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Multiple ionization of argon by helium ions

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Abstract

We apply the continuum distorted-wave eikonal initial state and the independent electron model to describe the multiple ionization of Ar by He^{2+} and He^{+} in the energy range 0.1–10 Mev amu^{-1}. Auger-like post collisional processes are included, which enhance the high energy multiple ionization cross sections via ionization of the inner shells. All Ar electrons (K, L and M-shells) have been included in these calculations. The results agree well with the experimental data at high energies, where the post-collisional ionization is the main contribution. At intermediate impact energies the description is also good though it tends to overestimate the triple and quadruple ionization data at intermediate energies. We analyze this by comparing the present results for He^{+2} in Ar, with previous ones for He^{+2} in Ne and Kr. It was found that the theoretical description improves from Ne to Ar and Kr, with the latter being nicely described even at intermediate energies. The present formalism is also tested for Ar inner shell and total ionization cross sections. In all the cases the results above 0.1 MeV amu^{-1} are quite reasonable, as compared with the experimental data available and with the ECPSSR values.

Keywords: ionization, multiple, CDW-EIS, inner-shell

(Some figures may appear in colour only in the online journal)

1. Introduction

The multiple ionization is a complex many-electron process where direct ionization and post-collisional electron emission contribute to the final charge state. Electron–electron correlation and changes in the target potential play a role [1]. For certain targets, such as He or even Ne, it may be decisive, for others as Kr or Xe it is negligible [2, 3]. The intermediate cases deserve a deeper study, this work is a step in this direction.

In the last years, very detailed calculations have been proposed to deal with the single and double ionization of He (a review can be found in [4]). However, with these calculations it would be almost impossible to tackle many electron targets. There are different approximations within the independent particle model (IPM) that give quite good descriptions of the multiple ionization experimental data. The continuous distorted wave eikonal initial state approximation (CDW-EIS) including the Auger-type contributions [2, 3, 5, 6] have been extensively tested, mainly for $|Z| = 1$ projectiles [3, 7]. This model managed to reproduce very well the high energy experimental data of the heaviest rare gases, Kr and Xe, even for the sextuple ionization of Kr (Xe), where L-shell (M-shell) contribution is decisive [8]. But it showed limitations for Ne target [2, 7, 9].

Another example within the IPM is the basis generator method (BGM) by Kirchner and coworkers [1, 10–13] applied to multiple ionization of Ne and Ar targets by bare and dressed ions. Recently this group [1, 12, 13] improved the theoretical description of the ionization by dressed ions by considering the two center electrons (projectile and target), and a time dependent interaction potential to include the changes in the target potential due to the subsequent loss of bound electrons. As expected, the changes (response) in the target potential weaken the multiple ionization, and lower cross sections are obtained. On the other hand, the inclusion of transfer and ionization processes (that leaves the projectile in the same final charge state) also decreases the cross sections at intermediate energies. This contribution produced a clear difference in the triple and quadruple ionization of Ne by multicharged heavy ions such as B^{+2} [12].

On the other hand, outside the IPM, recent calculations of multiple ionization of He^{2+} in Ne [14] and Ar [15] using the time dependent density functional theory (TDDFT) placed it as a promising alternative, at least for low to intermediate impact energies. The TDDFT triple and quadruple ionization cross sections of Ne by He^{+2} by Hong *et al* [14] are close to the experimental data in a region where the BGM [10] and the CDW-EIS [2] overestimate.

In the present contribution we study the multiple ionization of Ar (single to quintuple) by Helium ions, He^{+} and He^{+2}. We choose the He ions to compare with the recent TDDFT values by Zhang [15] and previous ones by Kirchner [11]. Besides, the He–Ar system has the additional interest of being in Tokamak plasmas, where highly charged Ar lines are observed due to the collision with the energetic alpha-particles generated in the fusion reactions [16]. The aim is to test the CDW-EIS as employed in [2], for this case of theoretical and experimental interest.

Different experimental measurements were carried out for the He–Ar system [17–22], with coincident measurement of projectile and target final charge state in order to have separate data of pure ionization (the target electron in the continuum, the ion charge unchanged) and electron transfer (the electron bound to the projectile). Also of interest are the measurements on multiple ionization of Ar by Li^{+2} ions by Sigaud and coworkers [23], which also add to the framework of present calculations.

The theoretical research on multiple ionization in the He–Ar system has been focused mainly on the low and intermediate energy region [11, 15], where direct ionization dominates the final target charge state. For higher energies the inclusion of the post-collisional ionization (PCI), such as the Auger and Coster-Krönig processes, or other electron shake-off mechanisms, proved to be decisive to describe the experimental multiple ionization cross sections [5, 6, 21, 24–26]. Thus, in certain cases PCI is the main contribution. For example, in this contribution we show that for 5MeV/amu alpha particles, the PCI contributes to 90% of the total cross section for Ar^{3+} formation, and only 10% is due to direct triple ionization.

