DS 25: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) Part II

Time: Friday 9:30–12:45 Location: H32

DS 25.1 Fri 9:30 H32

Reducing residual stress and dislocation density in AlN films grown on SiC by MOCVD for UV-C LED applications — •Christian J. Zollner[1], Abdullah Almogbel[1], Burhan Saif Addin[1], Michael Iza[1], Steven P. DenBaars[1,2], James S. Speck[1], and Shuji Nakamura[1,2] — [1]Materials Department, UC Santa Barbara, CA, USA — [2]Department of Electrical and Computer Engineering, UC Santa Barbara, CA, USA

In nitride optoelectronics, the most important figures of merit for buffer layers grown on foreign substrates are threading dislocation density (TDD) and residual stress. Residual stress can lead to polarization fields in GaN and AlN, as well as wafer bowing and film cracking. Threading dislocations are detrimental to optical emission efficiencies, laser lifetimes, and carrier mobilities, but growing low TDD nitride buffers has proven more challenging than in conventional semiconductors. I will discuss the tradeoff between low TDD and low stress in MOCVD grown AlN films, and how this tradeoff can be mitigated. As a result, TDD (measured by x-ray diffraction and TEM) has been reduced from 10^{10} cm^{-2} to 4×10^{8} cm^{-2}, and stress (measured with the x-ray radius of curvature method) has been reduced from nearly 2 GPa to below 500 MPa. The mechanisms of TDD and stress reduction are explored using TEM and secondary-ion mass spectroscopy, and theoretical contributions of different sources of stress are calculated and compared with experiment. Significant reductions in both TDD and stress yield higher performance in UV-C LED devices grown on improved AlN/SiC buffers.

DS 25.2 Fri 9:45 H32

Mass separated low-energy nitrogen ion assisted thin film growth — •Michael Mensing, Philipp Schumacher, Christoph Grüner, Jürgen W. Gerlach, and Bernd Rauschenbach — Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany

Ion beam or plasma assistance is consistently and increasingly utilized to enhance the capabilities of physical deposition techniques. The impact of their applications range from precise engineering of film properties to the alleviation of process constraints. Albeit the influence of the energetic particle flux has been extensively studied, the distinct contributions of individual ion species to film growth are typically not investigated due to the extensive efforts required. In this study the application of an energy and mass selected ion-beam assisted deposition (EMS-IBAD) setup is presented. It features a compact quadrupole mass filter system to separate the prominent ion species (N^+, N_2^+) involved in the growth processes of nitride thin films on the example of GaN. The thin films are deposited on 6H-SiC(0001) by employing different nitrogen ion species and compared with regards to their topography, crystalline quality and phase composition for different ion kinetic energies and ion-to-atom arrival ratios. The chosen hyperthermal ion energy range is <200 eV. The higher energy atomic nitrogen ions could be identified to impede the formation of the metastable zinc-blende GaN phase whereas the crystalline quality deteriorates. Molecular nitrogen ions are demonstrated to efficiently dissociate for kinetic energies as low as 20 eV, providing increased growth rates while preserving the crystalline quality.

DS 25.3 Fri 10:00 H32

Valence profiling of $LaMnO_3/SrTiO_3$ by use of resonant X-ray reflectometry and crystal field theory — •Michael Dettbarn[1], Volodymyr B. Zabolotnyy[1], Robert Green[2], Michael Zapf[1], Kirill Miller[1], Matthias Schmitt[1], Enrico Schierle[3], Michael Sing[1], Ralph Claessen[1], and Vladimir Hinkov[1] — [1]Universität Würzburg and Röntgen Center for Complex Material Systems (RCCM), Würzburg — [2]University of Saskatchewan, Saskatoon, Canada — [3]HZB, Berlin

We have measured resonant X-ray reflectivity (RXR) and X-ray absorption spectra (XAS) on a bulk stoichiometric $La_{7/8}Sr_{1/8}MnO_3$ sample and three thin $LaMnO_3$ films of 3, 12 and 30 u.c. thickness. The manganese in the $La_{7/8}Sr_{1/8}MnO_3$ sample can be modeled by a 3+ valence, whose line shape we fit theoretically by use of crystal-field theory, including a Jahn-Teller distortion.

We model the RXR spectra of the three $LaMnO_3$ films by a mixture of Mn^{3+} and Mn^{2+} contributions, and deduce the depth profiles of the two different valencies. We compare our results with previous microscopy studies, in which a preferred occurrence of Mn^{2+} near the interface and surface regions was observed.

