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Electron Impact Single and Double Ionization Cross Sections of Cr Ions and Atoms

Dharmendra Rai[1], Akhilesh Kumar Gupta[2,*], Geetanjali[3], Lalan Kumar Jha[4]

Abstract

The theoretical calculations of electron impact single and double ionization cross section of Cr ions/atom have been estimated from threshold 32 eV to 1000 eV and 40eV to 6000 eV impact energies respectively. The modified Binary Encounter Approximations (BEA) has been used in the aforesaid calculation. These theoretical electron impact ionization cross sections of Chromium ions or atoms are of pivotal importance in the several studies. The accurate expression of $\sigma_{\Delta E}$, cross sections for energy transfer ΔE and Hartree-Fock (HF) velocity distribution function for the target electron have been used throughout the calculations. The theoretical findings and experimental data of single ionization cross sections of Cr ions are compared. The calculated single ionization cross sections are in the excellent agreement with the experimental data throughout, particularly in intermediate to high impact energy range. In case of double ionization cross section of Cr atoms are compared with the result obtained from other theoretical approach and the results are in similar trend for intermediate to higher energy range. In case of electron impact double ionization, the ionization cross sections of Cr target atoms are calculated using the same theoretical method and the results are compared with the result obtained from other theoretical approach. On such comparison the results obtained are found in a suitable agreement and also following the similar trend of cross-sectional variation with impact energy for intermediate to higher energy range. The present theoretical estimation of electron impact single and double ionization cross sections of Cr ions and atoms respectively are in exemplary agreement with the data available.

Keywords: Electron impact, single ionization cross section, double ionization cross section, binary encounter approximations, chromium ions

INTRODUCTION

***Author for Correspondence**
Akhilesh Kumar Gupta
Email: akhil.inphy@gmail.com

[1]Research Scholar, Department of Physics, Patna University, Patna, Bihar, India
[2]Assistant Professor, Department of Physics, Patna University, Patna, Bihar, India
[3]Assistant Professor, Department of Physics, R. N. College, Hajipur, Bihar, India
[4]Professor, Department of Physics, B.R.A. Bihar University, Muzaffarpur, Bihar, India

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Collisions between electrons and atoms or ions are among the most fundamental interactions studied in atomic, molecular and plasma physics. Electron-impact ionization of atoms and ions is essential for processes in planetary atmospheres, pulsed-power switching, gaseous dielectrics, plasma physics as well as in many spectroscopic and collisional studies [1]. Ionization cross-sections obtained in the case of projectile-target atom interactions provides vital information about target atoms and their internal collisional dynamics. These ionization processes are important in fusion plasmas and gaseous environments rich in energetic electrons [2, 3]. Although cross-sections for multiple ionization are limited in the literature owing to mathematical complexities compared to those of single ionization and double ionization

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cross sections. Several quantal approaches have been successfully developed and implemented to obtain accurate values of electron impact ionization cross sections in different impact energy ranges for atoms/ions. However, these approaches have limitations for heavy atomic targets. Pindzola et al. [4] used a time-dependent close-coupling method to obtain the double ionization cross sections of He and this work was extended to obtain the electron-impact direct double ionization cross sections (DDI) for Mg, Be and Be^+ [5–7]. The Binary Encounter Approximation (BEA) has been successfully applied to calculate the electron-impact single and double ionization cross-sections for various atoms and ions.

In the past, the Binary Encounter Approximation has been used to calculate the ionization cross-sections of atoms and ions resulting from charged-particle impact [8]. The theoretical calculations showed good agreement with the experimental data [9]. The modified Binary Encounter Approximation has been successfully applied to calculate the single-ionization cross-sections for a range of atoms and ions under charged-particle impact [10]. Gryzinski made pioneering contributions by developing various theoretical approaches for rigorous investigations of atomic collision processes using the Binary Encounter Approximation [11–13]. Subsequently, several researchers have taken an interest in this approximation and introduced significant modifications for studies of ionization and charge-transfer processes [14, 15]. In the case of electron-impact ionization of atoms and ions, cross-section calculations have been successfully performed using the BEA [16–18]. Vriens derived an accurate expression for $\sigma_{\Delta E}$, the cross- section for energy transfer ΔE within the symmetrical model that is widely used in the calculation of ionization cross-sections [19].

