

Multi-charge-state molecular dynamics and self-diffusion coefficient in the warm dense matter regime

Yongsheng Fu^{1,2}, Yong Hou^{1,2}, Dongdong Kang^{1,2}, Cheng Gao¹, Fengtao Jin¹, Jianmin Yuan^{1,2}

1. Department of Physics, College of Science, National University of Defense Technology, 410073

Changsha, Hunan, P. R. China;

2. Graduate school, China Academy of Engineering Physics, Building 9, Beijing, 100193, P. R. China.

Warm dense matter (WDM) is the kind of intermediate state between condensed matter and ideal plasma. In this regime, the physical properties are crucial for modeling astrophysical objects and inertial confinement fusion experiments. Now, in the framework of density functional theory, many approaches are presented to calculate the WDM properties. However, the fine structure of the absorption or emission spectroscopy of WDM need detailed treatment of the multi charge states. From calculating atomic structure, detailed configuration accounting, unresolved transition array, super transition array, and detailed term accounting model could be used to describe different energy levels and ionic charge states in hot and rarefied plasmas, but in dense matter ion-ion coupling is very strong, these methods have not included ion-ion correlation effects on the electron structure and ionic charge-state distribution.

We present the multi-ion molecular dynamics simulation and apply to calculate the self-diffusion coefficients of different charge-state ions in the warm dense matter regime. Firstly, the method is used to self-consistently calculate electron structures of different charge-state ions in the ionic sphere, where the ion-sphere radii are determined by the plasma density and their charges. And then the ionic fraction is obtained by solving the Saha equation, which has included the interactions of different charge-state ions in the system and ion-ion pair potentials are computed by the modified Gordon-Kim method in the framework of the temperature-dependent density functional theory on the basis of the electron structures. Lastly, we perform the multi-ion molecular dynamics to calculate ionic self-diffusion coefficients through the velocity correlation function according to the Green-Kubo relation. Through comparing with the results of the average atom model, it is shown that different statistical processes will influence the ionic diffusion coefficient in the warm dense regime.

[1] Yong Hou, Jiayu Dai, Dongdong kang, Wen Ma, and Jianmin Yuan, *Phys. Plasmas* 22 , 022711 (2015).