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Electron impact single ionization of copper

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Abstract. Electron impact single ionization cross sections of copper have been calculated in the binary encounter approximation using accurate expression for $\sigma_{\Delta E}$ as given by Vriens and Hartree–Fock momentum distribution for the target electron. The BEA calculation based on the usual procedure does not show satisfactory agreement with experiment in this case but a striking modification is found to be successful in explaining the experimental observations. The discrepancy is linked with the ionization of the $3d^{10}$ electrons and probably effective single ionization does not take place from $3d$ shell of copper leading to smaller values of experimental cross sections.

Keywords. Electron impact ionization; binary encounter approximation; Hartree–Fock momentum distribution; copper.

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1. Introduction

Electron impact ionization of atoms and ions is one of the most fundamental problems in atomic and molecular physics. The study of this process finds important applications in different fields of current interest and is important from both experimental and theoretical points of view [1,2].

Shah *et al* [3] developed a crossed beam technique incorporating time of flight spectroscopy for measurement of the electron impact ionization cross section of atomic hydrogen with high precision over a wide energy range. Later on it was used successfully for studies of ionization of stable gas atoms [4,5]. By the use of a specially developed high temperature oven source, McCallion [6] and Shah *et al* [7] applied this method to study single and multiple ionization of metallic species. Many metallic species are important in fusion energy research and astrophysical applications [8]. Bolorizadeh *et al* [8] of the Belfast group have carried out accurate experimental measurements of single and multiple ionization of copper by electron impact at energies ranging from near threshold (7.8 eV for single ionization) to 2100 eV. The use of thermal energy copper beams in their measurements obviated metastable contamination ensuring that their experiment contained ground state copper atoms $(3d^{10}4s)$ only.

Unfortunately, theoretical calculations of even single ionization cross sections for copper have not been reported so far. Bolorizadeh *et al* [8] have compared their experimental measurements with the predictions based on the well-known Lotz [9] formula. The non-availability of theoretical calculations in case of copper is probably due to the complex nature of target as evidenced by Lotz's empirical calculations of single ionization cross sections. Calculations of ionization cross sections by quantal methods are difficult particularly for complex atomic targets. On the other hand, the binary encounter approximation developed by Gryzinski [10] has been successful in predicting ionization cross sections of atoms and ions. The model of Gryzinski using accurate expression of $\sigma_{\Delta E}$ as given by Vriens [11] and integrating the cross section over Hartree–Fock velocity distribution of target electrons has yielded satisfactory results in case of several atomic and ionic targets [12–14]. Keeping the above mentioned facts in view, we consider it worthwhile to use the BEA for a theoretical investigation of single ionization cross sections of copper by electron impact.

2. Theoretical methods

We have used the Vriens expression [11] in a symmetrical model including exchange and interference for calculating electron impact single ionization cross sections. In the unsymmetrical model of Gryzinski [10], if the incident and the target electron are at the same distance from the nucleus, it is assumed that because of the interaction with the nucleus, the atomic electron has finite potential energy whereas the incident electron has potential energy zero. On the other hand, the symmetrical model of Vriens [11] assumes that the incident electron with initial kinetic energy $\frac{1}{2}mV_1^2$ (m and V_1 being the mass and the velocity of the incident electron respectively) gains a kinetic energy $U + \frac{1}{2}mV_2^2$ (U, m and V_2 being the binding energy, the mass and the velocity of the atomic electron respectively) and simultaneously loses the same amount of potential energy before it interacts with the atomic electron which is bound with this potential energy. This ensures that the total energy of incident electron is conserved. By virtue of the above mentioned considerations, the Vriens expression in the symmetrical model includes exchange and interference (see Vriens [15]). Using dimensionless variables based on the work of Catlow and McDowell [16] the expression for cross section can be written in a convenient form as (see [12])

$$Q^i(s,t) = \frac{4}{(s^2+t^2+1)}\left[\frac{s^2-1}{s^2U} + \frac{2t^2}{3}\left(\frac{s^4-1}{s^4U^2}\right) - \frac{\Phi \ln s^2}{U^2(s^2+1)}\right](\pi a_0^2), \tag{1}$$

