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Single Crystal Plasticity in Ramp- and Cyclically-Loaded Aluminum[1]

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In recent years, there has been a great deal of interest in using large-scale atomistic simulations to model wave propagation in order to get a qualitative picture for inelastic deformation in materials. Although these simulations have provided a great deal of qualitative insight into the phenomena of high strain rate deformation in materials, there is an increasing need to be able to obtain quantitative continuum descriptions for the atomistic simulations in terms of stresses and strains so one can construct constitutive laws for plastic deformation. This presentation will be focused on recent work to develop this seamless approach from atoms to continuum and apply it shock compression of single-crystal Aluminum using very large-scale atomistic wave-propagation simulations. In the first part of this presentation, we discuss the performance of the available and newly developed interatomic potentials in terms of their ability to reproduce thermoelastic and plastic properties such as elastic moduli, specific heat, thermal expansion coefficient, thermal conductivity and gamma surface. We then describe recent large-scale simulations of ramp- and cyclically-loaded single-crystal Aluminum with varying initial defect concentrations. Using the method of characteristics, we impose a time-varying longitudinal force to generate ramp waves with specified shock-up locations in the material. Our calculations demonstrate that (1) the initial defect densities have a strong effect on the time-dependence and the maximum achieved equivalent stress, (2) shock-up consistently occurs earlier than expected due to the inherent inability for materials to sustain large gradients in the shock front at these micron length-scales, and that (3) the observed flow stress followed in the coarse-grained Lagrangian elements before shock-up are consistently higher than those after shock-up and those from shock-loading simulations. We discuss these differences in terms of continuum phenomenological models for plastic deformation constructed from coarse-grained analyses of these simulations, and consider future possible developments in large-scale atomistic simulations.

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