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Atomistic simulation of plasticity, spall damage and fracture of crystalline and polycrystalline metals under high strain rate[1]

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Modeling and simulation of dynamic atomistic phenomena and processes in condensed matter are considered, which accompany intensive shock compression and release, uniaxial and hydrostatic stretching. Standards are presented for molecular dynamics (MD) modeling and simulation of relaxation processes: (1) the choice of system sizes, particle numbers and boundary conditions is discussed with respect to the spatial and temporal requirements and restrictions imposed by correlation lengths and correlation times of the processes to be modeled; (2) instantaneous and time averaged diagnostics are considered, spatial resolution included. The diagnostics includes study of (a) time evolutions of distributions of macroparameters (stress, temperature etc.) and structural characteristics (dislocation motion, void growth); (b) deviations of atom velocity and position distributions from the equilibrium ones etc. A hierarchy of dynamic and stochastic processes is introduced by the comparison of time scales with the dynamic memory time (predictability limit) which appears as a result of the Lyapunov instability of particle trajectories. Some theoretical MD based multi-scale approaches are presented which could be used to extend the MD results to the larger spatial and temporal scales. Examples are presented for Al, Fe, pure and Al doped Cu, and some other species for both perfect and defected crystals. The EAM potentials are mostly deployed. Comparisons with the experimental data available as well as with the simulation results of other authors are given.