

DS 4: Thin Film Properties II

Time: Monday 16:30–18:15

Location: REC/C213

DS 4.1 Mon 16:30 REC/C213

Epitaxial Growth and Structural Characterization of Non-centrosymmetric B20-PtAl Thin Films — •AYUSA APARUPA BISWAL¹, DARIUS POHL², BERND RELLINGHAUS², EDOUARD LESNE¹, and CLAUDIA FELSER¹ — ¹Max-Planck-Institute für Chemische Physik fester Stoffe, Dresden, Germany — ²Dresden Center for Nanoanalysis (DCN), cfaed, TU Dresden, Dresden, Germany

Topological chiral semimetals with the non-centrosymmetric cubic B20 structure (space group P213) are distinguished by chirality in their crystal, magnetic, and electronic structures [1]. B20 compounds do not possess inversion or mirror symmetry but preserve rotational symmetries. Non-magnetic B20 compounds, such as CoSi, RhSi, PdGa, and PtAl, host multifold fermions originating from topological band crossings. These lead to large Chern numbers and produce Fermi arcs, alike those found in Weyl semimetals [2,3]. We report on the heteroepitaxial growth of crystalline PtAl thin-films with a non-centrosymmetric cubic B20 structure. We employ magnetron sputtering and explore the phase space of sample composition, growth temperature, post-annealing process, as well as resorting to suitable substrates and crystalline buffer layers. The samples are structurally characterized by a combination of X-ray diffraction and atomic-scale high-resolution transmission electron microscopy, which reveals a thickness-dependent microstructure of the B20 films, attributable to a combination of strain relaxation and the formation of extended defects, which are under detailed investigation. [1] B. Bradlyn et al., *Science* 353 (2016). [2] D. S. Sanchez, et al., *Nature* 567 (2019). [3] Z. Rao et al., *Nature* 567 (2019).

DS 4.2 Mon 16:45 REC/C213

high-quality Bi₂Te₃ TI thin films on [0001]-oriented sapphire substrate grown by MBE — •ISMET GELEN, AHMET YAGMUR, LUKE BENSON, and SATOSHI SASAKI — School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK

Over the past decades, topological insulators (TIs) have attracted great attention for their exotic property of being insulating in the bulk while conductive on the surfaces through topological surface states [1], offering promising prospects for future spintronic technologies [2]. Molecular beam epitaxy (MBE) growth method is very important to produce high-quality epitaxial thin film TIs samples. However, producing a high-quality thin film requires careful consideration of substrate preference, growth temperature, and growth rate. This study focuses on the systematic growth of high-quality Bi₂Te₃ TI thin films on a sapphire [0001] substrate with minimal lattice mismatch. We found that growth temperature has a big influence on the surface morphology, which can lead to small or large triangular terraces. When temperature is too low it can create pillars when it is too high it creates defects/holes in films. We will report our optimization of the Bi₂Te₃ growth in terms of X-ray reflectivity/diffraction, atomic force microscopy, Raman spectroscopy, and magnetotransport properties by measuring standard Hall-bar type devices at low temperatures. Finally, we obtain films with large grain size without defects/pillars, and with high mobility and low carrier density.

[1] Li, Y., et al. (2022). *ACS Nano*, 16(6), 9953–9959. [2] Hasan, M. Z., et al. (2010). *Reviews of Modern Physics*, 82(4), 3045–3067.

DS 4.3 Mon 17:00 REC/C213

exploring chalcogenide ABX₃ perovskites: challenges and insights from physical vapor deposition — •SEBASTIAN ZIMMERMANN¹, ROLAND SCHEER², and TORSTEN HÖLSCHER¹ — ¹B5 Photovoltaics, Just Transition Center, Martin Luther Universität Halle-Wittenberg — ²Photovoltaics Groups, Martin-Luther-Universität Halle-Wittenberg

The discovery of new solar cell materials is crucial for the next generation of multijunction systems in photovoltaics. This work focuses on synthesizing thin-film materials that are theoretically well suited for photovoltaic applications. To form these materials, we use physical vapor deposition (PVD). At the beginning, we aim to synthesize chalcogenide perovskites. Chalcogenide perovskites are crystals with a perovskite structure (typically ABX₃), where X stands for selenium or sulfur, A for group II metal like Ca or Ba and B for a transition metal like Ti or Zr. Compared to other perovskites, their advantages include lower toxicity and the predicted long-term stability of the layers. This talk presents results of microstructural analysis of PVD synthe-

sized chalcogenide perovskite films and discuss challenges encountered during synthesis. Our results provide new insights in the field of photovoltaic materials and are intended to open up new perspectives for multijunction thin-film solar cells.

