Kyiv, Ukraine
June 06-10, 2004

NATO Advanced Research Workshop

Fuel Cell Technologies: State and Perspectives

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Effect of Iron Oxide on Structural Features of Y-Stabilized Zirconia Ceramics

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Fully stabilized zirconium dioxide is widely used as oxygen conductor for solid state fuel cell. One of the basic requirements to this material is the thermal stability of the structure. The most effective stabilizer for zirconium oxide is yttrium oxide. However, the structure of Y-ZrO_2 degrades 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 (Y_2O_3 and Fe_2O_3) depending on chemical composition ($(1-x)ZrO_2 \cdot xY_2O_3 \cdot yFe_2O_3$, 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-ZrO_2 increases with yttrium content. Iron dissolves completely in Y-ZrO_2 at $Y/Fe \geq 2$. Increasing Y/Fe ratio in ZrO_2 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 ZrO_2. Mössbauer spectra of fully stabilized tetragonal Y-Fe-ZrO_2 showed that distribution of Fe^{3+} ions has a cluster topology. Two nonequivalent sites of Fe^{3+} with octahedral coordination in coprecipitated samples and three nonequivalent sites of Fe^{3+} 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-ZrO_2 stabilizes the structure and inhibits its degradation due to increase in Me-O binding energy. It has been shown that precipitated ZrO_2 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.

Keywords: stabilized zirconium dioxide, solid state fuel cell, thermal stability, combined dopant, Mössbauer spectra, soft easy-breaking aggregates