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ELECTRON IMPACT IONIZATION OF PLASMA IMPORTANT ATOMIC Be, B AND BX (X= N, O) TARGETS

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ABSTRACT

Electron impact cross sections on atomic boron and their compounds are required for understanding the erosion processes in fusion experiments [1]. The present paper reports comprehensive theoretical investigations on electron scattering with atomic Beryllium and Boron, and diatomic molecules containing boron viz, BX (X= N, O). Presently we determine the total inelastic cross section Q_{inel} and total ionization cross section Q_{ion}, in a complex potential quantum mechanical formalism [2]. We have started with the well-known spherical complex (optical) potential formalism (SCOP) [3], which provides total elastic cross section Q_{el} and its inelastic counterpart Q_{inel} that includes Q_{ion}. We employ our well established method to extract ionization cross sections Q_{ion} from calculated inelastic cross sections Q_{inel}, by introducing a ratio function as in [2, 3]. Since no experimental data are available, we calculate the Q_{ion} with two values of the peak position ratio R_p = 0.70 and 0.75. The calculated cross sections are tested against the available comparisons, and new results are also reported.

Keywords: electron, scattering, ionization, plasma

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INTRODUCTION

Electron impact ionization cross sections with atomic or molecular targets are widely used in modeling the structure and dynamics of plasmas [1], e.g. in the modeling of low- and high- temperature plasmas and in laser-plasma interactions. The boronization of the plasma exposed surfaces of tokomaks has proved to be an effective way to produce very pure fusion plasmas [2]. Apart from this, the ionization cross sections have wide applications in radiation physics, mass spectrometry, astrophysics etc. Therefore, we have carried out theoretical studies on the title targets, and the present paper reports our ionization and other cross sections for a class of plasma important targets.

Collision processes involving Beryllium atoms are important since Be has been chosen for first-wall plasma facing components in ITER, [4]. Boronization of the plasma exposed surfaces of tokomaks has proved to be an effective way to produce very pure fusion plasmas [5]. Hence, electron impact cross sections on atomic boron are required for understanding the erosion processes in fusion experiments. A look at relevant literature shows that, several authors [6-10] have calculated electron impact ionization cross sections for atomic boron under different theoretical approximations, but no experimental results are available, making it an exotic target.

Other Boron compounds are also important in the study of laboratory plasma as well as astrophysical plasma. Boron nitride as a solid has its own importance. Similar to carbon, it has both hexagonal (soft graphite-like h-BN) and cubic (hard, diamond-like c-BN) crystalline structures. While h-BN is used as a high temperature component and lubricant, c-BN also known under commercial name borazon [11], is a superior abrasive. Its hardness is only slightly smaller, but chemical stability is superior to that of diamond. Also BN is used in the formation of structural materials in space ion engines [12]. As per our knowledge there is no study of electron impact cross sections on free or gas-phase molecules Boron Nitride (BN) and Boron Oxide (BO), while there are no measured data on any of the present atomic and molecular targets, and hence the present research holds significance.

Thus we have enough motivation for studying the targets listed in the title. The present paper employs a theoretical approximation called 'Complex Scattering Potential – ionization contribution' (*CSP-ic*) method [13-18] to obtain total ionization cross sections of electron scattering with atomic Beryllium and Boron and boron compounds viz., BN and BO, at energies from ionization threshold (I) to 2000 eV.

THEORETICAL METHODOLOGY

In the following text, the total (complete) cross section of electron-atom/molecule collisions is denoted by Q_T, and is the sum of total elastic cross section Q_{el} and total inelastic cross section Q_{inel}. Thus

$$Q_T(E_i) = Q_{el}(E_i) + Q_{inel}(E_i) \quad (1)$$

Further,

$$Q_{inel}(E_i) = \Sigma Q_{ion}(E_i) + \Sigma Q_{exc}(E_i) \quad (2)$$

Where E_i is the incident electron energy. The quantity $\Sigma Q_{ion}(E_i)$ in the above equation shows the sum-total of first, second etc ionization cross sections of the target. For simplicity we denote the first term by Q_{ion}. The quantity $\Sigma Q_{exc}(E_i)$ shows the summed total electronic excitation cross sections.