DS 25.4 Fri 10:15 H32

HAXPES study of oxygen vacancies forming in thin film HfO_2-based MIM structures — •Thomas Szyjka[1], Ronja Hinz[1], Mai Hussein[1], Paul Rosenberger[1], Marek Wilhelm[1], Terence Mittmann[2], Uwe Schröder[2], and Martina Müller[1,3] — [1]PGI-6, FZ Jülich GmbH, Jülich, DE — [2]NaMLab gGmbH, Dresden, DE — [3]Fakultät Physik, TU Dortmund, Dortmund, DE

Hf-based dielectrics have replaced the traditional SiO_2 and SiON as gate dielectric materials for conventional CMOS devices. Due to the recently discovered ferroelectric properties in strained HfO_2, new applications like ferroelectric FETS are currently under development.

The ferroelectric properties are linked to the orthorhombic phase in HfO_2 which can be stabilized via doping or the creation of oxygen vacancies. In this context, it is crucial to understand the processes and engineering of the interface properties of strained-HfO_2 and electrode materials. Different thin film metal-insulator-metal (MIM) capacitors were fabricated with doped HfO_2 using different electrode materials (TaN, TiN, IrO_2) leading to various forming of oxygen vacancies. In addition, films with undoped HfO_2 and TiN electrodes were fabricated using either no or 2 sccm additional oxygen flow during the fabrication in order to reduce the amount of oxygen vacancies. Hard X-ray photoelectron spectroscopy (HAXPES) was performed at DESY (Hamburg) and BESSY (Berlin) to analyse the interface processes. The spectral features of the Hf4f, N1s and O1s core levels indicate an intermixing of the layers and provide a direct relation between the growth process and the formation of oxygen vacancies.

DS 25.5 Fri 10:30 H32

X-ray spectroscopic composition analysis of amorphous ZnSnOy grown by magnetron sputtering — •Ainur Zhussupbekova[1], Aitkazy Kaisha[1], Karsten Fleischer[1,2], Igor V. Shvets[1], and David Caffrey[1] — [1]School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College Dublin, Dublin 2, Ireland — [2]School of Physics, Dublin City University, Dublin 9, Ireland

The conductivity of Amorphous Transparent Conducting Oxide (a-TCO) materials is not dependent on their long range crystallographic order, making them ideal materials for flexible electronics. A potential candidate to take a prominent place in this field is amorphous ZnSnOy (a-ZTO) because, unlike amorphous InGaZnO4 (a-IGZO), it does not contain any non-abundant or expensive components such as indium.

In this study, X-ray Photoelectron Spectroscopy (XPS) is used to perform an extensive composition analysis of a-ZnSnOy grown by reactive and non-reactive magnetron sputtering. An identical maximum conductivity of 225 S/cm is achieved via both techniques. However, analysis of the a-ZnSnOy composition reveals that the distinct Zn/Sn ratios at which this maxima occurs varies depending on growth technique. The Zn/Sn ratios observed at each maxima have been found to correspond to theoretical unstable polymorphs of a-ZnSnOy. We confirm the existence of two corresponding distinct local bonding arrangements depending on deposition methodology via Raman spectroscopy.

DS 25.6 Fri 10:45 H32

MBE growth of oxide thin films on silicon — •Luqman Mustafa — ZIK SiLi-nano, Martin-Luther-University Halle-Wittenberg, Halle, Germany

Complex oxide thin films can exhibit many different physical properties. The epitaxial growth of these films on silicon enables the integration of their properties in silicon technology for the development of novel devices and optimizing existing technologies. Lately, ferroelectric oxide thin films has gained more interest in photonic applications, for example, waveguid structures made of BaTiO3 on silicon-on-oxide (SOI) wafers were developed exhibiting strong linear electro-optical effect, with effective Pockels coefficient higher than commercial optical modulators.

The greatest challenge in the epitaxial growth of oxides on silicon is the formation of amorphous silicon oxide layer at the interface once the

silicon surface is exposed to oxygen, making the intended heteroepitaxy of the film on silicon extremely difficult. Here we report on the optimized growth conditions of complex oxide thin films on SOI substrates. BaTiO3 thin films were grown using MBE technique. BaO,and SrTiO3 were used as a buffer layer to reduce strain. the thin film morphology, structural, and ferroelectric properties were investigated.

15 min. break.