Among the various multiple-ionization processes, double ionization is the most significant and has received considerable attention. In this case, electrons may be ejected either through direct interaction between the incident electron and the target electrons or due to the post-collisional relaxation of the residual target. Because of their wide range of applications and importance in understanding atomic collision dynamics, the study of single and double ionization processes is valuable from both experimental and theoretical perspectives [20]. Gryzinski [12] proposed two processes within a double binary encounter model for calculating the double direct ionization (DDI) cross-sections of atoms and ions. In the first process, it is assumed that the incident particle ejects two electrons through two successive interactions with the target material. The second process involves the incident particle ejecting one electron from the target, followed by the removal of a second electron by the first ejected electron. The cross-sections for these processes are referred to as Q_{sc}^{II} (scattered component) and Q_{ej}^{II} (ejected component). Roy and Rai [21] modified Gryzinski's mathematical framework by incorporating the necessary corrections into his expressions. They evaluated the double direct ionization cross-sections of atoms and ions by performing integrations over the energy transfers and velocity distributions of bound electrons in the expressions for Q_{sc}^{II} and Q_{ej}^{II}. Vriens [22] and Kara et al. [23] adopted the idea of a double binary encounter process as suitable.

In the electron impact ionization (EII) of Cr, the process involves an incident electron colliding with Cr (atom or ion) transferring sufficient energy to remove one or more bound electrons. For transition metals such as chromium (Cr), multiple ionization stages are possible owing to the partial filling of its 3d and 4s orbitals. The behaviour of each charge state depends directly on its specific configuration. The interaction is often denoted as

$$Cr^{q+} + e \rightarrow Cr^{(q+1)+*} + 2e$$

where Cr^{q+} is the initial charge state, the superscript $*$ denotes a possible excited state of the resulting ion and two electrons appear in the final state: the scattered projectile and the ejected electron.

The common charge states of chromium (Cr) in the case of electron impact ionization can form positively charged ionic species with various charges q with notable states as follows:

1. In electron impact ionization, positively charged ionic species with various charges q can be formed with notable states being Cr^0 (neutral chromium) that is the initial state before ionization

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and Cr^+ (singly charged ion), which is formed when one electron is removed, typically from the 4s or 3d orbitals. The electron-impact single ionization of the neutral Cr channel is therefore given as

$e^- + Cr^0 \rightarrow Cr^+ + 2e$ and for Chromium ion the channel is $e^- + Cr^+ \rightarrow Cr^{2+} + 2e$.

An incident electron knocks out one bound electron from the Cr atom/ion, producing Cr^+ and Cr^{2+} for Cr atoms and ions respectively.

2. The doubly ionized state of neutral chromium (Cr^{2+}) is formed by removing a second electron, often from the remaining 4s or 3d electrons. The channels are $e^- + Cr^0 \rightarrow Cr^{2+} + 3e$ and $e^- + Cr^+ \rightarrow Cr^{3+} + 3e$ for the Cr atom and ion respectively.

The ground state ionization channels are $e^- + Cr^+\left(6_{S_{\frac{5}{2}}}\right) \rightarrow Cr^{2+}\left(5_{D_0}\right) + 2e$

These channels are useful for electron impact ionization, plasma physics, and atomic collision studies. For the double ionization channel, singly ionized chromium is $e^- + Cr^+ \rightarrow Cr^{3+} + 3e$. Two bound electrons are removed from the target ion in a single collision. According to Moore's atomic energy level [24], the relevant chromium charge states are $e^- + Cr^+(3d^5 6_{S_{\frac{5}{2}}}) \rightarrow Cr^{3+}\left(3d^3 4_{F_{3/2}}\right) + 3e$. These are the standard charge states and ionization channels commonly quoted in atomic collision studies of chromium ions using Moore's level designations.

These ionic states of chromium (Cr) are achieved via electron impact ionization channels, namely direct ionization (DI) and excitation-autoionization (EA). In the DI processes, the incident electron directly ejects a bound electron into the continuum. In the case of Cr, this often involves the outer 4s electron first, followed by 3d electrons at higher energies. However, for EA processes an inner-shell electron (e.g.3p or 3s) is excited to a higher orbital creating an unstable state that subsequently ejects an electron contributing to higher charge states.

