

High-conductivity material demonstrates role of oxygen ions in enhancing their capabilities

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Yttria stabilized zirconia, also known as YSZ, is a material of great interest because of its relatively high oxygen-ion based conductivity. In particular, it finds applications in electrochemical devices, such as solid oxide fuel cells and oxygen sensors. In a study published in *European Physical Journal B*, Kia Ngai, from the University of Pisa in Italy, and colleagues from the Complutense University in Madrid, Spain, devised a model of the oxygen-ion dynamics that contribute to the conductivity of YSZ.

The problem is that fuel cells currently operate above 700 °C, which strongly limits their use. Understanding oxygen-ion diffusion is key to helping lower operating temperature down to room temperature. Previous attempts to do so were done with the so-called coupling model (CM), describing simple physical concepts related to ion-ion interaction. This helped uncover the importance of ion-ion correlation in limiting long-range ion mobility, and thus conductivity.

The trouble is that experiments show that ionic conductivity in YSZ requires an activation energy that is much higher than that supplied by [computer simulations](#) describing independent ion hopping. Relying on the CM model, the authors first established a quantitative description of the ion dynamics in YSZ. Then they compared the predictions of the CM with experimental results and with simulations, particularly those of nanometric-scale thin films, published in the last ten years.

Thus, in their model, they established the connection between the level

of the energy barrier for independent ion-hopping simulations and the level of activation energy measured experimentally for long-range movement of [oxygen ions](#). In addition, they attributed an increase of the conductivity in nanometers-thick YSZ films to a decrease in the ion-ion correlations. This model could also be used to study the conductivity relaxation of so-called molten, glassy and crystalline ionic conductors and ambient temperature [ionic liquids](#).

More information: Ngai K.L., Santamaria J. and Leon C. (2013), Dynamics of interacting oxygen ions in yttria stabilized zirconia: bulk material and nanometer thin films, *European Physical Journal B*, [DOI: 10.1140/epjb/e2012-30737-2](#)

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