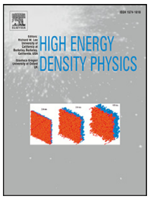
High Energy Density Physics 23 (2017) 217–222

Contents lists available at ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp



Ultrafast nonequilibrium ion and electron dynamics of a neon plasma produced by an ultra-intense x-ray pulse

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ARTICLE INFO

Article History:
Received 11 May 2017
Accepted 15 May 2017
Available online 16 May 2017

Keywords:
Electron energy distribution function
Rate equation
X-ray laser-matter interaction

ABSTRACT

Ultrafast nonequilibrium ion and electron dynamics of a neon plasma produced in the interaction with an ultra-intense x-ray pulse is investigated theoretically. Electron energy distribution function (EEDF) is obtained by solving Fokker–Planck equation, which is implemented self-consistently in a time-dependent rate equation in the framework of detailed-level-accounting approximation. Evolution dynamics of EEDF are presented at a variety of ion density in interaction with x-ray pulses of different laser intensities. Thermalization of free electrons is demonstrated after the x-ray pulses have turned off. The results are compared with two other simplified models, i.e., one is a relaxation model and the second uses the Maxwellian approach. Large discrepancies in the EEDF are found and the effects of detailed treatment of electron dynamics on population distributions are demonstrated and discussed.

1. Introduction

The investigation of light-matter interaction is expanding from the long-wavelength region into the short-wavelength region with the development of x-ray free electron lasers (XFEL) such as the Linac Coherent Light Source (LCLS) [1] and the Spring-8 Angstrom Compact free electron LAser (SACLA) [2]. Such ultra-intense and ultrafast x-ray pulses open new probabilities to study the ion and electron dynamics in the nonequilibrium plasmas produced. After the pioneering experimental work of Young et al. [3], considerable efforts have been devoted to understanding the interactions of ultra-intense x-ray pulses with atoms and molecules [3–9], clusters [10,11], and solid samples [12–15].

To theoretically understand the interaction mechanism of an ultra-intense x-ray pulse with atoms, the population evolution of atomic states and energy distribution of free electrons are of fundamental importance. At the current state of XFEL experiments, the coherent time of the x-ray pulses is usually very short [16] and therefore the Time Dependent Rate Equation (TDRE) approach is widely used to determine the population dynamic evolution [17–23]. In the interaction with an x-ray pulse, the inner-shell electrons of atoms are photoionized or resonantly excited, resulting in core-hole states which relax by Auger decay with ejection of an electron or by emitting a photon. For a dilute atom gas, the free electrons produced do not have pronounced effects on the ion and electron dynamics. For a dense plasma, however, the free electrons would further interact with atoms by impact excitation or ionization and thus control the dynamic processes. In such cases, the free electron energy distribution function (EEDF) plays an important role on level population distribution for collision dominated plasmas. Most past work assumed that the free electrons instantaneously equilibrate, which is not valid for such ultrashort x-ray pulses. A precise treatment relies on the accurate determination of EEDF. The nonequilibrium distribution of free electrons is reported in plasmas produced by electron beams [24], black-body radiative field [25], lasers in the optical regime [26–29], VUV and EUV wavelength range [30,31]. Few research efforts with detailed and accurate treatment on EEDF are reported in the x-ray FEL-matter interaction in literature [32,33]. Abdallah, Colgan, and Rohringer [32] investigated nonequilibrium effects of EEDF on populations and radiative properties of neon plasmas irradiated by an ultra-intense x-ray pulse by solving Fokker–Planck equation. The simulation is carried out at an ion density of 1.6×10^{19} cm^{-3}. Varga et al. [33] calculated the EEDF of neon plasmas at ion density of 1.0×10^{19} and 1.0×10^{22} cm^{-3} by utilizing a set of hydrogenic approximate formulas to obtain the rates of atomic processes within the framework of the super-configuration approximation. Three-body recombination is excluded to simplify their calculation. These investigations deepened our understanding of nonequilibrium electron dynamics in ultra-intense x-ray pulse interacting with matter.

In this paper, ultrafast dynamics of ion and electron is investigated for nonequilibrium plasmas produced in interaction with ultra-intense x-ray pulses by combining a TDRE with Fokker–Planck

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http://dx.doi.org/10.1016/j.hedp.2017.05.008
1574-1818/

equation, using neon as an example. The ion dynamics are implemented by solving the TDRE in the framework of detailed-level-accounting (DLA) approximation [34–36] and the EEDF is determined self-consistently by solving Fokker–Planck equation. Results for plasmas at different ion densities produced at variable laser intensities are compared with those obtained by the Maxwellian approximation and a relaxation model [37]. Effects of different treatments of EEDF on population distributions are demonstrated and discussed.

