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

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

Abstract

The theoretical calculations of electron impact single and double ionization cross section of Cr ion/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 ion or atom 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 ion 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 section of Cr ions/atoms 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

Collisions between electrons and atoms/ions are among the most fundamental interactional studied in atomic, molecular and plasma Physics. Electron-impact ionization of atoms and ions is essential to 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 case of projectile-target atoms interactions provides vital information about target atoms and their internal collisional dynamics. Such ionization processes are important in fusion plasmas and in gaseous environments rich in energetic electrons [2, 3]. Although cross-sections for multiple ionization are limited in literature due to mathematical complexities than those of single ionization and double ionization cross sections. Several quantal approaches have been successfully developed and implemented for obtaining accurate values of electron impact ionization cross sections in different

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

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

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impact energy range for atoms/ions. These approaches have the limitations for the heavy atomic targets. Pindzola et al. [4] used time dependent close coupling method for obtaining double ionization cross sections of He and this work have been 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 electron-impact single and double ionization cross-sections for a variety of atoms and ions.

In the past, the Binary Encounter Approximation has been used to calculate ionization cross-sections of atoms and ions resulting from charged-particle impact [8]. The theoretical calculations have shown good agreement with experimental data [9]. The Modified Binary Encounter Approximation has been successfully applied to calculate 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 took 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 previously been successfully carried out 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 various multiple-ionization processes, double ionization is the most significant and of considerable attention. In this case, electrons may be ejected either through direct interaction between the incident electron and the target electrons or due to post-collisional relaxation of the residual target. Because of their wide range of applications and their 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 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. 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), respectively. 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 energy transfers and the velocity distributions of bound electrons in the expressions for Q_{sc}^{II} and Q_{ej}^{II}. Vriens [22] and Kara et al [23] have been adopted this idea of double binary encounter process to be suitable.

In the electron impact ionization (EII) of Cr the process involved in which an incident electron collides 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 dueto 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.

Common charge states of Chromium (Cr) in 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 can form positively charged ionic species with varios charges q, with notable states are Cr^0 (neutral chromium) i.e. the initial state before ionization, Cr^+ (singly

charged ion) which is formed when one electron is removed, typically from the 4s or 3d orbitals. For electron impact single ionization of neutral chromium 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 Cr atom/ion producing Cr^+ and Cr^{2+} for Cr atom and ion respectively.

2. Double ionized state of neutral Chromium (Cr^{2+}) consequently 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 $e^- + Cr^+ \rightarrow Cr^{3+} + 4e$ for 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 very useful for electron impact ionization, plasma physics and atomic collision studies. For doubly ionization channel singly ionized chromium is $e^- + Cr^+ \rightarrow Cr^{3+} + 3e$. Where 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 state and ionization channels commonly quoted in atomic collision studies of chromium ion 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 case of Cr, this often involves the outer 4s electron first, followed by 3d electrons at higher energies while 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 Hartree-Fock velocity distribution function is used to obtain electron impact direct double ionization cross sections for ejection of both electrons of Cr atom targets. HF wave function includes electron-electron correlation to some extent through anti symmetrisation [25] which effect is insignificant in case of fast projectile [26]. Therefore, HF wave function for target electrons regarded reasonably appropriate in the study of DDI in BEA approximation. In the light of the above stated facts, it is worthy to estimate and analyse the electron impact single and double ionization cross sections of Cr ion and atoms respectively using modified BEA. We have chosen the experimental data of electron impact single ionization cross section of Cr ion reported by Maan et al. [27] for the present studies. The experiment was performed to measure the absolute electron impact single ionization cross section using cross beam technique. The experimental observation is compared with theoretical calculation which shows high degree of success of the theoretical method and model used. The DDI cross section of Cr atom reported by Bhatt et al [28] using semi empirical model. Direct double ionization (DDI) obtained using semi empirical model is compared with DDI Cross sections using present modified Binary Encounter Approximation. The present result shows the similar trend of DDI cross section and its coherency in the higher impact energy range except the cross-sectional peak obtained at lower impact energy. The resulting electron-impact single and double ionization cross sections for the Cr ion/atoms shows reasonably good agreement with the data available which shows 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 is due to physical assumption of the model and the input parameters such as orbital binding energy, shell radii and electron occupation number. Binary Encounter Approximation (BEA) assume that the projectile interacts primary with one target electron and many body correlation are neglected. Near the threshold the energy of the incident electron is very low and hence the impact parameter is large. In such a situation the magnitude of ionization cross section is large compare to the experimental measurements. Such a process is called distance encounter collision. With the increase in of the projectile the impact parameter gradually decreases. Hence, the magnitude of calculated cross sections are decreases. This process is called close encounter collision. Also due to exchange and interference phenomena the theoretical ionization cross sections overestimates at low impact energies and as a consequence of electron-electron correlation the ionization cross sections underestimate at higher impact energies.

Since modified Binary Encounter Model is valid for intermediate and high impact energy range therefore, it valid for close encounter.