With this background let us outline how the total cross sections Q_{ion} of electron scattering from these targets are deduced from Q_{inel} within a broad frame-work of complex potential formalism. In the present range of electron energy, many scattering channels that lead to discrete as well as continuum transitions in the target are

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open. Therefore we represent the electron-atom/molecule system by a complex potential, $V(r, E_i) = V_R(r, E_i) + i\, V_I(r, E_i)$, such that

$$V_R(r, E_i) = V_{st}\ r\ + V_{ex}(r, E_i) + V_P(r, E_i) \tag{3}$$

The RHS three terms of the equation (3) represent the static, the exchange and the polarization potentials respectively. These are obtained from the spherically averaged charge-density $\rho(r)$ of the target, where r is the radial distance of the incident electron. The atomic charge density for Beryllium as well as Boron is derived from the wave functions of Bunge and Barrientos [19]. The spherically averaged molecular charge density $\rho(r)$ is determined from the constituent atomic charge densities derived from the atomic wave functions of [20].

Now, the imaginary term V_I of the complex potential, also called the absorption potential V_{abs} is adopted here in a well-known non-empirical quasi-free model form given by Staszeweska et al [20; see also ref. 21, 22]. Thus,

$$V_{abs}(r, E_i) = -\rho(r)\sqrt{\frac{T_{loc}}{210}}\cdot\left(\frac{8\pi}{kE_{F\ i}^3}\right)\cdot\theta(p^2 - k_F^2 - 2\Delta)\cdot(A_1 + A_2 + A_3) \tag{4}$$

The local kinetic energy of the incident electron is denoted by T_{loc}. In equation (4), $p^2 = 2E_i$, $k_F = [3\pi^2\rho(r)]^{1/3}$ is the Fermi wave vector and Δ is an energy parameter. Further $\theta(x)$ is the Heaviside unit step-function, such that $\theta(x) = 1$ for $x \geqslant 0$, and is zero otherwise. The dynamic functions A_1, A_2 and A_3 occurring in the equation (4) depend differently on $\rho(r)$, I, Δ and E_i. Detailed expressions of these functions are given in [20] and also in [21, 22]. The energy parameter Δ is crucial, since it determines a threshold below which $V_{abs} = 0$, and the ionization or excitation is prevented energetically. We have modified the original absorption model, by considering Δ as a slowly varying function of E_i around I. The justification for the same is discussed in [13-18]. Briefly, a preliminary calculation is done with a fixed value $\Delta = I$, but the variable Δ accounts for the screening of the absorption potential in the target charge-cloud region and also yields better agreement with experimental and other data in many cases. Next, we set up the Schrödinger equation with our modified V_{abs}, and finds the complex phase shifts $\delta_l = Re\ \delta_l + i\ Im\ \delta_l$ for various partial waves l by following the Variable Phase Approach of Calogero [23].

The total elastic (Q_{el}), inelastic (Q_{inel}) and total (complete) cross sections (Q_T) are generated from the S-matrix as per the standard expressions given in [24].

Now, electron impact ionization corresponds to infinitely many open channels, as against the electronic excitation, which comes from a small number of discrete scattering channels. Therefore, starting from threshold I the ionization channel becomes dominating gradually as the incident energy exceeds I, thereby making Q_{ion} the main contribution to Q_{inel}. Thus from equation (2), we have in general

$$\mathrm{Q_{inel}(E_i) \geq Q_{ion}(E_i)} \tag{5}$$

There is no rigorous way to project out Q_{ion} from Q_{inel}. But in order to determine Q_{ion} from Q_{inel}, a reasonable approximation can be evolved by starting with a ratio function,

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)} \tag{6}$$

Perhaps a first ever estimate of ionization in relation to excitation processes was made, for water molecules, by Turner et al [25].

