The polarization impact on oxygen diffusion in zirconia

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Zirconium dioxide is used in many technological areas. Particularly, it is a catalyst for chemical reactions, thermal barrier coating material and the electrolysis process component. For high-temperature electrolysis, its resistance to high temperatures and high diffusion coefficient are essential. We study the influence of ion polarization on the diffusion coefficient at high temperatures. Buckingham-Coulomb potential simulated particles interaction, the polarization mechanism is reproduced by the Core-shell model [1]. Each ion is divided into two particles: a core and a shell, interacting with each other according to the equation of a harmonic oscillator. The diffusion coefficient is calculated using the Einstein-Smoluchowski formula, the temperature dependence is fitted using the Arrhenius relation. It is found that the temperature dependence of the diffusion coefficient for a system with polarization extrapolates the experimental data well [2]. The system without polarization is significantly further from experimental data. Also, in the system without polarization, melting is not observed at temperatures exceeding the real melting point.

[1] Zacate M O, Minervini L, Bradfield D J, Grimes R W and Sickafus K E 2000 *Solid State Ionics* **128** 243 – 254
[2] Pawel R E 1981 *J. Electrochem. Soc.* **128** 1999