DS 8: Thin Film Properties II

Time: Wednesday 9:30–12:30 Location: A 060

DS 8.1 Wed 9:30 A 060

Vacancy like defects in Cd3As2 — •Maciej Oskar Liedke[1], Anthony Rice[2], Maik Butterling[1], Eric Hirschmann[1], Nancy M. Haegel[2], Kirstin Alberi[2], and Andreas Wagner[1] — [1]Institute of Radiation Physics, Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstr. 400, Dresden 01328, Germany — [2]National Renewable Energy Laboratory, Golden, Colorado 80401, USA

Cd3As2 is a three-dimensional topological semimetal which can be transformed into exotic phases, e.g., Weyl semimetals, topological superconductors, or axion insulators. Using epitaxy provides an avenue for varying and controlling point defects during Cd3As2 growth. The knowledge of vacancy defects is essential for interpretation of electron transport behavior and guides growth efforts to develop materials with low defect concentrations. Point defects in Cd3As2 epilayers grown by molecular beam epitaxy with varying As/Cd flux ratios are probed by positron annihilation spectroscopy. We show that lower As/Cd flux ratios produce higher concentrations of point defects. Remarkably, the measurements indicate that the average defect size is larger than a monovacancy and vacancy complexes dominate [Rice et al. APL Mater 11, 061109 (2023)]. The evolution of defect microstructure as a function of temperature will be discussed as well.

DS 8.2 Wed 9:45 A 060

Towards high-throughput studies of gradient multi-component thin films — •Dmitry Lapkin, Alexander Gerlach, Alexander Hinderhofer, and Frank Schreiber — Institute of Applied Physics, University of Tübingen, Tübingen, Germany

Progress in the development of modern functional materials is indispensable for technological progress. In many cases, these materials are complex multi-component systems, with a rather non-trivial dependence of the properties on composition. A typically non-linear and non-monotonic composition dependence makes it mandatory to investigate the resulting properties with many points on the composition axis, and ideally within one given sample to ensure comparability, calling for suitable sample preparation techniques.

An example of such a preparation technique relevant for applications is organic molecular beam deposition (OMBD) of organic semiconductor thin films. A deposition chamber, recently developed in our group, makes it possible to overcome unintentional variations in deposition conditions for different samples and, importantly, to obtain a film with a composition gradient in one run.

In this work, we demonstrate the preliminary results of gradient two-component film deposition and how the spatial resolution of modern sample characterization methods can be effectively converted into compositional resolution using such gradient films. In combination with arising machine learning-based on-the-fly data treatment methods, this opens up horizons for high-throughput studies of the structure and properties of multi-component thin films.

DS 8.3 Wed 10:00 A 060

Structural and magnetic anisotropy in YBa2Cu3O7/ La0.67Sr0.33MnO3 bilayer film on SrTiO3 substrate — •Ankita Singh, Sawani Datta, Ram Prakash Pandeya, Srinivas C. Kandukuri, and Kalobaran Maiti — Department of Condensed Matter Physics & Material Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai-400005, India

We study the magnetic properties and emergence of superconductivity in YBa2Cu3O7 (YBCO)/ La0.67Sr0.33MnO3 (LSMO) heterostructures. Bilayer films of superconducting layer, YBCO and ferromagnetic layer, LSMO were grown on SrTiO3 (STO) (001) substrate using a home built ultrahigh vacuum (UHV) pulsed laser deposition (PLD) system. Magnetization data at 100 K as a function of applied field shows ferromagnetic behaviour due to the LSMO layer. Cooling below 100 K leads to superconductivity in this material; the onset of superconductivity occurs at a temperature TC(onset) of 86 K for Hext*c (in-plane) and Hext || c (out-of-plane) under 100 Oe applied field. In-plane magnetic measurements show significant suppression of diamagnetic behaviour as compared to the out-of-plane measurements. The susceptibility signals are higher for the out-of-plane direction. Such strong anisotropy in magnetism below the transition temperature reveal complex interplay of magnetism and superconductivity in this system and calls for further study in this direction.

