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# Electron impact ionization of multiply charged ion : a BE study

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Abstract : The electron impact ionization of multi-charged positive ions has been investigated in a binary encounter approximation which includes the effect of dipole interaction. Based on the geometry of the collision of electron with the target ions the model has been modified to provide a simple analytical expression for the ionization cross section. The modified expression has been used to calculate cross sections for single ionization of doubly and triply charged ions of noble gas atoms. The calculated cross sections are found to agree well with the available experimental measurements, especially in the higher energy region were hard collisions are expected to dominate. Comparison with experiment also shows that inclusion of inner shell contribution should further improve our results with respect to the measured values.

Keywords : Ionization cross section, electron impact, BED model

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## 1. Introduction

There exists much motivations for the sutdy of highly ionized atoms because they find wide applications in the field of astrophysics and fusion plasma [1,2]. They have applications in the interpretation of spectra from space, developments of X-ray lasers [3] and diagnostics of fusion plasma impurities [4]. Study of solar corona and flares [5], which affect our day to day life, also requires data on highly ionized systems. The availability of astrophysical and fusion data from the solar and heliospheric observatory (SOHO) and the Joint European Toras (JET) has provided further impetus to the study of multicharged ions. As a result many attempts have been made to provide simple theoretical models to calculate electron impact ionization of positive ions. The Mott theory [6] describing the collision of two free electrons has been improved upon by Vriens [7] by assigning a velocity distribution to the target electron so as to make it applicable for electron impact ionization of atoms and ions. This binary encounter theory, in its symmetric form, presents a simple analytical expression to calculate electron impact ionization cross sections of ionized targets. As it is an improvement over Mott theory, it suffers from the same shortcoming, namely it fails to account for distant collisions which take place essentially through the dipole interaction between the projectile and the target electron. As the dipole interaction dominates at high impact energies, the theory of Vriens fails to predict the correct asymptotic behaviour of the observed cross sections.

A number of attempts have subsequently been made, with varying success [8,9], to introduce the correct asymptotic

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nature in the binary encounter expression for the cross section by mixing the distant and close collision terms. Such an attempt has recently been mady by Kim and Rudd [10] to develope a model in which both the soft and hard collisions are mixed properly so that the calculated cross section agrees well with the experimental findings in the high energy region as well. As the scattered and ejected electrons become indistinguishable after an ionizing collission, they have also tried to retain the electron exchange effect in this model. They call their model '*Binary Encounter Dipole (BED) Model*' and have successfully used the same to calculate electron impact ionization cross sections for atoms, molecules and ions.

We attempt further improvement in this model keeping the collision geometry of the electron-ion interaction in mind. In the following section we describe the basic features of this model along with the modifications incorporated. We then apply the modified model to estimate the electron impact ionization cross sections of multicharged ions of noble gases. We also compare our calculated cross sections with the available experimental measurements. We finally end this article with a short concluding remark.

## 2. Theoretical method

Following Kim and Rudd [10], we define the following dimensionless variables :

$$t = \frac{T}{B},\ \overline{\omega} = \frac{W}{B},\ u = \frac{U}{B} \tag{1}$$

where $B$ is the binding energy of the target electron, $U$ is the average KE of the bound electron, $T$ is the KE of the projectile and $W$ is the KE of the ejected electron.

Taking $R$ as the Rydberg energy and $a_0$ as the first Bohr radius, we also define

$$S = 4\pi a_0^2 N\left(\frac{R}{B}\right)^2 \tag{2}$$

where $N$ is the number of bound electrons in the considered shell. The single differential cross section due to electron impact can then be expressed by the following expression :

$$\frac{d\sigma}{d\overline{\omega}} = S\sum_{n=1}^{n=3} F_n(t) f_n(\overline{\omega}) \tag{3}$$

where Kim and Rudd [10] have chosen the following values for $F_n$ in the symmetric binary encounter model.

$$F_1 = \frac{-F_2}{t+1},\ F_2 = \frac{2-\left(\frac{N_i}{N}\right)}{t+u+1},\ F_3 = \frac{\ln t}{t+u+1} \tag{4}$$

where various terms have been defined in Ref. 10. While arriving at this expression care has been taken to incorporate the direct, exchange and interference terms along with the dipole interaction. They have suggested that for $n = 1$ and 2, a simple expression

$$f_n(\overline{\omega}) = \frac{1}{(1+\overline{\omega})^n} \tag{5}$$

will be appropriate for the present purpose. However following Bethe theory, $f_3(\omega)$ has been taken as

$$f_3(\overline{\omega}) = \frac{1}{N(1+\overline{\omega})}\frac{df}{d\overline{\omega}} \tag{6}$$

