MS23-P9 Structural study of ceria-doped TiO_2 prepared at different conditions

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In our contribution we will present structural studies of titania oxide doped by ceria by means of X-ray diffraction at room and at elevated temperatures. Doping of Ce atoms in TiO_2 structure affects the photocatalytic properties. Sample have been prepared by hydrothermal synthesis at different temperatures and pressures. Using software package MStruct the real structure of investigated samples has been examined as well.

Keywords: X-Ray diffraction, nanostructured TiO2-Ce

MS23-P10 XRD characterization of structural evolution and morphology properties of silica-doped alumina aerogels

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Nanocrystalline aluminas are widely used as catalyst supports. A major advantage of aerogels compared to conventional alumina supports is their high specific surface area, high mesoporosity. Silica-doped alumina aerogels have a potential for high-temperature catalytic applications due to resistance to thermal coarsening and phase transformations. Structure and particle morphology are known to affect material properties. Thus, several studies revealed impact of morphology parameters on a thermal behavior of the alumina aerogels.

The objective of this work was study of phase transformations, morphology parameters of the silica-doped alumina aerogels by X–Ray Diffraction (XRD) analysis. To obtain information on the structure, dispersion, and morphology modeling XRD patterns was performed using the Debye Scattering Equation. The method allows calculating the XRD pattern from systems of nanoparticles with any structure, shape, and size. The aerogels with various molar Al:Si ratios were synthesized by the sol-gel method followed by supercritical drying. The pseudoboehmite phase was identified in the aluminium-rich aerogels calcined at 300°C. The XRD patterns featured anisotropic broadening of peaks. Modeling XRD patterns evidenced a plate shape of crystallites. The crystallites in the alumina aerogel were rectangular plates with average dimensions of 20x6.5x25 nm. The anisotropy was more pronounced in silica-doped alumina aerogel with Al:Si ratio of 9:1 (fig.1). Material consisted of pseudoboehmite plate-like crystallites with a thickness of one lattice constant in the [010] direction (14.0x1.2x14.5 nm in size). The pseudoboehmite structure is composed of octahedral oxygen layers packed in [010] direction. Formation of two-dimensional packets proceeded organization three-dimensional crystal structure. The results were supported by transmission electron microscopy.

It was shown that the silica dopant retarded the pseudoboehmite crystallization and its further transformation to γ-alumina phase upon calcination. The aerogels with high silica loading were X-ray amorphous within a wide temperature range. The morphology parameters were expected to be preserved at topotactic transition of the pseudoboehmite to alumina phase.

The work was performed in the framework of the Research and Educational Center for Energy Efficient Catalysis (Novosibirsk State University, Boreskov Institute of Catalysis). The structural studies were supported by the RSCF project №14-23-00037.

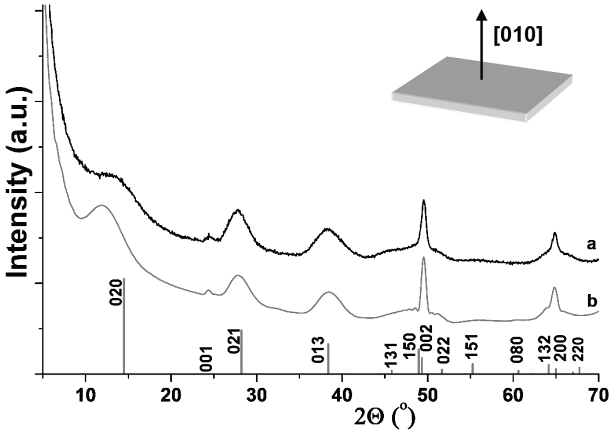

Figure 1. (a) - experimental XRD pattern of the aerogel sample (Al:Si=9:1); (b) – calculated diffraction pattern for AlO(OH) crystallites with dimensions of 14.0x1.2x14.5 nm (49x1x39 unit cells)

Keywords: nanostructure, alumina, pseudoboehmite, XRD, DSE

MS23-P11 Strain-relaxation in GaAs / InGaAs core-shell nanowire heterostructures grown by MBE onto Si(111)

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Semiconductor core-shell nanowires (NW) with different shell thickness can be grown onto [111] oriented silicon substrates without major structural defects due to the strain release towards the NW side planes [1]. This approach offers the possibility to form radial hetero-structures (HS) between highly lattice-mismatched materials but the process of strain relaxation is not fully understood.

We report on detailed investigations of anisotropic strain and strain relaxation mechanism in GaAs/$In_{0.25}Ga_{0.75}As$/GaAs NWHS grown by MBE onto Silicon (111) substrate. Independent from core-shell thickness ratio, x-ray diffraction measurements with scattering vector along the 111 growth direction shows no Bragg peak splitting but a single out-of plane lattice parameter explained by the strain balance between slightly expanded GaAs and compressed InGaAs shell. On the other hand, X-ray measurements along the NW side planes and edges show peak splitting between core and shell material confirming the appearance of in-plane lattice mismatch. The mismatch is different measuring along the (1-10) or the (2-1-1) directions that can be explained by a nominal In content of 22.5% and 18.5%, respectively. The difference can be related to strain induced segregation along the NW edges as it has been observed in AlGaAs/GaAs core-shell NWs [2]. Our data are interpreted in terms of finite element calculations revealing an insight into the complexity of strain relaxation mechanism in MBE grown core-shell nanowires.

Related publications

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Keywords: Strain relaxation, core-shell nanowires, finite element method, hetero-structures, x-ray diffraction.