In the following sections we present our CDW-EIS results for single to quintuple ionization cross sections of Ar bombarded by He^{2+} and He^{+} ions in the (0.1–10) MeV amu^{-1} energy range, including direct ionization and PCI. We compare these results with the experimental data available considering only *pure* multiple-ionization cross sections (no capture or capture and loss contributions, being the role of the He^{+} bound electrons just screening the nucleus potential). We also test our results for the ionization of the L and K shells of Ar by comparing them with the values of the ECPSSR approximation by Brandt and Lapicki [27, 28]. This is a semi empirical and very effective model based on the perturbed stationary state (PSS) approximation, with modifications to account for the enhanced binding energy of the target electrons, Coulomb (C) deflection, energy loss (E) and relativistic (R) wave functions. The inner-shell ionization cross sections and the total ionization cross sections are also compared with the experimental data available in order to test the model in a wide spectrum of possibilities.

2. Theoretical model

The theoretical developments have been extensively explained in our previous works [2, 3, 5, 7]. Briefly, within the IPM the direct multiple ionization is obtained as a multinomial combination of single ionization probabilities as a function of the impact parameter [29]. We combine the CDW-EIS ionization probabilities with the experimental branching ratios of single to multiple vacancy production. Another possibility might be to combine the IPM with the CDW [30], which has also been used with success for ionization of multi-electron targets.

In the intermediate and high energy regions, the CDW-EIS approximation [31–33] is one of the most confident ones within the IPM. The CDW-EIS ionization probabilities have been calculated as in [33, 34], by rigorously solving the radial Schrödinger equation for different angular momenta for both the initial bound and the final continuum states. Thus, we can assure the proper description of the continuum wave function and its mathematical orthogonality to the bound state. These values have already been tested in differential [33] and in total [34] ionization cross sections with good agreement with the experimental data.

The inclusion of the PCI is performed following [5, 24, 25] by considering the experimental branching ratios of charge state distribution after single ionization. The Auger-type processes are time-delayed electron emissions, they depend on the target initial vacancy and not on the projectile. This means that we can combine the ion-atom ionization probabilities with the branching ratios of charge state distribution after single-photoionization experiments. The branching ratios of the different processes are easily extracted from the experimental spectra due to the constant transmission of the spectrometer [35]. The experimental branching ratios employed in the present calculations are those tabulated in [5, 7], and correspond to data reported in [36–39].

3. Results and discussions

The single to quintuple ionization cross sections of Ar by He^{2+} and He^{+} have been calculated using the CDW-EIS and the first Born approximations. We have tested the high energy convergence of the CDW-EIS to the first Born values for projectile energies around 1 MeV amu^{-1}, from that on we employ the first Born approximation. The eighteen Ar electrons were considered. At high impact energies even the deep K and L-shells contribute to multiple ionization via single ionization followed by Auger decay and emission.

3.1. Inner-shell ionization

Our CDW-EIS results for the K and L-shell ionization cross sections by He^{+2} are displayed in figure 1 and compared with

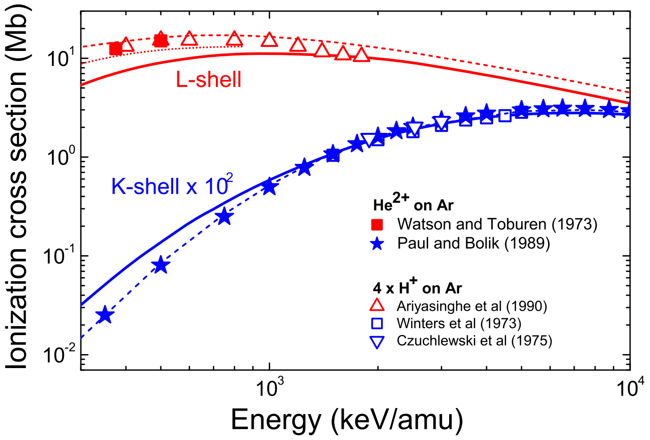

Figure 1. K and L-shell ionization cross section of Ar by He^{2+}. Curves: solid-lines, present theoretical results; dashed-lines, ECPSSR values [40]; dotted line, coupled states calculations by Martir *et al* [41]. Symbols, experimental data: full squares, Watson and Toburen [42]; full stars, Paul and Bolik [43]; open up-triangles, Ariyasinghe *et al* [44]; open squares, Winters *et al* [45]; open down-triangles, Czuchlewski *et al* [46]. Note: full symbols correspond to He^{+2}; open symbols are H^+ cross sections times 4.

