DS 6: Thin Film Application

Time: Wednesday 9:30–11:45 Location: H3

DS 6.1 Wed 9:30 H3

Fluorescent SiON-Doped Si Thin Films in Miniature Temperature Sensor Fabrication Using Machine and Deep Learning with Low Root Mean Square Error — Ali Karatutlu[1], Timuçin Emre Tabaru[2], •Zehra Gizem Mutlay[1], Esra Kendir Tekgül[1], Nurhan Güneş[2], and Bülend Ortaç[1] — [1]Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM) Bilkent University, Ankara, Türkiye — [2]Department of Electrical Electronics Engineering, Sivas University of Science and Technology, Sivas, Turkey

SiON-doped Si, discovered by our project team last year (DOI: Advanced Optical Materials, 2023, DOI: 10.1002/adom.20230009), has a special molecular matrix with a refractive index that can be controlled depending on the amount of SiON. The counterpart structures, such as SixNy, SiOxNy, or Si-rich Si3N4, are conventional structures with general properties such as mechanical durability, thermal stability, chemical resistance, electrical insulation, and optical transparency. We report that SiON-doped Si can have a relatively even higher refractive index from 2.07 to 2.56 near the telecom wavelength of 1310 nm, depending on the SiON content. In terms of application, SiON-doped Si thin films were tested at room temperature to 200°C using different packaging materials such as borosilicate glass and aluminum, and their use as miniature temperature sensors will be demonstrated. The preliminary temperature-fluorescence spectrum correlation was investigated using machine learning and deep learning methods that yield the root mean square error of this system to be as low as 2°C.

DS 6.2 Wed 9:45 H3

Electron-transparent free-standing ultrathin membranes for studying gas-solid and liquid-solid interfaces at high pressures — •Max Gertig[1], Carlos Morales[1], Andreas Schubert[2], Carlos Alvarado[2], Christian Wenger[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]IHP Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany

The chemical reactions of heterogenously catalyzed processes take place at the gas-solid and liquid-solid interfaces. Thus, significant efforts have been dedicated to developing new methods to study them under realistic conditions. In recent years, electron-transparent graphene windows have been used in ambient pressure X-ray photoelectron spectroscopy (AP-XPS) to separate liquids and gases at ambient pressure from a high vacuum. Following this design, we present free-standing ultrathin (up to 10 nm) Al_2O_3 membranes fabricated by atomic layer deposition (ALD) which are electron-transparent to tender and hard X-rays. Three different commercial supports are used: TEM SiN perforated membranes (1 μm), single-hole stainless steal apertures (20 μm), and TEM Cu-grids (80 μm). Their conformity has been examined by scanning electron microscopy (SEM) and atomic force microscopy (AFM), whereas their chemical composition and homogeneity by energy dispersive X-ray (EDX) mapping. Additionally, confocal μ-Raman microscopy complements the chemical and structural characterization. Conventional free-standing graphene membranes have also been fabricated for comparison purposes.

DS 6.3 Wed 10:00 H3

VO_2 Smart Windows for Applications: A Study of $Cu_xTi_{1-x}O_2$ Buffer Layers in Multilayer Thin Film Systems — •Hao Lu[1,2], Martin Becker[1,2], Jan Luka Dornseifer[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany — [2]Center of Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Giessen, Germany

Alloying the TiO_2 with CuO_2 yielding $Cu_xTi_{1-x}O_2$ may provide a suitable buffer layer for optical smart windows based on VO_2. Preliminary work in the literature suggests that the phase transition temperature of the anatase to rutile structural phase transition of TiO_2 is lowered for by alloying Cu. However, that the band gap of $Cu_xTi_{1-x}O_2$ decreases with increasing x compared with the wide band gap of TiO_2. We successfully grew polycrystalline $Cu_xTi_{1-x}O_2$ alloys with x up to 31% on quartz substrates by conventional rf-sputtering employing a TiO_2 ceramic target and Cu wires as Cu source. We determined the crystal phase of the deposited thin films by XRD and Raman spectroscopy and established a 2D phase map versus substrate temperature during growth and Cu content x. It shows that increasing Cu content considerably lowers the growth temperature where rutile $Cu_xTi_{1-x}O_2$ thin films can be obtained. Currently, we are assessing the trade-off between band gap, morphology, and growth temperature required for obtaining the most suitable rutile $Cu_xTi_{1-x}O_2$ buffer layer from the viewpoints of the best materials properties as well as a suitability for future commercialization in smart windows.

