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Dielectronic Recombination processes of \( \text{Xe}^{10+} \) ions

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Abstract. EUV light sources from compact plasmas are now intensively studied for the next generation of lithography. The multicharged Xe ions emit EUV emission and are now investigated extensively. However we do not know the detailed atomic processes for there Xe ions. We have calculated the energy levels, radiative transition probabilities (Ar), autoionization rates (Aa), and radiative recombination cross section for \( \text{Xe}^{10+} \) ions using the FAC code. The dielectronic recombination rate coefficient (\( \alpha_{DR} \)) from the \( \text{Xe}^{10+} \) ions and the related dielectronic satellitie lines are obtained. The dielectronic recombination processes for the \( 4d^8 + e \rightarrow 4d^7 4f^1 nl \rightarrow 4d^8 nl + h\nu \) and \( 4d^8 + e \rightarrow 4d^7 5p^1 nl \rightarrow 4d^8 nl + h\nu \) become important at low plasma temperature \( T_e \approx 10 \text{eV} \) for line intensities.

Keywords: dielectronic recombinaton, satellite line, \( \text{Xe}^{10+} \), radiative recombination

1. Introduction
Dielectronic recombination (DR) [1-5] is the dominant electron-ion recombination process for low charged ions in high-temperature and low density plasmas. Therefore, it is very important in determining the ionization balance. Another very important role of dielectronic recombination is connected with the presence of so-called satellite lines produced through the radiative decay of autoionizing states. Such spectral lines give information not only about ion structure but also about plasma parameters i.e., plasma density and plasma temperature, and therefore, play an essential role in X-ray spectroscopy and plasma diagnostics. The dielectronic recombination is a resonant, two step processes in which a multicharged ion \( \text{X}^{i-1} \) captures a free electron with simultaneous excitation of the target electron and creates a doubly excited ion \( \text{X}^{i-1} \), which then decays by a radiative transition.

\[ \text{X}^{i-1}(i_0) + e \rightarrow \text{X}^{i-1}(i) \rightarrow \text{X}^{i}(f) + h\nu \]  

(1)

where \( \text{X}^{i-1} \) expresses the autoionization state of the \( \text{X}^{i-1} \) ion and \( i_0, i, f \) denote the sets of quantum states of an ion in the initial state \( i_0 \), doubly excited target electron state \( i \), and final state \( f \). Another inverse process for the decay of an ion \( \text{X}^{i-1} \) is the autoionization process. As the interest about Xenon ions grows recently for EUV sources, many people are working on the research about Xenon ions. We need data about atomic collisional processes of Xenon ion to analyze Xenon spectra. However, as long as we know, there are few papers which give us enough data of the dielectronic recombination rate coefficient to each final bound state. These data are necessary to estimate the population of the excited states by a collisional radiative
model. In this paper, we calculated the data for the dielectronic recombination from $Xe^{10+}$ ions to the excited states of $Xe^{9+}$ ions. We investigate the $4d^75p^1nl$ and $4d^74f^1nl$ states as autoionizing states, which are important for the dielectronic recombination process. We use the Flexible Atomic Code (FAC)[6] for calculating the atomic data for dielectronic recombination rate coefficient. In section 2, we calculate the DR rate coefficient to the excited states and the total DR rate coefficients. In section 3, we obtain the dielectronic satellite lines through the radiative transitions of $4d^75p^1nl - 4d^8nl$ and $4d^74f^1nl - 4d^8nl$. In section 4, we calculate the total radiative recombination rate coefficient of $Xe^{10+}$ ions. Finally, in section 5, we summarize our result.