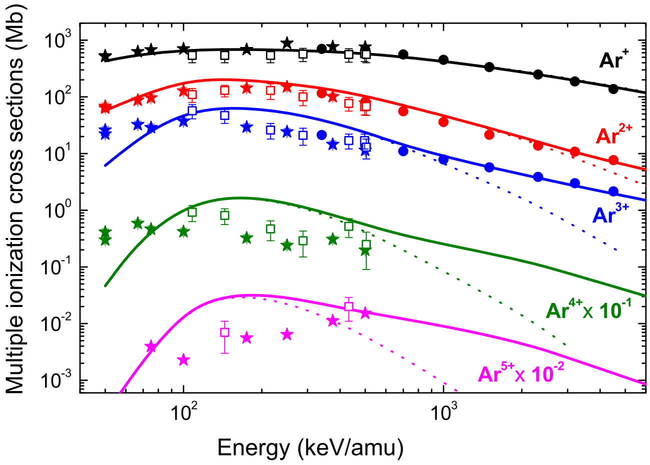

Figure 2. Multiple ionization cross section of Ar by He^{2+}. Curves: solid-lines, present theoretical results including direct ionization and PCI; dotted-lines, present results for direct ionization only. Symbols, experimental data: full circles, Andersen *et al* [17]; full stars, DuBois [20]; open squares, Li^{2+} impact data in [23].

the experimental data available. We also include in this figure the proton impact measurements times 4, in the high energy where the Z^2 behavior is valid. Other two theoretical curves are shown: the ECPSSR predictions [27, 28] obtained with the ISICS11 code [40], and the coupled-states results [41]. We obtained a good theoretical-experimental agreement above 1 MeV amu^{-1}, that is the sensitive region for the multiple ionization. Below this energy, our L (K) cross sections are a little below (above) the data, while the ECPSSR agree quite well with the measurements. The comparison performed in figure 1 is a relevant first test of the inner-shell ionization cross sections due to their participation in the multiple ionization at high energies. However, it is worth to remark that the good performance of the total ionization cross sections is necessary but not sufficient condition for a fair description of the multiple ionization, with the latter being a more demanding test as it depends on the impact parameter distribution.

3.2. Multiple ionization by He^{+2}

In figure 2 we display our results for the multiple ionization cross sections of Ar by He^{2+}. We display separately the direct multiple ionization values (dotted lines) in order to show explicitly the importance of PCI. It is clear in figure 2 that PCI contributes at very high energies to the Ar^{2+} formation ($E \geqslant$ 2 MeV amu^{-1}), but for higher Ar^{+q} charge states, this contribution is clear at much lower energies, i.e. 200 keV amu^{-1} for Ar^{5+}. It can be noted in this figure that above 5 MeV amu^{-1} the direct triple ionization cross section of Ar by alpha particles is more than 90% due to PCI (inner-shell contribution), as mentioned before.

The agreement with the experimental data is rather good, especially with Andersen *et al* [17] measurements in the high energy region where the PCI dominates. At intermediate energies the direct multiple ionization of the Ar outer shell is the main contribution. The present CDW-EIS results agree with DuBois data [20] for the single and double ionization cross sections, but overestimates the triple and higher multiple ionization. One of the reasons for this disagreement at intermediates energies could be the neglect of electron–electron correlation and of the capture contribution [12, 47].

The comparison with other theoretical calculations for the He^{+2}–Ar system [11, 15] is quite interesting. We find very good agreement with the BGM single to quintuple ionization cross sections by Kirchner *et al* in [11] in the 0.3–1 MeV amu^{-1} energy region (considering only direct multiple ionization). On the other side, the recent TDDFT values by Zhang *et al* [15] are closer to the experimental measurements for triple and quadruple ionization. Unfortunately, these TDDFT values go up to 300 keV amu^{-1}. The extension to higher energies could be very interesting.

We also include in figure 2 the recent measurements of multiple ionization cross sections of Ar by Li^{2+} by Sigaud and coworkers [23]. As already noted in [23], He^{2+} and Li^{2+} values are approximately the same, within the experimental uncertainties. This indicates that long distance collisions dominate, which is reasonable if the ionization of the Ar 3s and 3p electrons is the main contribution. The probabilities of ionization of Ar inner shells by Li^{2+} should be greater than by He^{2+}. This would end in higher triple ionization cross sections at high energies, where PCI plays an important role. New experimental measurements for multiple ionization of Ar by Li^{+2} above 1 MeV amu^{-1} could clarify this. For quadruple and quintuple ionization the Li^{2+} data is slightly but consistently greater than the He^{2+} values even at intermediate impact energy, seeming to confirm that most of the electron processes occur at small impact parameters [14].

