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Atomistic models of plasticity of metals and alloys under dynamic loading ALEXEY KUKSIN, ALEXEY YANILKIN, All-Russia Research Institute of Automatics, COMPUTATIONAL MATERIALS SCIENCE TEAM — The work presented is devoted to study the mechanisms and kinetics of plastic deformation of bcc and fcc metals and alloys under shock-wave loading (strain rates $> 10^5$ s^{-1}). To study the behavior of metals under conditions described the two scale approach is developed. It comprises molecular dynamics (MD) calculations of dislocation mobility and dislocations nucleation rate and continuum mechanics model with equations for description of elastoplastic deformation, kinetics and dynamics of dislocations. Dislocation velocities as functions of applied shear stress are calculated in Al, Cu, Fe, Mo from MD in a wide temperature range up to the melting point. Velocity-dependent drag coefficient is introduced to approximate the data obtained. The influence of Guinier-Preston (GP) zones on dislocation motion is analyzed. The results obtained are used to evaluate temperature dependence of dynamic flow stress and the evolution of dislocations subsystem under shock loading. Data on the attenuation of the elastic precursor and rare surface velocity profiles calculated for Al are in good agreement with the experiments. Simulation of the free surface velocity profiles during shock-wave loading of AlCu alloys is carried out.

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