where $df/d\overline{\omega}$ is the differential oscillator strength incorporated to let the $F_3 f_3$ term represent the dipole interaction. This enables them to write a very simple analytical expression for the single differential cross section due to electron impact, incorporating the important dipole interaction term, as follows :

$$\frac{d\sigma(\overline{\omega},t)}{d\overline{\omega}} = \frac{s}{(t+u+1)}\{A+B+C\} \tag{7}$$

with $$A = \frac{\left(\frac{N_i}{N}\right)-2}{t+1}\left(\frac{1}{\overline{\omega}+1}+\frac{1}{t-\overline{\omega}}\right)$$

$$B = \left[2-\left(\frac{N_i}{N}\right)\right]\left[\frac{1}{(\overline{\omega}+1)^2}+\frac{1}{(t-\overline{\omega})^2}\right]$$

and $$C = \frac{\ln t}{N(\overline{\omega}+1)}\frac{df(\overline{\omega})}{d\overline{\omega}}$$

We now proceed to use this relation for investigating electron impact ionization of a number of positively charged ions due to electron impact. As the incident electron will experience a Coulombic attraction (see also Kumar and Rai [1]) by the ionized target it is appropriate to obtain the total ionization cross section ($\sigma_i$) by carrying out the following intergration

$$\sigma_i = \int_0^{t/2}\frac{d\sigma}{d\overline{\omega}}d\overline{\omega} \tag{8}$$

The above change in the upper limit of the integration. along with some more simplifications, finally leads to a simple analytical expression for $\sigma(t)$ for all $t$ :

$$\sigma_i = \frac{S}{(t+2)}\left[\left\{\frac{1}{2}-\frac{2}{(t+2)^2}\right\}\right.$$

$$\left.\times \ln t + \frac{t}{t+2} + \frac{1}{t} - \frac{\ln(t+2)}{t+1}\right] \tag{9}$$

instead of evaluating the differential oscillator strength, we have used an approximate expression provided by Bethe [11] and used by Kim and Rudd in their simpler version of the binary encounter model. As the Virial theorem shows, $u = (U/B)$ is exactly equal to unit for any one electron atom. We also adopt this result for other targets as a first order approximation while deriving equation (9).

## 3. Results and discussion

We have used equation (9) to calculate electron impact ionization cross sections of multicharged ions of noble gases with charge state $q \geq 2$ upto impact energy 1 keV. In the following we however present a few selected results of ours and compare them with the available experimental measurements.

In Figure 1 the cross sections for ionization of $Ne^{2+}$ and $Ar^{2+}$ are plotted against the electron energy. The calculated cross sections are found to agree well with the experimental observations of Bannister [12] and Danjo *et al* [13]. For $Ne^{2+}$ our cross sections are in close agreement with those of Danjo *et al* in the lower energy range whereas at higher impact energies the recent measurements of Bannister exhibit better agreement. The estimated cross sections are found to be smaller than the measured values throughout the energy range, we have studied. Our calculated cross section is about 26% smaller than that of the measured value at 175 eV. This difference increases upto 32% at $E = 500$ eV, returning back to 26% at $E = 800$ eV. This type of systematic difference with respect to the experimental observations is quite expected because contribution from the inner shell of the target has not yet been taken into account. Before we make further comments on this aspect, we would like to point out that slightly improved agreement is obtained in case of electron impact ionization of $Ar^{2+}$; the present cross sections agree well with the measured value of Muller *et al* [14] and Man *et al* [15]. It is heartening to note that comparitively recent work Man *et al* shows better agreement with our calculated cross sectrions at $E = 300$ eV. In fact in this region the present cross sections nearly lie within the error bars of their measurements. For this system also the present cross sections are smaller than the measured values; this difference however decreases systematically from 31% at 175 eV to nearly 11% at 700 eV. As in case of $Ne^{2+}$, here also we have not included the contribution of 3*s* shell of $Ar^{2+}$ towards the process of target ionization.

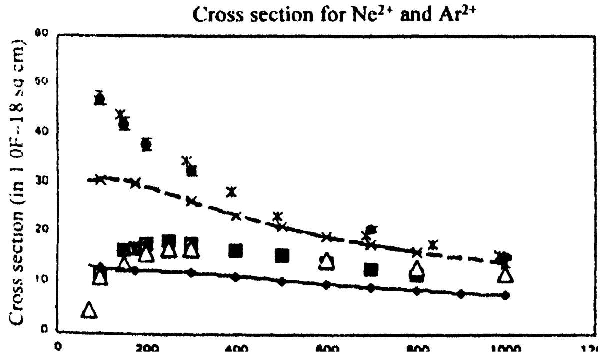

Figure 1. —— Present result for $Ne^{2+}$, ----- present result for $Ar^{2+}$ : Δ and □ are expts. for $Ne^{2+}$ (Refs. 13 and 12), X and O are expts. for $Ar^{2+}$ (Refs. 14 and 15)

