

A GENERALIZED QUASI-CONTINUUM METHOD FOR NANOSCALE OXIDE STRUCTURE

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A formalism of the quasicontinuum method suitable for atomistic-continuum modeling and nanoscale mechanics of complex oxide crystals is presented. Multiple, interacting quasicontinua, one per sublattice, which overlap in the physical crystal space are used to model complex oxide crystals. The Cauchy-Born hypothesis, which connects atomic coordinates in distorted crystals to the imposed deformation gradient, is assumed to be valid for the individual quasicontinua. Based on a Delaunay triangulation of the crystal and associated interpolation functions, the Cauchy-Born hypothesis is used to derive self-consistent coarse graining of the atomic forces of individual sublattices. Computation of forces and energy, however, takes into account the interaction among atoms on all sublattices. The method thus can be viewed as a numerical implementation of the theory of inner elasticity of crystals with basis. In this presentation, we show predictions of the structure of hematite (Fe_2O_3) crystal with and without imposed crystal distortions and compare with lattice statics method. A shell-type interatomic potential is used which accounts for the polarization of oxygen ions. In this case, the atomic shells associated with every oxygen sublattice are treated as separate sublattices, which amounts to doubling of the oxygen quasicontinua. Example applications of the generalized quasicontinuum method developed here to study problems of structure and nanoscale mechanics are also given