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Nonequilibrium molecular dynamics simulations of aluminum oxynitride N. SCOTT WEINGARTEN, U.S. Army Research Laboratory, ISKANDER G. BATYREV, BETSY M. RICE, U. S. Army Research Laboratory — Aluminum oxynitride, or AlON, is a crystalline ceramic material, whose transparency and high strength make it a potentially useful material for many structural engineering applications. The structure of AlON is 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 is not unique, nor are 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. Using this model, and crystal structures determined from first principles calculations, we have calculated a number of material properties and we compare these to experimental values. We present the results of nonequilibrium MD simulations of single crystal and bicrystal AlON systems under applied tension and compression, with a discussion of the yield and failure mechanisms of this material. Finally, we present preliminary observations of shock simulations, with comparisons to simulations of other crystalline ceramic material.

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