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Electron impact ionization of ground-state Be-like rare gas ions

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Abstract. Detailed calculations for electron impact ionization including direct ionization (DI) and excitation autoionization (EA) processes along the ground-state Be-like rare gas ions have been performed by using relativistic distorted wave (RDW) approximation. The DI contribution from 2s shell and the EA contributions from inner-shell electron impact excitations of $1s-nl$ ($n\leq 12$, $l\leq 4$) were considered. The contribution of DI is a little more than 90% to the total electron impact ionization cross section. The main EA contribution comes from $1s-2p$ electron impact excitation channel. The EA contribution relative to DI contribution first increased and then decreased as the atomic number Z increases in Be-like rare gas ion. The EA rate coefficients are given for all ground-state Be-like rare gas ions as a function of impact electron temperature.

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Key words: electron impact ionization, excitation autoionization (EA), relativistic distorted wave (RDW) approximation

1 Introduction

Rare gas ions are frequently introduced in tokamaks as density diagnostic elements for probing fusion plasmas. For this reason, a good knowledge of related spectroscopic and collisional atomic data is needed in order to interpret the observation of various plasma parameters. Among the processes playing a role in this field, electron impact ionization of atoms or ions is a fundamental one, because it governs the ion charge state distribution evolution in the plasma so that the corresponding ionization cross sections and rate coefficients are required for plasma modeling [1]. The indirect electron impact ionization processes such as excitation autoionization (EA), which consists of collisional excitation

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to a level above the ionization limit followed by autoionization, can dominate the total impact ionization cross section for many ions at energies above the threshold. Recently much attention has been paid to the electron impact ionization processes of ground-state Be-like rare gas ions, and the importance of EA process for Be-like rare gas ions has been shown in experimental measurements of total ionization cross sections and theoretical investigations [2-6]. Duponchelle *et al.* have clearly found the K-L excitation autoionization for Ne^{6+} contributes for some 7% of the total cross section at the corresponding threshold (888.3 eV) using animated crossed-beams method [2]. In previous theoretical researches [3, 5], the EA contributions of Ne^{6+} and Ar^{14+} have been shown clearly. However, no systematic analysis for the contributions of excitation to autoionizing intermediate states of Be-like rare gas ions was available prior to the present work. The above discussions motivate us to investigate the impact ionization including the direct ionization (DI) from $2s$ shell and EA contribution from all electron impact excitations of $1s-nl$ ($n\le 12$, $l\le 4$) for ground-state Be-like rare gas ions.

The remainder of the paper is arranged as follows. In Section 2 we give a brief outline of the theoretical method. In Section 3 the results of our calculations are presented and discussed. Finally a brief summary is contained in Section 4.

2 Theoretical method

In the present work, we consider the DI process of ground-state Be-like rare gas ions from $2s$ shell,

$$1s^2 2s^2 + e \to 1s^2 2s + 2e. \tag{1}$$

The direct ionization from $1s$ shell is not included in our calculations, for the direct ionization of the $1s$ electron in fact lead to a double ionization of Be-like ion [7]. The direct ionization (DI) cross sections are calculated by using the RDW approach implemented in the computer package FAC, which has been widely used to study the DI process [8, 9].

The EA from the ground level $g(1s^2 2s^{2\,1}S_0)$ of Be-like ion to all possible levels of Li-like ions is described by the inner electron impact excitation channels schematically as following,

$$1s^2 2s^2 + e \to 1s 2s^2 nl + e. \qquad 2\le n\le 12;\ 0\le l\le 4. \tag{2}$$

The total EA cross section for level g is,

$$\sigma_g^{EA} = \sum_j \sigma_{gj}^{ex}(E) B_j^a, \tag{3}$$

where $\sigma_{gj}^{ex}(E)$ is the cross section for electron impact excitation of inner-shell from level g to the autoionization level j as a function of the incident electron kinetic energy E, and B_j^a is the branching ratio for autoionization from the level j. B_j^a is given by