The usual complex potential calculations include ionization contribution within the inelastic cross section. In order to deduce the said contribution, we have introduced a method based on the equation (6). In our Complex Scattering Potential – ionization contribution (*CSP-ic*) method, the energy dependence of R (E_i) is given by the following relation [13-18].

$$R(E_i) = 1 - C_1\left[\frac{C_2}{U + a} + \frac{\ln(U)}{U}\right] \tag{7}$$

where the incident energy is scaled to the ionization potential I through a dimensionless variable,

$$U = \frac{E_i}{I} \tag{8}$$

Equation (7) involves dimensionless parameters C_1, C_2, and a, which are determined by imposing three conditions on the function $R(E_i)$ as discussed in our papers [13-18]. Briefly, we have $R = 0$ at the ionization threshold and the ratio takes up asymptotic value $R' \approx 1$ at high energies typically above 1000 eV, in view of equation (7). The third condition on R arises from its behaviour near the peak of ionization, and is expressed in the following manner.

$$R(E_i) = \begin{cases} 0, at\ E_i = I \\ R_p, at E_i = E_p \\ R', for\ E_i \gg E_p \end{cases} \tag{9}$$

Here, E_p stands for the incident energy at which our calculated inelastic cross section Q_{inel} attains its maximum, while R_p 0.7 stands for the value of the ratio R at $E_i = E_p$. The choice of this value is approximate but physically justified. The peak position E_p occurs at an incident energy where the dominant discrete excitation cross sections are on the wane, while the ionization cross section is rising fast, suggesting that the R_p value should be above 0.5 but still below 1. This behavior is attributed to the faster fall of the first term $\sum Q_{exc}$ in equation (2). An exact theoretical evaluation of R_p does not seem to be possible, but one can try to see the effect of a small change in this value. The choice of R_p in equation (9) is not rigorous and it introduces uncertainty in the final results. From equation (8) at high energies, the ratio R' approaches ~~to~~ unity which is physically supported by the low ionization cross sections in the same energy region. We employ the three conditions on R to evaluate the three parameters of equation (7) and hence deduce the Q_{ion} from the calculated Q_{inel} by using equation (6). Thus, the method of complex potential coupled with ionization contribution to inelastic scattering as explained above offers the

determination of different total cross sections Q_T, Q_{inel}, and Q_{ion} along with a useful estimate on electronic excitations in terms of the summed cross section $\sum Q_{exc}$.

All the cross sections are examined here as functions of incident electron energy.

RESULTS AND DISCUSSION

It is appropriate to calculate the ionization cross sections of electron scattering from Be, B, BN and BO targets in the same theoretical formulation, as has been done presently. The present work is also important in view of the energy range in which ionization is taking place along with elastic scattering as well as electronic excitations. Various input properties of the targets are shown in table 1.

Table 1:- Various input properties of the present targets

Property	Be	B	BN	BO
First Ionization energy (eV)	9.32	8.29	11.92	13.3
Bond length (Å)	-	-	1.28	1.23

We have organized the discussion of our present results along with comparisons, into two subsets, as follows.

Atomic targets

Beryllium

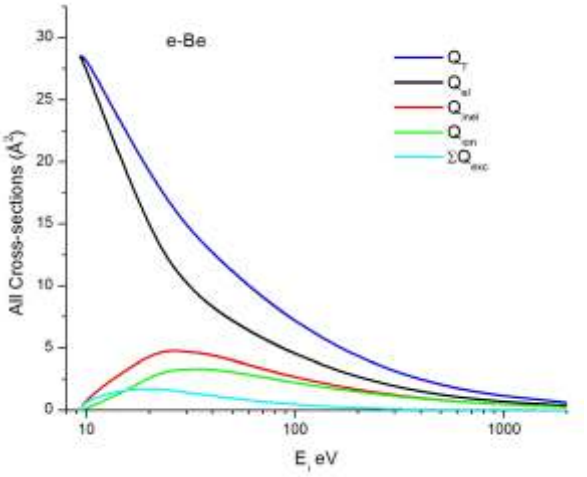
Turning to our theoretical results, we have shown all the present total cross sections of atomic beryllium as functions of electron energy in figure 1. This figure represents a comprehensive study not made so far on this atom. Total elastic cross sections of this target are higher than the inelastic cross sections even at high energies.

