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RESEARCH ARTICLE

Electron impact ionization cross-sections of Chromium

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Abstract

Abstract: The theoretical model, developed by S.P. Khare, has been modified to evaluate the total cross sections for ionization of Chromium atom due to electron impact at incident electron energy from ionization threshold to 6000 eV. The various calculated cross sections are in remarkable agreement with available experimental data and other theoretical cross sections. For Chromium atom, good agreement between theory and experiment is achieved. **Objective:** Our objective is to find the partial and total ionization cross sections for Chromium atom and its fragmentation ion at different energy levels and interpretation of results with other available data. **Method:-**The theoretical semi-empirical model, developed by S.P. Khare, has been remodeling to evaluate the total cross sections for ionization of Chromium atom due to electron impact at incident electron energy from ionization threshold to 6000 eV. **Findings:** A good agreement is observed when we compared our data for electron impact ionization cross section for Cr^{6+}, Cr^{7+}, Cr^{8+} and Cr^{10+} fragment ions. Also some disagreement is found between our data and other available data. Our results are higher for Cr^{7+}, Cr^{8+} fragment ions. For Chromium atom, good agreement between theory and experiment is achieved. **Novelty:** Electron impact ionization is engaged to produce positive and negative ions in many areas of physics and chemistry such as plasma studies, fusion modeling, radiation physics and gas discharges to more abstract applications such as astrophysical applications and modeling of planetary atmospheres.

Keywords: cross- section; impact; spectroscopy

1 Introduction

In fundamental physics, one of the critical issues is the few body problems where we need to deal with more than two particles. Since, we cannot solve the Schrodinger equation analytically for more than two particles; we need to use approximations for the theoretical models whose validity can only be checked by comparing with the experiments. One of the ways to study the few-body problem is through electron impact ionization of atoms or molecules. Electron impact ionization is referred as (e, 2e), in the initial channel we have one incident projectile electron and a target molecule, whereas in the final channel we have scattered projectile electron, ejected electron and ion, i.e., one electron in preliminary channel and two electrons in the final channel. As the world celebrates the 105th year of the Bohr atom model, the research field of electron interactions with of atoms and molecules, which has grown with atomic structure information, is equally old and yet developing. Bohr's atomic model had an immense impact on the history of atomic molecular physics and is a symbol of the scientific transformations of the 20th century(1). Quantization of atomic energy levels proposed in his model was exhibited in the famous experiment on inelastic scattering of electrons by mercury atoms(2). Scattering interactions of electrons and other charged particles got significant results with the growth of interest in their passage through gases in the context of particle detectors in nuclear physics. In this regard, Neils Bohr's book named 'The Penetration of atomic particles through matter' was a masterpiece in itself.While there have been extensive measurements of ionization potentials for many different atomic and molecular systems, the determination of absolute electron impact ionization cross sections for molecules has not received the same degree of attention. Theoretical and experimental research on electron scattering from atoms and molecules is thus a century old but active field of scientific endeavor and it continues to find a wide variety of applications in natural and man-made systems(3,4).

Electron collisional processes have gotten an extraordinary consideration due to applications in fields like gaseous electronics, gas discharges and lighting devices, dielectric applications, semiconductor etching, Mass-spectrometry, lasers, plasma and so on(5,6). Basically, elastic scattering of electrons by atoms/molecules results into deflections of the incident particles. Ionization induced by electrons results into energy loss of the incident projectiles while a variety of ionic (and neutral) species is produced from the target, and this is quite relevant in many of the environments of planets, satellites, comets and other astrophysical objects. In the ionospheres of the Earth and other planets the photoelectrons of sufficient energy can produce ions and also neutral species and give rise to ion as well as neutral chemistries(7). On planet Mars, the production of ions in its ionospheric E layer is mostly due to photoelectrons, which are produced by primary photo-ionization process(8). Different experimental and theoretical methods are used to determine various cross sections. Factors such as types of targets and relevant instrumentation, reliability (errors) of the results and speed of the output have restricted the observational study of some targets. The theoretical methods are needed to ponder data that experiments cannot determine (e.g. radical species, and compounds not easily prepared in the gas phase, bio-molecules). In theory also, for example, the electron ionization of atoms/molecules poses a difficult quantum mechanical problem, as it involves at least three charged species in the exit channel. Therefore, the need for approximation methods is imperative. A semi-empirical approach in this direction was developed over three decades ago in the form of Semi-Empirical formula. Two of the more successful recent theories for calculating the energy dependence of the electron impact ionization cross-section are the binary-encounter-dipole (BED) theory and Deutsch-Mark (DM). Both of these theories are relatively easy to apply to small molecules. They are generally applicable, with mixed success in accurately reproducing the ionization efficiency curves determined experimentally for molecular systems(9–11).

It is notable that electron is the most suitable projectile for scattering experiments and hence, electron impact collisions with atoms and molecules have been extensively studied by both experimentalists and theorists since the early years of the last century(12,13). We have seen a remarkable renaissance in both experimental and theoretical activities in the study of electron collision processes with molecules in the past ten years or so(14).

