MM 29: Topical Session TEM VIII

Time: Wednesday 15:45–17:00 Location: IFW B

MM 29.1 Wed 15:45 IFW B

Quantitative TEM-EDX analysis of compositional inhomogeneities in CIGS absorbers — •Isabel Knoke[1], Benito Vieweg[1], Stefan Jost[2], Jörg Palm[2], and Erdmann Spiecker[1] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Universität Erlangen-Nuürnberg, Cauerstraße 6, 91058 Erlangen — [2]AVANCIS GmbH & Co. KG, Otto-Hahn Ring 6, 81739 München

Thin film solar cells based on the chalcopyrite absorber material $Cu(In,Ga)(S,Se)_2$ are promising candidates for reducing the costs of photovoltaic [1]. However, depending on the fabrication process the absorber may show strong compositional inhomogeneities resulting in local variations of the band gap. Since these inhomogeneities occur on various length scales and both, in horizontal and vertical layer direction, characterization by TEM techniques is difficult because of missing depth information and limited thin area in conventional plan-view and cross-section samples, respectively. A new sample preparation technique overcomes these limitations by a double-wedge geometry that separates depth information in a continuous series of thin slices that are spread over a lateral distance [2]. Application of this preparation technique allows us to perform a significant number of EDX measurements at the same layer height and determine variations in the In/Ga resp. S/Se ratios. Corresponding changes in the lattice constant and band gap are calculated.

[1] J. Palm, V. Probst, F.H. Karg, Solar Energy 77, 757 (2004) [2] E. Spiecker et al., Acta Mater. 55, 3521 (2007)

MM 29.2 Wed 16:00 IFW B

Determination of Nitrogen Concentration in Dilute GaNAs by STEM HAADF Z-Contrast Imaging — •Tim Grieb[1], Knut Müller[1], Oleg Rubel[2], Rafael Fritz[2], Marco Schowalter[1], Kerstin Volz[2], and Andreas Rosenauer[1] — [1]Universität Bremen, D-28359 Bremen — [2]Universität Marburg, D-35032 Marburg

Incorporation of small amounts of nitrogen into III-V semiconductors such as GaAs reduces their band gaps which makes these alloys interesting for diverse applications. As only low N-concentrations are needed, composition analyses require highly sensitive methods. In this contribution we show that high-angle annular dark field (HAADF) scanning transmission electron microscopy (STEM) allows accurate determination of composition in diluted GaNAs, based on comparison of experimental with simulated reference images. HAADF intensity is affected by atomic number (Z-contrast), thermal-diffuse scattering (TDS), and Huang scattering at static atomic displacements (SADs). For GaNAs, conventional simulations based on frozen lattice multislice algorithms that include TDS let expect a lower HAADF-STEM contrast compared to pure GaAs, but experimental results show a contrary ratio. The observed contrast can be obtained by taking SADs into account that are caused by the comparatively small covalent radius of N atoms. The SADs are computed by relaxation of super cells via valence force field calculations and implemented into the STEMsim simulation software. Considering SADs we present quantitative evaluation of concentration in $GaN_{x<0.05}As_{1-x}$ quantum wells that agree with strain state analysis and X-ray diffraction measurements.

MM 29.3 Wed 16:15 IFW B

Quantitative local profile analysis of nanomaterials based on TEM diffraction — •Christoph Gammer, Clemens Mangler, Hans-Peter Karnthaler, and Christian Rentenberger — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

A method yielding a quantitative profile analysis from selected area electron diffraction patterns (PASAD, www.univie.ac.at/pasad) has been worked out. The results gained by PASAD can be combined with the local information from TEM images to study various nanomaterials. It can be used for the analysis of inhomogeneous materials, ultrathin nanocrystalline films, nanoparticles and nanosized ordered domains. As an example the grain size reduction by thermal annealing in nanocrystalline FeAl is shown in the present study. Nanocrystalline FeAl was made by severe plastic deformation resulting in the loss of the long-range order. Thermal annealing leads to the recurrence of the B2 superstructure, the recovery of dislocations, the sharpening of grain boundaries and an unexpected reduction in grain size. To study these processes, both the coherently scattering domain (CSD) size and the grain size were monitored during annealing by TEM methods. The CSD size was determined using PASAD and the grain size was determined from analysing dark field images: the CSD size increases by a factor of 2 while the grain size is reduced by a factor of 2. It is concluded that the decrease of the grain size during annealing is caused by the re-arrangement of dislocations forming new boundaries, that is linked to the recurrence of the long-range order.

MM 29.4 Wed 16:30 IFW B

Diffraction spots off the diffraction rings in severely deformed bulk nanocrystalline FeAl — •Anna Findeisen, Christoph Gammer, Christian Rentenberger, and Hans-Peter Karnthaler — University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Wien, Austria

The bulk intermetallic compound FeAl (processed with high purity Fe and Al) is made nanocrystalline by severe plastic deformation (SPD) applying the method of repeated cold rolling and folding. For the transmission electron microscopy (TEM) study thin foils were prepared by ion milling. TEM shows in the nanocrystalline structure grain sizes <100 nm. As expected the electron diffraction patterns show diffraction rings due to the different orientation of the nanograins. In addition to the diffraction spots lying on the rings, several spots are encountered that lie clearly off the rings. The TEM study reveals that these additional spots are not arising by an epitaxial oxide or other components. The analysis leads to the clear result that these spots are caused by moiré effects since their diffraction vectors can be constructed by adding the vectors of appropriate spots on the rings. Moiré effects are expected to occur in TEM of bulk nanocrystalline materials when the grain size is small and especially when the density of subgrainboundaries is high. The latter is confirmed by the fact that the occurrence of additional spots is more pronounced in the present case than in materials made nanocrystalline by other SPD methods. It also agrees with the results of differential scanning calorimetry showing in the present study higher values of enthalpies connected with the different peaks.

MM 29.5 Wed 16:45 IFW B

TEM Studies on Etch Pit Formation during the Nucleation of 3C-SiC on Si(001) — •Julian Müller[1], Philip Hens[2], Peter Wellmann[2], and Erdmann Spiecker[1] — [1]CENEM, University Erlangen-Nuremberg — [2]I-MEET, University Erlangen-Nuremberg

Due to its interesting electronic properties, cubic silicon carbide (3C-SiC) is widely investigated by many research groups. However, appropriate methods for bulk crystal growth are still lacking making it necessary to fabricate 3C-SiC in an epitaxial growth process. In view of microelectronic applications Si(001) is the most interesting substrate for epitaxial growth of 3C-SiC but the enormous lattice misfit (ca. 20%) leads to a high density of microstructural defects like dislocations, stacking faults and micro twins.

Within this work different heating rates have been applied during the growth of an initial 3C-SiC nucleation layer on Si(001) to investigate the impact on the final layer quality. It turned out that fewer grains nucleate at faster heating rates resulting in an improved layer quality. By TEM a new type of etch pit was detected, which differs from the well-known faceted voids reported in the literature. TEM investigations unambiguously revealed that the etch pits are filled with a continuous film of highly defective SiC. Both, the voids and the etch pits penetrate into the silicon. The etch pit formation can be ascribed to the contamination of the epitaxial deposition system with residual carbon, for which reason the cleanliness of the reaction chamber is proposed to be a crucial parameter for the growth of epitaxial 3C-SiC.