DS 3: Layer Properties

Time: Monday 15:00–18:00 Location: A 053

Invited Talk DS 3.1 Mon 15:00 A 053

Advances in AlN-based ternary alloy crystals with regard to their elastic, thermodynamic and piezoelectric properties — •Oliver Ambacher — Institute for Sustainable System Engineering, University Freiburg

The piezoelectric coefficient e33 from wurtzite AlN (wz-AlN), which is particularly interesting for high-frequency acoustic wave filters, can be increased up to 150% by alloying AlN with ScN or YbN. In addition, wz-ScAlN and wz-YbAlN layers show ferroelectric properties and large remanent polarizations up to very high temperatures. The ferroelectric effect enriches the dimension of polarization engineering in group-III-nitride based heterostructures and provides opportunities for the integration of novel functionalities into electronic and piezo acoustic devices. For this reason the piezoelectric, spontaneous, and ferroelectric polarization as wll as the structural, elastic, and thermodynamic properties of hexagonal GaN, ScN, YbN and AlN crystals as well as their ternary alloy will be presented.

DS 3.2 Mon 15:30 A 053

Eliminating oxygen in-diffusion for stabilization of electrical properties in CuI thin films — •Christiane Dethloff, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Felix-Bloch-Institut, Universität Leipzig, Deutschland

The p-type semiconductor CuI is of great potential for transparent opto-electronics due to an intrinsic charge carrier density of up to 10^{20} cm^{-3} combined with a direct band gap of 2.95 eV at room temperature and high transparency in the visible range [1,2]. The p-type behavior is attributed to Cu vacancies, but recently also to oxygen, which acts as a shallow acceptor. It was demonstrated that in particular ex-situ oxygen diffusion causes an increase of hole density and electrical conductivity, often resulting in degenerate thin films [2].
To access the full potential of CuI and its alloys for semiconductor thin film applications, it is crucial to prevent in-diffusion of oxygen. Although amorphous Al_2O_3 capping layers atop CuI thin films have already been shown to prolongate deterioration of the electrical properties, the influence of a full encapsulation has not yet been investigated. Therefore, we present completely *in-situ* encapsulated CuI thin films deposited by magnetron co-sputtering from a Cu target in a reactive iodine and argon atmosphere. We compare the efficiency of Al_2O_3 and SiN_x cappings that encapsulate the surface and the entire layers, respectively. For that, long-term resistivity and Hall effect measurements are performed over several days.
[1] Yang *et al.* Nat Commun **8**, 16076 (2017).
[2] Storm *et al.* APL Mater. **9** (5): 051101 (2021).

DS 3.3 Mon 15:45 A 053

Understanding of the Cu nanofilament behavior of Cu/HfO2/Pt with QPC model — •Taewook Kim[1], Enrique Miranda[2], Eszter Piros[1], Philipp Schreyer[1], and Lambert Alff[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany — [2]Universitat Autonoma de Barcelona, Barcelona, Spain

This study delves into the behavior of the Cu conducting filament in a Cu/HfO2/Pt MIM (Metal-Insulator-Metal) structure, specifically examining resistive switching mechanisms in filamentary-type memory. Utilizing the Quantum Point Contact (QPC) model, we analyze the Cu conducting filament's response to variations in oxide layer thickness. The investigation reveals distinct conducting filament behaviors associated with different oxide layer thicknesses. Thinner oxide layers result in a smaller energy barrier between ruptured filaments, while thicker oxide layers exhibit a higher energy barrier. Furthermore, thicker oxide layers show an increased ratio of broken parts, suggesting significant rupturing of the Cu conducting filament in thicker oxide layer sample. The study extends to examining the possible conduction mechanism post-rupturing, as evidenced by a comparison of the I-V curve between set and reset states. This research provides crucial insights into the intricacies of resistive switching in MIM structures, with potential applications in memory devices and contributions to the advancement of nanoscale electronics.

