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A Molecular Dynamics Study of Solid Gallium Using a Modified Embedded Atom Model FRANK CHERNE, KAI KADAU, TIMOTHY GERMANN, Los Alamos National Laboratory — Gallium is a complex material that has been simulated using the literature modified embedded atom method (MEAM) potential [Baskes et al., PRB 66, 104107 (2002)]. This potential captures some of the unique characteristics of this ubiquitous metal. Here we report on the structural transformations based upon the crystallographic direction. In order to characterize the nature of the transition we have performed both non-equilibrium and equilibrium molecular dynamics (MD) simulations. These simulations provide insight into the nature of the solid-solid and solid-liquid phase transitions in addition to the kinetic behavior of this complex material. The Hugoniot for solid gallium will be presented. This research is being done in collaboration with an experimental ultrafast X-ray diffraction effort here at Los Alamos National Laboratory. Supported by the US DOE under contract W-7405-ENG-36.

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