

MS23-P9 Structural study of ceria-doped TiO₂ prepared at different conditions

Tereza Brunatova¹, Lenka Matejova², Zdenek Matej¹, Stanislav Danis¹

1. Charles University, Faculty of Mathematics and Physics, Dept. of Condensed Matter Physics, Prague, Czech Republic
2. CNT – Nanotechnology Center, Technical University of Ostrava, 17. listopadu 15/2172, 708 33 Ostrava - Poruba, Czech Republic

email: brunatovat@centrum.cz

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 TiO₂ structure affects the photocatalytic properties. Samples 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

Vera P. Pakharukova^{1,2}, Dmiry A. Yatsenko^{1,2}, Anton S. Shalygin^{1,2}, Evgeny Y. Gerasimov^{1,2}, Sergey V. Tsybulya^{1,2}, Oleg N. Martyanov^{1,2}

1. Boreskov Institute of Catalysis, SB RAS, Pr. Lavrentieva 5, 630090 Novosibirsk, Russia
2. Novosibirsk State University, Pirogova Street 2, 630090 Novosibirsk, Russia

email: verapakharukova@yandex.ru

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.

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