15 min. break

DS 4.4 Mon 17:30 REC/C213

Molecule Adsorption at Me-polar and N-polar Sc(x)Ga(1-x)N Surfaces Investigated by Photo Electron Spectroscopy — •FABIAN ULLMANN^{1,2} and STEFAN KRISCHOK^{1,2} — ¹TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — ²Zentrum für Mikro- und Nanotechnologien, Gustav-Kirchoff-Straße 7, 98693 Ilmenau

ScGaN can occur in various crystal structures. The most important ones are wurtzite and rock salt formation. Depending on the scandium concentration, a phase transition between these orientations can be found. ScGaN surfaces with different scandium concentrations and orientations were grown by molecular beam epitaxy (MBE) to investigate the near-surface electronic structure. Two different substrates were used to achieve either Me-polar (SiC) and N-polar (sapphire) wz-ScGaN surfaces. The interaction of gas molecules (oxygen and water) in vacuum were analyzed by X-ray (XPS) and ultraviolet photoelectron spectroscopy (UPS).

DS 4.5 Mon 17:45 REC/C213

Molecular Beam Epitaxy of ferrimagnetic Mn₄N — •ADRIANO NOTARANGELO, MICHAEL HANKE, LUTZ GEELHAAR, OLIVER BRANDT, and PHILIPP M. JOHN — Paul-Drude-Institut für Festkörperphysik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany.

Mn₄N is a ferrimagnetic transition-metal nitride that crystallizes in the anti-perovskite structure. With its strong perpendicular magnetic anisotropy and high Curie temperature of ≈ 743 K, Mn₄N emerges as a promising material for rare-earth-free spintronics and other magnetic device applications. Since the magnetic properties of Mn₄N are sensitive to stoichiometry, strain, and lattice defects, achieving high-quality epitaxial growth is essential.

In this work, we grow 60 nm-thick Mn₄N layers by plasma-assisted molecular beam epitaxy on sub-1% lattice-mismatched SrTiO₃(001) substrates. After carefully calibrating the Mn/N flux ratio to achieve a 4:1 stoichiometric balance, we obtain phase-pure Mn₄N(001) films with no detectable secondary Mn_xN_y phases. X-ray diffraction reveals that optimal crystalline quality is achieved for growth temperatures between 300 and 400°C, while substantial Mn desorption hinders growth above 600°C. The out-of-plane lattice constant decreases from 3.854 to 3.828 Å as the growth temperature increases from 300 to 500°C, indicating an increased in-plane tensile strain imposed by the epitaxial constraint to SrTiO₃ with its larger lattice constant.

The optimization of Mn₄N film growth on SrTiO₃ is a solid basis for its growth on industry-relevant substrates such as Si, SiC, and GaN.

DS 4.6 Mon 18:00 REC/C213
Investigations of cubic boron nitride nucleation using in situ RHEED during pulsed laser deposition — •FALKO JAHN, LAURA DIENELT und STEFFEN WEISSMANTEL — Laserinstitut Hochschule Mittweida, Technikumplatz 17, 09648 Mittweida

Due to its outstanding properties such as second-highest hardness, the cubic allotrope of boron nitride (c-BN) has attracted significant interest from both academia and industry for decades. So far, challenges in the thin film deposition of this material have prevented a successful industrial application, for example as a wear-resistant coating for cutting tools. Although pulsed laser deposition (PLD) has enabled progress in this particular field, several aspects of the film formation process remain insufficiently understood. In particular, the process of nucleation from the hexagonal to the cubic phase still contains unanswered questions. In this work, the microstructure of the growing film is characterized in situ using reflection high-energy electron diffraction (RHEED). This enabled further insight into the nucleation process. The results provide support for the nucleation model of subplantation. These findings contribute to a deeper understanding of c-BN nucleation during PLD or similar PVD techniques.