Meshfree method for hybrid atomistic simulation of metals with hot electrons

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A new hybrid atomistic simulation technique is developed with the aim to make accurate representation of two-temperature (2T) states of metals with hot electron subsystem and its interaction with atoms, in which the molecular dynamics method for atoms is combined with the well-known smoothed particle hydrodynamics (SPH) method for electrons. The spatial distributions of electron energy, temperature and pressure are written as particle functions in a standard SPH form. Each SPH particle represents some number of conductive electrons, and its position is always assigned to its host atom, which guarantees the exact charge neutrality. Such an eSPH particle is assumed to be massless, which allows keeping only a conservation equation for electron energy balance in the SPH form. Both this equation and the atom motion equation have the terms of electron-atom energy exchange and work of electron pressure, which provides conservation of total energy in this hybrid method. Electron thermal conductivity between eSPH particles is also included in the energy balance equation.

The new meshfree MD+eSPH method is applicable without difficulties for material flow leading to formation of density jumps, cavities, and jets. MD+eSPH is tested in simulations of gold in 2T states by comparison with 2T hydrodynamics. The MD+eSPH results demonstrate a perfect agreement with 2T hydrodynamics results in several one-dimensional tests. Since the electron pressure always pushes apart atoms, it leads to effective reduction of cohesive energy with increase of electron temperature. It is also demonstrated that 2T physics manifests itself in a nonequilibrium distribution of electron temperature around a steady-state shock front in gold.