Ionization cross sections for electron scattering from metastable rare-gas atoms (Ne^* and Ar^*)*

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The optical-model approach has been used to investigate the electron-impact ionization of metastable rare-gas atoms. A complex equivalent-local polarization potential is obtained to describe the ionization continuum channels. We have calculated the cross sections for collisional ionization of the metastable atoms Ne^* and Ar^* by electrons in the energy range from threshold to 200 eV. The present results are in agreement with the available experimental measurements and other theoretical calculations.

Keywords: electron scattering, metastable rare-gas atom, ionization

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1. Introduction

Electron-impact ionization from ground and metastable states of rare-gas atoms is well known to be important in both fundamental studies and practical applications. The latter includes plasma modeling and the interpretation of astrophysical data. The electron impact on atoms may be considered as Coulomb three-body problems.[1] The break-up channel exhibits all the difficulties of many-body scattering theory coupled with the special problem of the infinite range of the Coulomb interaction. Therefore, significant experimental and theoretical efforts have contributed to this topic for several decades. Most of the investigations focus on the ionization of ground atoms by electron impact. A comprehensive review can be found in the article of Christophorou and Olthoff.[2]

The lower ionization threshold energies and the higher polarizabilities of the excited states of atoms significantly affect the ionization process in electron scattering and cause distinct cross sections compared with their respective ground states. These unique properties offer a new opportunity to understand the basic interactions in electron–atom collision, and consequently produce a challenging topic in theoretical research. For several decades, ionization of metastable rare gases by electron impact has become a subject of great interest, and there is a series of relevant research work that has been carried out.[3–11] However, the situation is much less satisfactory since significant differences can be seen between experimental observations and theoretical calculations.

In the experimental aspect, most of the measurements on electron-impact ionization of excited rare-gas atoms focus on helium.[3,6,12,13] For more complex rare-gas atoms, there are only experimental data for metastable neon and argon until now. In 1973, Dixon *et al.*[5] used the crossed electron and fast-atom beam technique and measured the ionization cross sections of metastable neon and argon respectively with the electron energy ranging from 5.6 eV to 500 eV; nevertheless, their data were not published. In 1996, Johnston *et al.*[4] carried out the crossed-beam experiment using a fast-neutral target formed by the charge transfer between a neon-ion beam and neon gas or sodium vapour, and then obtained the partial electron impact ionization cross sections of metastable neon in the energy range from threshold to 200 eV.

Theoretical studies of ionization in electrons and metastable rare-gas atoms collision have been performed by a number of approaches. In the early theoretical investigations,[11,14–17] the semi-empirical, the semi-classical, and the Born-approximations approach have all determined the electron-impact ionization cross sections of metastable rare-gas atoms. However, significant discrepancies among the above theoretical results exist. At the time, the available experimental data were very few, that was the measurement of Dixon *et al.*[5] Until the nineties of the last century, Johnston *et al.*[4] reported their measured ionization cross sections of metastable neon by electron impact. After that, several corresponding theoretical works were produced. In 1999, Deutsch *et al.*[10] used the semi-classical Deutsch–Märk (DM) formalism to calculate the absolute cross sections for the electron-impact ionization of metastable rare-gas atoms from threshold to 200 eV. In 2004, Ballance *et al.*[9] performed an *R*-matrix with pseudo-state (RMPS) calculation of ionization in electron scattering from metastable neon. In addition, they offered a configuration-average time-dependent close-coupling (TDCC) calculation and a distorted-wave (DW) calculation on

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this cross section. In 2007, using both RMPS and DW methods, Ballance *et al.*[8] calculated the electron-impact ionization cross sections of argon below 21 eV. In their RMPS calculations, there were 27 LS spectroscopic terms and another 282 LS pseudo-state terms to represent the high-Rydberg states.

