DS 1: Thin Film Characterisation: Structure Analyse and Composition (XRD, TEM, XPS, SIMS, RBS, ...) I

Time: Monday 10:15–12:00 Location: GER 37

DS 1.1 Mon 10:15 GER 37

Epitaxial growth of ZnO on $CuInS_2$(112) — Stefan Andres[1], •Carsten Lehmann[2], and Christian Pettenkofer[2] — [1]Oerlikon, Lichtenstein — [2]Helmholtz-Zentrum Berlin, Germany

We report on epitaxial growth of ZnO on (112) orientated $CuInS_2$ thin films. The preparation of the samples was performed in an ultra high vacuum system at the Helmholtz-Zentrum Berlin. An alternating step-by-step growth and investigation by photoelectron spectroscopy (PES) and low energy electron diffraction (LEED) provided insight on the growth dynamics and structure of the ZnO-$CuInS_2$-interface. We find that during the initial growth no ZnO is deposited. Instead a monolayer of ZnS is formed by depleting the $CuInS_2$ surface of excess sulfur. Thereafter, the ZnO growth starts on this ZnS buffer layer. Band alignment considerations show that the ZnS buffer layer is thin enough to provide a beneficial band alignment situation concering photovoltaic application.

DS 1.2 Mon 10:30 GER 37

Sputter deposition of vanadium pentoxide (V_2O_5) as electrode material in rechargable Li-ion batteries — •Tobias Gallasch, Tobias Stockhoff, and Guido Schmitz — Institut für Materialphysik, Westf. Wilhelms-Universität Münster , Wilhelm-Klemm-Str.10, 48149 Münster, Germany

V_2O_5 is a candidate as intercalation compound for rechargable Li-ion batteries due to its orthorhombic layered crystal structure, which allows reversible Li^+ intercalation. V_2O_5 thin films (thickness: 300nm) were deposited on silicon or glass substrates by ion beam sputtering from a sintered V_2O_5 powder target. The influence of different sputter parameters (such as: substrate material, temperature, oxygen partial pressure) and post-annealing conditions on the structure were investigated by XRD and TEM; Electronic properties were analysed by dc-conductivity measurements. It is demonstrated that the desired intercalation structure is only achieved by adding oxygen during sputtering and post-annealing under oxygen atmosphere. It is shown that the electronic conductivity spreads over several orders of magnitude depending on the preparation conditions.

Futhermore, electron energy-loss spectroscopy (EELS) was carried out to determine the V-oxidation state in dependence on sputter parameters and a comparison to well-defined powder materials is given. In first experiments using a liquid electrolyte ($LiClO_4$ as salt solved in ethylene carbonate/dimethyl carbonate mixtures) the efficiency of the sputtered V_2O_5 films for Li storage is demonstrated.

DS 1.3 Mon 10:45 GER 37

Photoactive TiO_2 Thin Films: Domination of Phase Formation or Microstructure — •Darina Manova, Jürgen Gerlach, Thomas Höche, and Stephan Mändl — Leibniz-Institut für Oberflächenmodifizierung, 04318 Leipzig

For several years, TiO_2 is receiving increasing scientific attention as one of the most promising photo catalysts with a huge potential for solving several different types of environmental problems. While TiO_2 powders and nanoparticles are well known and widely used, thin film surfaces are less investigated but still highly desired for applications. For TiO_2 polymorphs, anatase powder is reported to be a more potent photo catalyst than rutile. Metal plasma immersion ion implantation and deposition is employed to form titanium oxide films on different substrates at varying ion energies and substrate heating. At low temperatures, amorphous or nanocrystalline films were observed with TEM, while a columnar structure is present at 200 - 300 °C. XRD and Raman measurements indicate a transition from an anatase/rutile mixture at low temperatures and low ion energies towards pure rutile at high temperatures and high ion energies. It is shown that the photoactivity correlates closely with the phase formation and not with the microstructure of the thin films.

DS 1.4 Mon 11:00 GER 37

Formation of Ge NC's out of (GeO_x-SiO_2) superlattice structures — •Nicole M. Jeutter, Manuel Zschintzsch, Johannes von Borany, and Carsten Baehtz — Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, 01328 Dresden, Germany

Semiconductor Nanocrystals (NC), consisting only of a few hundred of atoms, are of great interest for new generations of light emitters, non-volatile memories or high efficiency solar cells [1]. However, it remains a remarkable challenge to achieve a high density ($>10^{12}cm^2$) of equal-sized, small (<5 nm) NC's of Ge or Si embedded in dielectric films. In this study we present the fabrication of Ge-NC's by decomposition of GeO_x (1<x <2) out of a (GeO_x -SiO_2) superlattice structure (SL). The SL was grown by dual reactive DC magnetron sputtering from elemental targets. Different Ge/O ratios in the SL structures were realized by the variation of oxygen flow and deposition temperature. Using *in-situ* x-ray reflectivity and grazing incidence diffraction at the CRG Beamline ROBL at ESRF we studied the deposition of the SL and the Ge NC's evolution during subsequent annealing. Depending on the GeO_x stoichiometry closed nanocrystalline films or separated Ge NC's with grain or particle sizes between 2-5 nm have been obtained with grazing incidence x-ray diffraction. The size of the NC's can be tuned with thickness of the GeO_x sublayer, its density exceeds $10^{12}cm^2$.