In the present calculation, the Hartree-Fock velocity distribution function is used to obtain the electron impact direct double ionization cross-sections for the ejection of both electrons of the Cr atom targets. The HF wave function includes electron-electron correlation to some extent through anti-symmetrization [25], which is insignificant in the case of fast projectiles [26]. Therefore, the HF wave function for the target electrons is considered reasonably appropriate for the study of DDI in the BEA approximation. In light of the above-stated facts, it is worthwhile to estimate and analyze the electron-impact single and double ionization cross sections of Cr ions and atoms respectively using the modified BEA. We chose the experimental data of the electron impact single ionization cross-section of Cr ions reported by Maan et al. [27] for the present studies. An experiment was performed to measure the absolute electron-impact single ionization cross section using the cross-beam technique. The experimental observations were compared with theoretical calculations which showed a high degree of success of the theoretical method and model used. The DDI cross-section of a Cr atom have been reported by Bhatt et al. [28] using a semi-empirical model. Direct double ionization (DDI) obtained using a semi-empirical model was compared with DDI Cross sections using the present modified Binary Encounter Approximation. The present results show a similar trend for the DDI cross section and its coherency in the higher impact energy range, except for the cross-sectional peak obtained at a lower impact energy. The resulting electron-impact single and double ionization cross-sections for the Cr ions/atoms show reasonable agreement with the available data, which shows the high degree of success of the method imposed.

In the present model adopted for the theoretical calculation of electron impact single and double ionization cross sections of Cr ions and atoms, the uncertainty and sensitivity involved are due to the physical assumption of the model and the input parameters such as orbital binding energy, shell radii

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and electron occupation number. The Binary Encounter Approximation (BEA) assumes that the projectile interacts primarily with one target electron and many-body correlations are neglected. Near the threshold, the energy of the incident electron is very low; hence, the impact parameter is large. In such a situation, the magnitude of the ionization cross-section is large compared to the experimental measurements. This process is called a distance-encounter collision. With an increase in the energy of the projectile, the impact parameter gradually decreased. Hence, the magnitude of the calculated cross sections decreases. This process is called a close-encounter collision. In addition, owing to exchange and interference phenomena the theoretical ionization cross-sections overestimate at low impact energies and as a consequence of electron-electron correlation the ionization cross-sections underestimate at higher impact energies.

The modified Binary Encounter Model is valid for intermediate and high-impact energy ranges. Therefore, it is valid for close encounters.

METHOD OF CALCULATION

The theoretical approaches used to calculate the electron-impact single and double ionization cross sections of atoms have been discussed previously [18]. For the reader's convenience, we find it helpful to provide a brief and organized overview of the underlying physical processes, along with the cross-section expressions used in this work. In our calculations of single and double ionization cross sections, we used Vriens' [19] accurate expression of $\sigma_{\Delta E}$ for the energy transfer ΔE, which accounts for both exchange and interference effects.

To simplify the calculations, we introduce two dimensionless variables *s* and *t* defined as follows: $s^2 = \frac{v_1^2}{v_0^2}$ and $t^2 = \frac{v_2^2}{v_0^2}$ where $v_1$and v_2 are the velocities in atomic units of the incident and target electrons respectively and $u = v^2$ is the ionization potential of the target in Rydbergs [29]. All other energies involved are expressed in Rydbergs. In terms of these variables, $\sigma_{\Delta E}$ is given by

$$\sigma_{\Delta E} = \frac{2}{(s^2+t^2+1)u}\left[\left(\frac{1}{\Delta E^2} + \frac{4t^2u}{3\Delta E^3}\right) + \left(\frac{1}{(s^2u+u-\Delta E)^2} + \frac{4t^2u}{3(s^2u+u-\Delta E)^3}\right) - \frac{\emptyset}{\Delta E(s^2u+u-\Delta E)}\right](\pi {a_0}^2) \quad (1)$$

Where, $\emptyset = \cos\{(s^2u+u)^{-\frac{1}{2}} \ln s^2\}$ [30].