METHOD OF CALCULATION

The theoretical approaches used to calculate electron-impact single and double ionization cross sections of atoms have already been discussed earlier [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 have 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 velocities in atomic units of the incident and the target electrons, respectively and $u = v^2$ is the ionization potential of the target in Rydbergs [29]. All other energies involved have also been expressed in Rydbergs. In terms of these variables, $\sigma_{\Delta E}$ is given as

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

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

In the same way, the expression for 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 is given by

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

expressions for Q_{sc}^{ii} and Q_{ej}^{ii} given by

The expressions for and given by Gryzinski [13] and modified by Roy and Rai [21].

Where,

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

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

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

The expressions for Q_{sc}^{ii} and Q_{ej}^{ii} were evaluated by numerically integrating over the energy transfers and the 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

$$f(t) = 4\pi t^2 u \rho_{nlm}(tu^{\frac{1}{2}}) \quad (7)$$

where, $$\rho_{nlm} = \frac{1}{2l+1}\sum_{m=-l}^{l}|\psi_{nlm}|^2 \quad (8)$$

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

$$\emptyset_{nlm}(r) = N_{nl}R_{nl}(r)Y_{nlm}(\Omega) \quad (9)$$

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

RESULT AND DISCUSSIONS

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

Single Ionization of Chromium ion

The computed values for the single ionization cross sections (SICS) of Cr ion are presented alongside the available experimental data in Table 1 and Figure 1. The electron-impact single-ionization cross section of the Cr ion has been calculated over the impact energy range of 32 eV to 1000 eV using modified BEA. The theoretical description is given in section 2. The theoretical ionization cross sections for the Cr ion have been calculated at impact energies for which experimental data are available. Comparison between the theoretical and experimental results supports the validity of the adopted theoretical framework. The Cross-sectional contribution of ejection of one electron leading to the single ionization from different shells (3d, 3p, 3s) for Cr ions are 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 occurs at an impact energy of 100 eV, while the experimental peak is observed at around 65 eV. The theoretical and experimental results are found to be nearly identical over the impact energy range of 90 eV to 1000 eV. The experiment reports an error of about 4.1%–4.6% for impact energies above 16.5 eV, while at low impact energies the error is much larger, reaching nearly 80%. At an impact energy of 90 eV, the theoretical ionization cross section matches the experimental observation.

Here, the theoretical and experimental ionization cross sections are in excellent agreement throughout when the contributions from the 3d and 3p shells are included in the total ionization cross section. The analysis and comparison with experimental cross sections [27] show that the BEA agrees well with experimental observations over a wide range of impact energies. However, it underestimates the values at low impact energies up to 80 eV, while at higher energies it closely matches the experimental data. Therefore, this theoretical calculation of electron impact ionization cross-section having 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, while 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 has been calculated over the energy range from its threshold of 40 eV up to 6000 eV. The total electron-impact double ionization cross sections are obtained by considering contributions from the (3d,3d), (3d,3p), and (3d,3s) shells. The maximum value of theoretical ionization cross section for Cr^{+2} ions calculated is 5.79 at 100 eV. While Bhatt et al. [28] cross section peak is reported at 150 eV impact energy. At higher impact energy the theoretical double ionization cross section of Cr gradually decreases. The present calculation of double ionization cross section of Cr atom is compared with 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 energy both theoretical calculations are in very good agreement. The binding energies of the different shells of Cr ions used in this theoretical analysis are taken from the tables of Clementi and Roetti.[32], and the shell radii are taken from Desclaux [33].

