DS 9: Thin Film Properties: Structure, Morphology and Composition (XRD, TEM, XPS, SIMS, RBS, AFM, ...) 3

Time: Tuesday 9:30–11:00 Location: H14

DS 9.1 Tue 9:30 H14

Structural properties of iron dichalcogenide thin films deposited by selenization process — •Luqman Mustafa[1], Andreas Kreyssig[1], Jill Fortmann[2], Aurelija Mockute[2], Alfred Ludwig[2], and Anna E. Böhmer[1] — [1]Institute for Experimental Physics IV, Ruhr-Universität Bochum, Germany — [2]Materials Discovery and Interfaces, Institute for Materials, Ruhr University Bochum, Germany

Transition-metal dichalcogenides with marcasite structure have been extensively studied for their applications in light energy conversion and photoelectrochemical devices. Lately this structure type has also gained interest for its magnetic properties as a candidate for the newly-predicted altermagnetic order.

We report on the formation of (Fe,X)Se_2, (X= Co, Mn, Cr....) thin films by ex-situ selenization of amorphous transition metal thin films. Using combinatorial deposition allowed to efficiently explore a wide range of substitution at the iron site with different transition metals (for example Co, Mn, Cr). The dependence of structural properties and phase stability on the selenization temperature and substitution level has been investigated. The process may be adapted for other transition metal dichalcogenides thin films, such as $FeSb_2$, and is therefore a unique tool to study a broad material family and its possible substitution ranges.

DS 9.2 Tue 9:45 H14

Structural and elastic properties of $Sc_xAl_{1-x}N$ — •Saskia Mihalic[1], Armin Dadgar[2], Niclas M. Feil[1], Christopher Lüttich[2], André Strittmatter[2], and Oliver Ambacher[1] — [1]Department of Sustainable Systems Engineering, University of Freiburg, Germany — [2]Department of Semiconductor Epitaxy, Otto von Guericke University Magdeburg, Germany

The hexagonal compound alloy scandium aluminum nitride ($Sc_xAl_{1-x}N$) shows an enhancement of the piezoelectric module d_{33}(x) by more than 300 % compared to aluminum nitride (AlN). Therefore, $Sc_xAl_{1-x}N$ is a highly promising material for the implementation of acoustic resonators for mobile communication systems, although usually a larger stiffness of the material is required. The direction-dependent elastic behavior of hexagonal $Sc_xAl_{1-x}N$ crystals is represented by the reciprocal Young's modulus S^*_{11}(x) and aids in identifying the best trade-off between piezoelectric and elastic properties of anisotropic $Sc_xAl_{1-x}N$ for microacoustic applications. To confirm the calculations with experimental results, thin films of $Sc_xAl_{1-x}N$(0001) and ScN(111) on Si-substrates were grown by reactive magnetron sputter epitaxy. The structural properties of thin films have been investigated by high-resolution X-Ray diffractometry (HRXRD) and high-resolution transmission electron microscopy (HRTEM). Furthermore, we will present a detailed comparison of theoretical and experimental results of the piezoelectric and stiffness coefficients achieved by the analysis of $Sc_xAl_{1-x}N$-based SAW resonators.

DS 9.3 Tue 10:00 H14

Structural analysis of $Sc_xAl_{1-x}N$ thin films — •Rebecca Petrich[1], Younes Slimi[1], Hauke Honig[2], Lorenz Steinacker[2], Katja Tonisch[1], Raphael Kuhnen[3], Dietmar Frühauf[3], and Stefan Krischok[1] — [1]TU Ilmenau, FG Technische Physik I, IMN MacroNano, 98693 Ilmenau — [2]TU Ilmenau, FG Werkstoffe der Elektrotechnik, IMN MacroNano, 98693 Ilmenau — [3]Endress+Hauser SE+Co. KG, TTD Technologieentwicklung, 79689 Maulburg

The further and new development of functional materials is an important and constant research approach for the optimization of microelectromechanical systems. In the field of piezoelectric materials, AlN stands out due to its good piezoelectric properties and its CMOS compatibility, its very good thermal stability and high sound velocity. While the basic research for this material is considered to be largely completed, research for the scandium-based alloy $Sc_xAl_{1-x}N$ is still in its infancy. The need for investigation is particularly high for alloys with scandium concentrations of more than x = 15%. For this purpose, $Sc_xAl_{1-x}N$ thin films were deposited and analyzed using pulsed magnetron sputtering in a concentration range between x = 15% and 35%. Starting with the crystal orientation (X-ray diffractometry) and the layer composition (energy-dispersive X-ray spectroscopy) through to the surface roughness (atomic force microscopy), optical parameters for determining the layer thickness and dielectric function (spectroscopic UV-Vis ellipsometry) were also examined and compared to pure AlN. In addition, the homogeneity of the layer properties was examined over different radii on 4" Si wafers.

