Effect of combined doping $(Y_2O_3+Fe_2O_3)$ on structural peculiarities of nanodispersed ZrO_2

A.G. Belous¹, E.V. Pashkova¹, O.I. V'yunov¹, V.P. Ivanitskii² and A.N. Makarenko¹

¹ V.I.Vernadskii Institute of General and Inorganic Chemistry, NAS of Ukraine

² Institute of Geochemistry, Mineralogy and Ore Formation, NAS of Ukraine

The most effective stabilizer for zirconium oxide is yttrium oxide. However, the structure of $Y-ZrO_2$ degraded at low temperature. Partial substitution of Fe^{3+} for Y^{3+} in system Y_2O_3 - ZrO_2 decreases both the crystallization and sintering temperature of zirconia ceramic. It is known that the content of monoclinic (M), tetragonal (T) and cubic (C) polymorphs determines the properties of ZrO_2 .

The aim of present work is the investigation of structural peculiarities (polymorphs, positions of atoms, site occupancies, local environment of Fe^{3+}) of zirconium oxide stabilized by combined dopant (Y₂O₃ and Fe₂O₃) depending on chemical composition ((1-x)ZrO₂.xY₂O₃.yFe₂O₃, where x+y=0.03-0.08), synthesis conditions (coprecipitation of hydroxides or successive precipitation of hydroxides) and heat treatment (970-1570 K).

It has been shown that solubility of iron in Y-ZrO₂ increases with yttrium content. Iron dissolves completely in Y-ZrO₂ at Y/Fe≥2. Increasing Y/Fe ratio in ZrO₂ doped with the same total amount of doping oxides stabilizes the structure and inhibits low-temperature degradation. Increasing the total amount of doping oxides extends the temperature range of existence of C and C+T polymorphs of ZrO₂. Mössbauer spectra of fully stabilized tetragonal Y-Fe-ZrO₂ showed that distribution of Fe³⁺ ions has a cluster topology. Two nonequivalent sites of Fe³⁺ with octahedral coordination in coprecipitated samples and three nonequivalent sites of Fe³⁺ with octa-, penta- and tetrahedral coordination in successively precipitated samples have been identified. Decrease in coordination number of iron ions in comparison with that of host cations in Y-ZrO₂ stabilizes the structure and inhibits its degradation due to increase in Me-O binding energy. It has been shown that precipitated ZrO₂ powders contain nanoparticles with grain size of 10-20 nm. Successively precipitated powders, in contrast to coprecipitated ones, consist of soft easy-breaking aggregates and do not require additional grinding.