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Atomic Scale Modeling of High Strain Rate Deformation and Failure of HCP Metals KAROON MACKENCHERY, GARVIT AGARWAL, AVINASH DONGARE, Department of Materials Science and Engineering, and Institute of Materials Science, University of Connecticut — A fundamental understanding of the microstructure effects on the defect evolution at the atomic resolution and the related contribution to plasticity at the macro-scales is needed to obtain a reliable performance of metallic materials in extreme environments. Large-scale molecular dynamics simulations are carried out to characterize the dynamic evolution of defect/damage structures during the deformation and failure behavior of HCP (Mg, Ti) metallic systems (single crystal and nanocrystalline at high strain rates as well as under shock loading conditions. The evolution of various types of dislocations, twins, faults, etc. and the related deformation and failure response (nucleation and growth of voids/cracks) will be discussed. The effects of strain rates on relationships between the microstructure and the strength of these materials at high strain rates and the underlying micromechanisms related to deformation and failure will be discussed.

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