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Evolution dynamics of charge state distribution in neon interaction with x-ray pulses of variant intensities and durations

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ABSTRACT

The level population and charge state distribution (CSD) of the neon atomic system interacting with x-ray pulses of variant intensities and durations at a central photon energy of 1110 eV are investigated by solving the time-dependent rate equations. The laser beam has a circular spot size with a Gaussian intensity pattern and the time history of the intensity is represented by Gaussian distribution in time. As an example, the CSD as a function of time is given at different distances from the spot center for an x-ray beam of intensity 1.5×10^{17} W/cm^2 and duration 75 fs (fs) for a spot size of 1 μm (full width at half maximum). The final CSD after averaging over the space and time is compared with a recent experiment and good agreement is found between the theory and experiment. Then systematic investigations are carried out to study the evolution of CSD with a wide range of intensity from 1.0×10^{15} W/cm^2 to 1.0×10^{19} W/cm^2 and duration from 30 fs to 100 fs. The results show that at intensities lower than 1.0×10^{15} W/cm^2, the CSD shows a typical physical picture of weak x-ray photoionization of the neutral atomic neon. At higher intensity, i.e., larger than 5.0×10^{16} W/cm^2, the dominant ionization stages are Ne^{7+} and Ne^{8+}, while the fractions of ions in the Ne^{3+}–Ne^{6+} stages are low for all laser durations and intensities.

1. Introduction

X-ray free-electron lasers such as the Linac Coherent Light Source (LCLS) [1] and the Spring-8 Angstrom Compact free electron LAser (SACLA) [2] open new possibility to investigate the physics of light-matter interaction in the short-wavelength regime at ultra-high intensity of ~10^{19} W/cm^2. A series of experiments [3–11] showed that the x-ray absorption is dominated by single photon ionization of deep inner-shell electrons yet resonance absorption [10,12] and two-photon absorption [6] play a role. These pioneering experiments investigated photoabsorption mechanisms by measuring the charge state distributions (CSD), which is of fundamental importance for any further studies such as equation of state and radiative property. These studies give us an understanding of the atomic response and absorption mechanism in the interaction of ultra-intense x-ray laser pulses with matters.

In the above experiments, there is a strong need to determine the physical parameters of the laser pulses such as the duration and intensity. However, accurate measurement of the duration and intensity of ultra-intense x-ray laser pulses is challenging. In the experiments, the duration of electron bunch and pulse energy can usually be accurately measured. Yet x-ray pulse duration is different from that of the electron bunch and their quantitative relation is difficult to measure. As a result, the intensity of x-ray laser pulses is usually difficult to be experimentally determined. Thus, it is necessary to develop reliable models with accurate atomic data as input to aid the experimental analysis and to infer or diagnose the x-ray pulse intensity. Such a requirement can easily be seen from the most recent experimental work on the interaction of high x-ray laser fluence with a liquid water jet [11]. Schreck et al. [11] reported on oxygen K-edge soft x-ray emission spectroscopy from a liquid water jet at LCLS. Significant changes in the spectral characteristics are found when they change the laser intensity. The authors explained these modifications are due to the reabsorption of x-ray emission by the quantum states generated by sequential Auger cascade. To quantify the reabsorption mechanism, one needs detailed and accurate model to describe the trend of population

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distribution with the variation of the laser intensity. However, such a quantitative and systematic theoretical investigations are lacking.

Hence it is worthwhile to systematically study the dynamics of atoms over a wide range of laser intensity and duration. In this work, we utilize a detailed level accounting (DLA) model to describe the interaction of x-ray radiation with atoms. A time-dependent rate equation (TDRE) approach [13,14] based on the collisional-radiative model is employed to obtain the CSD. The DLA method has been used to calculate the radiative opacity of hot dense plasmas in local thermodynamic equilibrium (LTE) [15–17]. Such a DLA formalism is also needed and more challenging for the highly transient plasmas produced by ultra-intense x-ray laser pulses. On one hand, more atomic data including the level-to-level excitation and ionization processes due to photons and electrons and Auger decay rate are required. On the other hand, the x-ray radiation excites and ionizes the deep inner-shell electrons and thus the atomic data such as Auger decay rates and photoionization cross sections for these highly excited states are difficult to be calculated accurately. Based on the DLA model, we systematically investigated the population dynamics for the interaction of x-ray laser pulses of different duration and intensity with neon. To have a more suitable description of the interaction of radiation and matters, we take the spatial distribution of the laser spot size and the energy spread of the incident x-ray laser beam into account. The energy spread of the laser beam is assumed to have a bandwidth of 0.5%.

