GRAIN SIZE DEPENDENT GRAIN BOUNDARY DEFECT STRUCTURE: CASE OF DOPED ZIRCONIA

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High purity 3 mol% Y_2O_3 doped ZrO_2 samples with average grain sizes of 120 nm to 1330 nm were prepared by sintering at different temperatures for various hours. The electrical properties were measured by impedance spectroscopy, and the microstructure studied by scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM). The grain boundaries of the high purity 3 mol% Y_2O_3 doped ZrO_2 samples were free of any second phase (Fig. 1); even so, the grain boundary conductivity was still ~2 orders of magnitude lower than the bulk conductivity, but increased with decreasing grain size. The low grain boundary conductivity, according to the Schottky barrier model,[1] is due to the depletion of oxygen vacancies in the grain boundary space charge layers. Within this framework the grain boundary space charge potential and the concentration of oxygen vacancies in the space charge layers were calculated. The electrical conductivities[2] of a 2.9 mol% Y_2O_3 doped ZrO_2 sample with an average grain size of 41 nm were similarly analyzed. It was found that the space charge potential decreased, but the oxygen vacancancy concentration increased with decreasing grain size (Fig. 2).

The literature results[3,4] for 8.2 mol% Y_2O_3 and 15 mol% CaO doped ZrO_2, respectively, were analyzed within the same framework, it was also disclosed that the space charge potential decreased and the oxygen vacancy concentration increased with decreasing grain size (Fig. 2).

Keywords: Zirconium oxide; Grain boundaries; Electrical conductivity; Space charge; Oxygen vacancy

Reference:

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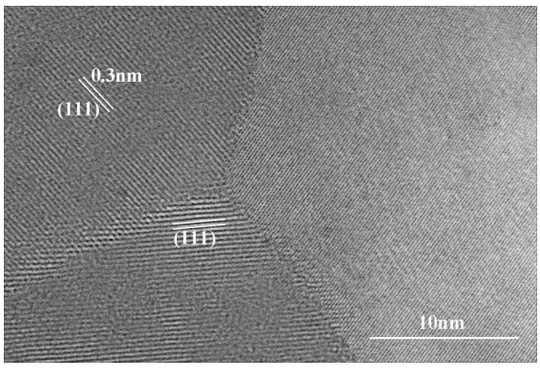

Fig. 1. HRTEM micrograph of 3 mol% Y_2O_3 doped ZrO_2 sample with an average grain size of 120 nm

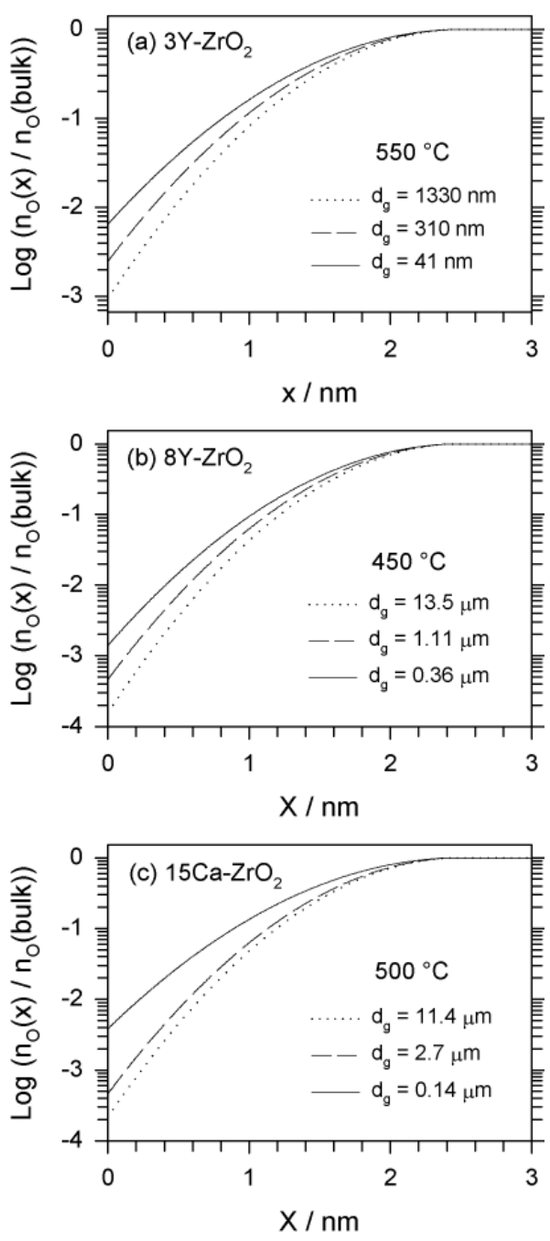

Fig. 2. Oxygen vacancy profiles in the space charge layers of (a) 3 mol% Y_2O_3 doped ZrO_2 at 550 °C, (b) 8.2 mol% Y_2O_3 doped ZrO_2 at 450 °C and (c) 15 mol% CaO doped ZrO_2 at 500 °C, respectively.