There have been only a few experimental efforts to obtain cross sections for excitation or ionization of beryllium or its ions, perhaps due to its toxic nature. On the theoretical side, there are plenty of calculations available for comparison. Studies of the electron - beryllium elastic scattering cross sections have been made by Fursa and Bray [26, 27] using the convergent close-coupling method at low energies. Also result of the DM (Deutch – Maerk) and BEB (binary encounter Bethe) calculations for the ionization cross section of Be [28] with predictions from CCC theory [29], R matrix with pseudostates (RMPS)[29], distorted wave method with electron scattering (DWIS) [30,31] and the plane-wave Born approximation or PWBA [32,33] methods are available. The details of these approaches can be found in the cited literature. For atomic Be the present Q_{ion} is calculated for two different values of R_p, viz 0.7 and 0.75. In Figure 2 both the present Q_{ion} are compared with all these theoretical calculations. We can see from the graph that there is no significant change in the cross section (apart from the peak) with the said change in ratio value. The DM and PWBA cross section maxima nearly coincide with each other but the PWBA curve falls off more rapidly at larger energies.

Boron

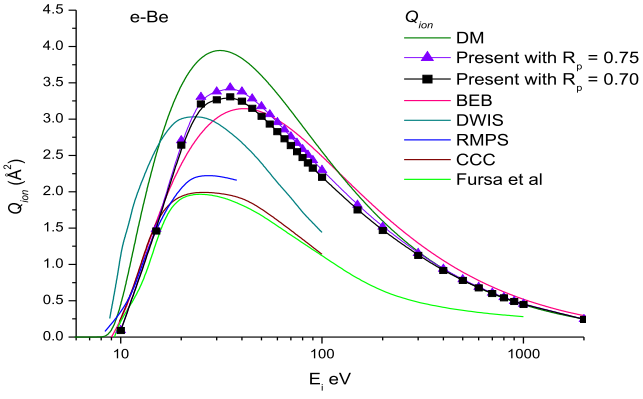
For atomic Boron the present Q_{ion} is calculated for two different values of R_p, viz 0.7 and 0.75. Our calculated ionization cross sections along with the compared data for electron scattering with B atoms are as shown in Figure 3. We can see from the graph that for Rp = 0.75, the cross section values are slightly higher than those for R_p = 0.70. Amongst the present targets atomic Boron finds the maximum of data-sets from the available literature, but all of these are theoretical results. The present Q_{ion} are compared with results from [5-9]. Kim and Stone [6] have calculated the ionization cross sections by BEB method, while Margreiter et al [7] performed theoretical calculations by an approximate DM formalism. Earlier Lotz [8] had derived the cross sections Q_{ion} by a semi-empirical formula. The ionization cross sections were also calculated by Stingl [9] using the Coulomb-Born Approximation. As one can see, the results of Margreiter et al [7] are quite large and correspond to the highest peak among the present comparison (figure 3). The peak position of Q_{ion} in our results is slightly shifted to lower energy with respect to the semi-empirical data from Stingl [9] and the BEB values of Kim and Stone [6]. On the other hand the theoretical estimates from Lotz [8] and recommended data by Moores [10] are underestimating.

Figure 1:- Various total cross sections (in Å^2) of electro scattering with Be atom



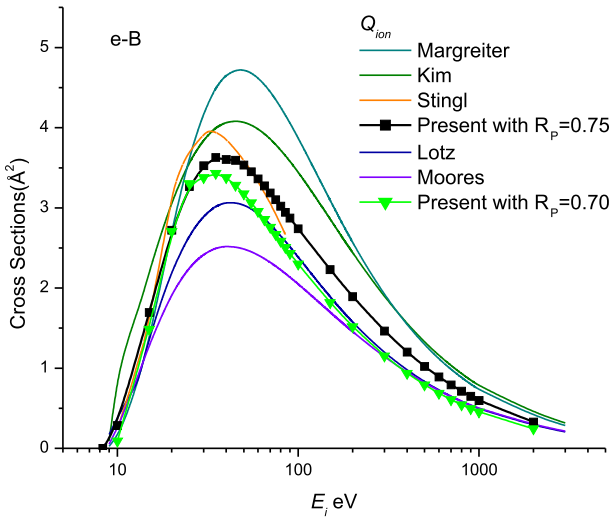
Blue solid line - Present $Q_{T;}$ Black solid line - Present $Q_{el;}$ Red solid line - Present $Q_{inel;}$ Green solid line - Present $Q_{ion;}$ Cyan solid line - Present