Similarly, the expression for the electron-impact single ionization cross-section is given as

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

Equation (2) has been numerically integrated over the Hartree–Fock velocity distribution of the target electron [31], leading to the following final expression for the ionization cross section:

$$Q^i(s) = n_e \int_0^\infty Q^i(s,t)\, f(t) U^{\frac{1}{2}} dt(\pi {a_0}^2) \quad (3)$$

The total direct double ionization cross section Q_D^{ii} is given by

$$Q_D^{ii} = Q_{sc}^{ii} + Q_{ej}^{ii}. \quad (4)$$

The expressions for Q_{sc}^{ii} and Q_{ej}^{ii} given by Gryzinski [13] and modified by Roy and Rai [21].

Where,

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$$Q_{sc}^{ii} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int_{U_i}^{E_q-U_{ii}}\sigma_{\Delta E}\left[\int_{U_{ii}}^{E_q-\Delta E}\sigma_{\Delta E'}d(\Delta E')\right]d(\Delta E) \quad (5)$$

$$Q_{ej}^{ii} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int_{U_i+U_{ii}}^{E_q}\sigma_{\Delta E}\left[\int_{U_{ii}}^{\Delta E-U_i}\sigma_{\Delta E'}d(\Delta E')\right]d(\Delta E) \quad (6)$$

Provided,

n_e-the number of electrons in the shell under consideration.

$\Delta E -$ energy transfer during first binary collision

r-denotes the mean distance between the electrons in the shell

$r = \frac{R}{n_e^{1/3}}$, where R is the radius of the target shell

The expressions for Q_{sc}^{ii} and Q_{ej}^{ii} were evaluated by numerically integrating over the energy transfers and Hartree–Fock velocity distributions of the two emitted electrons.

The function f(t) appearing in the above expressions is the momentum distribution function for the bound electron given by

$$f(t) = 4\pi t^2 u\rho_{nlm}(tu^{\frac{1}{2}}) \quad (4)$$

where, $\rho_{nlm} = \frac{1}{2l+1}\sum_{m=-l}^{l}|\psi_{nlm}|^2$ (5)

and

$\psi_{nlm}(\boldsymbol{X}) = \frac{1}{2\pi^{\frac{3}{2}}}\int \emptyset_{nlm}(r)e^{ix.r}dr$ is the Fourier transform of the one electron orbital

$$\emptyset_{nlm}(r) = N_{nl}R_{nl}(r)Y_{nlm}(\Omega) \quad (6)$$

Where, $R_{nl}(r)$-Hartree-Fock radial function.

RESULT AND DISCUSSIONS

We calculated the electron-impact single ionization of chromium ions (Cr ions) from their respective thresholds of 32 eV to 1000 eV impact energies using the modified BEA. The theoretical description is provided in Section 2. The ionization cross-section obtained using the modified Binary Encounter approximation tends to overestimate the values at low impact energies and underestimate them at higher impact energies. In the present study, this trend was observed from the threshold to 280 eV. To calculate the electron-impact single-ionization cross sections of the Cr ion, contributions from different shells were considered. The ejection of one electron leading to single ionization from different shells (3s), (3p), and (3d) of the Cr ion is considered in this work. The direct double ionization (DDI) cross-section of Cr atoms was also calculated using the method cited for the electron impact energy range of 40–6000 eV. The contributions of the double ionization cross sections are considered for the ejection of electrons from the (3d,3d), (3d,3p), and (3d,3s) shells. This result was compared with other theoretical cross sections reported in the literature.

Single Ionization of Chromium ion

The computed values for the single ionization cross sections (SICS) of Cr ions are presented alongside the available experimental data in Table 1 and Figure 1. The electron-impact single-ionization cross-section of Cr ions was calculated over an impact energy range of 32–1000 eV using a modified BEA. The theoretical description is provided in Section 2. The theoretical ionization cross sections for Cr ions were calculated at impact energies for which experimental data were available. A comparison between the theoretical and experimental results supports the validity of the adopted theoretical

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framework. The Cross-sectional contribution of the ejection of one electron leading to single ionization from different shells (3d, 3p, and 3s) for Cr ions was considered in the present calculation. At low impact energies up to 80 eV, the theoretical cross-sections underestimate the experimental data [27]. The theoretical peak occurred at an impact energy of 100 eV, whereas the experimental peak was observed at approximately 65 eV. The theoretical and experimental results were nearly identical over the impact energy range of 90–1000 eV. The experiment reported an error of approximately 4.1%–4.6% for impact energies above 16.5 eV, whereas at low impact energies, the error was much larger, reaching nearly 80%. At an impact energy of 90 eV, the theoretical ionization cross-section matched the experimental observation.

