electronic as well as photo-physical phenomena. For instance, dicyanoquinonediimine (DCNQI) coordinated by metal atoms forms a complex showing a pronounced metal-insulator transition from the quasi-1D metallic ground state to the Peierls insulating state upon cooling. This transition is accompanied by a conductivity change of up to seven orders of magnitude [1]. By photo-exciting the insulating phase, a reverse Peierls transition occurs back to the metallic state followed by a lattice rearrangement on picosecond time scale [2]. We characterize this photo-induced switching in $Cu(d_6\text{-DCNQI})_2$

single crystals by transient conductivity measurements as function of temperature and light intensity. The underlying mechanisms governing the dynamics of the reverse Peierls transition are characterized by a preliminary phenomenological model based on various decay processes for the excess energy upon photo-excitation. Finally, we will evaluate the potential of this material class for application as ultra-fast photo-switches.

[1] F. Karutz, et al., Phys. Rev. Lett. **81** (1998) 140
[2] B. Smit, et al., Adv. Mater. **31** (2019) 1900652

30 min. break

HL 40.7 Wed 11:30 POT 151

Large non-reciprocal transmission of surface acoustic waves in GaAs coated with epitaxial Fe_3Si film — •Alberto Hernández-Mínguez[1], Ferran Macià[2], Joan Manel Hernàndez[2], Jens Herfort[1], and Paulo Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]University of Barcelona, Barcelona, Spain

Non-reciprocal propagation of sound, that is, the different transmission of acoustic waves traveling along opposite directions, is a challenging requirement for the realization of devices like acoustic diodes and circulators. Here, we demonstrate the efficient non-reciprocal transmission of surface acoustic waves (SAWs) with 3.45 GHz frequency propagating along a GaAs substrate coated with a 50-nm-thick epitaxial Fe_3Si film. Fe_3Si is a binary Heusler-like ferromagnetic metal with potential applications in semiconductor-based spintronic devices. For well-defined orientations of the magnetization in the Fe_3Si film, the magneto-elastic (ME) coupling transfers energy from the acoustic into the magnetic system, thus inducing SAW attenuation. The strength of the ME coupling depends on the relative angle between magnetization and SAW wave vector, and leads to attenuation differences of up to 20% for SAWs propagating along opposite directions. We attribute the non-reciprocal behavior to the dependence of the magnetization dynamics on the helicity of the elliptically polarized ME field associated to the SAW. Our simulations confirm these results and show that Fe_3Si/GaAs is a promising platform for the realization of efficient on-chip, semiconductor-based non-reciprocal SAW devices.

HL 40.8 Wed 11:45 POT 151

Topological nanomechanical states by band inversion — •Martin Esmann[1], Fabrice R. Lamberti[1], Guillermo Arregui[2], Omar Ortiz[1], Carmen Gomez-Carbonell[1], Pascale Senellart[1], Clivia Sotomayor-Torres[2], Pedro David Garcia[2], Aristide Lemaitre[1], and Daniel Lanzillotti-Kimura[1] — [1]CNRS, Centre for Nanoscience and Nanotechnology (C2N), Palaiseau, France — [2]Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain

Many concepts studied in nanomechanics to control the confinement and propagation of acoustic phonons were inspired by their counterparts in optics and electronics. In these fields, the consideration of topological invariants has had a great impact for the generation of robust confined states. Here, we introduce this concept of topological invariants to nanophononics [1,2] and experimentally implement a GaAlAs heterostructure supporting a robust topological interface state at 350 GHz. The state is constructed through band inversion[3], by concatenating two semiconductor superlattices with inverted spatial mode symmetries. We experimentally evidenced the mode through Brillouin spectroscopy [1] and study its dynamics by picosecond optical pump-probe spectroscopy [3]. The reported robust topological interface state could become part of nanophononic devices requiring robust resonances such as mass sensors or phonon lasers.

[1] M. Esmann et al., PRB 97, 155422 (2018). [2] M. Esmann et al. PRB 98, 161109(R) (2018). [3] M. Xiao et al., Phys. Rev. X 4, 021017 (2014). [4] G. Arregui et al. APL Photonics 4, 030805 (2019).

HL 40.9 Wed 12:00 POT 151

Generation and propagation of superhigh-frequency bulk acoustic waves in GaAs — Diego H. O. Machado[1,2], •Antonio Crespo-Poveda[1], Alexander S. Kuznetsov[1], Klaus Biermann[1], Luis V. A. Scalvi[2], and Paulo V. Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]UNESP, Department of Physics, 17033-360 Bauru (SP), Brazil

Coherent superhigh-frequency (SHF) vibrations provide an excellent tool for the modulation and control of excitations in semiconductors. Here, we investigate the piezoelectric generation and propagation of longitudinal bulk acoustic waves (LBAWs) with frequencies up to 20 GHz in GaAs crystals using monolithic bulk acoustic-wave resonators based on piezoelectric thin ZnO films. The transducers are used to investigate the propagation of the LBAWs in the frequency and temperature ranges from 1 to 20 GHz and 10 and 300 K, respectively. We find that the acoustic absorption of GaAs in the temperature range from 80 K to 300 K is dominated by scattering with thermal phonons. In contrast, at lower temperatures, the acoustic absorption saturates at a frequency-dependent value. Experiments carried out with different propagation lengths indicate that the saturation is associated with losses during reflections at the sample boundaries. We also demonstrate devices with a high quality factor fabricated on top of acoustic Bragg reflectors. These findings prove the feasibility of high-quality acoustic resonators embedding GaAs-based nanostructures, opening exciting new technological opportunities, such as acoustic carrier control and nanomechanics in the SHF range.

HL 40.10 Wed 12:15 POT 151

Brillouin scattering in optophononic micropillar resonators at 300 GHz — •Martin Esmann[1], Fabrice R. Lamberti[1], Abdelmounaim Harouri[1], Isabelle Sagnes[1], Carmen Gomez-Carbonell[1], Ivan Favero[2], Olivier Krebs[1], Loïc Lanco[1], Aristide Lemaitre[1], Pascale Senellart[1], and Daniel Lanzillotti-Kimura[1] — [1]CNRS, Centre for Nanoscience and Nanotechnology (C2N), Palaiseau, France — [2]Matériaux et Phénomènes Quantiques, CNRS, Université Paris Diderot, Paris, France

Inelastic scattering of light by acoustic phonons has potential for tailored optical frequency combs, narrow-line lasers [1], and all-optical data storage [2]. To be efficient, these applications require strong optical fields featuring a large overlap with the acoustic modes. So far, patterned waveguides and photonic crystal fibers allow tailoring the acoustic spectrum up to few tens of gigahertz.

Here, we introduce a monolithic Brillouin generator [3] based on a high-frequency nanoacoustic GaAlAs resonator operating at 300 GHz, which is embedded inside an optical micropillar cavity. This decouples the design of the Brillouin spectrum and the optical device. We develop a free-space filtering technique to detect the generated Brillouin signals. The micropillars could be readily integrated into fibered and on-chip architectures, and are compatible with epitaxial quantum dots, making them relevant for quantum communication.

[1] N. T. Otterstrom et al. Science 360, 1113 (2018).
[2] M. Merklein et al. Nature Commun. 8, 574 (2017).
[3] M. Esmann et al. Optica 6, 854 (2019).