



Average-atom model for two-temperature states and ionic transport properties of aluminum in the warm dense matter regime



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ABSTRACT

The average-atom model combined with the hyper-netted chain approximation is an efficient tool for electronic and ionic structure calculations for warm dense matter. Here we generalize this method in order to describe non-equilibrium states with different electron and ion temperature as produced in laser-matter interactions on ultra-short time scales. In particular, the electron-ion and ion-ion correlation effects are considered when calculating the electron structure. We derive an effective ion-ion pair-potential using the electron densities in the framework of temperature-dependent density functional theory. Using this ion-ion potential we perform molecular dynamics simulations in order to determine the ionic transport properties such as the ionic diffusion coefficient and the shear viscosity through the ionic velocity autocorrelation functions.

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1. Introduction

Ionic transport properties of warm dense matter (WDM) are crucial input parameters in hydrodynamic simulations for inertial confinement fusion (ICF) experiments and in modeling astrophysical objects [1–4]. However, due to the strong ion-ion coupling and electron degeneracy in the WDM regime, it is difficult to describe the electronic and ionic structure simultaneously in theoretical calculation [5]. In particular, when an ultra-short, femtosecond laser pulse interacts with the dense matter, a non-equilibrium state with different electron and ion temperature is generated [6,7]. According to a two-temperature model, the relaxation time in the electron-ion system is more longer than for the pure electron and ion subsystem due to great mass difference between electrons and ions [8,9]. This two-temperature state is usually treated by assuming that electrons and ions are in local thermodynamic equilibrium having different temperatures, T_i and T_e [10]. However, it is still a challenge to improve such simple models and to describe WDM under non-equilibrium conditions consistently [11,12].

Quantum molecular dynamics (QMD) simulations, which calculate the electron structure in the framework of density functional theory (DFT) and solve the Newton equation to describe the ionic motion, have become a powerful tool for computing the properties of WDM in the low temperature region [13–17]. QMD can also be

applied to describe the properties of hot dense matter by using quantum Langevin molecular dynamics (QLMD) simulations [18,19], which consider the ion moving in dense electronic system, as the motion of Brownian particle, and electronic random collision yields friction force. Alternatively, orbital-free molecular dynamics (OFMD) [20–24] and pseudo-atom molecular dynamics (PAMD) simulations [25,26] were developed to describe the warm and/or hot dense plasma region. These methods use the Thomas–Fermi approximation or Khon–Sham equation to compute the electron structure and molecular dynamics simulation to give the ionic structure. The hyper-netted chain (HNC) approximation within the Ornstein–Zernike (OZ) equation can also be solved to describe the ion structure if the ion-ion pair potential is obtained consistently from the electron structure calculations [27–31]. Recently, we have combined the average-atom model [32,33] with the HNC approximation (AAHNC) to calculate the electronic and ionic structures of Al and the x-ray Thomson scattering (XRTS) spectrum in the WDM regime [34]. In this method, ion structure is determined in HNC approximation, where the ion-ion pair potential is obtained from the electron distribution in the framework of temperature-dependent DFT [35,36], and the electron structure is calculated through Dirac equation through considering the ion and free electron correlation effects. The electron and ion structure are described through different approximation and solved self-consistently.

In the present study, we investigate the ionic structure and transport properties considering difference temperatures for ion and

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electron subsystems using the AAHNC method. The electron structure is obtained by solving the Dirac equation in the average-atom model which has considered the effects of ions interacting via an ion-ion pair correlation function [34]. The ionic pair potentials are obtained from the electronic density distributions of two isolated ions based on a modified temperature- and density-dependent Gordon–Kim model [35,36]. When we calculate the electronic structure, the ionic structure is considered and, at the same time, the electronic structure is needed when calculating the ion-ion pair potential. This problem is solved self-consistently [34]. Subsequently, classical (CMD) and Langevin molecular dynamic (LMD) simulations based on the ion-ion pair potential derived from the AAHNC method are performed to compute the ionic self-diffusion coefficient and the viscosity of Al according to the velocity autocorrelation function [37]. When solving the Dirac and Newton equation, we use different temperatures for electron and ion, T_e and T_i , respectively.

2. Theoretical methods

2.1. Two-temperature AAHNC model

In the Born–Oppenheimer approximation, the electronic and nuclear structures can be described separately. The electronic motions can be described by the Schrödinger or Dirac equation in the central-field approximation. In local thermal equilibrium, for an isolated ion we have computed the electronic structures through the modified average atom (AA) model [32,33]. It considers the electron energy level broadening due to the density effect on the electronic distributions in a statistical way. In Ref [34], we also included the effects of interactions with the surrounding free electrons and ions through the correlation function. Here we try to include the effects of different temperatures for the electrons and ions. Each bound electron is considered in the ion-sphere, and wave function is obtained by solving the Dirac equation:

$$\frac{dP_{n\kappa}(r)}{dr} + \frac{\kappa}{r}P_{n\kappa}(r) = \frac{1}{c}[\epsilon_{n\kappa} + c^2 - V(r)]Q_{n\kappa}(r), \quad (1)$$

$$\frac{dQ_{n\kappa}(r)}{dr} - \frac{\kappa}{r}Q_{n\kappa}(r) = -\frac{1}{c}[\epsilon_{n\kappa} - c^2 - V(r)]P_{n\kappa}(r). \quad (2)$$

