Computer Simulation of Disorder in Ceramic Materials

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by
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Abstract

This thesis is concerned with disorder in ceramics; both the mechanisms via which disorder arises and the impact this has on properties of the ceramic. Two atomic scale computer simulation techniques have been used, one based on a classical effective potential description of forces between ions, the other based on a quantum mechanical plane wave density functional model.

Work on gadolinia doped ceria establishes a mechanism for the calculation of the energies associated with the clustering of defects by considering large clusters as the sum of their smaller constituents. We find that in almost all evaluated cases energies of large clusters can be accurately estimated from the sum of the interactions of each constituent pair of defects (termed the pair deconvolution technique).

Cation inversion in magnesium aluminate spinel has been investigated using a variety of competing techniques, namely mean field theory, defect volume analysis and a novel combined energy minimization - Monte Carlo (CEMMC) approach. It was found that the CEMMC technique accurately reproduces the experimental data. Intrinsic defect structures and energies for both isolated and clustered defects have also been evaluated in spinel and used to establish models for cation and anion migration via vacancy and interstitial mechanisms. This has resulted in the prediction that aluminium migrates on the magnesium sublattice in this material, a new concept in oxides with two or more cation sublattices.

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Contents

List of Tables

List of Figures