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Molecular dynamics simulation of the shock-induced wurtzite-to-rocksalt transition in CdSe and CdS[1] AIDAN THOMPSON, MARCUS KNUDSON, Sandia National Laboratories — The shock-induced wurtzite-to-rocksalt structural transformation is studied using large-scale molecular dynamics simulation. The primary goal is to understand the atomistic mechanisms underlying the interesting transformation kinetics observed in the case of cadmium sulfide [M. D. Knudson and Y. M. Gupta, J. Appl. Phys, v. 91, p. 9561, 2002]. Since the mechanical and structural properties of CdS are very similar to those of CdSe, we have performed multi-million atom MD simulations of the shock-induced phase transformation in CdSe single-crystals using the well-established interatomic potential of Rabani, which has been shown to correctly describe the wurtzite and rocksalt phases and the transformation pressure. In MD simulations of shock along the wurtzite c-axis, the elastically-compressed wurtzite transforms directly to grains of rocksalt. Along the a-axis, a three-wave structure is observed; the wurtzite first transforms to a tetragonal crystal phase, which in turn transforms to rocksalt grains.

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