$P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are, respectively, the large and small components of wave function of orbital $n\kappa$, c is the speed of light, and $V(r)$ is the self-consistent potential which has the form [34,38]:

$$V(r) = -\frac{Z}{r} + \int \frac{\rho_b(r')}{|\vec{r}-\vec{r}'|} d^3r' + V_{xc}(\rho_b(r) + \rho_e^0) - V_{xc}(\rho_e^0) - \frac{\rho_e^0}{\beta_{ee}} \int C_{ee}(\vec{r}-\vec{r}') h_{ie}(r') d^3r' - \frac{\rho_i^0}{\beta_{ie}} \int C_{ie}(\vec{r}-\vec{r}') h_{ii}(r') d^3r'. \quad (3)$$

Where the first four terms constitute the single ionic contribution, and the last two terms in Eq. (3) represent interactions with the surrounding free electrons and ions, respectively. Because the central potential, $V(r)$, depends on the electron density and the correlation functions, the solution of Eqs. (1)–(3) has to be done self-consistently if we know the correlation functions. When the electron and ion structures are solved, the different temperatures for electron and ion, T_e and T_i , respectively, are considered, and β_{ee} is equal to $(k_B T_e)^{-1}$ and β_{ie} is $(k_B \sqrt{T_e^2 + T_i^2})^{-1}$, where k_B is the Boltzmann's constant. In order to obtain the same electron density at the boundary for all ions, the central potential at the ion-sphere boundary is chosen as the common reference point in the AA model. In this way we define electrons with energies larger than zero as *free* and with negative energies as *bound*. In our AA model, the boundary conditions are the same as Eqs. (3) and (4) in Ref. [32] when we solve the Eqs. (1) and (2), which the bound state orbitals are broadened to energy bands, and the density of bound electrons is computed through

wave functions in the central-field approximation. Free electrons are described much simpler using the TF approximation and the free electron density is calculated with a Fermi–Dirac distribution in momentum space, as described in the Ref [34].

In our calculation, the ion-ion correlation functions extend to the whole space through the pair correlation function, however, we only consider correlation effects inside the ion-sphere when calculating the electron structure of the isolated ion. The ion-ion pair potential is calculated using the modified Gordon–Kim (GK) model [35],

$$V(R) = V_{Coul}(R) + V_k(R) + V_e(R) + V_c(R), \quad (4)$$

where R is the distance between the two nuclei, $V_{Coul}(R)$ is their static Coulomb interaction, $V_k(R)$ is the kinetic energy, $V_e(R)$ and $V_c(R)$ are the exchange and correlation energies, respectively, which depend on the electron density $\rho(r)$ and temperature. The static Coulomb potential can be calculated directly from the electron density according to the GK model [36]. The difference between the present model and the original GK model is that the electronic density of the single ion is divided into two parts, the uniformly distributed free-electron sea $\rho(r_b)$ and the quasi-localized electrons $\rho_i^{loc}(r)$, see Ref. [35]. The kinetic energy $E_k(\rho)$, exchange energy $E_e(\rho)$, and correlation energy $E_c(\rho)$ [36] are computed based only on the electron densities in the spheroidal coordinate system, $\lambda_1 = (r_1 + r_2)/R$, $\lambda_2 = (r_1 - r_2)/R$.

The ion-ion and free electron-electron correlation functions are calculated using the HNC approximation ($a = e, i$),

$$h_{aa}(r) = \exp[-\beta_{aa} V_{aa}(r) + h_{aa}(r) - C_{aa}(r)] - 1 \quad (5)$$

and the Ornstein–Zernike relation in Fourier space

$$h_{aa}(k) = C_{aa}(k)[1 + \rho_a^0 h_{aa}(k)], \quad (6)$$

where ρ_a^0 is the average density for the electrons or ions. The free electron potential is considered using the Deutsch formula [27], which includes quantum effects such as the uncertainty principle and exchange interactions which lead to its temperature dependence. The ion-electron pair correlation function is defined via the excess free electron density,

$$h_{ie}(r) = \frac{\rho_f(r)}{\rho_e^0} - 1, \quad (7)$$

where ρ_e^0 is the uniform electron density given by $\rho_e^0 = \rho(r_b)$.

When we calculate the electronic structure, the pair correlation functions of electrons and ions are needed. On the other hand, ion-ion pair potentials are based on the electron density distribution. We obtain the electronic and ionic structure using the self-consistent calculations, see Ref [34]. After reaching converged electronic and ionic structures, we obtain the ion-ion pair potentials, which depend on the electronic density distribution and temperature. Based on this results, we can perform the molecular dynamics to calculate the ionic transport properties.

2.2. Langevin molecular dynamics simulation

In the dense matter regime, collisions between electrons and ions are important. In particular, for the high-Z elements, this electron-ion collisions become more important with increasing ionization. We have discussed the effects in Ref. [18,19] using quantum Langevin molecular dynamics (QLMD), which considers the ion moves in dense electronic medium, as the motion of Brownian particle. Random electronic collisions lead to friction force. When simulating ionic motion, we use the Langevin equation [18]

$$m_i \frac{d^2 \mathbf{r}_i(t)}{dt^2} = \mathbf{F} - \gamma m_i \frac{d\mathbf{r}_i(t)}{dt} + \mathbf{N}_i, \quad (8)$$

where m_i is the ionic mass, \mathbf{r} , the ionic positions, \mathbf{F} , the force calculated for the ion-ion pair potential, \mathbf{N}_i the Gaussian random noise, and γ is the Langevin friction coefficient, which is estimated by the

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