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Structure modification of Pr - doped ZrO_2-Y_2O_3 after heat treatment at 1200°C

E. Werner-Malento [1*], W. Paszkowicz [1], J. Fidelus [2], M. Godlewski [1] and S. Yatsunenko [1]

[1] *Institute of Physics, Polish Academy of Sciences, al .Lotników 32/46, 02-668 Warsaw*

[2] *Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokołowska 29/37, 01-142 Warsaw*

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**) e-mail: ewerner@ifpan.edu.pl*

Yttria-stabilized zirconia (YSZ) is one of the most studied metal oxides [1, 2]. It is a relatively hard and chemically inert material. YSZ is characterized by wear resistance, high-temperature stability and corrosion resistance, superionic conductivity at high temperature. The material is mostly used in jet engines to determine oxygen content in exhaust gases, to measure pH in high-temperature water, as membranes for high temperature solid oxide fuel cell, as a component of waveguides, laser mirrors and optical filters, as well as for electrolytes or insulators in microelectronic devices.

Several zirconia polymorphs are known (monoclinic, tetragonal, cubic and rhombohedral ones). Among them, those of the highest symmetry are of most interest due to their attractive properties. To achieve this goal, thermal treatment and/or doping with yttrium or other dopants are typically used.

Nanocrystalline zirconium dioxide powder samples were characterized by X-ray diffraction using a Philips X'pert MRD diffractometer. The changes in ZrO_2 structure due to annealing, praseodymium trioxide doping (~ 0.4 mol %) and yttria doping (0 mol % Y_2O_3, 3.56 mol % Y_2O_3, and 4.79 mol % Y_2O_3) are studied. Rietveld analysis is performed using the FullProf program, based on the structure of the component phases [3]. The calculations permitted for for quantitative phase analysis and structure refinement.

The phase composition and structure of $(Zr,Y)O_2$ nanocrystals prepared by treatment at 70°C and 1200°C are studied and compared with pure ZrO_2 samples. Changes in the structure and phase composition due to addition of yttria, Pr doping and annealing are observed. The unannealed undoped sample contains the tetragonal (78%) and monoclinic (22%) phases. The addition of yttria results in disappearing of the minority monoclinic component, in agreement with literature data. The axial ratio of the tetragonal phase shows a clear decreasing tendency. Some of the observed trends are similar to those observed in Ref. 4. The effect of the Pr doping on the phase content and lattice parameters is marginal.

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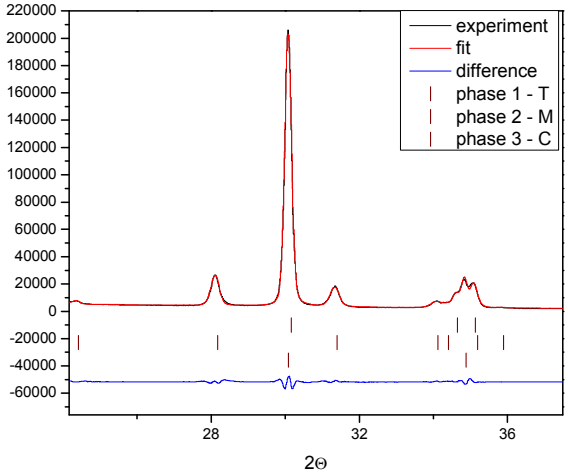

Figure 1. Experimental X-ray diffraction patterns of Pr-doped YSZ (4.79 mol % of yttria). The vertical bars show the peak positions for the tetragonal phase (upper), monoclinic phase (center) and cubic phase (lower).

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