In Figure 2, we present our calculated cross sections for $Ne^{3+}$ and $Ar^{3+}$ alongwith the available experimental results of Gregogy *et al* [16]. The present calculation for $Ne^{3+}$ exibits satisfactory agreement with the experimental observations in the energy range of our interest. As expected, our calculated cross sections are smaller in magnitude as compared to the measured values; the deficit is around 40 ± 5%. Agreement is bound to improve a lot if we include contribution from the next inner shell of the target in our calculation. It is desirable at this juncture to make some pertinent comments on the role of inner shell ionization on the process of single ionization of the target. Comparing $Ne^{3+}$ with $Ne^{2+}$ we find that disagreement with the experimental observations has increased by 10% or more in the investigated energy range. This is hardly surprising. In $Ne^{2+}$, 2*p* is the outer most shell which contains 4 electrons; the next inner shell 2*s* has only 2 electrons. Obviously contribution from the inner shell in this target is bound to be much smaller than what the valence shell contributes. But in case of $Ne^{3+}$, as 2*p* and 2*s* shells contain 3 and 2 electrons respectively, the role of inner shell ionization will be definitely more significant. This is very transparently exhibited through our calculations even without including the contribution of inner shells. We however plan to look into this aspect of target ionization in near future so that a more realistic comparison may be carried out with the experiments.

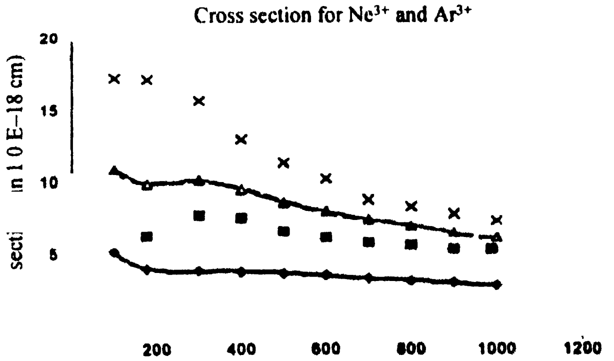

Figure 2. —— Present result for $Ne^{3+}$, ----- present result for $Ar^{3+}$ : □ is expt. for $Ne^{3+}$ (Refs. 16), X is expt. for $Ar^{3+}$ (Refs. 16).

In case of $Ar^{3+}$ (see Figure 2) also our calculated cross sections are found to be smaller than the measured values throughout the energy range of investigation; the deficit systematically decreases from 37% to 11% as we go to higher electron velocities. This discripancy, slightly larger than what we obtained for $Ar^{2+}$, can again be explained on the basis of relative contributions of valence shell and inner shell ionizations of the target. At this point it must be noted that the ions of Ne behave somewhat differently as compared to the ions of Ar. This may be partly due to the reason that a binary encounter description is not very suitable for Ne target. As noted by Bates and Kingston [17], the total ionization cross sections for this atom is expressed as the sum of partial ionization cross sections associated with continuum states of different angular momenta. As this target has certain special features associated with itself, and the BEA fails to take into account these features, the above sum often leads to a total ionization cross section much different from what should have been obtained (see also Ref. 1). It appears that different ions of Ne are also behaving in the same way and that is why results for $Ne^{2+}$ and $Ne^{3+}$ do not seen consistant with those for Ar ions.

Although we do not present our calculated cross sections for similar ions to Kr and Xe, we would like to mention that the estimated cross sections for these targets are on expected track. One major difference these ions have with those of Ne and Ar emanates from the difference in their atomic structure. For the ions of Ne and Ar, the inner shell is $2s$ which contains only two electrons. On the other hand the inner shell of Kr and Xe ions is $nd^{10}$, $n$ being 3 and 4 respectively for them. Consequently, contribution from the inner shell towards the process of single ionization of the target is bound to be large; it may even dominate over the outer shell stripping cross section in certain energy region. Our preliminary calculations for these ions confirm such a scenario as valence shell ionization cross sections turn out to be much smaller than their measured counter parts.

## 4. Conclusion

We have thus introduced a very simple modification in a binary encounter model, including the high energy dipole interaction term, so as to make it suitable for investigating the electron impact ionization of positively charged ions. The modified analytical expression has been sucessfully used to calculate cross sections for single ionization of doubly and triply charged ions of Ne and Ar. The obtained cross sections, agree well with the experimental results and the observed discripancy can very well be explained in terms of contributions from inner shell of the target. The method provides a very convenient way to make quick and satisfactory estimate of ionization cross sections; inclusion of inner shell contributions is expected to further improve agreement with experiments.

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