Wave packet molecular dynamics density functional theory simulations of shock-compressed deuterium

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A new wave packet molecular dynamics (WPMD) density functional theory (DFT) simulation method is applied to study the shock-compressed deuterium. The method is based on the WPMD and DFT. It allows to study nonideal plasmas and warm dense matter accounting for simultaneous dynamics of electrons and ions, electron–ion relaxation, plasma conductivity and interaction of plasma with the laser irradiation. In this report, we condenser mainly thermodynamic properties of the shock-compressed deuterium to validate the WPMD-DFT method. In this approach, the electrons are represented as Gaussian wave packets whereas the Hartree approximation for the many-body wave function is used. The exchange and correlation effects are treated using an additional energy term taken from DFT. This term is determined by an exchange-correlation functional and a correction to the kinetic energy. It is calculated via integration over the mesh values of the function that depends on the electron density. The local electron density distribution is determined by the positions and widths of the wave packets. The proposed approach is meant as a replacement for the antisymmetrized WPMD (AWPMD) method which is more time consuming. The WPMD-DFT method is applied for direct simulation of deuterium shock compression. The simulation is performed as a series of compression and relaxation stages. The convergence of simulation results as a function of compression speed is studied. In addition, the WPMD-DFT method is used for isentrope calculation via Zel'dovich's approach. The results are compared with experimental data and other quantum molecular dynamics simulations.