DS 13: Layer Properties

Time: Wednesday 15:00–16:15 Location: REC/B214

Invited Talk DS 13.1 Wed 15:00 REC/B214

Tailored thermal treatments for multi-layer, multi-material polymer devices — •Katherina Haase, Shaoling Bai, Mike Hambsch, Vojtech Millek, and Stefan C. B. Mannsfeld — Faculty of Electrical and Computer Engineering & Center for Advancing Electronics Dresden (cfaed), TUD Dresden University of Technology, 01069 Dresden, Germany

Thermal annealing constitutes an important processing step during the fabrication of organic semiconductor-based devices as it removes residue solvent and often leads to improved structural order. Recently, we have explored an additional aspect of thermal annealing - its impact on the dissolution of conjugated polymer (CP) thin films. We could show that thermal annealing induces physical cross-linking in a wide range of CPs,[1] which distinctly increased their stability in the original solvent. Hence, we suggested that tailored thermal treatments could enable polymer heterojunction devices though simple sequential coating.

In this presentation, we discuss the important finding that the thermal physical cross-linking (TPC) effect produces solvent-resistant thin films for a wide variety of CPs that could be combined into a multitude of novel devices, and explore the fabrication of solution-coated, polymer heterojunction-based synaptic transistors - devices that could not have been realized without the application of cross-linking.

[1] S. Bai, K. Haase, J. Perez Andrade, M. Hambsch, F. Talnack, V. Millek, A. Prasoon, J. Liu, K. Arnhold, S. Boye, X. Feng, S. C. B. Mannsfeld, Adv. Electron. Mater. 2024, 10, 1.

DS 13.2 Wed 15:30 REC/B214

Mechanical Stress Evolution in Polycrystalline Ge Thin Films under MeV Ion Irradiation — •Karla J. Paz Corrales[1], Aaron Reupert[2], Kevin Lubig[2], Frank A. Müller[2], Berit Marx-Glowna[3], Ralf Röhlsberger[3], Till Weickhardt[1], Giancarlo Soavi[1], Martin Hafermann[1], Elke Wendler[1], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, 07743 Jena, Germany — [3]Helmholtz-Institut Jena, Fraunhoferstr. 8, 07743 Jena, Germany

Polycrystalline Ge thin films were deposited by magnetron sputtering, annealed at 600 °C for 1 h, and irradiated with 1.8 MeV Au ions over a broad fluence range. Structural, optical, and in-situ mechanical stress analyses were performed to investigate irradiation-induced property modifications. At low fluences, the films show a reduction of the initial tensile residual stress from the preparation process. This stress compensation is linked to the formation of point defects, which also decrease the optical band gap. These defects can migrate to grain boundaries, where recombination enhances the resistance to amorphization compared with single-crystalline Ge. At higher fluences, defect accumulation increases tensile stress and leads to the formation of mixed polycrystalline-amorphous phases. With further irradiation, the films fully transform into an amorphous phase, as evidenced by changes in both structural and optical properties. In this amorphous state, additional stress relaxation occurs, attributed to plastic flow or to interface effects between the film and substrate.

DS 13.3 Wed 15:45 REC/B214

Optical tuning of Sr(Mo,Ti)O_3 thin films through solid solution — •Anjima Kallam Valli, Juliette Cardoletti, and Lambert Alff — Institute of Materials Science, TU Darmstadt, Darmstadt, Germany

Transparent conductive oxides are key materials in display technology and renewable energy applications, being used as transparent electrodes in solar cells and optoelectronic devices. Perovskite oxides such as $SrMoO_3$, $SrVO_3$, and $SrNbO_3$ exhibit exceptional metallic conductivity combined with optical transparency. Among them, bulk $SrMoO_3$ shows a conductivity of $2 * 10^7$ S m $^{-1}$ exceeding that of platinum at room temperature; however, its optical transparency is limited to the UV visible range (300 to 500 nm). This work investigates the broadening of the transparency window of $SrMoO_3$ through partial B-site substitution of molybdenum by titanium. Titanium incorporation modifies the carrier density and thereby tunes the plasma frequency, shifting the optical reflection edge toward longer wavelengths. Epitaxial Ti-substituted $SrMoO_3$ thin films have been grown by pulsed laser deposition. Structural analysis was performed by XRD, and their electrical transport properties, including resistivity and carrier density, were characterised using van der Pauw and Hall-effect measurements. Optical transparency has been evaluated by spectroscopic analysis. Through tailoring of the transparency with varying Ti concentration, this work opens the door to various optoelectronic device applications.

DS 13.4 Wed 16:00 REC/B214

Automating calculations for advancing the simulations of solid interfaces — •Elisa Damiani, Margherita Marsili, and Maria Clelia Righi — Dipartimento di Fisica e Astronomia, University of Bologna, Italy

Solid-solid interfaces are ubiquitous and simulations help understanding their properties, and may represent powerful screening and designing tools. Often first-principles electronic structure methods must be used: for example to characterize their transport, electronic, optical and magnetic properties, and also their adhesion and friction. Nevertheless, these approaches comes along with computational complexity and costs. In this talk I will present how we address these computational challenges by developing TribChem, a software that automates the creation of interface models, the identification of the optimal computational parameters, job submission, and data retrieval and storage. I will also show how this code has been successfully applied to the systematic study of different classes of interfaces such as metal-metal, metal-semiconductor, and metal-2D-materials ones, and illustrate the current developments that carried out to increase the complexity of the systems that can be addressed (amorphous and molecular solids) employing a Bayesian Optimization approaches.

These results are part of the SLIDE project that has received funding from the European Research Council (ERC) under the European Union*s Horizon 2020 research and innovation program (Grant agreement No. 865633).