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Non-LTE kinetics modeling of krypton ions: Calculations of radiative cooling coefficients

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Abstract

For plasmas containing high-Z ions the energy loss due to radiative processes can be important in understanding energy distributions and spectral characteristics. Since high-Z plasmas occur over a wide range of temperature and density conditions, a general non-LTE population kinetics description is required to provide a qualitative and quantitative description for radiative energy loss. We investigate radiative properties of non-LTE krypton plasmas with a collisional–radiative (CR) model constructed from detailed atomic data. This work makes two extensions beyond previous non-LTE kinetics models. First, this model explicitly treats the dielectronic recombination (DR) channels. Second, this model allows one to investigate the higher electron density regimes found commonly in laboratory plasmas. This more comprehensive approach enables the study of population kinetics in a general manner and will provide a systematic guide for reducing a complex model to a simpler one.

Specifically, we present the calculations of radiative cooling coefficients of krypton ions as a function of electron density in the optically thin limit. Total, soft X-ray (1.6 keV $\leq E \leq$ 12 keV), and hard X-ray ($E \geq$ 12 keV) radiative cooling coefficients are given for the plasma conditions of 0.6 keV $\leq T_e \leq$ 10 keV and 10^{14} cm^{-3} $\leq N_e \leq 10^{24}$ cm^{-3}. The ionic radiative cooling coefficients provided are sufficient to allow users to construct the total rate from given charge state distributions. Steady-state calculations of the average charge state at given T_e and N_e values are also presented.

Keywords: Collisional–radiative modeling; Non-LTE kinetics; Plasma spectroscopy; Radiative cooling rates; Radiative loss rates; Krypton; Power loss

1. Introduction

Radiation emitted from high-Z plasmas is of importance to astrophysical and laboratory plasma researchers. For example, emission of radiation plays a role in evolution of tokamak plasmas in the divertor region [1,2], in astrophysical blast waves [3,4] and for the development of light sources [5–13]. In particular, krypton has been used recently in studies of EUV and X-ray generation [5–13] using electron-beam ion trap (EBIT) [5,6], pulsed-power devices [7,8], laser-produced plasmas [9], and laser absorption in gas clusters or droplets [10,11]. These krypton plasmas range from temperatures T_e of a few eV to a few keV and from electron densities $N_e < 10^{14}$ cm^{-3} to $N_e \sim 10^{23}$ cm^{-3}. Moreover, the maximum plasma density achievable in the laboratory should increase even further when the National Ignition Facility begins to operate at full power [14]. To study energy distributions and spectral characteristics one requires quantitative information on emission intensities over this large plasma condition parameter space.

For plasmas in the coronal limit the steady-state cooling rate coefficients have been available for decades [15,16]. Recently, radiative cooling coefficients for krypton were provided by Fournier et al. [1] for the coronal limit, i.e., low-electron-density plasmas ($\leq 2 \times 10^{14}$ cm^{-3}) and validated by comparison with krypton cooling rates derived from tokamak experiments. At low densities, the population in each ion is concentrated in its ground state, and one calculates

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populations of excited levels by collisional excitation from the ground level so that these populations are proportional to N_e. This leads to a linear dependence on N_e for the emitted radiation. On the other hand, at sufficiently high electron densities, the plasma should approach local thermodynamic equilibrium (LTE). In the LTE limit, the relative bound state population densities are given by the Boltzmann distribution for the bound states and Saha–Boltzmann distribution for the relative populations of the ions. Thus, the radiative properties of LTE plasmas can be determined without the need to calculate collisional processes.

On the other hand, in the regime between these two limits level population densities do not depend linearly on electron density, as ionization from the excited states will modify the total ionization process. As the density increases beyond the coronal limit, partial LTE will be established amongst excited levels of an ionization stage and possibly these excited levels come into Saha–Boltzmann equilibrium with the ground state of the next ionization stage. In order to study radiative properties of plasmas with intermediate electron densities, a population kinetics model needs to account for both collisional and radiative processes. In the previous work by Apruzese and Kepple [17] only a sufficient number of excited states (≤13 per ion) were included to provide qualitatively correct behavior beyond coronal limit and excitation–autoionization and dielectronic recombination were not included in a manner that permits detailed balancing, but was included in a bulk rate. However, to study the convergence of the kinetics model to provide the correct *quantitative* behavior more detailed set is required. Indeed, the model presented here permits not only the study of the number of states required for convergence but also maintains the strict detailed balancing of all processes required for the general descriptions.