where

$$\Phi = \cos\left\{\left(\frac{1}{s^2U+U}\right)^{1/2}\ln s^2\right\}.$$

In the above expression $s^2 = V_1^2/V_0^2$, $t^2 = V_2^2/V_0^2$ where V_1 and V_2 are the velocities in atomic units of the incident and target electron respectively. V_0 is the root mean square velocity in atomic unit of the target electron corresponding to the binding energy of the shell under consideration. The equality of the magnitudes of the binding energy and the

mean kinetic energy of the target electron predicted by the virial theorem for the Coulomb potential gives the relation $\frac{1}{2}mV_0^2 = U$. Thus, in atomic units we have $\frac{1}{2}V_0^2 = U$ and hence $V_0^2 = U$ where U is the ionization potential of the shell of the target in Rydbergs [16].

The above expression for $Q^i(s,t)$ has been integrated numerically over the Hartree–Fock velocity distribution for the target electron to obtain the ionization cross section. Thus, the expression for electron impact single ionization cross section for a particular shell of the target is given by

$$Q^i(s) = n_e \int_0^\infty Q^i(s,t) f(t) U^{1/2} \mathrm{d}t. \tag{2}$$

Here n_e is the number of equivalent electrons of the atomic shell and $f(t)$ is the momentum distribution for the target electron. The momentum distribution function $f(t)$ is given by (see [16])

$$f(t) = 4\pi t^2 U \rho_{nl}(tU^{1/2}). \tag{3}$$

Here

$$\rho_{nl} = \frac{1}{2l+1} \sum_{m=-l}^{m=+l} |\psi_{nlm}(\mathbf{x})|^2,$$

where

$$\psi_{nlm}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int \phi_{nlm}(\mathbf{r}) \mathrm{e}^{i\mathbf{x}.\mathbf{r}} \mathrm{d}\mathbf{r}$$

is the Fourier transform of the one electron orbital

$$\phi_{nlm}(\mathbf{r}) = N_{nl} R_{nl}(r) Y_{lm}(\Omega)$$

in which $R_{nl}(r)$ is the Hartree–Fock radial function. In the present work, we have used ionization thresholds and Hartree–Fock radial wavefunctions of $4s$ and $3d$ shells of copper as given by Clementi and Roetti [17].

At this stage we would like to mention that the use of Hartree–Fock wavefunction does not properly take into account the correlation between the electrons in an atom. There are methods by which correlation between electrons can be properly taken into account e.g. configuration interaction approach based on Slater–Condon theory, multiconfiguration Hartree–Fock approach. Calculations using these wavefunctions become very complicated, particularly for heavier targets. With the use of correlated wavefunctions in the BEA the aim of adopting a simplified theoretical approach will not be achieved. In this connection, we would like to mention that Hartree–Fock wavefunctions consider the electron–electron correlation to some extent through antisymmetrization [18]. Moreover, for fast projectiles the effects of electron–electron correlation may not be significant [19]. Thus, the use of Hartree–Fock wavefunction in studies on ionization process using the BEA may be considered to be reasonable.