Recently, fully *ab initio* methods have been developed and applied to the direct ionization of one-electron (hydrogen-like) and two-electron (helium-like) atoms and ions. These methods include grid-based approaches such as exterior complex scaling and TDCC, as well as the convergent close-coupling (CCC) approach. Extension of these methods to more complex targets has not been achieved to date.[7] The straightforward extension of these methods to the calculation of cross sections for ionization from metastable excited levels has some limitations. Most recently, a large-scale pseudostate calculation of *R*-matrix has been carried out for the ionization cross section of Ne initialized in ground and metastable states.[7] These calculations, however, are computationally more challenging in comparison to the ionization from the ground state, due to the additional partial-wave symmetries involved and the overall slower convergence of the partial-wave expansion because of the smaller threshold energy. Their calculation results exhibit a good agreement with the experimental data over a wide impact energy region, except for the near threshold range of energies from 15 eV to 20 eV in which their two pseudostate calculation results were very close and underestimated the experimental data of Johnston *et al.*[4]

In the present paper, we demonstrate a new calculation for the total ionization cross sections of electron impact on metastable neon and argon at intermediate energy from the ionization threshold up to 200 eV by applying an optical model,[18] that is an *ab initio* calculation. In this model, an equivalent local complex optical potential is employed to describe the target continuum and the orthogonalized Born-Oppenheimer approximation is used for the ionization amplitude.[19] Total cross section of ionization is closely proportional to the imaginary part of the momentum space optical potential. This method has been used in predicting the ground-state ionization cross sections for electron scattering from various targets,[20–26] and the positron scattering from atoms.[27,28] The approach allows for a straightforward extension to the calculation of cross sections for ionization from metastable excited levels.[6,29] In this paper, we have used the optical potential model to calculate the electron-impact ionization cross sections for the metastable states of neon and argon, and have compared the results with experimental measurements and other theoretical calculations.

2. Model and method

The approximation used for the total ionization cross section is[18]

$$\sigma_{\rm I} = \frac{2}{\boldsymbol{k}}(2\pi)^3 W(0), \tag{1}$$

where $\boldsymbol{k}$ is the momentum of the incident electron, and $W(0)$ is the imaginary part of the momentum space optical potential $W(P)$ at $P=0$, which is[19]

$$\begin{aligned} W(0) &= \pi \sum_i n_i \int \mathrm{d}^3 q_1 \int \mathrm{d}^3 q_2 A \langle \boldsymbol{k}\phi_i | v | \chi^{(-)}(\boldsymbol{q}_<)\boldsymbol{q}_> \rangle \\ &\quad \times \delta(E - \frac{1}{2}(q_1^2 + q_2^2)) \langle \boldsymbol{q}_> \chi^{(-)}(\boldsymbol{q}_<) | v | \phi_i \boldsymbol{k} \rangle, \end{aligned} \tag{2}$$

where ϕ_i is the orbital for the independent-particle state i which is occupied by n_i electrons, A is the antisymmetrization operator, E is the total energy, $\chi^{(-)}(\boldsymbol{q})$ is a time-reversed Coulomb wave orthogonalized to ϕ_i, $\boldsymbol{q}_<$ and $\boldsymbol{q}_>$ are, respectively, the one of $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ which has the lesser or greater magnitude, and v is the electron–electron potential. The contributions from heavy-particle knockout and autoionization are ignored. For computational convenience, an equivalent-local approximation[18] is made, and consequently, the amplitude for ionization of an electron in an orbital ϕ_{lm} resulting in a slow electron of momentum $\boldsymbol{p}$ and a fast electron of momentum $\boldsymbol{k}'$ is approximated by

$$\begin{aligned} \langle \boldsymbol{k}' \chi^{(-)}(\boldsymbol{p}) | v | \phi_{lm} \boldsymbol{k} \rangle &= \langle \boldsymbol{k} \phi_{lm} | v | \chi^{(+)}(\boldsymbol{p}) \boldsymbol{k}' \rangle \\ &= (2\pi^2 K^2)^{-1} \Delta_{lm}(\boldsymbol{K}, \boldsymbol{p}), \end{aligned} \tag{3}$$