2. Dielectronic recombination rate coefficients for $Xe^{10+}$

The DR rate coefficients, $\alpha_{DR}(i_0, f; T_e)$, for electrons in the Maxwellian distribution can be expressed as

$$\alpha_{DR}(i_0, f; T_e) = \left( \frac{h^3}{2\pi m_e k_B T_e} \right)^{3/2} \sum_i \frac{1}{2g_{i_0}} Qd(i_0, i, f) e^{-\frac{E_{i,i_0}}{k_B T_e}}, \text{[cm}^3\text{s}^{-1}] \tag{2}$$

where $T_e$ is the electron temperature, $m_e$ is the electron mass, $h$ is the Planck constant, $k_B$ is the Boltzmann constant, $g_i$ and $g_{i_0}$ are the statistical weights of the autoionizing state $(i)$ formed by dielectronic capture and the target state $(i_0)$ before dielectronic capture, $E_{i,i_0}$ is the resonance energy calculated from the ionization limit. The intensity factors ($Qd$) for the dielectronic satellite lines from $i$ to $f$ are given by

$$Qd(i_0, i, f) = \frac{g_i Aa(i, i_0) Ar(i \rightarrow f)}{\sum_{i'} g_{i'} Aa(i, i') + \sum_{f'} Ar(i \rightarrow f')}. \tag{3}$$

where $g_i$ and $g_{i_0}$ are the statistical weights of the intermediate(autoionization) state $i$ and initial states $i_0$ of $Xe^{10+}$, $Ar(i \rightarrow f)$ is the radiative decay rate from level $i$ to level $f$, $Aa(i, i_0)$ is the autoionization rate from level $i$ to level $i_0$. The sum over $i_0'$ runs over all the levels in the next higher ion reachable from level $i$ by autoionization, and the sum over $f'$ runs over all bound levels reachable from $i$ by radiative decay. The autoionizing states formed by dielectronic capture may either autoionize, or radiatively decay. The radiative decay to the states below the ionization limit completes the recombination process. The radiative branching ratio for dielectronic recombination can be expressed as $\sum Ar(i \rightarrow f')$. For estimating contributions from autoionizing states with higher $n$ levels for $n > 15$, we use empirical scaling laws ($Aa_{ij}^{15} \approx Aa_{ij}^{10}(15/n)^3$). We extrapolate $Aa$ and $Aa$ values from $n = 15$ for the scaling. When we calculate the dielectronic recombination rate coefficients, we calculate the data of $n \leq 15$ and $l \leq n - 1$ by FAC code. Figure 1 and 2 show the dielectronic recombination rate coefficients summed over all $l$ but for each different $n$ as a function of electron temperature. The maximum values of the dielectronic recombination rate coefficients for the $4d^8 \rightarrow 4d^74f^1nl \rightarrow 4d^8nl$ and $4d^8 \rightarrow 4d^75p^1nl \rightarrow 4d^8nl$ move from 10eV to 50eV for high $T_e$. The difference of the values between $n$ and $n + 1$ of the dielectronic recombination rate coefficient for the $4d^8 \rightarrow 4d^74f^1nl \rightarrow 4d^8nl$ and $4d^8 \rightarrow 4d^75p^1nl \rightarrow 4d^8nl$ decreases as $n$ value increase as shown in figure 1 and 2. We can see that the result of the dielectronic recombination rate coefficient for the $4d^8 + e \rightarrow 4d^74f^1nl \rightarrow 4d^8nl + h\nu$ and $4d^8 + e \rightarrow 4d^75p^1nl \rightarrow 4d^8nl + h\nu$ at $n = 4$ and 5 are different from other levels, because the values of $E_{i,i_0}$ of $4d^74f^1nl$ and $4d^75p^1nl$ at $n = 4$ and 5 are much smaller than other. The total dielectronic recombination rate coefficient is given by

