POPULATION KINETICS MODELING FOR NON-LTE AND NON-MAXWELLIAN PLASMAS GENERATED IN FINITE TEMPERATURE DENSE MATTER EXPERIMENTS ARISING FROM SHORT PULSE X-RAY SOURCES

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Abstract. *The short pulse x-ray sources will provide a major advance in dense matter studies important to understand implosion physics for ICF as a generator of warm dense matter or a probe of finite temperature dense matter. The interaction of such a high-energy photon pulse with the initially solid matter creates highly transient states of plasmas initially whose relaxation processes are of interest to the equation of states or spectral properties of these matter. For these plasmas, assumptions such as LTE population distributions or Maxwellian electron energy distributions should be tested by employing a method that does not make these assumption a priori.*

Our goal is to present a model that can be used to simulate the electron distributions, the ionization balance and the spectral output of transient systems generated in the future ICF experiments. We report on the progress in developing a non-LTE atomic population kinetics code integrated with Boltzmann equation solver to provide a self-consistent time-dependent solution of the level populations and the particle energy distributions.

I. INTRODUCTION

Recent advances in lasers e.g. long-pulse National Ignition Facility (NIF), short-pulse high-power (petawatt) lasers or short-pulse x-ray free electron lasers (XFEL) will play a critical role in finite temperature dense matter studies. Warm dense matter is defined as a region between a solid and a plasma and will be found in virtually every plasma device where a solid is heated up rapidly, including inertial fusion devices. While the equation of states and spectral properties of such matter are of fundamental interest, they have not been confirmed. By creating warm dense matter or as a probe of such matter, the x-rays from short pulse laser plasmas or next generation light sources will provide an experimental test-bed for the existing theories. In addition to warm and hot dense matter studies, the short-pulse x-rays from XFEL will be used in a wide range of applications including studies of biology and material structure.

The interaction of the high-energy photons with the initially solid density matter proceeds predominantly by the creation of inner-shell ionization. This is followed by Auger decay and then by interaction of lower energy electrons with the atoms. The timescales for these various processes affecting population distributions as well as electron energy distributions are comparable to the duration of the short pulse x-ray sources being developed, i.e., in the sub-picosecond regime. The highly transient nature of the system, the strongly non-Maxwellian nature of the electron energy distributions, and the coupling of the electrons with the initially structured solid density material requires the development of a novel approach for the study of the properties of these systems. For example, the petawatt laser interaction with solids of interest to the fast ignitor concept the development of a tool that can be used to simulate the spectrum of these highly transient states is important so that one can study the effects of the non-thermal transient processes on the equation of states and ionization distributions.

The goal of this effort is a model that can be used to simulate the electron distributions, the ionization balance and the spectral output of these transient systems. We report on the progress in developing a non-LTE atomic population kinetics code integrated with Boltzmann equation solver to provide a self-consistent time-dependent solution of the level populations and the par-

ticle energy distributions. First, we develop a code FLYCHK by extending the K-shell spectroscopy code FLY to include L- or M-shell models for near-neutral species. Schematic level structures are applied for L- or M-shell models with appropriately scaled atomic cross-sections. Second, we incorporate Boltzmann equation solver (ZELDA) into FLYCHK to obtain self-consistent velocity distribution and population kinetics solutions. Finally, we will apply the new model to study examples of non-LTE and non-Maxwellian plasmas generated by intense sub-picosecond x-ray sources.

II. POPULATION KINETICS MODEL

II.A. FLYCHK

The K-shell spectroscopy code FLY has been widely used as a useful and reliable tool to study hot dense plasmas. [1] Both steady-state and time-dependent population distributions of K-shell ions and Li-like ions can be calculated from rate equations using highly accurate atomic data for all relevant collisional and radiative processes. The FLY suite is not only easy-to-use but also provides graphics tools to plot line ratios and synthetic spectra for on-line analysis of x-ray measured data. The code has been validated and benchmarked over the past two decades by numerous experiments generating highly ionized plasmas such as laser-produced plasma or radiatively-driven implosion experiments. Although FLY has been used successfully for hot dense plasmas, it will not be adequate to study near-neutral species found in warm dense matter due to the simple model of species less ionized than Li-like. In order to improve and make FLY applicable to plasmas that are colder and/or less ionized, the extended code FLYCHK has been proposed. It is our goal to make FLYCHK general and portable and eventually available for researchers interested in studying highly non-equilibrium states of hot and warm dense matter.

