DS 9: Thin Film Characterisation: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS, ...) II

Time: Monday 12:00–13:00 Location: GER 38

DS 9.1 Mon 12:00 GER 38

The interface of epitaxial bixbyite-structured rare-earth sesquioxides on Si(111) — •Michael Niehle, Tatsuro Watahiki, and Achim Trampert — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin

Rare-earth oxides (RE_2O_3) are promising high-κ materials for replacement of SiO_2 as insulator in CMOS technology. They are required for further downscaling. Recently, the possibility to grow single domain RE_2O_3 in the cubic bixbyite structure on Si(111) with atomically smooth, chemically stable and crystalline interfaces has been demonstrated by molecular beam epitaxy. Understanding the interface's microstructure is necessary to optimize growth conditions and to estimate applicability in future devices. Binary Gd_2O_3 or an adequate ternary alloy like $(La,Lu)_2O_3$ allow for a nearly lattice matched epitaxial growth. High-resolution transmission electron microscopy (HRTEM) is used to demonstrate that a coherently grown heterostructure is feasable. Two models for the atomic configuration at the interface are proposed and incorporated in a supercell which serves as input for HRTEM image simulation applying the multi-slice algorithm. Results of the simulation are confirmed by comparison to experimental HRTEM-images of $(La_{1-x}Lu_x)_2O_3$ and $(Gd_{1-x}Lu_x)_2O_3$ with $x \approx 0.5$ and $x \approx 0$, respectively. Competing crystal structures to the bixbyite phase are excluded.

DS 9.2 Mon 12:15 GER 38

Structure of heteroepitaxial type-B oriented CeO_2(111) on cubic- and hexagonal-Pr_2O_3/Si(111) supports — •Marvin Zoellner[1], Joachim Wollschläger[2], Marcus Bäumer[3], Michael Reichling[2], Peter Zaumseil[1], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany. — [2]Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany. — [3]Universität Bremen, Leobener Str. 2, 28359 Bremen, Germany.

Single crystalline epitaxial cerium oxide is of interest for model catalysis. Furthermore, a combination with praseodymium oxide exhibits an enhanced oxygen storage capability. Therefore, CeO_2(111) thin films were grown on cub-Pr_2O_3(111)/Si(111) and hex-Pr_2O_3(0001)/Si(111) by molecular beam epitaxy (MBE). The cub-CeO_2(111) lattice has an ABCABC... and the hex-Pr_2O_3(0001) lattice an ABABAB... stacking sequence. In such oxide heterostructures stacking twins can occur, which influence catalytic activity. Reflection high energy electron diffraction (RHEED) was used for in-situ monitoring of the layer orientation. To gain a global and local insight of the heterostructures, X-ray diffraction (XRD) and transmission electron microscopy (TEM) were performed ex-situ. Finally, synchrotron radiation-grazing incidence X-ray diffraction (SR-GIXRD) gives a surface sensitive twin analysis. A twin-free, exclusively type-B oriented CeO_2[1-10]||Si[-110] epitaxial relationship of the CeO_2(111) film on the cub- as well as on the hex-Pr_2O_3 was detected. Theoretical ab initio calculations were carried out to gain an understanding of the unexpected twin-free growth mechanism.

DS 9.3 Mon 12:30 GER 38

Epitaxial growth of GeTe on Si(111) and in-situ compositional analysis — •Karthick Perumal, Wolfgang Braun, and Raffaella Calarco — Paul Drude Institut für Festkörperelektronik, Berlin, Deutschland

GeTe is an important phase change material lying on one end of the pseudobinary line of Ge-Sb-Te alloys, with Sb_2Te_3 at the other end. The complex growth behaviour of ternary Ge-Sb-Te alloys requires better understanding of the binary component GeTe. Here, we report on the molecular beam epitaxy of GeTe on Si(111) substrates and the use of desorption mass spectroscopy as an in-situ technique for compositional analysis during the growth. The source fluxes of Ge and Te are kept at a ratio of 2:5. The GeTe samples grown at different substrate temperatures were continuously monitored by a quadrupole mass spectrometer and an algorithm was made to subtract the observed background pressure, thereby deducing the incorporation ratio of various atomic species. With the assumption that the sensitivity of the mass spectrometer is one, we calculate the Te to Ge ratio of incorporating atoms. The compositional results lie within 10% of the values confirmed by XRF measurements. X-ray diffraction analysis was performed on the grown samples and the crystal structure was found to be hexagonal. We find that the growth of GeTe is independent of Te as long as there is an excess tellurium flux, which shows that GeTe behaves like III-V materials: with higher Te flux, the growth is Ge limited.

DS 9.4 Mon 12:45 GER 38

Electron microscopy study of amorphous SiCN hard coatings — •Andrea Sendzik, Steffen Schulze, Marcus Günther, Frank Richter, and Michael Hietschold — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

The two-component systems Si-C, Si-N and C-N have been studied in terms of their mechanical, electrical and optical properties. The goal for the ternary amorphous SiCN compounds is to unite the positive properties of the binaries, such as chemical stability, hardness and large band gap. We have characterized thine layers by scanning electron microscopy (SEM) and transmission electron microscopy (TEM), through the studies of diffraction patterns and the analysis of electron energy loss spectra (EELS).The layers were produced by plasma enhanced chemical vapor deposition PECVD. For this a mixture of following gases was used: Ttrimethylsilane ($SiH(CH_3)_3$), N_2 and Ar. A series of samples has been prepared, differing in terms of gas composition and pressure. All SiCN films were deposited on silicon or on NaCl(100) substrates. By SEM the morphology of the layers were characterized. The atomic structure was investigated by TEM. By analyzing diffraction patterns and EELS-spectra findings about the short-range order of atoms, the atomic composition, and the chemical bonding were made. By comparing the experimentally obtained scattering curves with model distributions earlier structural ideas could be expanded and systematized in accordance with the deposition conditions. In addition the first results of mechanical tests are presented, such as E-Modul and stress values of the layer.