DS 8.4 Wed 10:15 A 060

Calcium Made Interesting — •Kai Bröking[1,2,3], Stephan Brückner[1], Daniel Tasche[1,2], and Christoph Gerhard[1,4] — [1]Hochschule für Angewandte Wissenschaft und Kunst, Göttingen, Germany — [2]Technische Universität Clausthal, Fakultät für Natur- und Materialwissenschaften, Clausthal-Zellerfeld, Germany — [3]Max-Planck-Institut für multidisziplinäre Naturwissenschaften, Göttingen, Germany — [4]School of Industrial and Information Engineering, Politecnico di Milano, Milano, Italy

During manufacturing, optical glass components come into contact with a variety of process agents. An exchange between the glass and these chemical compounds leads to the accumulation of some of their ingredients in surface and sub-surface defects, and, by diffusion, in the glass itself [1]. On the other hand, a depletion of glass constituents near the glass surface takes place as well. As can be expected, these processes lead to unwanted changes in glass properties near the surface [2] and may facilitate its deterioration. We investigate both depletion and accumulation of metal ions near the surfaces of multi-component glasses and explore the scaling behaviours of the transport processes involved.

[1] Gerhard &al., Applied Surface Science Volume 537, 30 January 2021, 147984, doi:10.1016/j.apsusc.2020.147984

[2] Gerhard, Köhler, Opt Mater Expr Vol. 12, Issue 9, pp. 3658-3666 (2022), doi:10.1364/OME.458227

15 min. break

DS 8.5 Wed 10:45 A 060

Study of self-organized structures at metal-organic interface In/CuPcFx — •Olga Molodtsova[1], Dmitrii Potorochin[1,2], Sergey Babenkov[1,3], Serguei Molodtsov[2,4], Anna Makarova[5], Dmitry Smirnov[6], and Victor Aristov[1] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]TUBergakademie Freiberg, D-09599 Freiberg, Germany — [3]CEA-Saclay, 91190 Gif-sur-Yvette, France — [4]Europian XFEL GmbH, D-22869 Schenefeld, Germany — [5]Institute of Chemistry and Biochemistry, Free University of Berlin, D-14195 Berlin, Germany — [6]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany

The start and development of molecular electronics has attracted particular attention to molecular semiconductors such as metal phthalocyanines. They have unique properties and are technologically advanced in production. Using ultrathin films as a matrix, it is possible to create metal-organic composites containing metal nanoparticles that self-organize in an organic matrix. The technologies for creating the described nanocomposites are quite simple and relatively cheap; therefore, such materials can find a prominent place in practical applications in various electronic devices. However, despite the growing interest in hybrid systems, numerous questions about their properties and the processes occurring during their formation remain unanswered. For example, interfacial phenomena can radically change the electronic properties of organic wide-gap matrices.

DS 8.6 Wed 11:00 A 060

Stability and Elasticity of Ultrathin Sphere-Patterned Block Copolymer Films — •Le Qiao[1], Daniel A. Vega[2], and Friederike Schmid[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, D55099 Mainz, Germany — [2]Instituto de Física del Sur (IFISUR), Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Universidad Nacional del Sur, 8000 Bahía Blanca, Argentina

Sphere-patterned ultrathin block copolymers films are potentially interesting for a variety of applications in nanotechnology. We use self-consistent field theory to investigate the elastic response of sphere monolayer films with respect to in-plane shear, in-plane extension and compression deformations, and with respect to bending. The relations between the in-plane elastic moduli is roughly compatible with the expectations for two-dimensional elastic systems with hexagonal symmetry, with one notable exception: The pure shear and the simple shear moduli differ from each other by roughly 20%. Even more importantly, the bending constants are found to be negative, indicating that free-standing block copolymer membranes made of only sphere

monolayer are inherently unstable. Our results are discussed in view of experimental findings.

DS 8.7 Wed 11:15 A 060

Defect break-down in systematically disordered Cr_2AlC — •Joao S. Cabaco[1,6], Maciej O. Liedke[2], Javier Pablo-Navarro[3,4], Fabian Ganss[1], Cesar Magen[3], Manuel R. Ibarra[3,4], Ulrich Kentsch[1], Maik Butterling[2], Andreas Wagner[2], Jurgen Lindner[1], Jurgen Fassbender[1,5], Christoph Leyens[6], Richard Boucher[6], and Rantej Bali[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Germany — [2]Institute of Radiation Physics, HZDR, Germany — [3]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Spain — [4]Laboratory of Advanced Microscopies, University of Zaragoza, Spain — [5]Institute of Solid State and Materials Physics, TU Dresden, Germany — [6]Institute of Materials Science, TU Dresden, Germany

The presence of open-volume defects, such as vacancies, can influence the structural, magnetic, and transport properties. This study uses ion irradiation to investigate the evolution of defects in MAX-phase Cr_2AlC. Thin-films of 50 nm and 500 nm were irradiated at increasing fluences, using both inert ions and transition metal ions. Through the combined use of positron annihilation and *ab-initio* simulations, it was possible to distinguish different types of defects, determine their size and concentration. Large clusters of 9-15 vacancies, originally present in the as-grown films, transform into Al mono-vacancies and Cr-Al di-vacancies upon ion irradiation. Furthermore, an overall reduction in open-volume defect concentration and size due to irradiation was observed. **Grant:** (DFG) TRANSMAX no. 456078299.

