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Development of an interatomic potential for aluminum oxynitride

N. SCOTT WEINGARTEN, ISKANDER G. BATYREV, BETSY M. RICE, U. S. Army Research Laboratory — Aluminum oxynitride (AlON, or $Al_{23}N_5O_{27}$) is a ceramic whose transparency and high strength make it a potentially useful material for many structural engineering applications. AlON is a cubic spinel, with anions forming a close-packed structure, and aluminum atoms occupying the tetrahedral and octahedral interstitial sites, with one site remaining vacant. However, the location of the vacancy has not been determined experimentally, nor have the positions of the nitrogen atoms, which replace oxygen atoms in the close-packed structure. We have developed an interatomic potential, based on the Buckingham model, for use in classical molecular dynamics (MD) simulations of AlON. The adiabatic shell model can be used to polarize atoms, which allows for a more accurate description of dielectric and defect properties of the material. Using crystal structures determined from first principles calculations, we have calculated a number of material properties using this model, including the lattice parameter and elastic constants, both with and without the shell model, and we compare these to experimental values.

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