Figure 2 Total ionization cross sections (in Å^2) of atomic Be by electron impact



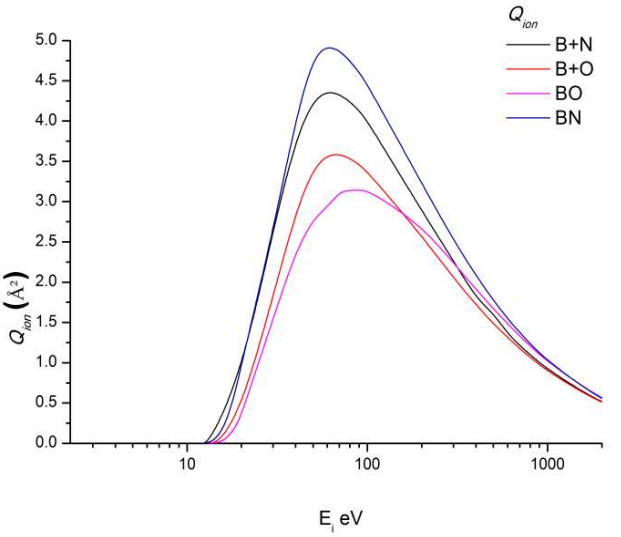
Olive line– DM [28] $Q_{ion,}$ Black Squares– Present Q_{ion} with Rp = 0.70, Violet triangles – Present Q_{ion} with Rp = 0.75, Pink line – BEB[28], Dark Cyan line – DWIS[30,31] $Q_{ion,}$ Blue line – RMPS[29] $Q_{ion,}$ Maroon line - CCC[29] $Q_{ion;}$ Green line – Fursa at al[26,27] $Q_{ion.}$

Figure 3: Electron scattering ionization cross sections (in Å^2) of atomic Boron



Dark cyan line – Margreiter[7]$Q_{ion;}$ Green line – Kim[6]$Q_{ion;}$ Orange line Stingl[9]$Q_{ion;}$ Black Squares– Present $Q_{ion;}$ Blue line – Lotz[8]$Q_{ion;}$ Red line – Moores[10]$Q_{ion.}$

Figure 4: Electron scattering ionization cross sections (in Å^2) of BN and BO



Black solid line – Present Q_{ion} (B+N); Red solid line – Present Q_{ion} (B+O); Magenta solid line – Present Q_{ion} (BO); Blue solid line – Present Q_{ion} (BN)

Molecular targets

BN and BO

As discussed above, the boron compounds BN and BO are of much importance in the field of plasma Physics and technology. But there is hardly any electron impact cross sectional data available for them. Both these are linear polar molecules. Their electron impact ionization cross sections determined presently are shown in figure 4. Due to the higher ionization potential the Boron nitride target gives very high values of Q_{ion} as compared to Boron oxide. The peak Q_{ion} values of the molecules are in accordance with their molecular bond lengths. For the comparison purpose, we have also applied simple additivity rule as indicated in the figure 4. The present CSP-*ic* results (with R_p = 0.70) are lower than the additivity values, and that is expected on theoretical grounds.

CONCLUSIONS

In conclusion we have reported here our theoretical cross sections of electron collisions with two light atoms Be and B, and two lesser known molecules BN and BO for which there are no experimental measurements so far. For e – Be ionization discrepancies are found among the present and compared theoretical data. We believe that, in view of small ionization thresholds the atomic ionization peaks would not be so small as indicated by some of the compared results in figures 2 and 3. Our atomic cross sections are in an overall agreement with the BEB theory, which is known for its successes in many cases. Further, the present method with chosen R_p= 0.70 has also met with success in a number of atomic and molecular targets. Our molecular results are also in keeping with their size or bond-length and ionization threshold.

It would be interesting to examine isoelectronic molecules BN and C_2, and also extend these calculations to electron scattering in solid phases of BN and BO.

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