Here, the theoretical and experimental ionization cross sections are in excellent agreement when the contributions from the 3d and 3p shells are included in the total ionization cross section. The analysis and comparison with the experimental cross-sections [27] show that the BEA agrees well with the experimental observations over a wide range of impact energies. However, it underestimates the values at low impact energies up to 80 eV, whereas at higher energies, it closely matches the experimental data. Therefore, this theoretical calculation of the electron impact ionization cross-section has a high degree of success for intermediate and high impact energy ranges.

Double Ionization of Chromium atoms

The computed values for the theoretical double ionization cross sections (DICS) of Cr atoms are presented alongside the available Bhatt et al. data in Table 2 and Figure 2. The electron-impact double ionization cross-section is denoted as (e, 3e). In the initial channel, a single projectile electron interacts with a target atom or ion, whereas in the final channel, there is one scattered projectile electron, two ejected electrons, and the resulting target ion. The cross-section for producing Cr^{2+} ions via electron-impact double ionization of Cr was calculated over the energy range from its threshold of 40 eV to 6000 eV. The total electron-impact double ionization cross sections were obtained by considering contributions from the (3d, 3d), (3d, 3p), and (3d, 3s) shells. The maximum value of the theoretical ionization cross-section for Cr^{+2} ions was calculated as 5.79 at 100 eV. However, Bhatt et al. [28] reported a cross-section peak at 150 eV impact energy. At higher impact energies, the theoretical double ionization cross section of Cr gradually decreased. The present calculation of the double ionization cross section of Cr atoms is compared with the theoretical calculation reported by Bhatt et al. [28]. For impact energies below 1000 eV, the ratio of the present calculated cross-section to that of Bhatt et al. is beyond 1.8. At higher impact energies, both theoretical calculations are in good agreement. The binding energies of the different shells of Cr ions used in this theoretical analysis were obtained from the tables of Clementi and Roetti.[32], and the shell radii are taken from Desclaux [33].

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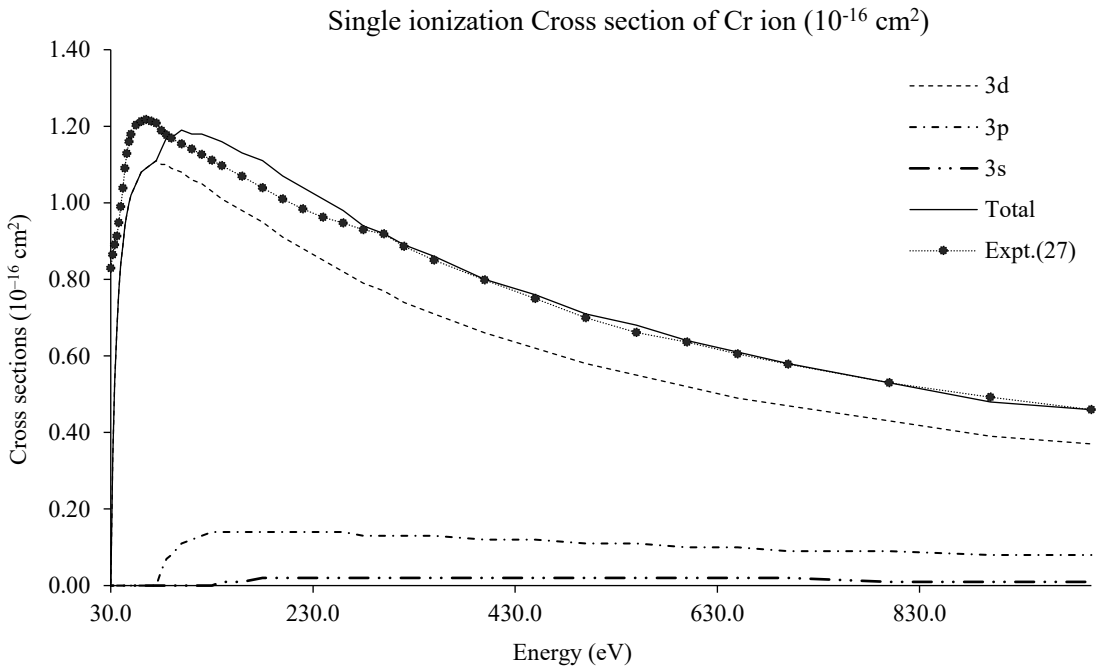


Figure 1. Electron impact single ionization cross sections of Cr ion (in the units of 10^{-16} cm^2).