DS 25.7 Fri 11:15 H32

Orbital character of the mobile and localized electron states at the LAO/STO interface — •Alla Chikina[1,2], Frank Lechermann[3], Marius-Adrian Husanu[1,4], Marco Caputo[1], Claudia Cancellieri[5], Thorsten Schmitt[1], Milan Radovic[1], and Vladimir N. Strocov[1] — [1]Swiss Light Source, Paul Scherrer Institute, Villigen CH-5232, Switzerland — [2]IFW Dresden, P.O. Box 270116, Dresden D-01171, Germany — [3]Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, Hamburg DE-20355, Germany — [4]National Institute of Materials Physics, Atomistilor 405A, Magurele RO-077125, Romania — [5]Empa, Swiss Federal Laboratories for Materials Science & Technology, Ueberlandstrasse 129, Duebendorf CH-8600, Switzerland

Interfacing different transition-metal oxides opens a route to functionalizing their rich interplay of electron, spin, orbital, and lattice degrees of freedom for electronic and spintronic devices. Electronic and magnetic properties of a mobile two-dimensional electron system (2DES) of SrTiO3-based interfaces are strongly influenced by oxygen vacancies, where strongly correlated localized electrons in the in-gap states (IGSs) coexist with noncorrelated delocalized 2DES. Here, we use resonant soft-X-ray photoelectron spectroscopy to prove the eg character of the IGSs, as opposed to the t2g character of the 2DES in the paradigmatic LaAlO3/SrTiO3 interface. Supported by a self-consistent combination of density functional theory and dynamical mean field theory calculations, this experiment identifies local orbital reconstruction that goes beyond the conventional eg-vs-t2g band ordering.

DS 25.8 Fri 11:30 H32

PFM and SHG study of ferroelastic twin domain crossings in $PbZr_{0.2}Ti_{0.8}O_3$ — •Philippe Tückmantel[1], Grégory Taupier[2], Kokou D. Dorkenoo[2], Joshua C. Agar[3], Lane W. Martin[3], Patrycja Paruch[1], and Salia Cherifi-Hertel[2] — [1]DQMP University of Geneva, Geneva, Switzerland — [2]University of Strasbourg CNRS, IPCMS, Strasbourg, France — [3]University of California, Berkeley, DMSE, USA

Domains walls in ferroelectrics can exhibit properties absent from their parent material, such as a higher electric conductivity, photovoltaic effect, and ferromagnetic ordering, leading to a surge in interest in potentially using these nanoscale interfaces as active device components. Both theoretical and experimental studies have recently focused on the complex structure of these domain walls, underlying the rich functional behaviour. For example, SHG experiments have confirmed the non-Ising character of 180° domain walls in $PbZr_{0.2}Ti_{0.8}O_3$ and $LiTaO_3$ which locally show Néel and Bloch like polarisation, respectively. However, relatively little is known about how such domain walls respond to disorder, variations of electrostatic boundary conditions or strain, which strongly influence polarisation in bulk and thin film samples, and which could affect the emergent properties of the domain walls.

Here, we report on the interplay of disorder and electromechanical effects, using SHG and PFM to focus on the crossings of 180° domain walls and ferroelastic twin domain walls in $PbZr_{0.2}Ti_{0.8}O_3$ grown by PLD on a $DyScO_3$ substrates, highlighting their complex polarisation patterns and the key role of strain.

DS 25.9 Fri 11:45 H32

Topotactic transition mechanisms in $SrCoO_{2.5+x}$ films — •Patrick Schöffmann[1], Sabine Pütter[1], Anirban Sarkar[2], Amir Syed-Mohd[1], Markus Waschk[2], Tanvi Bhatnagar[2], Paul Zakalek[2], and Thomas Brückel[2] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Jülich, Germany

Strontium cobaltite ($SrCoO_{3-\delta}$) exists in two topotactic phases, depending on the oxygen content. $SrCoO_3$ is a ferromagnetic metal (T_C=305K) with perovskite structure while $SrCoO_{2.5}$ is an antiferromagnetic insulator(T_N=570K) with brownmillerite structure. Because of the multivalent Co states and high oxygen mobility it is a promising material for energy and information applications [1]. To control the oxygen content, several possibilites exist. We focus on annealing in oxidising conditions and applying variable strain with a piezoelectric substrate to the film.

We grow thin films of $SrCoO_{2.5}$ by molecular beam epitaxy on various substrates including a piezoelectric with a conducting buffer layer.