15 min. break

DS 8.8 Wed 11:45 A 060

Phase-Selective Epitaxy of Trigonal and Orthorhombic Bismuth Thin Films on Si (111) — •Xiao Hou[1], Abdur Rehman Jalil[2], Peter Schüffelgen[2], Claus Michael Schneider[1], Lukasz Plucinski[1], and Detlev Grützmacher[2] — [1]Peter-Grünberg-Institute (PGI-6) — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Over the past decades, the growth of Bi thin films has been extensively explored due to their potential applications such as thermoelectrics, ferroelectrics, and recently in topological and neuromorphic areas. The strong spin-orbit coupling renders some Bi allotropes topologically non-trivial [1], offering opportunities to explore topological devices. Besides, due to its thermal instability, Bi is a suitable candidate for phase-change and low-power neuromorphic applications. Despite significant research efforts, achieving reliable and controllable growth of high-quality Bi thin-film allotropes has remained a challenge [2].
This study is dedicated to achieve well-controlled high-quality growth of Bi epilayer on Bi-terminated Si (111) 1×1 surfaces using MBE. With systematic growth, this work yields a phase map that demonstrates the realization of trigonal, orthorhombic, and pseudo cubic thin-film allotropes of Bi. In-depth characterization through XRD techniques and STEM analysis provides a comprehensive understanding of phase segregation, phase stability, phase transformation, and phase-dependent thickness limitations in various Bi thin film allotropes.
[1] Jalil A R. PhD thesis. RWTH Aachen, Germany (2022). [2] Jalil A R, Hou X, et al. Nanomaterials (2023).

DS 8.9 Wed 12:00 A 060

Design of a polymeric thin film for 2D material printing — •Sebastiaan Haartsen[1], Pantelis Bampoulis[1], Harold Zandvliet[1], Johannes Aprojanz[1,2], Inga Wille[2], and Harald Jasper[2] — [1]University of Twente — [2]Actega Metal Print GmbH

In this talk, we present a method of printing 2D materials based on flexographic printing. In this method, 2D materials are transferred to a polymeric surface. Using additives, we show that the adhesive properties of a polymeric thin film can be modified to enhance the transfer of the 2D material.

Crossectional atomic force spectroscopy together with surface spectroscopy allows for a greater understanding of the enhancements caused by the additive. Using low concentrations of the additive, we record a segregation of the additive towards the surface of the thin film, shown by an increase in the adhesive force and energy. Increasing the concentration of the additive from 1 to $10wt\%$ enhances the adhesive properties at the surface while concentrations higher than $10wt\%$ reduce the adhesive properties. Above 10

Results from this research are used for the design of a polymeric thin film suitable for 2D material printing.

DS 8.10 Wed 12:15 A 060

Atomic imaging of the critical nucleus size of multilayer hexagonal ice growth — •Dong Guan, Tiancheng Liang, Zixiang Yan, Li-Mei Xu, En-Ge Wang, and Ying Jiang — International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China

Multilayer water ice growth is widespread and plays a significant role in various natural phenomena. An essential aspect of water ice growth is the elusive nature of the critical ice nucleus, attributed to its transient and delicate characteristics. We present the precise atomic size of the critical ice nucleus in hexagonal water ice (ice Ih) through the utilization of qPlus-based cryogenic noncontact atomic force microscopy (NC-AFM) equipped with a CO-terminated tip. Freezing samples during the growth process allows us to capture the intermediate structures involved in the growth of Ih ice. Our investigation reveals that pentamers and hexamers are the most prevalent intermediate structures, and their combination gives rise to the 3-5 cluster, which we define as the critical ice nucleus. Combined with density functional theory, we might show that the structure alteration of the 3-5 cluster results in the formation of a new core for Ih ice. This new core can expand by incorporating additional water molecules along its periphery. This research is the first achievement in elucidating the exact atomic structure of a critical ice nucleus in water. It provides valuable insights into the water freezing process and holds the potential for application to other nucleation processes.