In this work, we present a systematic study of a general non-LTE kinetics model and radiative cooling coefficients in the optically thin limit. The level population distribution is calculated by using the collisional–radiative (CR) approach where atomic two and three-body processes are considered in detail. We describe the atomic data and CR model in Section 2 and review assumptions made to construct the model in Section 2.3.[1] When line trapping is important, the level population should be solved self-consistently with the radiative transport equation for the particular problem and hence it is beyond the scope of this work. Thus, the results from the CR model for the radiative cooling rate coefficients of krypton ions and charge state distributions for electron temperatures in the range 0.6 keV $\le T_e \le$ 10 keV and densities, 10^{14} cm^{-3} and 10^{17} cm$^{-3} \le N_e \le 10^{24}$ cm^{-3} in the optically thin limit, are presented in Section 3. Radiative yields, i.e. energy per second per atom, in X-ray energies between 1.6 keV and 12 keV and greater than 12 keV are presented along with the total yield integrated overall energies. We discuss population kinetics at various electron densities together with the validity and limitation of the present model in Section 3.3.

[1] As demonstrated in the non-LTE kinetics workshop [18], charge state distributions and spectral calculations for high-Z plasmas can vary significantly depending on assumptions made for CR models.

2. Theoretical method to determine radiative rates

The emitted radiation for ion i at T_e and N_e is obtained from

$$L^i(T_e,N_e) = \sum_{jf} I^i_{jf}(T_e,N_e) \quad [\mathrm{eV/s/ion}] \tag{1}$$

where I^i_{jf} is the photon emission coefficient for a transition from level j to level f. Assuming the plasma is optically thin, I^i_{jf} is given by

$$I^i_{jf}(T_e,N_e) = h\nu_{jf} A_{jf} n^i_j(T_e,N_e) \tag{2}$$

where the $h\nu_{jf}$ is the transition energy, A_{jf} is the spontaneous decay rate of a transition $j \rightarrow f$ and n^i_j is a fractional population density of the upper level j within the ionization stage i where $\sum_j n^i_j = 1$. The total radiative loss rate for line radiation from an atom for given plasma conditions is obtained from the sum of the radiative cooling coefficients of each ion weighted by charge state distribution

$$P(T_e,N_e) = \sum_i L^i(T_e,N_e) \times y_i(T_e,N_e) \tag{3}$$

where y_i is the fractional density for ionization stage i of an atom and $\sum_i y_i = 1$.

In addition, the total radiative loss rate from atoms in a plasma must include contributions from the bound–free and free–free continuum radiation. The intensity of a radiative recombination transition from a bound state k of an ionization stage i to a bound state f of the ionization stage $i-1$ is given by integrating the free–bound emissivities over the relevant photon energy range. That is,

$$I^i_{kf}(T_e,N_e) = n^i_k(T_e,N_e) \times \left[\frac{n^{i-1}_f}{n^i_k}\right]^{\mathrm{LTE}} 4\pi \int_{\nu_0}^{\infty} \mathrm{d}\nu \left(\frac{2h\nu^3}{c^2}\right) \exp\left(\frac{-h\nu}{kT_e}\right) \alpha_{fk}(\nu) \tag{4}$$

where $\alpha_{fk}(\nu)$ is the photoionization cross-section from the state f to the state k and ν_0 is the threshold frequency, and the LTE population ratio $[n^{i-1}_f/n^i_k]^{\mathrm{LTE}}$ is obtained from Saha equation. Total energy loss coefficients [eV/s/atom] for radiative recombination radiation are obtained from Eqs. (1), (3) and (4). The energy emitted from free–free transitions, i.e., bremsstrahlung radiation, is given for a pure Coulomb field as following [19]:

$$P(T_e,N_e) = 9.55 \times 10^{-14} N_e T_e^{1/2} \sum_i Z_i^2 y_i \left\langle g_{ff} \right\rangle \quad [\mathrm{eV/s/atom}] \tag{5}$$

where T_e is in the unit of eV and $\langle g_{ff} \rangle$ is the free–free gaunt factor [20].