$$\alpha_{DR}^{tot}(T_e) = \frac{1}{2} \left( \frac{h^3}{2\pi m_e k_B T_e} \right)^{3/2} \sum_{i,f} \frac{g_{i_0} Qd(i_0, i, f) / g_i}{\sum_{i_0} g_{i_0}} e^{-\frac{E_{i,i_0}}{k_B T_e}}, \text{[cm}^3\text{s}^{-1}] \tag{4}$$
where \( g_i \) and \( g_0 \) are the statistical weights of the intermediate (autoionization) state \( i \) of \( Xe^{9+} \) and initial states \( i_0 \) of \( Xe^{10+} \). Figure 3 shows the total dielectronic recombination rate coefficient calculated for the following processes of \( 4d^8 \rightarrow 4d^7f^1nl \rightarrow 4d^8nl \) and \( 4d^8 \rightarrow 4d^75p^1nl \rightarrow 4d^8nl \) processes. The numbers I and II represent the transition of \( 4d^8 \rightarrow 4d^7f^1nl \rightarrow 4d^8nl \) and \( 4d^8 \rightarrow 4d^75p^1nl \rightarrow 4d^8nl \) including, respectively, \( n = 4-100 \), \( l = n-1 \) for \( n \leq 15 \), and \( l = 0-6 \) for \( n > 15 \). The I' and II' represent the transitions including \( n = 1-15 \) and \( l = n-1 \). The total dielectronic recombination rate coefficients have the maximum values at around 50eV and the temperatures at maximum values increase towards higher electron temperature with larger \( n \) and \( l \).

3. Satellite lines of \( Xe^{10+} \)

The satellite lines [7,8] for \( Xe^{10+} \) parent emissions of the types \( 4d^8 - 4d^7f^1f \) and \( 4d^8 - 4d^75p^1 \) are emitted by the radiative stabilization from the doubly excited states in the \( Xe^{9+} \) ions: \( 4d^7f^1nl - 4f^6nl \) and \( 4d^75p^1nl - 4f^6nl \). These satellite lines are of great interest in fields of study involving laboratory, astrophysics and particularly in diagnostics of plasmas, where they are used to determine the electron temperature or electron density through intensity ratios. The doubly excited states are populated by the processes of dielectronic capture:

\[
\begin{align*}
\text{e}^- + Xe^{10+} (4d^8) & \rightarrow Xe^{9+} (4d^7f^1f) \rightarrow Xe^{9+} (4d^8nl) + \nu \quad (5) \\
\text{e}^- + Xe^{10+} (4d^8) & \rightarrow Xe^{9+} (4d^75p^1) \rightarrow Xe^{9+} (4d^8nl) + \nu \quad (6)
\end{align*}
\]

The dielectronic recombination processes is resonated by the incident electron energy, the required being equal to the energy of the doubly excited state relative to the ionization energy of the \( Xe^{9+} \) ion. The autoionization takes place only when the energy of the doubly excited states is above the threshold energy. The ionization energy from the ground state \( 4p^64d^9 \) of \( Xe^{9+} \) ion is about 1,627,000 cm\(^{-1}\) (201.7 eV)[9]. The emissivity of a dielectronic satellite transition from the autoionizing state \( i \) to a final state \( f \) is proportional to a \( Qd(i_0, i, f) \) factor which expresses the rate of dielectronic capture into the autoionizing state followed by radiative decay to the final state.

Thus, the intensity of a satellite lines produced by dielectronic recombination can be expressed by

\[
\alpha_{DR}^{tot}(T_e) \approx \frac{1}{2} \left( \frac{\hbar^3}{2\pi m_e k_BT_e} \right)^{3/2} e^{-\left(\Delta E_x/k_BT_e\right)} \sum_{i,f} <Qd(i_0, i, f)/g_0 > [cm^3s^{-1}] \quad (7)
\]

where \( g_i \) and \( g_0 \) are the statistical weights of the intermediate (autoionization) state \( i \) of \( Xe^{9+} \) and initial states \( i_0 \) of \( Xe^{10+} \), \( \Delta E_x \) and \( <Qd(i_0)/g_0 > \) represent the average value over all initial state the \( Xe^{10+} (4d^8) \). When the satellite lines of \( Xe^{9+} \) are observed, the satellite lines appear near the parent emissions of \( Xe^{10+} \). The parent emission lines are generally produced by an excitation process. It is necessary to know the contribution of satellite lines on the excitation processes. It is necessary to known the contribution of satellite lines on the excitation process. It is necessary to known the contribution of satellite lines on the excitation process.
Figure 1. Dielectronic recombination rate coefficient for $4d^8 - 4d^74f^1nl - 4d^8nl$ calculated with different $n$ values as function of the plasma temperature