DS 6.4 Wed 10:15 H3

VO_2 Smart Windows for Applications: A Study of $Cu_xTi_{1-x}O_2$ Buffer Layers in Multilayer Thin Film Systems — •Hao Lu[1,2], Martin Becker[1,2], Jan Luka Dornseifer[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany — [2]Center of Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Giessen, Germany

Alloying the TiO_2 with CuO_2 yielding $Cu_xTi_{1-x}O_2$ may provide a suitable buffer layer for optical smart windows based on VO_2. Preliminary work in the literature suggests that the phase transition temperature of the anatase to rutile structural phase transition of TiO_2 is lowered for by alloying Cu. However, that the band gap of $Cu_xTi_{1-x}O_2$ decreases with increasing x compared with the wide band gap of TiO_2. We successfully grew polycrystalline $Cu_xTi_{1-x}O_2$ alloys with x up to 31% on quartz substrates. We determined the crystal phase of the deposited thin films by XRD and Raman spectroscopy and established a 2D phase map versus substrate temperature during growth and Cu content x. It shows that increasing Cu content considerably lowers the growth temperature where rutile $Cu_xTi_{1-x}O_2$ thin films can be obtained. Furthermore, we find that the morphology of the $Cu_xTi_{1-x}O_2$ thin films changes with increasing x. Currently, we are assessing the trade-off between band gap, morphology, and growth temperature required for obtaining the most suitable rutile $Cu_xTi_{1-x}O_2$ buffer layer from the viewpoints of the best materials properties as well as a suitability for future commercialization in smart windows.

session break

DS 6.5 Wed 10:45 H3

Achieving superconductivity in infinite-layer nickelate thin films by aluminum sputtering deposition — •dongxin zhang[1], A. Raji[2], L. M. Vicente-Arche[1], A. Gloter[2], M. Bibes[1], and L. Iglesias[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, 91405, France — [2]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, 91405, France

After decades of research, the recent discovery of superconductivity in hole doped infinite-layer nickelates (ABO2) has offered new perspectives to deepen the understanding of high-temperature superconductivity. infinite-layer (IL) nickelates are synthesized by topotactic reduction that selectively removes all apical oxygens of the precursor perovskite ABO3 phase. This is typically achieved by an ex-situ complex annealing using CaH2 as a reducing agent. However, the progress in this field is hampered by significant challenges in materials synthesis and the limited number of research groups capable of producing high-quality superconducting (SC) samples.Here, we present a new method to synthesize SC IL nickelates Pr0.8Sr0.2NiO2 thin films using an aluminum overlayer deposited by sputtering as a reducing agent. We optimized the aluminum deposition conditions and achieved SC samples reduced either in-situ or ex-situ. In-situ Al reduction enhances the quality of the SC Pr0.8Sr0.2NiO2 films, with a maximum transition temperature Tconset of 17 K. This simplified synthesis approach, more accessible than existing ones, enables more research groups to produce high-quality SC nickelate samples, Possibly advancing experimental understanding of superconductivity in IL nickelate.

