WPMD–DFT SIMULATIONS OF DYNAMIC AND RELAXATION PROCESSES IN NONIDEAL ELECTRON–ION PLASMAS

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A new WPMD–DFT simulation approach [1] is applied to study the isentropic compression and electron–ion relaxation rate in nonideal plasmas of hydrogen and helium. The method of wave packet molecular dynamics (WPMD) is based on the representation of electrons as Gaussian wave packets whereas ions are treated as classical particles. Compared to the classical molecular dynamics it improves the representation of electron–ion bound states without involving pseudopotentials and allows to account for electron degeneracy. In the latest modification of this method called WPMD–DFT, the exchange and correlation effects are determined by calculating the functional of the total electron density provided by the density functional theory (DFT) approach within the LSDA approximation. It provides an optimal balance between the code performance and precision of account for quantum effects compared to other WPMD modifications such as electron force field (eFF) and dynamics of antisymmetrized wave packets (AWPMD).

The main feature of the original molecular dynamics and WPMD methods is the ability to study simultaneous dynamics of electrons and ions, particularly for non-equilibrium states. This feature is missing in the Monte–Carlo simulations including PIMC as well as in the quantum molecular dynamics bases on the Born–Oppenheimer adiabatic approach. At the same time, the study of relaxation processes and non-isothermal nonideal plasmas is of great interest as such states are observed in the plasma generated by short laser pulses, particle beams, shock waves, etc.

In this work, we demonstrate the ability of WPMD–DFT to study dynamic compression and electron–ion relaxation of nonideal plasmas in different conditions for electron number densities up to 10^{24} cm^{-3} which is far above the limit of the classical molecular dynamics and the original WPMD approach. The simulations of isentropic compression are compared with the latest experimental data, QMD simulations, and SAHA–D chemical model [2].

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2. Mochalov M. A., Il'kaev R. I., Fortov V. E., et al // J. Exp. Theor. Phys. 2021. V. 133. No. 5. P. 630.