Figure 2. Dielectronic recombination rate coefficient for $4d^8 - 4d^75p^1nl - 4d^8nl$ calculated with different $n$ values as function of the plasma temperature
Total dielectronic recombination rate coefficient is obtained by the summation of the each dielectronic recombination rate coefficient for these autoionizing states of $I$, $II$, $I'$, and $II'$.

$I : 4d^8 - 4d^7 \, 4f^{1nl} - 4d^8 \, nl \, (n = 4 - 100, l = 0 - 6),$ $II : 4d^8 - 4d^7 \, 5p^{1nl} - 4d^8 \, nl \, (n = 5 - 100, l = 0 - 6),$ $I' : 4d^8 - 4d^7 \, 4f^{1nl} - 4d^8 \, nl \, (n = 5 - 15, l = n - 1),$ $II' : 4d^8 - 4d^7 \, 5p^{1nl} - 4d^8 \, nl \, (n = 5 - 15, l = n - 1)$

4. Radiative recombination rate coefficients for $Xe^{10+}$

In radiative recombination[10,11], a free electron is directly captured by a target, releasing its kinetic energy and binding energy of the final bound state to the emitted photon. Radiative recombination is an important contributor to the total recombination rate coefficients at least in some temperature ranges.

\[ e^- + Xe^{10+}(4d^8) \longrightarrow Xe^{9+}(4d^8 \, nl) + h\nu \] (8)

Radiative recombination is obtained from the photoionization cross sections through the Milne relation. The photoionization cross sections for the $n < 10$ shell and $E_e < 10E_{th}$, where the $E_{th}$ values are the ionization thresholds for corresponding shells are calculated in the distorted-wave approximation, taking into account the electronic dipole operator. The atomic code (FAC) used in the computation is developed by the M. F. Gu [10]. But the photoionization cross sections for the $n < 10$ shell and $E_e > 10E_{th}$ are calculated by using a simplified version of the formula suggested by Verner et al.[11] until 10000eV,

\[ \sigma_{PI}(E_e) = \sigma_0 x^{-3.5 - 1 + p/2} \left( \frac{1 + b}{\sqrt{x + b}} \right)^p \text{[cm}^2\text{]} \] (9)

where $x = (E_0 + E_e)/E_0$, $l$ is the orbital angular momentum of the photoionized shell, and $\sigma_0$, $E_0$, $p$, and $b$ are fit parameters. The radiative recombination cross section for $n > 10$ shells are estimated using the semiclassical Kramers formula.

\[ \sigma_n(x) = 2.1 \times 10^{-22} \, \frac{n}{x(x + 1)} \text{[cm}^2\text{]} \] (10)
Figure 4. Satellite lines produced by dielectronic recombination \((4d^8 \rightarrow 4d^7 4f^2 \rightarrow 4d^8 4f^1)\) of \(Xe^{9+}\) ion and radiative line that is obtained by radiative decay \((4d^8 \rightarrow 4d^7 4f^1)\) of \(Xe^{10+}\) ion.

