Enhancement of Effective Excitation Rate Coefficients of Ions in Dense Plasma through Doubly Excited States

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We constructed a collisional-radiative model including doubly excited states for a two electron ion. We study the density effects on the effective rate coefficients and the n -dependence of the population densities where n is the principal quantum number. The effective $1s$ - $2l$ excitation rate coefficients increase with increasing electron density due to the indirect process. We also found that for $2s$ - $1s$ de-excitation, l -changing transitions, $2snl$ - $2pnl$, are important at intermediate densities. The population densities per statistical weight for doubly excited states attain a scale of n^{-4} at very high density in ionizing plasmas.

Keywords: collisional-radiative model, dense plasma, population density, effective rate coefficient

The effective rate coefficients in hot dense plasma where ladder-like excitation-ionization processes are important were studied by Fujimoto and Kato[1]. They examined $1s$ - $2s$ excitation / de-excitation using a collisional-radiative model (CRM) including doubly excited $2snl$ states as well as $1s$ - $2p$ excitation / de-excitation including doubly excited $2pnl$ states. They found an enhancement of the excitation and de-excitation rate coefficients with increasing electron density. Approximate descriptions for the effective rate coefficients are important in treating the large number of excited states. Thus study for systematic treatment of the effective rate coefficients is required.

We constructed a new CRM including $1snl$, $2snl$, $2pnl$, $3snl$, $3pnl$, and $3dnl$ doubly excited states. Our model contains a total of 255 levels. Our CRM includes $1s^2$, $1s$, $2l$, and $3l$ states and 60 singly excited $1snl$ states, 118 doubly excited $2l'nl$ states and 70 doubly excited $3l'nl$ states, where n is up to 20. The atomic processes considered in our model are excitation/de-excitation by electron impact, ionization/three-body recombination, radiative transitions, radiative recombination and autoionization/dielectronic capture. Atomic data used in our CRM for $1snl$ and $2l'nl$ states are the same as those described in ref.[1]. For $3l'nl$ states

we calculated the data using HULLAC code[2]. We used the excitation rate coefficients taken from hydrogen-like ions for $1snl$ - $2l'nl$ [3], $1snl$ - $3l'nl$, $2l'nl$ - $3l'nl$, and $2snl$ - $2pnl$ [2] transitions.

We solved rate equations for singly and doubly excited states assuming a quasi steady state for these excited states. The population densities can then be expressed as a sum of independent contributions from each $1s^2$, $1s$, $2l$, and $3l$ state, as follows:

$$N_i = \sum_y r_i^{(y)} N_e N_y, \quad (1)$$

where N_i is the population density of an excited i -th state, $r_i^{(y)}$ is a population density coefficient of an i -th state for the contribution from a y state, N_e is the electron density, and N_y is the population density of an independent state y ($1s^2$, $1s$, $2l$, and $3l$). The effective rate coefficients from the y to the y' state are derived from rate equations of the y state and are written as follows:

$$C_{y,y'}^{CR} = \sum_i W_{y,i} r_i^{(y)}, \quad (2)$$

where $W_{y,i}$ is a transition rate from the i state to the y state.

Indirect contributions to effective $1s$ - $2s$ and $1s$ - $2p$ excitation rate coefficients exceed each direct excitation rate coefficient at $N_e \sim 10^{19} \text{ cm}^{-3}$ for $Z = 6$ ions as shown in Fig.1. Indirect contributions

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through autoionization ($3l'nl$ to $2l$) after dielectronic capture ($1s - 3l'nl - 2l$), which is a resonance contribution, are important at low density. This resonance contribution decreases with increasing electron density at $N_e > 10^{21} \text{ cm}^{-3}$, as predicted in Ref.[4] by ladder-like excitation-ionization process $1s \rightarrow 3l'nl \rightarrow 3l'n''l'' \rightarrow 3l'$. With increasing density, indirect contributions through dielectronic-capture ladder-like excitation-ionization, $1s \rightarrow 2l'nl \rightarrow 2l'n''l'' \rightarrow 2l'$ increase. At very high density ($> 10^{21} \text{ cm}^{-3}$), indirect processes $1s - 1snl - 2l'nl \rightarrow 2l'$ increase the effective rate coefficients proportionally to N_e [5]. We also found that for $2s$ - $1s$ de-excitation, l -changing transitions, $2snl$ - $2pnl$, are important at intermediate densities.

Fig.1. The effective $1s$ - $2p$ excitation rate coefficients for $Z = 6$ at $T_e = 3.5 \times 10^5 \text{ K}$. Solid lines: indirect contribution including $2l'nl$ and $3l'nl$ states, dotted lines: without $3l'nl$ states, dot-dashed line: dielectronic capture resonances through $3l'nl$ states, dot-dot-dashed lines: direct $1s$ - $2p$,

Two population mechanisms are considered for doubly excited states at high density in ionizing phase ($N_{Is} = 1$). The first one is dielectronic capture ladder-like excitation-ionization, $1s \rightarrow 2l'nl \rightarrow 2l'n''l'' \rightarrow 2l'$, where contributes to the increase in the effective excitation / de-excitation. The second one is indirect process $1s - 1snl - 2l'nl \rightarrow 2l'$ where the excitation $1snl - 2l'nl$ process is important to produce the population densities of $2l'nl$ states. At high density, a population density for a high- n doubly excited state q ($2l'nl$) can be written approximately using the method described in Ref.[4],

Fig.2 population density per statistical weight for doubly excited states $2snl$ for $Z = 6$ at $T_e = 3.5 \times 10^5 \text{ K}$.

$$N_q \sim \frac{C_{q-1,q}}{C_{q,q+1}} N_{q-1} + \frac{C_{i,q}}{C_{q,q+1}} N_i. \quad (3)$$

The excitation rate coefficients are scaled as $C_{q-1,q} \propto (n-1)^7/n^3$, $C_{q,q+1} \propto n^7/(n+1)^3$. The excitation rate coefficients $C_{i,q}$ for $1snl$ - $2l'nl$ do not depend on a principal quantum number n . We can derive $N_q \propto n^{-4}$ or $N_q/g_q \propto n^{-6}$ from the first term in eq.(3), as is shown in Ref.[6], where g_i is a statistical weight. The second term in eq.(3) corresponds to the second population mechanism, and $N_q \propto n^{-2}$ or $N_q/g_q \propto n^{-4}$ is derived since $N_i \propto n^2$ in LTE. At very high density, the second process has a stronger effect than dose the first. So n -dependence of the population density per statistical weight changes from n^{-6} to n^{-4} at very high density as shown in Fig.2.

The results in this paper are obtained from the definition in Eq.(2). A different definition might produce less dramatic enhancement of the effective rates. Our model still contains several problems that remain to be solved. These include 1) the treatment of high Rydberg states near the continuum states, and 2) the lowering of the levels by pressure ionization, etc. In future study we will examine the effect of these factors on our effective rate coefficients.

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