

Nanocomposites and nanomaterials

Effect of raw materials on structural properties of ZrO₂-based composites doped with Cu and Y

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Zirconia-based nanopowders attract considerable attention due their promising catalytic properties. Recently, we have revealed that raw materials used for the powders' production can play important role in the structural and optical properties of final powders. In present work, the effect of nature of Zr-based precursors on the structural properties of Cu-doped Y-stabilized ZrO₂ (Cu-YSZ) nanopowders is discussed.

The powders were prepared by co-precipitation technique. As Zr source, the Zr nitrate (N-set) or oxychloride (Cl-set), while for Cu and Y sources, their nitrates were used. The powders were doped with 1 mol % (Cu1-Cl(N)) or 8 mol % Cu (Cu8-Cl(N)) upon synthesis process and after washing and drying were calcined at T_c=500-1000C during 2 h in the air. Their structural properties were studied by X-ray diffraction (XRD).

It was observed that whatever the Zr precursor and Cu content, the powders calcinated at T_c=500-700C show the formation of ZrO₂ tetragonal phase predominantly. The T_c increase stimulates phase transformation. For Cu1-Cl samples the noticeable increase of monoclinic phase is observed, but for Cu8-Cl only slight monoclinic phase concentration changes were observed. Besides, for the Cu1-N and Cu8-N powders this transformation is more prominent.

The coherent domain sizes, *d*, were found to increase gradually for both phases. For tetragonal phase this increase is mostly independent on CuO content, while for monoclinic phase *d*-values for Cu8-Cl are slightly lower, than for Cu1-Cl. The XRD peaks for Cu1-Cl samples shifted to lower angles distinctly, while for Cu8-Cl samples they have very slight shift. The peak shift, observed on Cu1-Cl samples is alike to the behavior of Cu1-N samples. At the same time, the behavior of XRD peak positions of Cu8-Cl samples differs from that of Cu8-N ones. The peak shift to the low angles and increase of monoclinic phase content in Cu1-Cl is obviously caused by Cu out-diffusion from nanocrystals. At the same time in Cu8-Cl this process is hampered in contrast to Cu8-N samples. This effect is considered to be caused by the formation of Cu-Cl bonds in ZrO₂ nanocrystals.