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The effect of configuration complex on dielectronic recombination process in highly ionized plasmas*

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This paper analyses the effect of configuration complex on dielectronic recombination (DR) process in highly ionized plasmas (Xe^{26+}, Dy^{38+}, W^{46+}) by using the multiconfiguration relativistic Hartree–Fock method. Resonant and nonresonant radiative stabilizing transitions and decays to autoionizing levels followed by radiative cascades are included. Collisional transitions following electron capture are neglected. The remarkable difference between the isoelectronic trend of the rate coefficients for DR through $3d^9 4l4l'$ and through $3d^9 4l5l'$ is emphasized. The trend of DR through $3d^9 4l4l'$ shows irregularities at relatively low temperature due to the progressive closing of DR channels as atomic number Z increases.

Keywords: dielectronic recombination, autoionization, radiative-decay
PACC: 5225，3480L

1. Introduction

The knowledge of accurate ionization and recombination rates of heavy ions is crucial for the study of ionization balance of highly ionized elements in hot plasmas.[1−3] This knowledge is also important for the research of x-ray lasers, specifically for calculating the populating and depopulating of lasing levels.[4,5] It finds that the position of 3d-inner-shell excited configurations is above or below the ionization limit depending on the atomic number Z.[6] In order to complete the accurate ionization balancing, precise data on recombination rates are needed. The main recombination process in highly ionized plasmas is the dielectronic recombination (DR). Previous works on this sequence were performed only for Gd^{36+}[7] and Ta^{45+}[8] by using the multi-configuration Dirac–Fock model. In the present work, we consider the two Cu-like configurations $3d^9 4l4l'$ and $3d^9 4l5l'$ which are expected to give the strongest contributions to DR. All calculations assume that no collisional transitions occur after the initial electron capture. The resonant radiative transitions and nonresonant stabilizing transitions are considered. Since in the CuI isoelectronic sequence some inner-shell excited levels (of the $3d^9 4l4l'$ configuration complex) lie below the ionization limit, nonresonant decays from the autoionizing levels towards these levels constitute a stabilizing channel for the effective DR process, and thus might be of significant importance to the DR rates.

2. Theory and formulas

We consider the DR of a Ni-like ion in its ground state $3d^{10}$, through a Cu-like $3d^9 4ln'l'(n' = 4, 5)$ inner-shell excited level lying above the ionization limit, to any final state below the ionization limit. This process can be schematically represented by

$$\begin{aligned}&[\text{Ar core}]3d^{10} + e^- \leftrightarrow \\ &[\text{Ar core}]3d^9 4ln'l' \quad (n' = 4, 5),\end{aligned} \tag{1}$$

$$\begin{aligned}&[\text{Ar core}]3d^9 4ln'l' \rightarrow \\ &[\text{Ar core}]3d^{10} n''l'' + h\gamma,\end{aligned} \tag{2a}$$

or

$$\begin{aligned}&[\text{Ar core}]3d^9 4ln'l' \rightarrow \\ &[\text{Ar core}]3d^{10} 4l4l'' + h\gamma,\end{aligned} \tag{2b}$$

where $[\text{Ar core}]3d^{10}$ represents a Ni-like ion , [Ar core] symbolizes the full $1s^2 2s^2 2p^6 3s^2 3p^6$ electron inner shells, e^- is the interacting free electron and $h\gamma$ is the emitted photon. The first process is the electron capture which is reversible by autoionization, whereas processes (2a) and (2b) are the resonant and nonresonant radiative stabilizing transitions, respectively. Nonresonant stabilizing transitions refer to radiative

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decays from autoionizing levels to inner-shell excited levels below the ionization limit. In case where the radiative decay from the $3d^9 4ln'l'$ level is to another inner-shell excited level above the ionization limit, the stabilization can be reached after several consecutive radiative transitions.

In the present work, neglecting electron collision processes for depletion of excited level, we find that the inner-shell excited Cu-like ion in level d can either autoionize back to Ni-like ion or decay radiatively. The configurations that we considered are $3d^{10}4s$, $3d^9 4s4p$, $3d^9 4s4d$, $3d^9 4p^2$, $3d^9 4p4d$, $3d^9 4s4f$, $3d^9 4p4f$, $3d^9 4s^2$, $3d^9 4p^2$, $3d^{10}5s$, $3d^9 4s5s$, $3d^9 4s5p$, $3d^9 4s5f$, $3d^{10}5f$. The mean DR rate coefficient for a given configuration c is defined by

$$\overline{\alpha_c^D} = 1.656 \times 10^{-22} kT_e^{-3/2} \times \exp\left(\frac{-\overline{\Delta E_c}}{kT_e}\right) \frac{1}{g_k} \frac{\left(\sum_d g_d A_{dk}^a\right)\left(\sum_d \sum_i A_{di}\right)}{\left(\sum_d \sum_{k'} A_{dk'}^a + \sum_d \sum_i A_{di}\right)},$$

