The boundary impact on oxygen diffusion in zirconia

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Zirconium dioxide is widely used in power engineering for electrolysis due to its high conductivity and high melting point [1]. We studied the impact of the polarization mechanism on the diffusion coefficient of oxygen ions in zirconium dioxide [2] and started to research the boundary effects. The Buckingham-Coulomb potential is used for ion interactions. A polarisation effect is imitated by the Core-Shell model [3]. We use the model of a bicrystal consisting of two cubic monocrystals rotated relative to each other at different angles. In a system without polarisation, an asymmetry of the transport properties of oxygen is observed. It is found that oxygen ions move along the boundary easier than perpendicular to it. The total diffusion coefficient in a bicrystal is higher than in a monocrystal. In a system with polarization, asymmetry of the diffusion coefficient is not observed. Still, there is a general increase of conductivity when an angle between single crystals is not equal to zero. Boundary effects make collected data closer to real experiments [4].

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