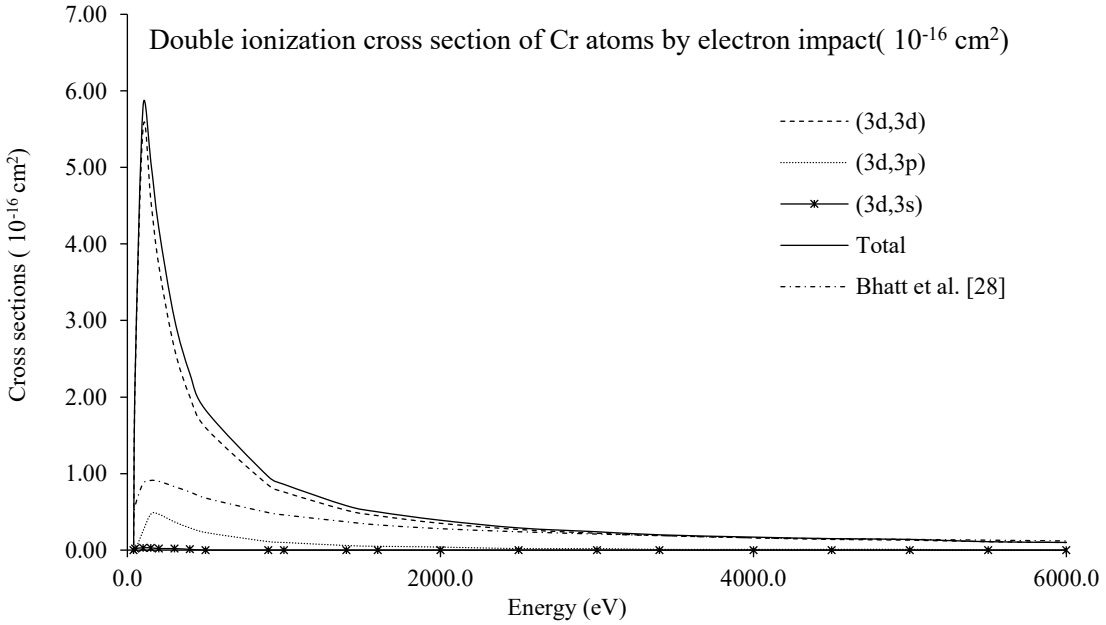


Figure 2. Electron impact double ionization cross sections of Cr atoms (in the units of 10^{-16} cm^2).

Table 1. Electron impact single ionization cross section of Cr ion (in the units of 10^{-16} cm^2).

Energy (eV)	3d	3p	3s	Total	Expt. [27]
32.0	0.33	0.00	0.00	0.33	0.864
34.0	0.53	0.00	0.00	0.53	0.890
36.0	0.67	0.00	0.00	0.67	0.913
38.0	0.77	0.00	0.00	0.77	0.948
40.0	0.84	0.00	0.00	0.84	0.990
42.0	0.89	0.00	0.00	0.89	1.038
44.0	0.94	0.00	0.00	0.94	1.090