where $\overline{\Delta E_c} = \overline{E_c} - E_I$, $\overline{E_c}$ is the statistically weighted average energy of the configuration and E_I the ionization energy. $\overline{\Delta E_c}$ and kT_e are expressed in eV. Here $\sum\sum A_{dk'}^a$ is the sum of the coefficients for autoionization to all possible Ni-like states, $\sum g_d A_{dk}^a$ is the statistically weighted sum of the coefficients for autoionization to $3d^{10}$ and $\sum\sum A_{di}$ represents the sum of the radiative decay coefficients for all the transitions. The formulas about autoionization rate coefficients and radiative decay coefficients is in Ref.[9].

3. Conclusion

The detailed level energies were computed using the relativistic multi-configuration Hartree–Fock method.[10] The autoionization and radiative-transition rate coefficients are computed in the model of SOSA (spin-orbit-split-array) and then we obtain the value which is needed in the calculation formulas. In the process of calculating autoionization rate coefficients, the relativistic Slater integrals are calculated in the procedures of RCG and RCN.[11] In order to prove the feasibility of this method, we compare the results of Bauche–Arould in Ref.[9] who used means of a relativistic parametric potential central-field code to compute the autoionization coefficients of Ta^{45+} with the results of this method under the same condition and the DR coefficients of Xe^{26+} ions at T=200eV in Ref.[12]. The results are very close with each other.

Figure 1 displays the total rate coefficients for DR through the whole $3d^9 4l4l'$ configuration complex as a function of the electron temperature in the 20eV$\leq kT_e \leq$ 200eV range for the three ions (Xe^{26+}, Dy^{38+}, W^{46+}) considered. The configuration interaction is considered in the $3d^9 4l4l'$ case.[13] The interactions between $3d^9 4s4d$ and $3d^9 4p^2$, $3d^9 4p4d$ and $3d^9 4s4f$, and $3d^9 4p4f$ and $3d^9 4d^2$ are particularly important. For this reason the summed coefficients for DR through the mixed configurations are given in these cases. The influence of configuration mixing on DR rate has been checked for the $3d^9 4l5l'$ configuration complex as well, and is found to be much less crucial than for $3d^9 4l4l'$ complex. Figure 2 displays the total rate coefficients for DR through the whole $3d^9 4l5l'$ configuration complex as a function of the electron temperature in the 200eV$\leq kT_e \leq$ 2000eV range for the three ions considered.

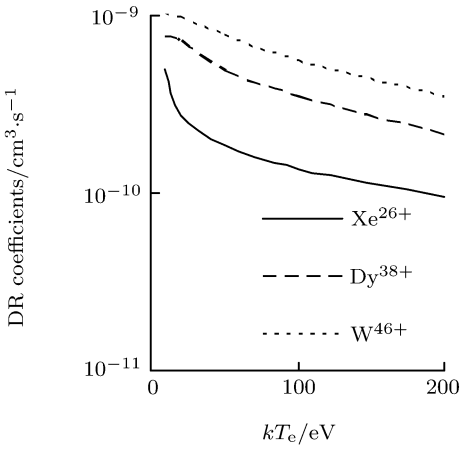


Fig.1. Rate coefficients for DR of Ni-like through the whole Cu-like $3d^9 4l4l'$ complex as a function of the electron temperature.

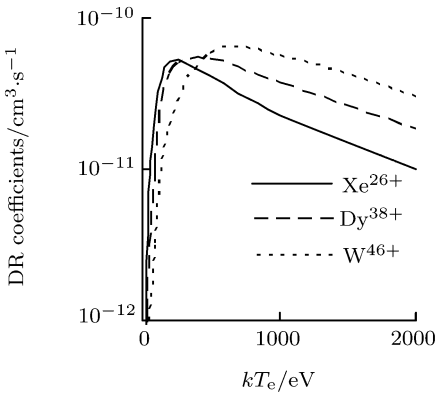


Fig.2. Rate coefficients for DR of Ni-like through the whole Cu-like $3d^9 4l5l'$ complex as a function of the electron temperature.

In the temperature range exhibited, DR through $3d^9 4l4l'$ is the prevalent DR process especially for heavy element due to the exponential dependence on $-\overline{\Delta E_c}/(kT_e)$. As can be seen in Fig.1, at low electron temperature the DR coefficients show a rather complex dependence on electron temperature, which is different from ion to ion. This is explained by the fact that some autoionizing levels very close to the ionization limit can considerably enhance the DR rate. In this case, only detailed calculations including configuration mixing are reliable. For the $3d^9 4l5l'$ configuration complex, in which all levels are above the ionization limit and configuration interaction are relatively unimportant.

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