$$B_j^a = \frac{\sum_k A_{jk}^a + \sum_{j'} A_{jj'}^r B_{j'}^a}{\sum_k A_{jk}^a + \sum_i A_{ji}^r}, \tag{4}$$

where A^a_{jk} is the Auger rate for autoionization from level j to level k of the Li-like ion; A^r_{ji} is the radiative rate for spontaneous emission from level j to any lower-lying Be-like level i; $A^r_{jj'}$ is the radiative rate from level j to some other level j', which can further autoionize. $B^a_{j'}$ is the branching ratio for further autoionization from level j', defined as B^a_j . This allows one to take into account all the possible further autoionizations following cascading, until the radiative decay reaches a level m below the first ionization limit such that $B^a_m = 0$. In the present work, the contribution of further autoionization is negligible, and the B^a_j is given by

$$B^a_j = \frac{\sum_k A^a_{jk}}{\sum_k A^a_{jk} + \sum_i A^r_{ji}}. \tag{5}$$

The rate coefficient for the EA process from a specific level g is

$$S^{EA}_g(T_g) = \sum_j Q^{ex}_{gj}(T_e) B^a_j, \tag{6}$$

where Q^{ex}_{gj} is the impact excitation rate coefficient from level g to level j. Assuming a Maxwellian velocity distribution corresponding to an electron temperature T_e, the Q^{ex}_{gj} is given by

$$Q^{ex}_{gj} = \int_0^\infty v f(v) \sigma^{ex}_{gj} dv, \tag{7}$$

where v is the electron velocity and $f(v)$ is the electron velocity distribution.

3 Calculational procedure and discussion

Detailed calculation of impact ionization parameters should include determination of energies, radiative transition probabilities and autoionization rates for atomic states in the recombined ion. These parameters are obtained by using the fully relativistic configuration-interaction code, i.e., the flexible atomic code (FAC) [10-12]. The atomic structure calculation in FAC is based on the relativistic configuration interaction method. The continuum processes, such as direct excitation and autoionization, are treated in the relativistic distorted-wave (RDW) approximation. Recently, the FAC has been widely used to deal with atomic process [13-18]. In the present work, full configuration mixing within each complex is included. For example, all possible configurations of $1s2s^2nl$ with given n are included in one configuration interaction (CI) calculation to obtain the energy levels and wave functions. Mixings among complexes are of no importance and therefore was neglected. The radiative decays of $nl \to 1s$ and the decays among the levels of the above inner-shell excited configurations, i.e., the radiative decays of $nl \to n'l'$, are considered. All stabilizing electric dipole radiative decays are taken into account. The final autoionization configuration included is $1s^2nl$.

3.1 Ne^{6+} cross section

The calculated total electron impact ionization cross sections for Ne^{6+} together with other theoretical and experimental results are shown in Fig. 1.

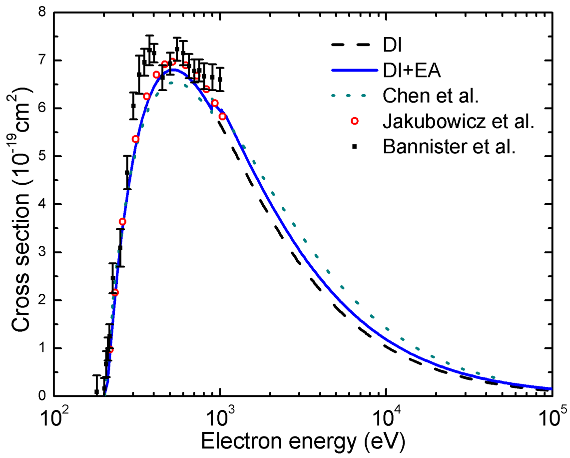

Figure 1: Total ionization cross section for Ne^{6+} as a function of incident electron energy. The dashed line and solid line represent DI cross section, DI plus EA cross section, respectively. The data with error bars are experimental results of Bannister *et al.* [19]. The dotted line and open circles denote theoretical calculation of Chen *et al.* [3] and Jakubowicz *et al.* [20], respectively.