[1] A.Rogach (ED.), Semiconductor nanocrystal quantum dots, Springer, Wien 2008, ISBN 978-3211752357

DS 1.5 Mon 11:15 GER 37

Characterization of Sr-Ta-O/TiN/Si stacks by means of XPS, AES and TOF-SIMS — •Canan Baristiran Kaynak, Mindaugas Lukosius, and Christian Wenger — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Strontium tantalate (STA) films has been deposited on TiN/Si(100) substrates by Atomic Vapor Deposition (AVD) technique using a single source $Sr[Ta(OEt)_5(methoxyethoxide)]_2$ as precursor for metal-insulator-metal (MIM) applications. The deposition of STA films was investigated in dependence on different deposition conditions. X-Ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES) and Time of Flight Secondary Ion Mass Spectrometry (TOF-SIMS) were used for chemical and interface characterization of STA thin layers. The AES and TOF-SIMS depth profiles revealed a uniform and homogeneous STA films. Furthermore, electrical properties have been investigated in MIM capacitors after deposition of Au as top electrode. The correlation between chemical compositions of STA based MIM capacitors and their electrical properties are presented.

DS 1.6 Mon 11:30 GER 37

Characterization of the diffusion process in Al_2O_3 thin films based on ToF-SIMS measurements — •Pawel Piotr Michalowski[1], Malte Czernohorsky[1], Volkhard Beyer[1], Gert Jaschke[2], and Steffen Teichert[2] — [1]Fraunhofer-Center for Nanoelectronic Technologies, Königsbrücker Strasse 180, D-01099 Dresden, Germany — [2]Qimonda Dresden GmbH & Co. OHG, Königsbrücker Strasse 180, D-01099 Dresden, Germany

In next generation charge trapping non-volatile memory devices the blocking oxide material (currently SiO_2) has to be replaced by a high-k dielectric thin film. The appropriate selection of a suitable material from a large variety of potential candidates requires precise analytical characterization techniques. This work focuses on Secondary Ion Mass Spectroscopy (SIMS) of Al_2O_3 thin films which were fabricated by atomic layer deposition on Si(001) wafers. These samples were treated by rapid thermal annealing in wide range of temperatures ($750 - 1100°C$) and gas ambiences (N_2, O_2, H_2). SIMS depth profiles indicate that Si diffuses from the substrate through the alumina during annealing which leads to a segregation of Si on the Al_2O_3 layer surface. Grain boundary diffusion was identified to have the most significant impact in the diffusion process. Furthermore the activation energy of the diffusion was found to be 0.6 eV/atom and 2.3 eV/atom for amorphous and crystalline samples, respectively. The influence of different Al_2O_3 sublayers (e.g. SiO_2, Si_3N_4) and annealing conditions on the diffusion process will be discussed.

DS 1.7 Mon 11:45 GER 37

Structural and magnetic properties of CoFeB/MgO multilayers — •Kirill Zhernenkov[1], Miriana Vadala[1], Boris Toperverg[1], Hartmut Zabel[1], Hitoshi Kubota[2], and Shinji Yuasa[2] — [1]Department of Physics and Astronomy, Ruhr-Universität

Bochum 44780 Bochum, Germany — [2]National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1, Umezono, Tsukuba, Ibaraki 305-8568, Japan

CoFeB/MgO/CoFeB tunnel junctions display one of the highest TMR values at room temperature[1], only surpassed by Fe/MgO/Fe(001) MTJs. In the latter case, it is argued that the giant TMR effect is due to the textured epitaxial growth properties which leads to a coherent tunneling process instead of a diffuse tunneling. However, CoFeB films are amorphous and the MgO layer is microcrystalline. Nevertheless, very high TMR values of more than 350% have been achieved. We have investigated multilayers of CoFeB/MgO fabricated by different preparation procedures and annealed at temperatures between 240 - 360°C. High resolution x-ray scattering, polarized neutron reflectivity (PNR) and MOKE measurements have been done. It was found that the multilayers have different interfacial sharpness and structural quality depending on the way of preparation. At certain conditions the interfaces remain sharp up to the highest annealing temperature, whereas recrystallization or texturization is not observed. PNR experiments indicate a dependence of the CoFeB layer magnetization upon annealing temperature and method of MTJ sample fabrication. 1. S. Yuasa and D. D. Djayaprawira, J. Phys. D: Appl. Phys. 40 (2007) R337