MS39-O2

Complete structure analysis of single cores shell nanowires by X-ray methods

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It is known that core-shell-shell semiconductor nanowires (NW) grow pseudomorph along the growth direction, i.e. the axial lattice parameters of core and shell materials are the same. Therefore, both structural composition and interface strain of the NW are encoded along directions perpendicular to the growth axis. In this work, we determine the complete structure of single GaAs/(In,Ga)As/GaAs core-shell-shell NW heterostructres with core diameter of 50 nm and (In,Ga)As shell thickness of 20 nm with nominal indium concentration of 15% capped by 30 nm GaAs outer shell MBE grown on prepatterned silicon (111) substrates by means of x-ray nano-diffraction using synchrotron radiation. In order to access single NWs by x-ray nano beam being incident parallel to the surface of the substrate, a single row of holes with seperation of 10 µm was defined by electron beam lithography to act as nucleation centers for MBE NW growth. These well separated NWs were probed sequencially by X-ray nano diffraction recording 3D reciprocal space maps (RSM) of Bragg reflections with scattering vectors parallel (out-of-plane) and perpendicular (in-plane) to the NW growth axis. From the out-of-plane (111) Bragg reflection, we derived deviations from the hexagonal symmetry and diameters of the probed NWs grown under the same conditions. The radial NW composition and interface strain became accessible measuring the 2D scattering intensity distributions of the in-plane (2-20) and (22-4) reflections exhibiting well pronounced thickness oscillations perpendicular to the NW side planes (truncation rods - TR). Quantitative values of thickness, composition and strain acting at the (In,Ga)As and GaAs shells were obtained via finite element modelling (FEM) of the core-shell-shell NW and subsequent Fourier transformation simulating the TRs measured along the three different directions of the hexagonally shaped NWs simultaneously. Considering the experimental constraints of the current experiment, thicknesses and In content have been evaluated with uncertainty of ± 2 nm and ± 0.01%, respectively. Comparing data taken from different single NWs, the shells thicknesses differ between one and the other.

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MS39-O3

Novel usage of neutron scattering: holography for observations of local atomic structures of light elements

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As a new view point of structural physics, understanding of three-dimensional (3D) local atomic structures, such as slight changes of atomic structures around dopants in functional materials, or local lattice distortions in mixed crystals, must generate breakthroughs in novel materials science Atomic resolution holography (ARH) is a quite unique and indispensable probe for local atomic structure investigations, because it has following important advantages: (a) 3D local structures without translation symmetry can be directly observed without models (b) Observable range is ~20 Å, which is much longer than lattice constants of most inorganic materials. (c) The central atom can be selected In particular, neutron ARH is the best probe to visualise local structures of materials which include light elements, such as H, B, or O.

Neutron holography was firstly proposed by Cser *et al.*[1], and was demonstrated using a single crystal of $Al_4Ta_3O_{13}(OH)$ by Sur *et al.* in a reactor facility in 2001[2]. The authors also succeeded in neutron holography in a reactor facility in Japan in 2008. However, in reactor facilities, holograms with only one wavelength could be obtained; accuracy of obtained atomic images by such single-wavelength ARH measurements is insufficient because of many ghost images or artifacts. To avoid these, multi-wavelength ARH, which uses many holograms with different wavelengths, is quite effective for reconstructions of accurate atomic images. Thus, the authors have developed white neutron ARH in the pulsed neutron facility, Japan Proton Accelerator Research Complex (J-PARC) at Tokai, Japan because one can obtain over 100 holograms with different wavelengths by time-of-flight method, and succeeded in visualising local atomic structures around Eu in 1 % Eu doped CaF_2, which is a typical scintillation crystal, and have found that local distortion of Ca and excess F around Eu[3].

By the development of the white neutron ARH, the authors have also succeeded in visualising clear images of local atomic structures around dopants in many materials, such as B doped Si, Sm doped RB_6 (R=Yb, La) already. These recent results indicate that white neutron ARH will be an indispensable probe for structural circumstances of various materials with light elements, for instance, hydrides or B doped functional materials. In our presentation, recent results of white neutron ARH will be reported as well as its brief principle and advantages.

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MS39-O4

Analysis of short range phenomena in novel materials using the PDF-method

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In the present contribution, we will show results and further progress in analysis of pair distribution function (PDF) studies on amorphous materials containing crystalline domains. The materials are of stoichiometry $(SiO_2)_x(TiO_2)_y$. - The synthesizers' ([1]) aim was to prepare a material that is similar to the zeolithe TS-1 (titanium silicalite), which exhibits catalytic properties (eg phenol hydroxylation) but is amorphous and thus mechanical more stable. - The focus of this work is not on catalytical activity but on structural features.

A big research question concerns the coordination number of the Ti-atoms with respect to oxygen. Extensive studies (Rietveld analyses and neutron scattering using isotope substitution) have been done on TS-1 (see [2]). Literature states that 4-fold coordination is necessary for the material to exhibit catalytic properties and that incorporation of Ti-atoms into the bulk-SiO_2, thereby substituting Si, happens only at low Ti-contents ([3]). The origin of catalytic properties of TS-1 is still an open topic and no consesus has been reached in literature.

The experimental PDF could be modelled with a contribution by amorphous SiO_2 and small spherically shaped crystalline TiO_2-particles in the Rutile modification, i.e. Ti in six-fold coordination. A model based on a pure glass phase with Si partially substituted by Ti in four fold coodinatikon did not result in as good an agreement. The features in the difference PDF indicate interaction between the particles and the surrounding matrix. TEM and SAXS measurements indicate a structure of elongated pores, but due to electrostatic charging in the TEM no magnification sufficient for the detection of the small TiO_2 particles could be achieved.

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