It can be shown from Fig. 1, the calculated results of Ne^{6+} agree well with theoretical results of Jakubowicz *et al.* [20] and experimental results of Bannister et al. [19] in the direct ionization range. The dashed line in Fig. 1 shows the DI cross section is a smooth function of incident electron energy. The solid line is the total ionization cross section including DI and EA cross section. The present total cross section and the results of Chen *et al.* [3] using distorted-wave Born exchange (DWBE) approximation both sharply increase at about 890 eV, which is due to the $1s-2p$ inner-shell electron impact excitation. Only the resonant $1s-2p$ inner-shell electron impact excitation was taken into account by Chen *et al.*[3], while the $1s-nl$ ($n \leq 12$, $l \leq 4$) electron impact excitation considered in present calculations. The 1s-nl excitation spans 890.5 to 1093.3 eV energy range, and the main excitation channels are $1s-2p$ and $1s-3l$ electron impact excitations. The $1s-2p$ and $1s-3l$ excitations span 890.5 to 897.1 eV energy range and 1009.3 to 1021.4 eV energy range, respectively. The enhancement of the total cross section from $1s-nl$ relative to DI cross section at 1093.3 eV is about 4.03×10^{-20} cm^2. The ratio of $1s-nl$ EA cross section to DI cross section is 7.4%.

3.2 Cross sections for heavier rare gas ions

The total electron-impact ionization cross sections for Ar^{14+}, Kr^{32+}, Xe^{50+} and Rn^{82+} are shown in Fig. 2.

From Fig. 2(a) we can see our calculated cross sections of Ar^{14+} give a good description of the theoretical data of Zhao *et al.* [5] and Lennon *et al.* [21] in the direct ionization range. Both our calculation and the result of Zhao *et al.* [5] using distorted-wave Born exchange (DWBE) show the EA contribution at about 3076.2 eV. For only the main $1s-2p$ excitation channel was considered in Zhao *et al.* [5], the total cross sections in higher electron energy were lower than that of our calculation. The $1s-nl$ excitation spans 3076.2 to 3912.2 eV energy range. The $1s-2p$ excitation spans 3076.2 to 3092.0 eV energy range and enhances the cross section about 2.43×10^{-21} cm^2. Relative to DI cross section at 3912.2 eV, the enhancement of the total cross section from $1s-nl$ is about 3.16×10^{-21} cm^2,which corresponds to a ratio of $1s-nl$ EA cross section to DI cross section 9.3%.

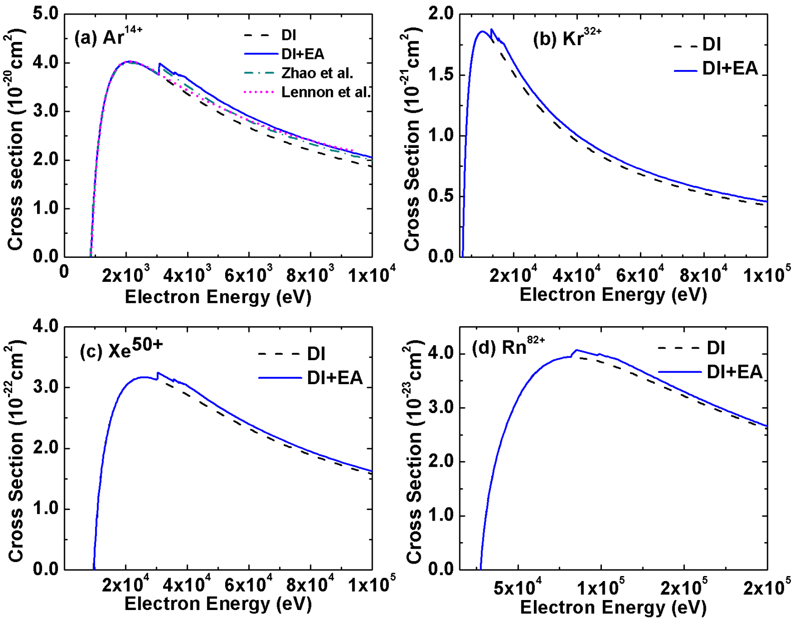

Figure 2: Total DI cross section (dashed line), DI plus EA cross section (solid line) as a function of the incident electron energy for the Ar^{14+}, Kr^{32+}, Xe^{50+} and Rn^{82+} ions. The dash dotted and short dotted lines denote theoretical calculation of Zhao *et al.* [5] and Lennon *et al.* [21]for Ar^{14+}, respectively.