DS 9.4 Tue 10:15 H14

Phase behavior of dumbbell monolayers obtained via Langmuir-Blodgett-like Brownian dynamics simulations — •Anton Lüders, Rouven Stuckert, Ellen Zander, Alexander Wittemann, and Peter Nielaba — Universität Konstanz, Konstanz, Deutschland

We explore the structure formation and the phase behavior of thin films of dumbbell colloids. For this, we first determine empiric formulas for the microscopic diffusion coefficients of dumbbells using a bead-shell approach. These diffusion coefficients are used to perform two-dimensional Brownian dynamics (BD) simulations where the area fraction of the system is adjusted via movable barriers at the boundaries of the simulation box. The results of the simulations are compared to Langmuir-Blodgett experiments with dumbbell monolayers at the air/water interface. Using Voronoi diagrams and the Voronoi cell shape factor, the influence of the area fraction on the structure of the monolayers is investigated. The simulations and the experiments show - in excellent agreement with each other - that an increase of the area fraction leads to a higher percentage of domains containing particles with six nearest neighbors. Especially in dense systems, these domains can consist of aligned particles with uniform Voronoi cells. Thus, the increase of the area fraction enhances the order of the monolayers. The remarkable qualitative agreement of the simulations and the experiments indicates a versatile way of characterizing colloidal monolayers by BD simulations which opens up perspectives for application to a broad range of nanoparticle-based thin film coatings.

DS 9.5 Tue 10:30 H14

Thermal Laser Epitaxy of Refractory Metals — •Lena Nadine Majer, Hongguang Wang, Wolfgang Braun, Peter A. van Aken, Jochen Mannhart, and Sander Smink — Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

In thermal laser epitaxy, both the substrate and the individual evaporation sources are heated by high-power continuous-wave lasers. This method combines the advantages of MBE and PLD, allowing the efficient thermal evaporation and epitaxial deposition of practically any combination of elements from the periodic table. We demonstrate and discuss the epitaxial growth of refractory metals on c-cut sapphire. As examples we present Ru and Ta growth, because they are of particular interest for many technological applications. We have optimized the growth parameters to obtain epitaxial films of superior quality, which are apparently devoid of defects over large areas. The films have been characterized by AFM, RHEED, STEM, and X-ray analysis, revealing that the layers grow single phase, with a low surface roughness and that the interface between the layer and the substrate is atomically sharp.

DS 9.6 Tue 10:45 H14

Temperature-dependent C-AFM measurements on rhodium paddle-wheel coordination polymers — Daniel Steinbach, Sophie Gersdorf, and •Florian Mertens — Institute of Physical Chemistry, TU Bergakademie Freiberg, Germany

To overcome one of the disadvantages of most coordination polymers and metal-organic frameworks being insulators, conjugated coordination polymers are investigated regarding their electrical conductivity. To obtain a potentially conductive system paddle-wheel structures with a documented metal-metal bond, here rhodium derivates, were linked via conjugated organic molecules like pyrazine. Coordination polymers of this type were first synthesized as bulk materials, characterized using XRD, TG-DSC and XPS and then deposited as coatings on gold surfaces. Subsequently, the topography of the deposited layers was determined. The morphological properties of the coatings were correlated with the properties of the basic coordination polymer com-

ponents.

The conductivity was investigated via temperature-dependent C-AFM measurements. As expected no conductivity is measurable for coordination polymers containing acetates based paddle-wheels even if they are linked with a tridentate conjugated ligand. For the $[Rh_2(acam)_4(pyz)]_n$ (Hacam = acetamide) coordination polymer a strong temperature and field dependency of the conductivity was observed. From the corresponding measurements an arrhenius type activation energy of app. 0.3-0.4 eV was derived. In addition, various conduction mechanisms were discussed.