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Deformation near grain boundaries in rocksalt structured ceramics at high strain rates JAMES PALKO, University of Michigan, JOHN KIEFFER, University of Michigan — The rocksalt structure is one of the most basic ceramic crystal structures, and provides a useful model to study the deformation processes that occur near grain boundaries in ceramic materials. We used molecular dynamics and electronic structure calculations to explore the structure and deformation modes of high angle tilt grain boundaries in these materials, particularly NaCl, under various stress states at high strain rates. These simulations show the effects of dislocation impingement and emission on the structure of these grain boundaries, and the nucleation of cracks via the Zener-Stroh process. Lower dimensional structures are found to play a role in strength retention during fracture and grain boundary sliding processes. The stability of these structures was verified using ab-initio electronic structure calculations. Finally, an expanded hexagonal phase was discovered as a unique stress relief mechanism for a particular grain boundary structure.

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