EQUILIBRIUM PROPERTIES OF WARM DENSE DEUTERIUM CALCULATED BY THE WAVE PACKET MOLECULAR DYNAMICS

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A joint simulation method based on the wave packet molecular dynamics and density functional theory (WPMD-DFT) is applied to study warm dense deuterium and helium (nonideal plasmas). This method was developed recently [1-3] as an extension of the wave packet molecular dynamics (WPMD) in which the equations of motion are solved simultaneously for classical ions and semiclassical electrons represented as Gaussian wave packets. Compared to the classical molecular dynamics and WPMD simulations the method of WPMD-DFT provides a more accurate representation of quantum effects such as electron-ion coupling and electron degeneracy. In the WPMD-DFT, the Hartree approximation for the many-body wave function is used but the exchange and correlation effects are determined by a functional taken from DFT. It is calculated via integration of the function that depends on the electron density over the mesh. The local electron density distribution is determined by the positions and widths of the wave packets.

The compression isentrope and principal Hugoniot curves are obtained by WPMD-DFT and compared with available experimental data and other simulation approaches to validate the method. The isentrope calculation are 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 isoentrope calculation via Zel'dovich's approach. For both isentropic and shock compression of deuterium, the WPMD-DFT results are compared with experimental data and other more accurate QMD simulations. The results are in a good agreement, except for some overestimation of the pressure.

[1] Lavrinenko Ya.S., Levashov P.R., Minakov D.V., Morozov I.V., Valuev I.A. // Phys. Rev. E. 2021. V. 104. P. 045304.
[2] Lavrinenko Ya.S., Morozov I.V., Valuev I.A. // J. Phys. Conf. Ser. 2021. V. 1787. P. 012043.
[3] Lavrinenko Ya.S., Morozov I.V., Valuev I.A. // Contrib. Plasma Phys. 2019. V. 59. P. e201800179.