4th International Symposium on
Energy Challenges & Mechanics
- working on small scales

11-13 August 2015
Aberdeen, Scotland, UK

Anisotropy effects in solid oxide fuel cells

Udo Schwingenschlögl

King Abdullah University of Science and Technology, Physical Science and Engineering Division, Thuwal 23955-6900, Saudi Arabia

Accepted for publication on 4th April 2015

Anisotropy effects in solid oxide fuel cells are typically not considered because of the high operating temperatures. We demonstrate by means of numerical simulations that such an approximation is no longer valid when the operating temperature is reduced. We also discuss the consequences of this fact for the material properties and practical applicability. Choosing $LaMnO_3$ as a prototypical material, we have performed first-principles calculations to develop an understanding of the governing mechanisms on an atomic level. At reduced operating temperatures, local distortions become relevant in perovskite oxides, which is shown to have dramatic implications for the oxygen vacancy formation and diffusion. We also find that strain and Sr doping are capable of further increasing the anisotropy of the oxygen vacancy formation. The energy difference between the undistorted and distorted structures turns out to be reduced from 2.92 eV in $LaMnO_3$ to 1.84 eV in $La_{0.75}Sr_{0.25}MnO_3$. In addition, tensile strain promotes the oxygen vacancy formation as well as the diffusion of oxygen atoms in both pristine and Sr doped $LaMnO_3$. On Sr doping the oxygen vacancy formation energy decreases, which is advantageous for solid oxide fuel cells. Importantly, in both $LaMnO_3$ and $La_{0.75}Sr_{0.25}MnO_3$ the diffusion of oxygen atoms is strongly favorable in the [011] and [0-11] directions at reduced operating temperatures, due to weaker La-O bonding and additional space for migration. The structural and electronic similarities in the class of perovskite oxides suggest that the findings of our work are generally applicable to perovskite solid oxide fuel cell cathodes. Reference: Journal of Materials Chemistry A 2, 19733 (2014).

Keywords: O vacancy; formation; diffusion; anisotropy