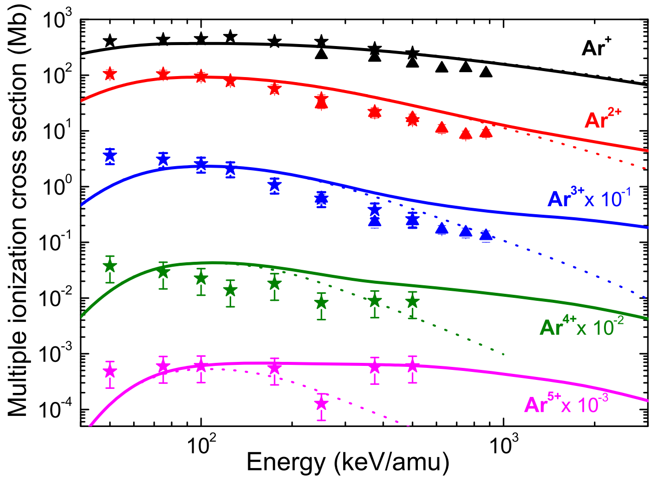

Figure 3. Multiple ionization cross section of Ar by He$^+$. Curves: solid-lines, present theoretical results including direct ionization and PCI; dotted-lines, present results for direct ionization only. Symbols, experimental data: full stars, DuBois [18]; full triangles, Santos *et al* [21].

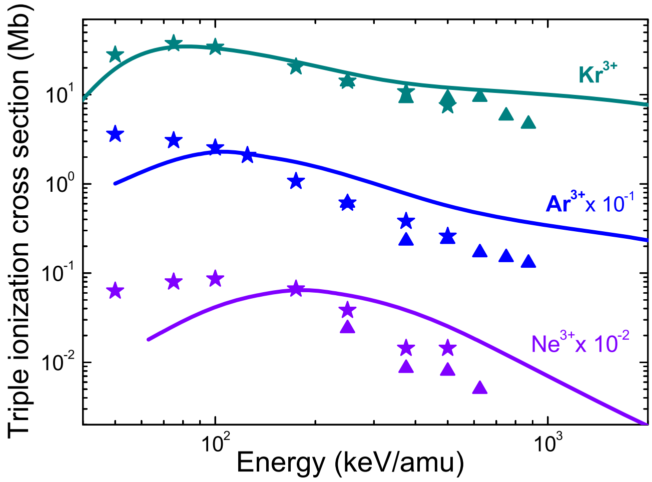

Figure 4. Triple ionization of Ne, Ar and Kr by He$^+$. Symbols, experimental data: full stars, DuBois [18]; full triangles, Santos *et al* [21].

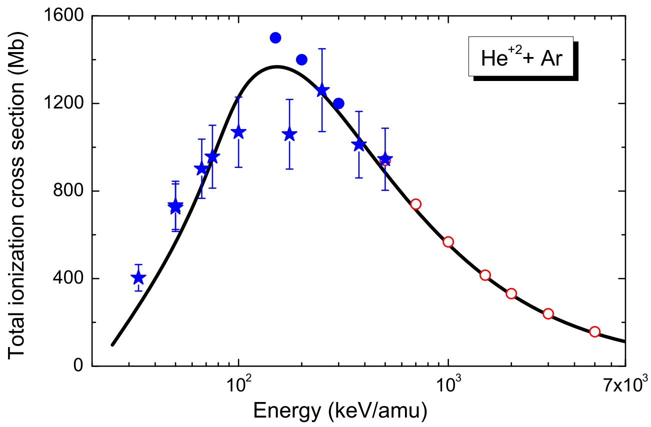

Figure 5. Total ionization cross section of Ar by He^{+2}. Curves: present results for *pure* ionization. Symbols, experimental data: full stars, DuBois [20]; full circles, Rudd [22]; empty circles, Rudd *et al* [48] for proton impact ×4.

3.3. Multiple ionization of Ar by He$^+$

The case of He$^+$ ion with one electron bound is different. We calculate the multiple ionization cross sections of Ar by He$^+$, with frozen He$^+$, no capture, no electron loss, only pure ionization of the Ar target [34]. This is different from Kirchner proposal [12] that considers all the electrons active.