where the momentum transfer $\boldsymbol{K} = \boldsymbol{k} - \boldsymbol{k}'$, and

$$\begin{aligned} \Delta_{lm}(\boldsymbol{K}, \boldsymbol{p}) &= \int \mathrm{d}^3 q \langle \phi_{lm} | \boldsymbol{q} \rangle [\langle (\boldsymbol{q} + \boldsymbol{K}) | \psi^{(+)}(\boldsymbol{p}) \rangle \\ &\quad - \sum_n \langle (\boldsymbol{q} + \boldsymbol{K}) | \phi_{ln} \rangle \langle \phi_{ln} | \psi^{(+)}(\boldsymbol{p}) \rangle], \end{aligned} \tag{4}$$

where $\psi^{(+)}(\boldsymbol{p})$ is a Coulomb wave for an incident particle with momentum $\boldsymbol{p}$ that is orthogonalized to the relevant target state and n is the magnetic quantum number of the bound state $|\phi_{ln}\rangle$.

The orthogonalized Coulomb-plane-wave overlap Δ is expressed in terms of functions that are easily computed

$$\Delta_{lm}(\boldsymbol{K}, \boldsymbol{p}) = D_{lm}(\boldsymbol{K}, \boldsymbol{p}) - \sum_n D_{ln}(\boldsymbol{K}, \boldsymbol{p}) F_{mn}(\boldsymbol{K}), \tag{5}$$

where

$$F_{mn}(\boldsymbol{K}) = \int \mathrm{d}^3 p \langle \phi_{lm} | \boldsymbol{q} \rangle \langle (\boldsymbol{q} + \boldsymbol{K}) | \phi_{ln} \rangle \tag{6}$$

and $D_{lm}(\boldsymbol{K}, \boldsymbol{p})$ is a bound-free transition form factor in the Slater expansion of ϕ_{lm}, which is obtained from the following formula given by Belkić[30]

$$D_{lm}(\boldsymbol{K}, \boldsymbol{p}) = (2\pi)^{-3} \int \mathrm{d}^3 r \phi_{lm} e^{-\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}} \psi^{(+)}(\boldsymbol{p}, \boldsymbol{r}). \tag{7}$$

3. Results and discussion

With the optical model, we have calculated the electron-impact ionization cross sections of metastable neon and argon from threshold to 200 eV. Our calculation results are displayed in Figs. 1 and 2, together with the available experimental measurements[4,5] and the theoretical calculation results.[7–11,16,17]

In the case of metastable neon, figure 1 exhibits the present ionization cross sections σ_I compared with the available measurement data of Dixon *et al.*[5] and Johnston *et al.*[4] together with the previously published theoretical results. It can be found in Fig. 1 that the present calculation results agree well with the experiment data of Dixon *et al.*[5] and Johnston *et al.*[4] in the whole impact energy region. At about 7 eV, there is a relatively obvious difference between our results and both of the above measurement data. However, the present results lie in their systematic error bars of the experimental results. For earlier theoretical calculations,[11,16,17] there is a detailed comparison with the available experimental data in the recent paper of Johnston *et al.*[4] and we will not describe them here. For the semi-classical calculation of Deutsch *et al.*[10] shown in Fig. 1, we can see that their results are about 60% higher than the available experiments above about 10 eV. The recent RMPS calculations of Ballance *et al.*[9] and Zatsarinny and Bartschat[7] show good agreement with the available experiment,[4,5] whereas at about 15 eV the RMPS results appear to be about 20% lower than the available measurement data.

