Microsymposia

the size-property correlation in these MoS2 nanosheets. Our results imply that nanostructured films with a high density of edge spins can give rise to magnetism even though the bulk material is nonmagnetic. For the first time, we show that Arsenic(ii) sulfide nanocrystal could be fabricated by a wet process of cluster-mediated nucleation method from the bulk material. Arsenic sulfide nanocrystals can show sizedependent fluorescences ranging from 287nm to 450 nm as well as two-photon upconverion. In China, realgar was also reported to be used as a drug in traditional Chinese medicine for more than 1500 years although arsenic is well known to be a highly toxic material. Preliminary pharmakinetic studies showed that arsenic sulfide quantum dots may afford good potential in anti-cancer treatment.

Keywords: nanocrystals, arsenic sulfide, molybdenum sulfide

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In-situ transmission electron microscopy and theoretical studies on the coalescence of nanoparticles

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The production of low-cost nanoparticulate devices based on a bottom-up approach is subject of current research activities. One of the important questions on the way to sustainable devices concerns the question of their mechanical, thermal or electrical stability. Several routes of bottom-up integration of nanoparticulate systems are under investigation, including chemical linking, hybrid integration in a stable matrix and thermal processing. This presentation will focus on aspects of the thermal processing of nanoparticulate films and demonstrate a variety of different processes, which are directly related to the chemical bonding of the material. The thermally activated densification and sintering processes have been studied using time resolved in-situ hot-stage transmission electron microscopy of self-supporting films. The experiments were documented as live stream with a TV-rate CCD camera on a hard disc recorder. Varying mechanisms were found for the different materials: a) for ionic ITO particles, an adjustment of the crystal orientation prior to the coalescence is observed at temperatures well below of half the melting temperature; b) for covalent silicon, a melting and subsequent wetting process of the nanoparticles is observed; c) metallic silver particles form area defects during their coalescence, which migrate out of the particles afterwards. These observed mechanisms go clearly beyond the models of classical sintering theory. Our experiments clearly demonstrate that a more sophisticated treatment is necessary in order to understand the sintering processes in nanoparticles, which needs to takes into account the chemical bonding and crystallographic orientation. DFT and KMC and MD Simulations support and substantiate the presented experimental results.

Keywords: nanoparticles, sintering / coalescence, *in-situ* transmission electron microscopy

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Structural and magnetic properties of MBE grown MnSb layers

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We present results, which open the way towards generating novel materials utilizing the electron spin. We propose to create such materials, by producing the appropriate inclusions in a semiconductor matrix. Bulk MnSb has a TC of 587 K, being therefore a good candidate to form ferromagnetic nano-inclusions in the semiconductor. To establish the best growing condition for MnSb layers and for multiphase materials, we present results of a characterization of MnSb layers grown on GaAs (100) or GaAs (111) substrates by the MBE method. To determine the crystallographic orientation and the local atomic order of the layers, w -2q scans and x-ray absorption studies of the Mn K- edge were performed at DESY-Hasylab. The phase analysis of the near surface region was performed in glancing incidence geometry (2q scan). In the layer grown on (100) GaAs the existence of two hexagonal MnSb domains with 10.1 and 11.0 orientations and polycrystalline inclusions of zinc-blende GaSb and hexagonal MnSb was detected. The diffraction peaks, observed for a layer grown on (111) GaAs, were indexed as 00.1 MnSb and 111 GaSb. No diffraction peaks originating from polycrystalline inclusions were found. The EXAFS analyze has shown that MnSb layers grown on (100) and (111) substrates have slightly different stoichiometries and/or the number of defects. The magnetic properties were examined by x-ray magnetic circular dichroism at MAX-lab (beamline D-1011). The spin magnetic moment per Mn atom was found to be 1.5 muB for both layers but large differences between layers were observed in x-ray reflectivity data, probably produced by a different morphology of these layers. This work was partially supported by a national grant of the Polish Ministry of Science and High Education N202-052-32/1189.

Keywords: synchrotron diffraction, ferromagnetic semiconductor, X-ray absorption spectroscopy

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Leverage analysis: A statistical tool to enhance the control on the crystal structure refinement

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The least-squares crystallographic refinement can be a nontrivial task because of the occurring of some statistical outliers in the data set. This is due to a number of causes: intrinsic noise in the experimental data, not suitable weighting schemes, not valid refinement strategies, problems in the crystallographic model employed and so on. In order to adjust the refinement protocol, a suitable detection of the actually influent outliers is needed. The