Alternative ion-ion pair potentials applied to molecular dynamics simulation
for hot, dense Fe and Al plasmas*

Yong Hou and Jianmin Yuan★

Department of Physics, National University of Defense Technology, Changsha, China

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With the development of the laser technique, it is possible to produce the hot, dense plasmas in the laboratory, and so constructing theoretical models of thus region to simulate the properties, such as the equation of state, radiative transfer, is necessary. The properties are of the importance in the inertial confinement fusion (ICF) and astrophysics. We present a method to calculate the ion-ion pair potential which is based on the density function theory (DFT) at hot, dense plasma region. The electronic structure is calculated using the average-atom (AA) model, and the electronic number density around the nuclear is divided into the two parts: the electronic sea $\rho(r,h)$, is equal to the density of the ion-sphere boundary; the second $\rho^{2nd}(r)$ is the total density minus to the first ones. And the electron densities of system is taken as the sum of densities of the two separate atoms or ions, the pair potential is obtained through integrating out the electron densities. And then we performed molecular dynamics simulations for ions on base of the pair potentials in the wide regime of density and temperature. As an example, hot, dense Fe and Al plasmas are simulated, and the equation of state and ion-ion pair distribution function are obtained. The results are in agreement with that of the other theoretical models.

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★Email: jmyuan@nudt.edu.cn