\[(a) : \text{Satellite line, (b) : radiative line}\]
Figure 5. Satellite lines produced by dielectronic recombination \((4d^8 \rightarrow 4d^75p^15d^1 \rightarrow 4d^85d^1)\) of \(Xe^{9+}\) ion and radiative line that is obtained by radiative decay \((4d^8 \rightarrow 4d^75p^1)\) of \(Xe^{10+}\) ion. [(a) : Satellite line, (b) : radiative line]
where n is the principle quantum number, $E_0 = \frac{z^2 Ry}{n^2}$, Ry is the Rydberg energy, and z is the residual charge of the ion. Contributions up to n = 1000 are taken into account. The Maxwellian averaged rate coefficients of the partial n shells are calculated numerically using the cross sections in the temperature range $10^{-3} - 10^3$ eV

$$K_{rr}^{nl}(T_e) = 6.6941 \times 10^{-14} \sqrt{E_{nl}} \beta^{3/2} \int_0^\infty u \sigma_{nl}(u) e^{\beta u} du, \quad [cm^3s^{-1}] \quad (11)$$

where $\beta = \frac{E_n}{kT_e}$ and $\sigma_{nl}(u)$ is calculated by FAC code and Eq. (9). Thus, the total radiative recombination rate coefficient into all states of the Xe$^{10+}$ ions can be written in the form

$$K_{rr}^{10d}(T_e) = \sum_{n=4}^{10} K_{rr}^{nl}(T_e) + \sum_{n=11}^{1000} 5.18 \times 10^{-14} z \beta'^{3/2} e^{-\beta' } E_1(\beta'), \quad [cm^3s^{-1}] \quad (12)$$

where $\beta' = \frac{z^2 Ry}{n^2 kT_e}$. Figure 6 show the total radiative recombination rate coefficient represented by the solid line and the total dielectronic recombination rate coefficient represented by the dotted lines. Through this figure, we know that the values of the radiative recombination rate coefficient are smaller than the values of the dielectronic recombination processes in our temperature region of interest at $T_e = 1$ eV - 1000 eV.

5. Summary
We calculate the energy levels, the radiative transition probability (Ar), Autoionization rate (Aa), the intensity factor(Qd) of the dielectronic satellite spectra of Xe$^{9+}$, the dielectronic recombination rate coefficient ($\alpha_{DR}$), and radiative recombination rate coefficient of Xe$^{10+}$ ion with use of FAC. We took into account the $4d^7 4f^1 nl$ states and the $4d^7 5p^1 nl$ states of Xe$^{9+}$ ions. For the small value of $n < 15$, the value of Aa from the $4d^7 4f^1 nl$ and $4d^7 5p^1 nl$ levels

\[
E_0 = \frac{z^2 Ry}{n^2}
\]

\[
\beta = \frac{E_n}{kT_e}
\]

\[
\sigma_{nl}(u) = \text{calculated by FAC code and Eq. (9)}
\]

\[
K_{rr}^{nl}(T_e) = 6.6941 \times 10^{-14} \sqrt{E_{nl}} \beta^{3/2} \int_0^\infty u \sigma_{nl}(u) e^{\beta u} du, \quad [cm^3s^{-1}]
\]

\[
K_{rr}^{10d}(T_e) = \sum_{n=4}^{10} K_{rr}^{nl}(T_e) + \sum_{n=11}^{1000} 5.18 \times 10^{-14} z \beta'^{3/2} e^{-\beta' } E_1(\beta'), \quad [cm^3s^{-1}]
\]

\[
\beta' = \frac{z^2 Ry}{n^2 kT_e}
\]
are much larger than the value of $Ar$. The values of $Aa$ decrease as $l$ increases for large $l$, but the values of $Ar$ keep almost constant for large $l$. Therefore, we did not take into account the dielectronic recombination processes with $l \geq 7$ for large $n > 15$. For the small value of $n > 15$, we used these dependences for the extrapolation. We obtained dielectronic recombination and radiative recombination rate coefficient of $Xe^{10+}$ using the FAC code and compared these results. Through these results, we could know that the dielectronic satellite lines are important for the temperature of plasma smaller than 10eV comparing to the line produced by excitation and the radiative recombination rate coefficient are smaller than the values of the dielectronic recombination processes in our temperature region of interest at $Te = 1eV - 1000eV$.

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