15 min. break

DS 3.4 Mon 16:15 A 053

Are Xenes excitonic insulators? — •Olivia Pulci[1], Paola Gori[2], Davide Grassano[3], Marco D'Alessandro[4], and Friedhelm Bechstedt[5] — [1]Department of Physics, and INFN, University of Rome Tor Vergata, Italy — [2]Department of Industrial, Electronic and Mechanical Engineering, Roma Tre University, Italy — [3]Theory and Simulation of Materials (THEOS), Ecole Polytechnique Federale de Lausanne, Switzerland — [4]Istituto di Struttura della Materia-CNR (ISM-CNR), Rome, Italy — [5]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany

Using a variational approach, the binding energies Eb of the lowest bound excitons in Xenes under varying electric field are investigated. The internal exciton motion is described both by Dirac electron dispersion and in effective-mass approximation, while the screened electron-hole attraction is modeled by a Rytova-Keldysh potential with a 2D electronic polarizability α2D. The relation between Eb and the spin-orbit gap Eg is ruled by the screening. The values of Eg and α2D are strongly modified by a vertical external electric bias U, which defines a transition from the topological into a trivial insulator at U = Eg /2, with the exception of plumbene. The existence of an excitonic insulator phase with Eb>Eg sensitively depends on the chosen α2D. Many-Body perturbation theory, applied to stanene, confirm the absence of an excitonic insulator phase, thus validating our results obtained by ab initio modeling of α2D.

DS 3.5 Mon 16:30 A 053

Electrical characterization of the pseudo-binary line In_3SbTe_2-SnTe — •Christian Stenz, Thomas Schmidt, Michael Dappen, and Matthias Wuttig — I. Institute of Physics (IA) RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen

Materials can be categorized by examining their properties, including band gap, effective coordination number, electrical and optical conductivity, Born effective charge, and more. Based on such properties and quantum chemical bond identifiers a classification into metallic, covalent, ionic, and metavalent bonding (MVB) appears appropriate. MVB is defined by a competition between electron localization and delocalization resulting in a unique property portfolio. SnTe and In_3SbTe_2 are identified to be metavalent and metallic, respectively. However, both occur in a rocksalt-like structure with similar lattice constants allowing for isostructural alloying. Investigating the property portfolio of the pseudo-binary line yields insights about the pronounced changes in properties by crossing the tipping point towards complete electron delocalization and closing the band gap. In this study several alloys on the pseudo-binary line In_3SbTe_2-SnTe are produced by sputter deposition. Properties like crystallization temperature T_x, electrical conductivity and superconducting transition temperature T_c are investigated. Upon the transition from MVB to metallic bonding a change in charge carrier type as well as a remarkable increase of T_c by 85 % and 1200 % compared to the pure compounds In_3SbTe_2 and SnTe, respectively, has been found.

DS 3.6 Mon 16:45 A 053

Mesoscale modeling of deformations and defects in crystalline sheets — •Lucas Benoit–Maréchal[1], Ingo Nitschke[1], Axel Voigt[1,2], and Marco Salvalaglio[1,2] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany

We present a self-consistent mesoscale description of deformations and defects in thin, flexible sheets with crystalline order using a coarse-grained Phase-Field Crystal (PFC) model which aims at bridging atomistic and continuum approaches.

The PFC model describes crystals at diffusive timescales through a continuous periodic field representing the atomic number density. In its amplitude expansion (APFC), a coarse-grained description featuring slowly varying fields retaining lattice deformation, elasticity, and dislocations is achieved. We introduce the surface APFC (sAPFC) model in a convenient height formulation encoding normal deformation.

This framework is proven consistent with classical aspects of strain-induced buckling, defect nucleation on deformed surfaces, and out-of-plane relaxation near dislocations obtained from atomistic and continuum descriptions. By considering the mutual interaction of elas-

tic/plastic relaxation and variations in the height profile as accessible within the sAPFC model, we outline the complexity of the resulting phenomenology.