In figure 3 we display the present results and the experimental data [18, 21]. We note certain overestimation of the double and triple ionization in the energy region 200–500 keV amu^{-1}. Surprisingly, the quadruple and quintuple ionization cross sections agree quite well with the data. Perhaps because above 200 keV amu^{-1} the single ionization of inner shell followed by PCI dominates. We remark again that in our calculations, the He$^+$ electron plays a role of screening the ion nucleus and it is not active in the collision (no capture and loss processes have been included). For heavier ions the inclusion of the capture channel within the multiple ionization calculations is important, even when the final ion charge remains unchanged as shown in [12] in comparison with B^{+2} in Ne experiments [9].

It can be said that at high energies our model correctly describes the experimental multiple ionization cross sections of the rare gases by low charged projectiles, i.e. for Ne and Ar up to triple ionization [2, 3], and for Kr and Xe [7] up to sextuple ionization. However, at intermediate energies the results show a tendency to overestimate. To analyze the dependence of the theoretical description with the target we compare the present results for He$^+$ on Ar, with previous ones for He$^+$ on Ne and Kr [2]. In figure 4 we display the triple ionization cross sections of Ne, Ar, and Kr by He$^+$. Clearly, the CDW-EIS description improves with higher target atomic numbers. It would be reasonable to say that changes in the target potential due to the removal of three bound electrons affect more to Ne (with 10 electrons) than to Kr (with 36 electrons), at least if we accept that relaxation takes place in the collision time. The inclusion of certain kind of response or time-dependent potential reduces the cross sections, as shown for He^{+2} in Ne and Ar [10, 11], and also by the TDDFT calculations [14, 15]. However, the increase in the theoretical and computational complexity versus the possibility within the IPM of obtaining multiple ionization results for multi-electron targets at high energies, involving all the target electrons and for high final charge states (quintuple, sextuple ionization), is something to evaluate in each case of study.

3.4. Total ionization of Ar by He$^+$ and He^{+2}

Finally, in figures 5 and 6 we show the total ionization cross section $\sigma = \sum n\ \sigma_n$, where σ_n is the n-fold pure ionization cross section. In figure 5 we compare our CDW-EIS values for the ionization of Ar by He^{+2} with the measurements by DuBois [20], and Rudd *et al* [22]. For energies above 500 keV amu^{-1} we also include the proton impact total ionization cross sections by Rudd [48] (times Z_P^2). The CDW-EIS describes quite well the measurements even at lower energies than expected. Around the maximum, Rudd

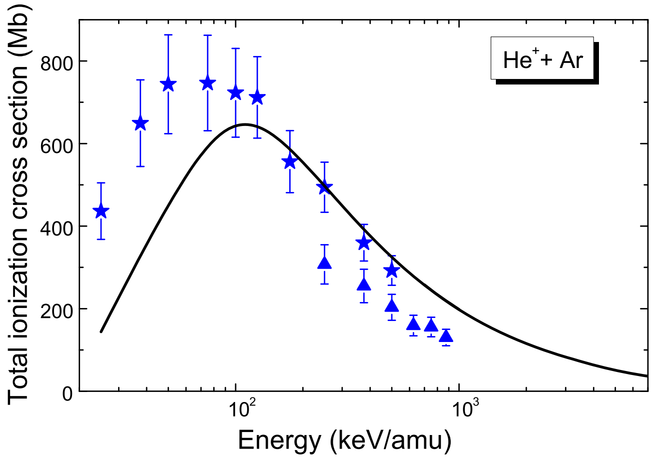

Figure 6. Total ionization cross section of Ar by He^+. Curves: present CDW-EIS ionization cross section. Symbols, experimental data: full stars, DuBois [18]; full triangles, Santos *et al* [21].

experimental values [22] include capture and separate from DuBois [20] pure ionization measurements. In the case of ionization of Ar by He^+, in figure 6, the theoretical results only describe the data by DuBois [18] above 100 keV ($v \sim Z$). This is the range of validity of the CDW-EIS approximation. The values by Santos [21] are low, even compared with previous DuBois measurements [18].

4. Concluding remarks

In this contribution we study the pure ionization of Ar by Helium ions, considering three aspects, inner-shell ionization, n-fold ionization including PCI, and total ionization. We combine the independent particle approximation CDW-EIS with empirical branching ratios of final charge state. The present single to quintuple ionization cross sections are rather good, especially for high impact energies where the PCI dominates. We found an overestimation of the triple and quadruple ionization cross sections in the intermediate energy region. The multielectron direct ionization dominates in this energy region over the PCI. The lack of inter-electronic correlation, not included in the independent electron model, and of electron capture contribution could be the reason for this difference. The K and L-shell ionization cross sections and also the total ionization cross sections show the good performance of the present proposal above 0.1 MeV amu^{-1}.

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