DS 6.6 Wed 11:00 H3

Deposition and characterisation of NbTiN thin films for application in SRF cavities — •Bharath Reddy Lakki Reddy Venkata, Aleksandr Zubtsovskii, and Xin Jiang — Chair of Surface and Materials Technology, University of Siegen, Germany

Superconducting radio frequency (SRF) cavities are key components for modern particle accelerators. While bulk niobium (Nb), with the highest lower critical magnetic field, Hc1 (0.18 T), and transition temperature, Tc (9.23 K), among elemental superconductors, has dom-

inated SRF applications, the performance of bulk Nb cavities has reached theoretical limits. Recent research focuses on the use of superconducting thin films of Nb or other alternative higher Tc materials, such as NbN, NbTiN, Nb3Sn, MgB2, etc, to enhance SRF cavity performance and cost efficiency. However, their lower Hc1 limits high accelerating gradients and quality factors. Gurevich's SIS multilayer theory offers a breakthrough to shield an underlying superconductor from the applied magnetic fields, thus increasing the maximum accelerating gradient beyond the bulk Nb limits. This study investigates NbTiN thin films deposited on Si substrates using reactive DC- and HiPIMS techniques. Deposition parameters were optimised to achieve improved microstructure and superconducting properties, enabling their integration into SIS structures. To understand the microstructural characteristics of NbTiN films, positron annihilation spectroscopy (PAS) was employed alongside SEM, XRD, AFM, and EDX, offering deeper insights into how deposition techniques and parameters affect material performance.

DS 6.7 Wed 11:15 H3

T-dependent switching of molecular spin-crossover (SCO) monolayers — •Fabian Streller[1], Kirill Gubanov[1], Stephen Goodner[2], Marat Khusniyarov[2], and Rainer Fink[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich Alexander Universität Erlangen Nürnberg — [2]Lehrstuhl für Anorganische und Allgemeine Chemie, Friedrich Alexander Universität Erlangen Nürnberg

Spin-crossover (SCO) complexes are regarded as promising materials in spintronics, molecular electronics and ultra-high-density memory systems applications. Switching between diamagnetic low-spin (LS) and paramagnetic high-spin (HS) species is triggered by external stimuli, e.g., change of temperature, pressure, or illumination with light.[1] One major challenge is the transfer from solution or bulk towards thin films or even monolayers on well-defined surfaces without quenching of the switching behaviour. Six-coordinate iron(II) complexes have been used as SCO materials. This material is attached to the surface via a bidental phenanthroline ligand containing moieties suitable for bonding to the substrate. We report on a step-by-step formation of SCO-active single-layer films on Au(111) surfaces. Thus created specimens were characterized by atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS) and temperature dependent near edge x-ray absorption fine structure (NEXAFS) to follow the molecular switching. Research is funded by the BMBF (contract 05K22WE2)
[1] B. Rösner, M. Milek, A. Witt, B. Gobaut, P. Torelli, R. H. Fink, M. M. Khusniyarov Angewandte Chemie. 2015, 127, 13168-13172.

DS 6.8 Wed 11:30 H3

High Accuracy Reflection Prediction Model for Multi-Layer Anti-Reflection Coatings Using Deep Learning and Machine Learning — •Iremnur Duru, Semih Oktay, and Timuçin Emre Tabaru — Department of Electrical Electronics Engineering, Sivas University of Science and Technology, 58000 Sivas, Turkey

In order to optimize the thickness parameters, this work employs Machine Learning (ML) and Deep Learning (DL) approaches to develop an accurate reflection prediction model that will direct the design of filters with multilayer Anti-Reflection Coating (ARC). A dataset of information derived from 3000 (1500 Ge- Al2O3, 1500 Ge- SiO2) computer simulations based on the thicknesses of multilayer structural materials has been used to create this model. Al2O3 and SiO2 served as the second layers in both coatings, with Ge serving as the substrate. Reflectance values for wavelengths ranging between the 3-5 *m and 8-12 *m bands characteristic of the mid-wave infrared (MWIR) and long-wave infrared (LWIR) bands are included in the data set. The average reflectance in the given 2-layer data set was at least 0.36 at thicknesses of 515 nm Ge and 910 nm SiO2. In terms of predicting reflectance values, the results demonstrate that machine learning (ML) models*specifically, decision tree, random forest and bagging methods perform better than the DL model and offer a useful guide for conceptualizing and manufacturing optical thin-film filters.