To be able to transfer strain from the substrate to the film, a high sample quality and epitaxy is mandatory, thus we present the results of the film growth and quality, as well as first results of the magnetic characterisation by SQUID and neutron reflectometry.

[1] H. Jeen et al., Nature Materials 12, 2013

DS 25.10 Fri 12:00 H32

Effect of Interfaces in the Oxide Transport Process in Platinum Coated Porous Frameworks of Yttria-Stabilized Zirconia (YSZ) — •Michele Bastianello[1], Jan-Ove Söhngen[1], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Institute of Experimental Physics I, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 16, 35392 Gießen — [3]Institute of Physical Chemistry, Justus-Liebig-University Gießen, Germany, Heinrich-Buff-Ring 17, 35392 Gießen

Mixed ionic and electronic conductors (MIEC) are used for many applications, i.e. as electrolyte for oxygen separation membranes. Here we present the preparation of artificial MIECs. Different YSZ-Pt-YSZ multilayered thin films were prepared as model systems using pulsed laser deposition (PLD) together with porous YSZ thin films subsequently coated with a thin layer of metallic platinum using atomic layer deposition (ALD). The as-prepared materials were structurally charachterized using grazing incidence X-ray diffraction (GIXRD) and scanning electron microscopy (SEM). The electrical transport properties were investigated performing electrochemical impedance spectroscopy (EIS) at different temperatures and oxygen partial pressures to determine the conductivity as well as the activation energy of the thin films.

DS 25.11 Fri 12:15 H32

Structure evolution of hydrogenated TiO_2 by means of Perturbed Angular Correlation — •Dmitry Zyabkin[1], Juliana Schell[2,3], Ulrich Vetter[1], and Peter Schaaf[1] — [1]Chair materials for Electronics, Institute of Materials Engineering and Institute of Micro- and Nanotechnologies MacroNano®, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau, Germany — [2]European Organization for Nuclear Research (CERN), CH- 1211 Geneva, Switzerland — [3]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany

Hydrogenated titania has been recently attracting plenty of attention due to its promising properties. Not quite long ago some results proved that H is able to create a bond with Ti via Ti-OH and stays connected up to 530-550 K when it starts to dissociate and leave, additionally V_0 start to rearrange. To study this phenomena we applied recent perturbed $\gamma\gamma$-angular correlation (PAC) studies of TiO_2:H thin films using the probe ^{111m}Cd, which was implanted at the online isotope separator ISOLDE at CERN. The films were produced by reactive magnetron sputtering on Si substrates. The subsequent H_2 plasma treatment was performed at various temperatures up to 663K. After implantation with 10^{11} probe atoms the samples were transported to a PAC setup and measured in various atmospheres (O_2, air and vacuum) and in a range of temperatures to follow structure refinement. In order to preserve H-boundings no after implantation annealing was done. Time-differential R(t) spectra were fitted against electric quadrupole interaction parameter sets corresponding to fractions of probes.

DS 25.12 Fri 12:30 H32

Epitaxial growth of Ba_2SiO_4 thin films on Si(001) — •Julian Koch and Herbert Pfnür — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

Ba_2SiO_4 is a very promising candidate as a high-k dielectric [1]. Previously, Ba_2SiO_4 films were grown by diffusion of Si from the Si(001) substrate into a deposited BaO layer [1]. These films featured a high interface trap density, which was most likely a result of the diffusion.

This study aims to improve the structural quality of the Ba_2SiO_4 films by employing a co-deposition growth method, in which Ba and Si are evaporated simultaneously in an oxygen atmosphere. This eliminates the need for the Si diffusion and allows for control of the interface and the exact stoichiometry.

The chemical composition and the crystallinity of the films are investigated using XPS and SPA-LEED, respectively. The chemical shift of the O 1s peak in XPS enables the detection of excess Ba or Si and can thus be used to adjust the Si/Ba deposition ratio. The films are grown at RT to avoid Si diffusion from the substrate. Growth at higher temperatures is also possible, but the Si deposition rate has to be reduced to offset the diffusion. The epitaxial growth succeeded without any surface passivation or interface layer. However, even with correctly adjusted deposition rates, annealing to 680°C is needed in order to obtain crystalline films. During the annealing process the film is partially evaporated but the relative concentration of Ba to Si remains unchanged.

[1] S. Islam et al. Phys. Rev. Applied 5, 054006 (2016)