In order to make the atomic model general while maintaining the computational efficiency, a screened hydrogenic model is applied to describe the ground and excited states of L-shell and M-shell ions. Autoionizing inner-shell excited levels are also included since they are essential to study the relaxation processes of photo-electrons and Auger electrons after x-ray pumping. The bound level structure of the model is defined by ionization potentials of individual levels. The ionization potential of the ground state is taken from the empirical values [2] and that of an excited level with a outermost bound electron of principal quantum number n is computed using the hydrogenic approximation with relativistic corrections [3, 4]. The difference between the two ionization potential defines the excited level energy with respect to the ground state. The energy of the first inner-shell excited level with respect to the ground state of its ionization stage is obtained as the difference between the ionization energy of the inner-shell electron obtained with the screening coefficients [3, 4]. and that of the ground state of the next ionization stage.

For collisional and radiative data, scaled hydrogenic formula are applied. An absorption oscillator strength of a transition from a level n to a level m is defined with hydrogenic oscillator strength multiplied by the occupation number of the level n. We use collisional excitation cross-sections based on the absorption oscillator strength for the allowed transitions [5]. For bound-free processes, Kramers' quasi-classical photoionization cross-sections are used [6]. A semi-empirical formula of Burgess and Chidichimo [7] is used for collisional ionization from a level n. For the photoionization and autoionization processes involving inner-sell excited levels, more accurate cross-sections are required. Hence, the K-shell and L-shell photoionization cross-sections are computed for hydrogenic levels by using Hartree-Fock-Slater wave functions [8, 9]. Autoionization rates calculated by perturbation theory in the Dirac-Hartree-Slater approach [10, 11]. Details of atomic data implemented in FLYCHK can be found in the previous publication [12]

Dielectronic recombination(DR) processes are implemented by using effective DR recombination rates from the ground state of the recombining ion to an excited state of the recombined ion via autoionizing states not explicitly included in the model. In order to insure the detailed balance of DR processes, excitation autoionization(EA) processes are similarly implemented by using effective EA rates from an excited state of an ion to the ground state of the next ion. The effective EA and DR rates are computed with scaled hydrogenic cross-sections and in general the DR rates are comparable to Burgess-Mertz formalism [13] within a factor of two .

II.B. ZELDA

A Boltzmann equation solver for Z-scaled electron distribution function, also known as ZELDA, calculates the electron energy distribution. For a given ion population distribution and electron-ion collisional cross-sections, ZELDA calculates the time-dependent electron energy distribution function from the Boltzmann transport equation including following processes: (1) Elastic losses to phonon (deformation potential) scattering (2) Inelastic (excitation) and superelastic (de-excitation) scattering of bound states (3) Sources such as photo and Auger electrons or collisionally ionized electrons (4) Sinks by 3-body, dielectronic, and radiative recombina-

tion (5) Electron thermalization due to collisions with other electrons The theoretical and numerical details of this solver can be found in the previous publication [14]. More details on the coupling to population kinetics code as well as assumptions on source and sink distributions will be given elsewhere.

II.C. Ct27

The kinetics code FLYCHK requires an electron energy distribution function as an input in order to compute atomic level population distributions on which the distribution function itself depends. The new code, tentatively called Ct27, is a kinetics code based on FLYCHK incorporated coupled with a Boltzmann solver ZELDA, and calculates time-dependent population distributions self-consistently to the electron energy distribution.

Stewart-Pyatt formalism overestimates an ionization potential depression (IPD) at low temperatures for near-neutral system in solid states where ions are in lattice structure. In order to take an account of solid structures at the very beginning of the interaction between the solid matter and x-ray pulse, a quadrature formalism is proposed for the IPD. The formalism using the ion-sphere radius (r_i), debye length (r_d) and the lattice constant (r_a) will give an IPD at both low and high Te limits for finite temperature dense matter and is written as following.

$$IPD(eV) = 1.45 \times 10^7 Z/(r_a^2 + r_i^2 + r_d^2)^{1/2} \qquad (1)$$

where Z is the ionization stage of the ion (e.g. 1 for neutral atom) and

$$ra = 10^{-8}/Z^2 + 0.3 \times 10^{-8} Z \qquad (2)$$

The validity of this formalism will be investigated in the future publication.

