

Doping of CeO₂ as a tunable buffer layer for coated superconductors: A DFT study of mechanical and electronic properties

Ceramic superconductors (CSC) are, just like roof tiles and flower pots, brittle by nature. To fabricate flexible superconducting wires, they are grown as a layered architecture on a metal substrate. Buffer layers are used to prevent metal diffusion and improve lattice matching between the CSC and the substrate. CeO₂ is one example of such a buffer layer. To prevent the formation of micro cracks during the fabrication process, doping of CeO₂ has been suggested.

In this work, we study the influence of dopants (both tetravalent and aliovalent) on the mechanical and structural properties of CeO₂ by means of density functional theory (DFT). For tetravalent dopants, a clearly different behavior is found for the group IVa and IVb elements – with the latter acting as stable dopants (i.e. leading to uniform doping) and the former as unstable. This difference is linked to the dopant electronic structure. For all dopants, an inverse relation is observed between the bulk modulus and thermal expansion coefficient. The presence of charge compensating oxygen vacancies is found to modify the dopant influence significantly, often counteracting it. Oxygen vacancies lead to non-linear lattice parameter modifications and strongly reduce the material's bulk modulus.

Based on the study of these idealized systems, new dopants are suggested for applications.