Tuning of CeO2 buffer layers for coated superconductors through Metal doping

Danny E. P. Vanpoucke(1,3), Stefaan Cottenier(2), Veronique Van Speybroeck(2), Patrick Bultinck(3), Isabel Van Driessche(1)

(1)Department Inorganic and Physical Chemistry, Solid State Chemistry, Ghent University, Belgium

(2) Center for Molecular Modeling, Ghent University, Belgium

(3)Department Inorganic and Physical Chemistry, Ghent Quantum Chemistry group, Ghent University, Belgium

Abstract(1500max→WC=1556)

Cerium oxide-based materials have been of increasing interest over the last two decades. This is mainly due to their remarkable properties which are used in a number of industrial applications: Three-Way-Catalysts, oxygen sensors, solid oxide fuell cells, etc. More recently, cerium oxide has been used as thin film buffer layer in coated superconductors. However, the layer thickness of these buffer layers is limited by the formation of cracks during deposition. This behavior has been linked to internal stress due to lattice mismatch and different thermal expansion coefficients (TEC) of the substrate and the buffer layer. A simple way to reduce these mismatches is though metal doping.

Using ab-initio atomistic calculations we study the behavior of the lattice parameter (LP), bulk modulus (BM) and TEC of ceria due to metal doping. A Vegards Law behavior is found for the LP, and the Shannon radii of the dopants are retrieved from the lattice expansion. Metal doping is found to decrease the BM and increase the TEC. In addition, the introduction of charge compensating oxygen vacancies is shown to have a strong influence on the BM, while the heat of formation is only slightly modified. As a practical result, optimum dopant concentrations for LP-and BM-matching with a lanthanumzirconate substrate are found to be roughly 5% for Cu and Zn, in good agreement with the concentrations used in experiments. In contrast, simulaneous matching of the BM and TEC is shown to be impossible.