2. Theoretical method

The TDRE approach is employed to study the dynamics of level population and CSD in the interaction of x-ray radiation with matters, where the rate coefficients are determined by the cross sections of microscopic processes due to photons and electrons [18,19]. The evolution of the population for level i in the matter system is determined by

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

where n_i is the population of level i and R_{ij} and R_{ji} represent the rate coefficients which depopulate and populate for the level i, respectively, and N_L is the total number of levels included in the rate equation. In this work, the levels of all ionization stages from the neutral to the fully stripped neon ions are included. The details of included levels in this work will be given in the following. Explicitly, photo-excitation, photoionization, electron impact excitation, electron impact ionization, Auger decay and their inverse processes are taken into account.

The rate coefficients contributed by the photo-excitation and photoionization processes are closely related with the radiation intensity. As we know, the intensity is in general a function of space, time and frequency of x-ray pulses. In principle, the intensity distribution with the space, time and frequency can be determined experimentally. However, such measurements are challenging at the level where femtosecond x-ray pulses are being used. In the present work, we assume the laser intensity has a Gaussian profile on space, time and frequency

$$I(r,t,h\nu) = I_0 e^{-\ln 2\left(\frac{r}{\Delta}\right)^2} e^{-\ln 2\left(\frac{t-t_0}{\tau}\right)^2} \sqrt{\frac{\ln 2}{\pi\Gamma^2}} e^{-\ln 2\left(\frac{h\nu-h\nu_0}{\Gamma}\right)^2}, \tag{2}$$

where I_0 is the peak intensity, t_0 is the center of temporal profile and $h\nu_0$ is the central photon energy of the x-ray pulse. Δ, τ and Γ are the half width at half maximum (HWHM) of Gaussian profile of the x-ray pulse for the distribution with respect to space, time and photon energy, respectively. Note that the dependence of intensity on photon energy (frequency) has been multiplied by a constant quantity to satisfy the normalization (to 1). The pulse energy of x-ray beams can be obtained by the integration over space, time and photon energy. The quantitative connection of pulse energy and intensity can help us better understand the physics of the interaction.

The rate coefficients used in the rate equation are determined by the cross sections of microscopic processes due to photons and electrons. The photoexcitation and photoionization rates $R_{ij}(r,t)$ from level i to level j irradiated by an x-ray pulse with intensity $I(r,t,h\nu)$ at spatial position r from the center of the laser spot and time t are obtained by Ref. [20].

$$R_{ij}(r,t) = \int \frac{I(r,t,h\nu)}{h\nu} \sigma_{ij}(h\nu) d(h\nu), \tag{3}$$

where $\sigma_{ij}(h\nu)$ is the photoexcitation or photoionization cross section at photon energy $h\nu$.

For electron impact excitation and ionization, the rate can be written

$$R_{ij}^e = n_e \int v(\varepsilon) f(\varepsilon) \sigma_{ij}^e(\varepsilon) d\varepsilon, \tag{4}$$

where $\sigma_{ij}^e(\varepsilon)$ means the cross section of electron impact excitation or ionization at electron energy ε, n_e is the electron density, and $f(\varepsilon)$ is the electron energy distribution function. In principle, $f(\varepsilon)$ should be obtained by solving the Boltzmann equations for the electrons that is coupled to the rate equations [21,22]. The evolution of $f(\varepsilon)$ with time is expressed as

$$\frac{df(\varepsilon)}{dt} = S(f(\varepsilon), \mathbf{N}), \tag{5}$$

where $\mathbf{N}$ is the population distributions of levels obtained by solving rate equation and S is the source function which is contributed by elastic and inelastic collisions. The elastic electron-electron contribution can be evaluated by using the Fokker–Planck equation and the inelastic contribution includes the microscopic atomic processes involving photons and electrons as mentioned above for the rate equation. The detailed descriptions for the construction of S can be found in Ref. [22].

3. Atomic model and atomic data

To consider all possible channels due to photo-excitation, photoionization and Auger decay, we include the quantum states of excitation of up to two 1s electrons from the respective ground configuration for all ionization stages from the neutral atom to bare ion in the rate equation. Explicitly, the fine structure levels belonging to the configurations of respective neon ions given in Table 1 are used to construct the rate equation. In this table, we have used a simplified notation to designate the configurations. $(N)^M$ means possible arrangement of the M electrons in the orbital with principle quantum number N. For examples, $(1)^2(2)^6(3)^1$ in Ne^{1+} includes configurations of $1s^22s^22p^43l$, $1s^22s2p^53l$, and $1s^22p^63l$ (l=s, p, and d), which has a total number of 9 configurations. The designations beginning with $(1)^1$ and $(1)^0$ in Table 1 means single and double K-shell core-hole states. The x-ray radiation effectively photoionizes the inner-shell electrons and then the single core-hole states relax dominantly by Auger decay. If the intensity is large enough, the K-shell electron of the single core-hole