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Kinetic Monte Carlo Simulation of Cation Diffusion in Yttria-Stabilized Zirconia BRIAN GOOD, NASA Glenn Research Center — Yttria-stabilized zirconia (YSZ) is of interest to the aerospace community, notably for its application as a thermal barrier coating. In such an application, the inhibition of oxygen diffusion is a major concern, and this issue has been addressed via molecular dynamics and kinetic Monte Carlo simulation. However, the mechanical integrity of such coatings can be affected by processes involving diffusive motion on the cation lattice. In this work, we perform kinetic Monte Carlo simulations to investigate cation diffusion in YSZ. We obtain diffusive migration barrier energies ab initio calculations; these barriers are considerably larger than those for oxygen diffusion, and consequently the calculated cation diffusivities are much smaller than oxygen diffusivities from earlier KMC simulations. We report on the effects on cation diffusivity of cation sublattice vacancy concentration, and of Y concentration (and the related oxygen vacancy concentration).

Brian Good
NASA Glenn Research Center

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