15 min. break

DS 3.7 Mon 17:15 A 053

Multiscale Simulation Framework for Functional Polymers — •Steffen Kampmann[1], Alexander Croy[2], Arezoo Dianat[1], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TU Dresden, Dresden, Germany — [2]Chair of Theoretical Chemistry, Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany

Functional mechanically resilient polymer films, such as films of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), play an important role for strain gauges or organic light-emitting diode (OLED) displays [1-2]. The modeling and simulation workflow presented here enables the generation of disordered polymers and the linking of the mechanical and electronic properties from the atomistic to the microscopic size scale. Here, the focus is on the relationship between deformation and conductivity behavior. To calculate the multi-scale material behavior, we use density functional tight binding (DFTB) calculations, molecular dynamics simulations, and the finite element method. The in-situ processing, evaluation as well as the exchange of the generated data across simulation methods is performed using our Python framework. The multi-scale computational workflow indicated here represents a computationally efficient assessment of material properties at different scales. [1] R. Luo, et al., Progress in Organic Coatings, (2022) [2] M. Cinquino et al., Journal of Science: Advanced Materials and Devices, (2022)

DS 3.8 Mon 17:30 A 053

Controllable phase transition of two-dimensional ferromagnetic chromium telluride thin films grown by molecular beam epitaxy — •Haili Huang — Shanghai Jiao Tong University

Two-dimensional (2D) Cr(1+δ)Te2 materials exhibit strong magnetic ordering and high Curie temperatures, making them attractive for various applications. However, it is crucial to achieve controllable synthesis for their successful integration into device technologies. In this study, we present the synthesis of phase-controllable 2D Cr(1+δ)Te2 films on the Si (111) substrate via molecular beam epitaxy. The composition and phase transition of the as-grown Cr(1+δ)Te2 films are characterized by using in-situ reflection high-energy electron diffraction, scanning tunneling microscopy, ex-situ X-ray photoelectron spectroscopy, X-ray diffraction, and theoretical calculations. By carefully adjusting the film thickness, we achieve precise control over the phase and growth mode of Cr(1+δ)Te2. These changes are attributed to interfacial effects and the phase stability of Cr(1+δ)Te2 compounds. The magnetic measurements reveal that the 30-nm Cr2Te3 film exhibits ferromagnetic behavior with a Curie temperature of about 180 K. Our work offers a robust method for the controllable growth of high-quality 2D Cr(1+δ)Te2 films on Si substrates, providing an ideal platform for investigating their intrinsic properties and advancing the development of 2D magnet-based spintronics devices.

DS 3.9 Mon 17:45 A 053

Combinatorial study of BaCu2Se2 thin films for photovoltaics — •Marin Rusu[1], José A. Márquez[1], Hannes Hempel[1], Leo Choubrac[1], Galina Gurieva[1], Rene Schwiddessen[1], Pablo Reyes-Figueroa[1], Robert Wenisch[1], Markus Schleuning[1], Christian A. Kaufmann[1], Iver Lauermann[1], Susan Schorr[1,2], and Thomas Unold[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

BaCu2Se2 thin films with earth-abundant elements are investigated for application in photovoltaics. We apply the combinatorial approach for the study of BaCu2Se2 thin films with a lateral gradient in the [Cu]/[Ba] atomic ratio, which were synthesized on areas as large as 5x5 cm2 by selenization of Cu-BaO precursors from pulsed laser deposition. Close to the the 1:2:2 stoichiometric point, the optical measurements revealed a direct band gap with an energy of 1.89 eV in perfect agreement with the observed bright photoluminescence centered at 1.9 eV. An absorption coefficient of 1.5 x 105 cm-1 was determined and a theoretical open-circuit voltage of 1.3 eV was calculated. By using optical-pump terahertz-probe spectroscopy mapping, as well as a combined Kelvin probe with a photoelectron yield spectroscopy method, we find that the equilibrium charge carrier concentration can be tuned over five orders of magnitude. Surface photovoltage measurements revealed a p-type conductivity of the films. The charge carrier mobility reaches a maximum value of ~60 cm2 V-1s-1. Thus, BaCu2Se2 thin films are very attractive for application in tandem photovoltaics.