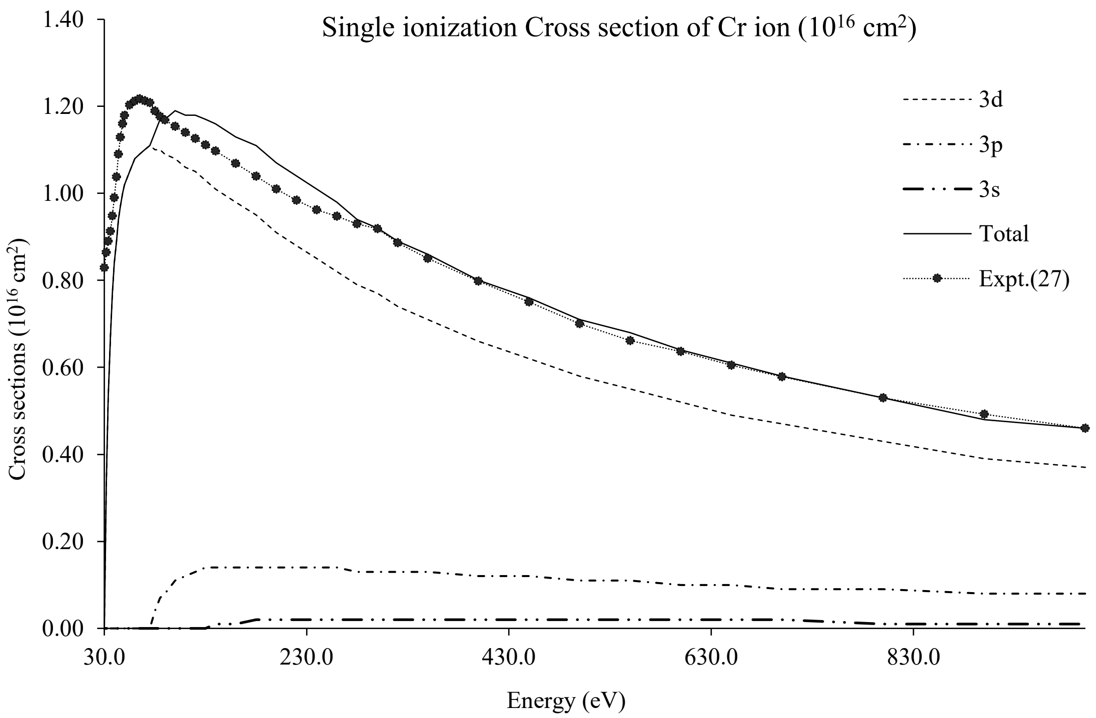

Figure 1. Electron impact single ionization cross sections of Cr ion (10^{-16} cm^2).

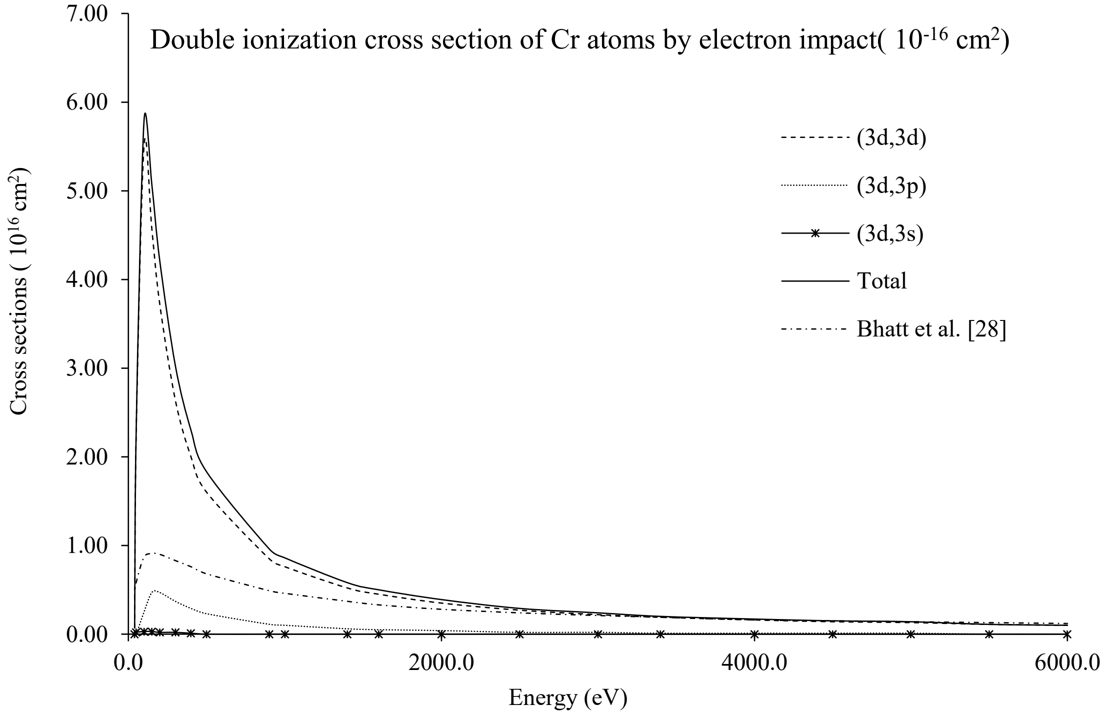

Figure 2. Electron impact double ionization cross sections of Cr atoms (10^{-16} cm^2).

Table 1. Electron impact single ionization cross section of Cr ion (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
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 (10^{-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
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 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. are in excellent agreement with experimental observation at the intermediate and higher impact energy range. At low impact energies up to 80 eV, the theoretical cross sections are lower than the experimental observations. The theoretical and experimental results are found to be nearly identical over the impact energy range of 90 eV to 1000 eV. The experimental observations report an error of about 4.1%–4.6% beyond 16.5 eV impact energy. Overall, the theoretical and experimental cross sections are in excellent agreement across the entire energy range up to 1000 eV. The cross section for producing Cr^{2+} ions via electron-impact double ionization of Cr atom has been calculated over the energy range from the threshold of 40 eV up to 6000 eV. The present calculation of direct double ionization cross section of the Cr atom is compared with the result obtained from other theoretical results. At higher impact energy the theoretical double ionization cross section of Cr atoms gradually decreases. At intermediate and higher impact energy both theoretical calculations are in very good agreement and showing similar trend of cross section variation with impact energy.

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