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Dynamics of Plastic Deformation in Atomistic Shock Compression Simulations[1] WILHELM WOLFER, ALISON KUBOTA, Lawrence Livermore National Laboratory — Dynamics simulations of shock compression of aluminum are evaluated in terms of a continuum mechanics descriptions to obtain detailed stress and strain distributions behind shock fronts. The equivalent or von Mises stress reaches steady values that coincide with the dynamic yield strength obtained by Huang and Asay from the analysis of particle velocity profiles of release and reshock experiments. This agreement is all the more significant as the experimental results are indirect, while the atomistic simulation results extract the dynamic strength directly. Additional information is obtained when the evolution of the von Mises stress is viewed in the Lagrangian frame. Different material elements experience nearly the same stress evolution: a rapid rise, as the elastic wave front passes the material element, followed by an exponential decline of the von Mises stress. This evolution implies a constitutive law for plastic deformation that can be used as is in finite element codes, and/or it can be further interpreted by the dislocation mechanisms that the atomistic simulations so vividly reveal and display. Temperature can also be extracted directly from the atomistic simulations and be separated into adiabatic and plastic heating.

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