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46.0	0.97	0.00	0.00	0.97	1.129
48.0	1.00	0.00	0.00	1.00	1.160
50.0	1.02	0.00	0.00	1.02	1.179
55.0	1.05	0.00	0.00	1.05	1.203
60.0	1.08	0.00	0.00	1.08	1.212
65.0	1.09	0.00	0.00	1.09	1.217
70.0	1.10	0.00	0.00	1.10	1.213
75.0	1.11	0.00	0.00	1.11	1.208
80.0	1.10	0.04	0.00	1.14	1.189
85.0	1.10	0.07	0.00	1.17	1.177
90.0	1.09	0.08	0.00	1.17	1.169
100.0	1.08	0.11	0.00	1.19	1.154
110.0	1.06	0.12	0.00	1.18	1.140
120.0	1.05	0.13	0.00	1.18	1.126
130.0	1.03	0.14	0.00	1.17	1.111
140.0	1.01	0.14	0.01	1.16	1.097
160.0	0.98	0.14	0.01	1.13	1.069
180.0	0.95	0.14	0.02	1.11	1.039
200.0	0.91	0.14	0.02	1.07	1.010
220.0	0.88	0.14	0.02	1.04	0.984
240.0	0.85	0.14	0.02	1.01	0.962
260.0	0.82	0.14	0.02	0.98	0.947
280.0	0.79	0.13	0.02	0.94	0.930
300.0	0.77	0.13	0.02	0.92	0.919
320.0	0.74	0.13	0.02	0.89	0.886
350.0	0.71	0.13	0.02	0.86	0.850
400.0	0.66	0.12	0.02	0.80	0.798
450.0	0.62	0.12	0.02	0.76	0.750
500.0	0.58	0.11	0.02	0.71	0.700
550.0	0.55	0.11	0.02	0.68	0.661
600.0	0.52	0.10	0.02	0.64	0.636
650.0	0.49	0.10	0.02	0.61	0.605
700.0	0.47	0.09	0.02	0.58	0.578
800.0	0.43	0.09	0.01	0.53	0.530
900.0	0.39	0.08	0.01	0.48	0.492
1000.0	0.37	0.08	0.01	0.46	0.460

Table 2. Electron impact double ionization cross section of Cr atoms (in the units of10^{-16} cm^2).

Energy (eV)	**(3d,3d)**	**(3d,3p)**	**(3d,3s)**	**Total**	**Bhatt et. al. [28]**
40.0	0.07	0.00	0.00	0.07	0.41
50.0	2.27	0.00	0.02	2.29	0.58
100.0	5.51	0.25	0.03	5.79	0.87
150.0	4.57	0.47	0.03	5.07	0.91
200.0	3.73	0.47	0.02	4.22	0.90
300.0	2.64	0.37	0.02	3.03	0.83
400.0	2.00	0.29	0.01	2.30	0.76

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500.0	1.60	0.23	0.00	1.83	0.68
900.0	0.85	0.11	0.00	0.96	0.49
1000.0	0.76	0.10	0.00	0.86	0.46
1400.0	0.52	0.06	0.00	0.58	0.37
1600.0	0.45	0.05	0.00	0.50	0.33
2000.0	0.35	0.04	0.00	0.39	0.28
2500.0	0.27	0.02	0.00	0.29	0.24
3000.0	0.22	0.02	0.00	0.24	0.21
3400.0	0.19	0.01	0.00	0.20	0.19
4000.0	0.16	0.01	0.00	0.17	0.16
4500.0	0.14	0.01	0.00	0.15	0.15
5000.0	0.13	0.01	0.00	0.14	0.14
5500.0	0.11	0.00	0.00	0.11	0.13
6000.0	0.10	0.00	0.00	0.10	0.12

CONCLUSIONS

The calculated electron-impact single-ionization cross-sections of the Cr ion over impact energies from the threshold up to 1000 eV indicate that the dominant contribution to the total ionization cross-section arises from the 3d shells. The theoretical ionization cross section using B.E.A. is in excellent agreement with the experimental observation in the intermediate and higher impact energy ranges. At low impact energies up to 80 eV, the theoretical cross sections were lower than the experimental observations. The theoretical and experimental results were nearly identical over the impact energy range of 90–1000 eV. The experimental observations reported an error of approximately 4.1%–4.6% beyond 16.5 eV impact energy. Overall, the theoretical and experimental cross sections were in excellent agreement across the entire energy range of up to 1000 eV. The cross-section for producing Cr^{2+} ions via electron-impact double ionization of Cr atoms was calculated over the energy range from the threshold of 40 eV to 6000 eV. The present calculation of the direct double ionization cross section of the Cr atom is compared with the results obtained from other theoretical results. At higher impact energies, the theoretical double ionization cross-section of Cr atoms gradually decreased. At intermediate and higher impact energies, both theoretical calculations are in very good agreement and showing similar trend of cross-section variation with impact energy.

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