

Investigation of tunable buffer layers for coated superconductors

Ceramic superconductors are, just like roof tiles and flower pots, brittle by nature. To fabricate flexible superconducting wires, they can be deposited as thin films on a metal wire or tape. However, the metal atoms in such substrates tend to diffuse into the superconducting thin film, destroying the superconductivity. One way to prevent this diffusion is through the deposition of one or more buffer layers in between the substrate and the superconducting layer. Recently, cerium oxide (CeO_2) has been used as such a buffer layer for architectures with the $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$ high temperature superconductor. However, the layer thickness of these CeO_2 buffer layers is limited by the formation of cracks during deposition, limiting their interest for industrial applications. The formation of these microcracks has been linked to internal stress, and metal doping has been suggested as a means of reducing this internal stress, by alleviating the lattice mismatch and mismatch of the thermal expansion coefficients between the different layers.

The introduction of dopants in CeO_2 generally gives rise to the formation of charge compensating vacancies, which also contribute to the changes in the CeO_2 properties. To have a clear understanding of the influence dopants have on the properties of CeO_2 , it is important to separate the contributions of these two structural changes; *i.e.* to distinguish between the consequences of doping and subsequently those of the introduced charge compensating vacancies. Theoretical calculations are ideally suited to separate these different contributions.

We have studied the influence of dopants on the mechanical and structural properties of cerium oxide. Since cerium is tetravalent in CeO_2 , we focus on tetravalent dopants in a first step. In a second step aliovalent dopants are studied without the presence of charge compensating vacancies, while in a third and final step the charge compensating vacancies are included.

Our study of the tetravalent dopants shows a clear difference exists between the group IVa and group IVb elements, indicating that the specific electronic structure of the dopant (p-block compared to d-block) may be more important than its oxidation state. We find that the group IVa elements are unstable dopants (unlikely to form uniformly doped CeO_2) while the group IVb elements are stable dopants (rather likely to form uniformly doped CeO_2). Similar differences are also found for the calculated bulk moduli and thermal expansion coefficients.

The introduction of aliovalent dopants without charge compensating oxygen vacancies is found to show generally similar trends as those found for the group IV dopants. The introduction of charge compensating vacancies, on the other hand, changes the picture rather radically. Where the lattice parameter of the doped CeO_2 formerly showed a Vegard's law behavior, the addition of oxygen vacancies introduces a nonlinear behavior of the lattice parameter. Furthermore, lattice contractions are often for a large part compensated, resulting, in some cases, in lattice expansions. The introduced vacancies also have a very strong influence on the CeO_2 bulk modulus, and it is this strong influence which allows for both lattice parameter matching and bulk modulus matching, for example, between CeO_2 and $\text{La}_2\text{Zr}_2\text{O}_7$ at low dopant concentrations (~5%) in a layered high temperature superconductor architecture.

This shows that theoretical calculations on idealized systems provide a wealth of information and insight in the general behavior of dopants on the properties of a host system. From these insights, new dopants are suggested for experiments, as are doping ranges for bulk modulus matching or lattice matching.

[1] D. E. P. Vanpoucke, S. Cottenier, V. Van Speybroeck, P. Bultinck, and I. Van Driessche, *Appl. Surf. Sci.* 260, 32-35 (2012)

[2] D. E. P. Vanpoucke, "*Investigation of tunable buffer layers for coated superconductors*", PhD thesis, Ghent University 2012.