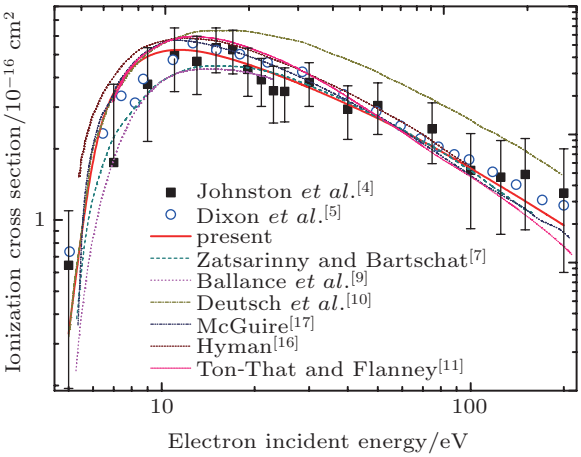


Fig. 1. (color online) Electron-impact ionization cross section for metastable neon. The present results are compared with experimental data[4,5] and other theoretical predictions.[7,9–11,16,17]

In Fig. 2, we present our calculated ionization cross sections from the metastable argon in comparison with other theoretical results[8,10,11,16,17] and the available measurement data of Dixon *et al.*[5] which are the only reference data to date. However, we can find an obvious disagreement between all of the above available data from Fig. 2. The present results show the general consistency with the experiment of Dixon *et al.*[5] over all of the energy range. Especially at higher impact energy region (above about 20 eV), there is an excellent agreement between our results and the data of Dixon *et al.*[5] At lower impact energy region (approximately 7 eV–20 eV), the present calculations lie 30% higher than the measurement results of Dixon *et al.*[5] However, we note that our results do not exceed the error range of the experiment data of Dixon *et al.*[5] which is about 50%. For other theoretical calculations[8,11,16,17] shown in Fig. 2, there are also certain differences between them and the available data of Dixon *et al.*[5] From Fig. 2, we can see that their calculated cross sections are lower than the measurement values in different energy ranges. In the impact energy region below 7 eV, the results of McGuire[17] based on a scaled Born approximation and the RMPS calculation of Ballance *et al.*[8] are both nearly 40% lower than the measurement of Dixon *et al.*[5] On the other hand, over the above energy range, the ionization cross sections calculated by using the semi-classical Deutsch–Märk formalism of Deutsch *et al.*[10] are also 30% lower than the experiment of Dixon *et al.*[5] At higher incident energy above 20 eV, the available theoretical results of McGuire,[17] Hyman,[16] Ton-That and Flannery[11] are all lower than the measurement values of Dixon *et al.*[5] and the maximal deviation is up to 50%. All of the above discrepancies among the experiment data and the theoretical results indicate that more theoretical research and experiment investigations are expected.

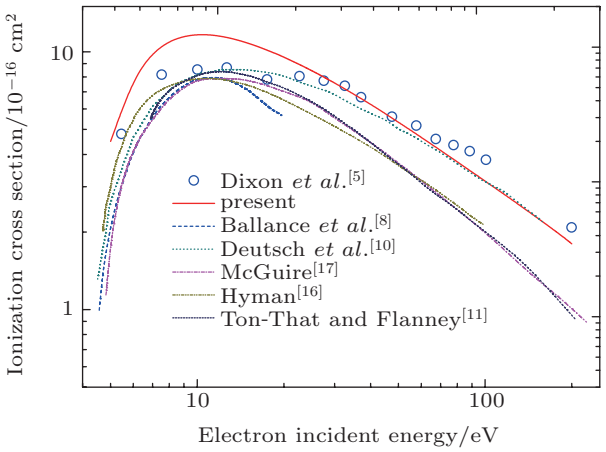


Fig. 2. (color online) Electron-impact ionization cross section for metastable argon. The present results are compared with the experimental data[5] and other theoretical predictions.[8,10,11,16,17]

4. Conclusions

In the present work, an equivalent-local optical potential approach has been used to study the ionization cross sections in the electron scattering from metastable rare-gas atoms (Ne* and Ar*) in the energy range from threshold to 200 eV. For Ne*, present results are in good agreement with the available experimental data and other theoretical calculations. We believe that the present method is a useful tool to investigate the

collision between electrons and metastable atoms. For Ar*, our calculations agree fairly well with the experimental data, except for in the case when the collisional energy ranges from 6 eV to 25 eV. Further theoretical studies as well as experimental measurements are much needed.

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