3. Results and discussion

In order to obtain electron impact single ionization cross sections for copper, we have considered ionization from $4s$ and $3d$ shells only. Ionization from deeper inner shells $(3p, 3s, 2p, 2s)$ have not been included in the present calculations as a single vacancy in the shells leads to Auger emission as discussed by Bolorizadeh *et al* [8]. The present results along with experimental data [8] and empirical calculations of Lotz [9] have been shown in figure 1 and table 1. In the figure we have plotted the single ionization cross sections considering ionization from $4s$ shell including contribution due to only one electron of $3d$ shell. The reason of adopting this type of approach would be discussed below. The contribution from $4s$ and $3d$ shells have been shown separately in the table. Firstly, we would like to discuss our results by considering ionization from $4s$ shell only. At low incident energies the present results overestimate the cross sections and at 10 eV impact energy the calculated result is two times larger than the experimental value. With increase in energy the calculated results become closer to experimental data up to 20 eV. Beyond this energy value the calculated results underestimate the cross sections but are within a factor of two up to 70 eV impact energy. At still higher energies the discrepancy goes on increasing and at 1000 eV the experimental result is about 4.5 times larger than the calculated value. The peaks obtained in our calculation and experiment appear at 20 and 30 eV respectively. The magnitudes of the peaks are 2.55×10^{-16} and 3.21×10^{-16} cm^2 respectively, the theoretical cross section being about 20% smaller than the experimental value. The calculations of Lotz show a peak at 50 eV which is much shifted in position as compared to the present calculations and the experiment. If the contribution of 10 electrons of $3d$ shell is included in the calculations, the cross sections becomes 5 to 6 times larger than the experimental data at all incident energies above 25 eV. In this connection it may be

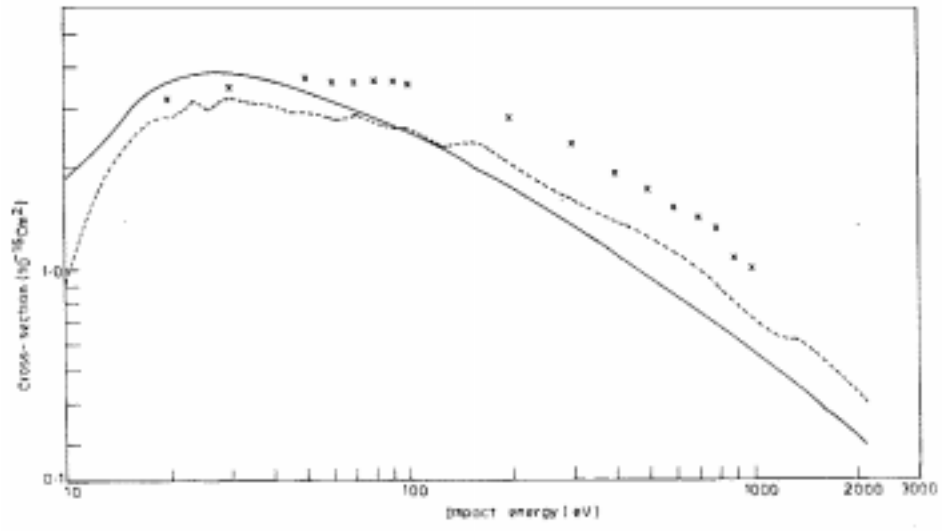

Figure 1. Electron impact single ionization cross sections of copper in units of 10^{-16} cm^2. Present results ———; experimental results [8] - - - - ; empirical calculation of Lotz [9] xxxx .

Table 1. Electron impact single ionization cross section for copper in unit of 10^{-16} cm^2.

Energy (eV)	Present result			Experimental result [8]	Empirical calculation of Lotz [9]
	$4s$ contribution	One $3d$ electron contribution	Total		
20	2.55	1.06	3.61	2.80	3.2
30	2.33	1.47	3.80	3.21	3.5
40	2.05	1.56	3.61	3.08	3.6
50	1.81	1.56	3.37	2.90	3.7
60	1.62	1.54	3.16	2.77	3.6
70	1.46	1.50	2.96	2.89	3.54
80	1.31	1.46	2.77	2.76	3.6
100	1.12	1.38	2.50	2.55	3.5
200	0.64	1.07	1.71	2.05	2.8
300	0.46	0.89	1.35	1.63	2.3
400	0.33	0.72	1.05	1.43	1.9
500	0.28	0.65	0.93	1.20	1.7
600	0.24	0.58	0.82	1.12	1.5
700	0.21	0.52	0.73	0.97	1.4
900	0.18	0.46	0.64	0.73	1.07
1000	0.15	0.41	0.56	0.66	1.0

noted that calculations of single ionization cross sections in the binary encounter approach show good agreement with experimental data in high energy region, being always within a factor of two.