To our knowledge, both experimental and theoretical cross sections for Kr^{32+}, Xe^{50+} and Rn^{82+} are scarce in literature. For Kr^{32+}, the $1s-nl$ excitation spans 12923.8 to 16798.8 eV energy range. The $1s-2p$ excitation spans 12923.8 to 13009.5 eV energy range and enhances the cross section about 0.85×10^{-22} cm^2. The $1s-3l$ excitation spans 15154.3 to 15235.7 eV energy range and enhances the cross section about 0.09×10^{-22} cm^2. Relative to DI cross section at 16798.8 eV, the enhancement of the total cross section from $1s-nl$ is about 1.15×10^{-22} cm^2. The ratio of $1s-nl$ EA cross section to DI cross section at 16798.8 eV is 7.0%.

For Rn^{82+}, the $1s-nl$ excitation spans 82113.2 to 109005.1 eV energy range. The ratio of $1s-nl$ EA cross section to DI cross section at 109005.1 eV is 4.0%.

The EA contribution relative to DI contribution first increased and then decreased as the atomic number Z increases in Be-like rare gas ion. This is due to excitation cross sections decrease approximately as $(1/Z)^2$, while ionization cross sections decrease more rapidly as $(1/Z)^4$; the rates for radiative decay increase rapidly as Z^4, while the autoionization rates are independent on Z.

3.3 EA rate coefficients

In many situations, EA ionization rate coefficients, rather than cross sections, are needed. The EA rate coefficients for the Be-like rare gas ions are displayed in Fig. 3 as a function of electron temperature in the $0.1E_I \leq kT_e \leq 10E_I$ range, where E_I is ionization energy for each Be-like rare gas ion.

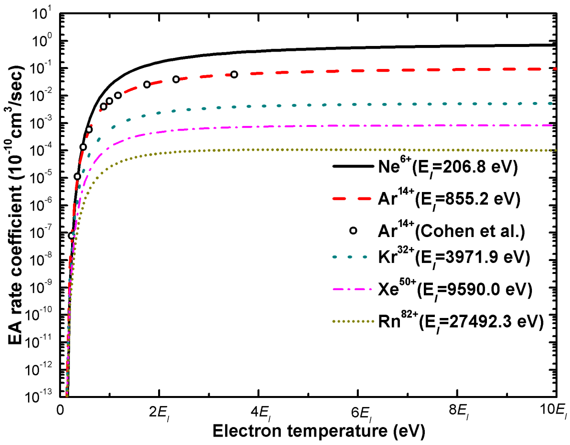

Figure 3: EA rate coefficients for ground Be-like $(1s^2 2s^2)$ rare gas ions as a function of impact electron temperature. The open circles are theoretical results of Cohen *et al.* [6] for Ar^{14+}. E_I is ionization energy for corresponding Be-like rare gas ion.

In Fig. 3, we compare the present results with the available rate coefficients given by Cohen *et al.* [6]. The comparison shows that the agreement is very good.

4 Conclusions

In this work, the electron impact ionization cross sections including direct ionization and electron-impact excitation to autoionizing intermediate states are computed by using RDW approximation along the Be-like rare gas ions. The contribution of direct ionization is a little more than 90% to the total electron-impact ionization cross sections. The computed total ionization cross sections have been compared with the available theoretical and experimental results. The main EA contribution comes from $1s-2p$ electron impact excitation channel. The EA contribution relative to DI contribution first increased and then decreased as the atomic number Z increases in Be-like rare gas ion. The EA rate coefficients are given for all Be-like rare gas ions as a function of electron temperature.

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