## Nanocomposites and nanomaterials

# Impurity-governed structural modification of $ZrO_2$–based composites doped with Cu and Y

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In recent years Cu-doped Y-stabilized $ZrO_2$ (YSZ) composites are intensively investigated due to their excellent properties (such as environmental degradation, catalytic activity, tribologocal behavior). These latter were found to be depended on spatial Cu localization in the YSZ grains.

In present work, structural properties of Cu-doped YSZ nanopowders were studied by X-ray diffraction (XRD) and high-resolution transmission microscopy methods.

The powders were synthesized by a co-precipitation technique and doped with 1 mol % or 8 mol % Cu upon synthesis process. These nanopowders were calcinated at $T_c$=500-1100C during 2 h.

Whatever the Cu content, the powders calcinated at $T_c$=500-600C show the formation of $ZrO_2$ tetragonal phase predominantly. Besides, for these samples the XRD peak positions are shitted to higher angles in comparison with those of Cu-free YSZ powders, this shift is being more pronounced for higher Cu content in the samples and testifies to the Cu incorporation in YSZ grains.

The $T_c$ increase stimulates two main processes. One of them is the non-monotonic shift of XRD peak positions with $T_c$ that gives the information on the change of Cu localization in the composite, i.e. either its incorporation in YSZ grains (the shift of XRD peaks towards higher angles) or Cu outward diffusion (in the case of opposite XRD shift).

Another process is the YSZ phase transformation, i.e. from tetragonal to cubic and both of them to monoclinic. This latter appears at $T_c$=700-800C, being dependable on Cu content, and its contribution increases with $T_c$. This can be explained by the Cu replacement from lattice sites to interstitials that stimulates its outward diffusion via interstitials and promotes Y outward diffusion through the Cu vacancies. These results are confirmed by TEM experiments.

The ways to control Cu localization in YSZ nanopowders are proposed.