III. PRELIMINARY RESULTS

Recent advances in laser and beam technology have led to the generation of near-neutral plasmas with low temperatures of a few eV and near-solid density. Plasma states of such warm dense matter are not very well understood so far [15, 16] and there is a growing interest in plasma, condense-matter and statistical physics communities. It is our goal to apply the L- and M-shell model in Ct27 to study warm dense plasmas as well as hot dense plasmas. Here, we show that Ct27 is a potential tool to study population relaxation and ionization distributions of such plasmas.

As the first step, we study a case where a 20 μ thick solid Al target is illuminated by a 200 fs pulse with 10^{12} photons each of 200 eV, a case relevant to the XUV-FEL at DESY [17]. We have demonstrated in our previous publication [12] that the inner-shell ionization energy deposition model in FLYCHK is reasonable and the population distributions correctly reach the equilibrium value if electrons reach the thermalization instantaneously. Under this assumption, initially T_e corresponds to the energy of the ejected electron. As electrons are liberated by Auger processes and collisional ionization, T_e decreases rapidly as the energy deposited by laser is distributed to electron kinetic energy and the internal energy of ions. While the internal energy rises as excited and ionized levels are populated from the ground state by electron collisions, the levels also reach the collisional equilibrium and hence the growth rate of internal energy slows down. Once equilibrium is set up, T_e rises since photo-absorbed energy is passed to electron kinetic energy.

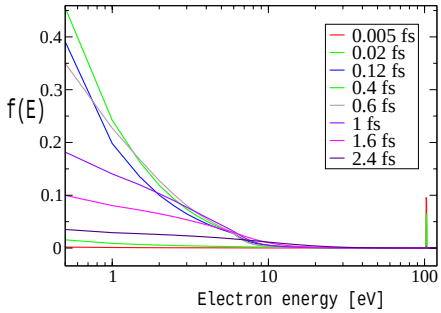

FIGURE 1. Electron energy distribution function during the fi rst few femtoseconds

In this paper, we would like to investigate the relaxation of electron energy distribution for the first few femto-seconds. Fig.1 shows that initially electrons photoionized by x-ray pulse have energies at 105 eV and then get thermalized to the lower electron energies within the tenth of femto-seconds. It is noted that the ion density is assumed to be solid density and hence within the tenth of femto-seconds, the electron density has already reached at 10^18 cm^3 leading to a fast thermalization.

The mean average energy of electrons is shown in Fig.2 by electron temperature. The temperature (or 2/3 of mean average energy) decreases as secondary electrons are liberated by collisions and Auger processes before rising after 1 femtosecond. It is encouraging to see that the new code allows one to study the electron energy relaxation with time in detail and the results so far are consistent to what we observed with our previous study of instantaneous thermalization. It should be noted, however, we made several assumptions that need more investigation for these results. They include the validity of the IPD model, electron sink or source distributions due

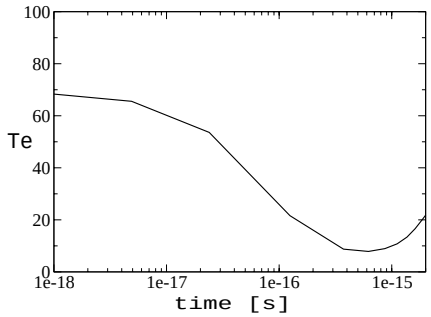

FIGURE 2. Electron temperatures during the first few femtoseconds. Note that the temperature is defined as 2/3 of average energy.

to ionization and recombination, sensitivities of energy grid on results. More investigations will be on the way.

SUMMARY AND FUTURE WORK

The new development of x-ray free electron lasers will lead to a new regime of finite-temperature dense matter studies. We have been developing a capability to study the electron distributions, the ionization balance and the spectral output of dense matter. Here, we introduce the physics and applications of our new code Ct27 which calculate self-consistent population distributions and electron distributions as a function of time. There is more work to be done to validate and benchmark this code for realistic results of dense matter studies.

ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

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