At this stage it is worth mentioning the observation made by Lotz who calculated electron impact ionization cross sections of atoms with the help of his empirical formula and found satisfactory agreement with experimental data in most of the cases. In absence of theoretical calculation, experimental data are often compared with the results obtained by Lotz formula, as done by Bolorizadeh *et al* in case of copper. Lotz has mentioned that he had to reduce the cross section of $3d^{10}$ electrons drastically for copper target in order to get reasonable agreement with experiment. Almost similar difficulties have been observed by Lotz in case of silver $(4d^{10}5s)$ [9] which has electronic configuration of similar nature as that of copper. Keeping in view the observation of Lotz, we have made an ad hoc assumption to include contribution of one $3d$-electron in order to examine the results. It can be seen from the figure and table that the results so obtained are in good agreement with the experimental data throughout the energy range investigated. The peaks appear in the calculation and the experiment at 26 and 30 eV respectively being close to each other. The magnitudes of the peaks are 3.81×10^{-16} and 3.21×10^{-16} cm^2 respectively, the theoretical cross section being about 19% larger than experimental value.

From the facts given above it is apparent that one faces difficulty in calculation of $3d$ shell single ionization cross section of copper if contributions from all the ten electrons are taken into account. Similar difficulties have been experienced by earlier workers in case of other atoms and ions involving ionization from fully occupied d-shells. Bell *et al* [20] have observed difficulties in calculation of electron impact ionization of In^+. In

order to obtain satisfactory agreement with experiment the contribution to the ionization cross sections from electrons in the $4d$ shells was added in at only one half of its calculated value in configuration averaged distorted wave (CADW) approximation. Use of only half of the d-subshell contribution was proposed by Rogers *et al* [21] earlier and was found to fit the experimental data better in case of other experiments [22,23]. In case of electron impact ionization of gallium, Patton *et al* [24] have discussed the observation made by Vainshtein *et al* [25] that autoionization is the dominant Ga^{2+} production mechanism since removal of a $3d$ electron leads mainly to double ionization. Later on Thomason *et al* [26] have mentioned about the calculation of Younger [27] for electron impact ionization of $4d$ electron in Cs^+ which leads to autoionization and hence double ionization.

Now we would like to discuss the possibilities of different physical processes consequent upon ionization of $3d$ electron in case of copper. After removal of one electron from $3d$ shell, the target is left in $3d^9 4s$ state. This state is not an autoionizing state and hence autoionization is not possible. At the same time removal of a $3d$ electron will not lead to an Auger decay since there is only one electron in state higher than $3d$. However, it is quite likely that there may be a high probability of immediate de-excitation of the target from $3d^9 4s$ configuration to $3d^{10}$ configuration. In other words, the ionization of a $3d$ electron in copper may lead to the immediate capture of the $4s$ electron. This might be due to hybridization of d and s electrons during the scattering. Thus, the consideration of pure s electrons and pure d electrons during the ionization has no physical justification.

At this stage we would like to mention that the probability of the above mentioned process may not be unity. However, it is not possible to estimate this probability in the BEA. From the discussion given above it is probable that large number of $3d^{10}$ copper ions and only a small number of $3d^9 4s$ copper ions might have been detected in the experiment. The former case corresponds to effective single ionization of $4s$ shell only whereas the latter case corresponds to a small probability of single ionization of $3d$ shell. The entire discussion suggests that the actual probability of single ionization of d shell in case of copper may be much smaller as compared to the probability obtained by usual method leading to a small contribution from ionization of d shell.

We have also calculated electron impact single ionization cross section of scandium (with a single d electron) and found that depending on the binding energies of d and s shells, ionization cross sections are consistent with those obtained in case of copper. Due to non-availability of experimental data in the literature it is not possible to draw any conclusion regarding single ionization of d shell of scandium and hence the results are not presented here.

The discussion given above explains why the inclusion of contribution of one $3d$ electron brings our calculated result in good agreement with the experiment. More elaborate theoretical investigation is required for quantitative understanding of the process of single ionization from $3d$ shell of copper. It is expected that this work will stimulate other theoretical workers to take up further study of this problem.

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