2. Theoretical method

In the present work, a TDRE based on a DLA approximation is employed to determine level population dynamics,

$$\frac{dn_i}{dt} = \sum_{j \neq i}^{N_L} n_j R_{ji} - n_i \sum_{j \neq i}^{N_L} R_{ij}, \tag{1}$$

where R_{ij} and R_{ji} represent the rates which depopulate and populate the level i by level j, N_L is the total number of levels included in the rate equation. Microscopic atomic processes due to interaction of photons and electrons are included, namely photoexcitation, photoionization, electron impact excitation, electron impact ionization, Auger decay and their inverse processes. The detailed methods for calculation of the rates can be found in a previous work (see Ref. [38]). The rates due to photon interaction is expressed by

$$R_{ij}(r,t) = \int \frac{I_\nu(r,t)}{h\nu} \sigma_{ij}(h\nu) d\nu, \tag{2}$$

where σ_{ij} is photoionization or photoexcitation cross section for the transition from levels i to j and $I_\nu(r, t)$ is laser intensity. The laser beam is assumed to have a circular spot size on which the intensity has a Gaussian distribution, and the temporal distribution of the intensity is also assumed to be Gaussian. The intensity has a Gaussian distribution with respect to photon frequency to account for bandwidths of laser pulses [3]. Explicitly, the XFEL intensity $I_\nu(r, t)$ at spatial position r from the center of the laser spot, time t and photon frequency ν is written by

$$I_\nu(r,t) = I_0 e^{-\ln 2\left(\frac{r}{\Delta}\right)^2} e^{-\ln 2\left(\frac{t}{\tau}\right)^2} \sqrt{\frac{\ln 2}{\pi \Gamma^2}} e^{-\ln 2\left(\frac{h\nu - h\nu_0}{\Gamma}\right)^2}, \tag{3}$$

where I_0 is the peak intensity, $h\nu_0$ is the central photon energy of the x-ray pulse, Δ, τ and Γ are the half width at half maximum (HWHM) of the Gaussian distribution profile with respect to space (on laser spot), time and photon energy, respectively.

The rates caused by electron impact reads

$$R_{ij}(r,t) = \int \sqrt{\frac{2E}{m}} f(E) \sigma_{ij}(E) dE, \tag{4}$$

where m is electron mass, σ_{ij} is the electron impact excitation or ionization cross section, and $f(E)$ is EEDF. In the present work, EEDF is obtained by solving the Fokker–Planck equation [39],

$$\frac{\partial f(E)}{\partial t} = -\frac{\partial}{\partial E}[a(E)f(E)] + \frac{1}{2}\frac{\partial^2}{\partial E^2}[D(E)f(E)] + S, \tag{5}$$

where S represents all creation and destruction of electron population by photon-atom and electron-atom impact, $a(E)$ and $D(E)$ are electron energy exchange rate and diffusion rate, respectively,

$$a(E) = \int a(E, E_1) f(E_1) dE_1, \tag{6}$$

$$D(E) = \int D(E, E_1) f(E_1) dE_1, \tag{7}$$

where $a(E, E_1)$ is energy exchange rate coefficient for two electron impact with energy E and E_1, and $D(E, E_1)$ is diffusion rate coefficient [39].

3. Results and discussions

In this work, we investigate the x-ray interaction with neon at a photon energy $h\nu_0$ = 2000 eV with pulse duration of τ = 50 fs (HWHM), which is close to the experiment condition carried out by Young et al. [3]. We chose the time when the laser intensity arrives at maximum as t = 0 fs and calculation is carried out from $t = -2\tau$ fs to $t = 2\tau$ fs. Initially the neon atoms are all in the ground state.

3.1. Atomic model

X-rays effectively photoionize K-shell electrons of neon leaving inner-shell holes that dominantly relax by Auger decay. The resulting photo-electrons and Auger-electrons further impact with atoms (including ions). In the present work, the main microscopic atomic processes due to photons and electrons are included. Explicitly, they include photoexcitation, photoionization, electron impact excitation, electron impact ionization, Auger decay and their inverse processes. The atomic configurations of neon atom and ions are the same as those listed in Ref. [22], i.e., the ground configurations, singly excited configurations from valence shells, and single and double K-hole configurations. Such a choice of configurations is appropriate to balance the precision of calculation and cost of computation for the simulation of ultra-intense x-ray pulse interacting with neon atoms [22,37,42]. A complete set of atomic data including energy levels, spontaneous radiative decay rates, photoionization cross section, electron impact excitation and ionization cross section, and Auger decay rates is obtained in the framework of DLA approximation. The detailed theoretical method for calculating these basic atomic data is given in Ref. [38]. Briefly, the radial wave functions are obtained by solving Dirac–Fock equation, which are used to construct configuration state functions. Atomic wave functions are constructed by the linear combination of configuration state functions. The continuum wavefunctions are obtained by using the relativistic distorted wave methods [43]. High-order atomic processes such as double Auger decay rates are also included and determined by using simplified formulas under the approximation of knock-out and shake-off mechanisms [44–46]. In the present work, the ion density of neon plasmas is restricted to be no more than 1.0 × 10^{21} cm^{-3}. Under such conditions, plasma environmental effects are weak and it is valid to use atomic data based on isolated atomic approximation.

3.2. EEDF and population distribution

Fig. 1 shows time evolution of EEDF obtained by solving Fokker–Planck equation at ion number density of 1.0 × 10^{19}, 1.0 × 10^{20} and 1.0 × 10^{21} cm^{-3} respectively. The peak intensity of the x-ray pulse is $I_0 = 4.0 \times 10^{16}$ W/cm^2. The electron population around 1100 eV originates from the K-shell single photoionization of neon atoms, whose K-shell threshold is 870.3 eV [47] and those around 1900 eV are caused by L-shell photoionization of neon atom. Obviously, the K-shell photoionization is much stronger than that of L-shell. With increasing time, more electron population is found at a lower electron energies. This is because more and more higher ionization stages are produced, which have higher ionization thresholds and consequently more lower energy electrons are produced. The electrons around 600–800 eV are due to Auger decay of K-shell hole states. The electrons located around 2800 eV are produced by electron impact, where an electron impacts an atom or ion in a highly excited state and then it de-excites to a lower state. However, the population is eight orders of magnitude smaller than the peak