2 Theory

The BEB model is a simplified version of the more detailed binary-encounter-dipole (BED) model of Kim and P M Stone(15). The BED model combines a modified form of the Mott cross section(16) with the Bethe theory(17). The BED model calculates the singly differential cross section, or the energy distribution of secondary (ejected) electrons, and requires the continuum oscillator strength, df/dE, where E is the photon energy, for each atomic orbital.

In modified Khare Model, the ionization cross section is given by

$$\sigma_C = \sigma_{CBB} + \sigma_{CMB} + \sigma_t \tag{1}$$

Where the Bethe cross section σ_{CPB} is given

$$\sigma_{CBB} = \frac{ST_r^2}{(t+j)} \int_{I_r}^{E_r} \frac{1}{\xi^3} \ln\left(\frac{\xi}{P_-}\right) d\xi \tag{2}$$

Mott cross section ($\sigma_{CMB)}$ due to traverse interaction is given

$$\sigma_{CMB} = \left(\frac{S}{t+j}\right) \times \left[\left(1 - \frac{2}{t+1} + \frac{t-1}{2t^2}\right) + \left(\frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)} - \left(\frac{t+1}{t^2} \ln\left(\frac{t+1}{2}\right)\right)\right)\right] \tag{3}$$

And the cross section due to transverse interaction (σ_t) is

$$\sigma_t = \frac{ST_r^2}{\mathrm{NR}(t+j)} K^2 \left(\ln\left(1-\lambda^2\right)+\lambda^2\right) \tag{4}$$

Where t and S is

$$t = \frac{E_r}{T_r} \quad S = \frac{4\pi R^2 N a_0^2}{T_r^2}$$

Here R is the Rydberg energy. λ is the ratio of the incident velocity v, and the velocity of light c and K^2 is equal to the total dipole matrix squared for the ionization. It is given by

$$K^2 = \int_{I_{nl}}^{\phi_{\max}} \frac{Rdf(\phi,0)}{\phi d\phi} d\phi \tag{5}$$

For the incident electron of the rest mass 'm' and velocity 'v', the relativistic energy E_r is

$$E_r = \frac{1}{2}mv^2 = \frac{1}{2}mc^2 \left(1 - \frac{1}{\left(1+\frac{E}{mc^2}\right)}\right) \tag{6}$$

$$T_r = \frac{1}{2}mv_b^2 = \frac{1}{2}mc^2 \left(1 - \frac{1}{\left(1+\frac{I}{mc^2}\right)}\right) \tag{7}$$

Where T_r is the kinetic energy of an electron with speed v_b and I is the binding energy of the atom.

The relation between K^2 and Bethe collision parameter (b_{nl}) is given by

$$b_{nl} = \frac{T_r K^2}{Z_{nl} R} \tag{8}$$

Where Z_{nl} is the number of electrons in the (nl) subshell of the atom. Taking Z_{nl} = N and putting the value of K^2 from Eq. (5) in Eq. (4), we get

$$\sigma_t = -\frac{Sb_{nl}}{(t+j)} \left(\ln\left(1-\lambda^2\right)+\lambda^2\right) \tag{9}$$

With COOS (Continuum Optical Oscillator Strengths) df/dφ=N I /φ^2, we get the value of Bethe collision parameter (b_{nl}) is equal to 0.5 for all atoms that does not depend on Z . This is because at present the appropriate form of the COOS is not known. It will be convenient to take the value of the Bethe parameter b_{nl} in the Khare parameters. The value of b_{nl} in the Khare parameters is given by

$$b_{nl} = \alpha a^{-\gamma} \tag{10}$$

Where a = T/ T_s , $T_s = Z_s{}^2 R$, Z_s = Z −s is the effective atomic number and the Khare parameters are α = 0.285 and γ = 1.70.

The recoil energy P_- is given by

$$P_- = 0.5mc^2 \left(\left(E_r\left(E_r-\xi\right)\right)^{\frac{1}{2}} - \left(\left(E_r-\xi\right)\left(E_r-\xi+2mc^2\right)\right)^{\frac{1}{2}} \right)^2 \tag{11}$$

For ξ << E due to the assumption that a large contribution to the integral comes from the small values of ξ, we obtain from Eq. (11)

$$P_- = \frac{\xi^2}{4}\left(\frac{1}{2}mc^2 + \frac{1}{E_r}\right) \tag{12}$$

Now putting this into Equation (2) and evaluating the integral we obtain

$$\sigma_{CBB} = \left(\frac{S}{t+j}\right) \times \left(0.4431\left(1-\frac{1}{t^2}\right) - 0.5\ln\left(\frac{1}{t}+\frac{T_r}{2mc^2}\right) + \frac{1}{2t^2}\ln\left(1+\frac{E_r}{2mc^2}\right)\right) \tag{13}$$

After putting the values of σ_{CMB} , σ_t and σ_{CBB} from Eqs. (3), (9) and (13) into Eq. (1), the ionization cross sections are obtained for the chromium atom.

3 Results and discussion

The values of all ten calculated partial ionization cross-sections (Cr^+ to Cr^{10+}) for Chromium are given in Table 1. The absolute total single-ionization cross-section, which has been obtained as the sum of the partial ionizations of the parent Chromium atom is also given in Table 1.

Table 1. Partial ionization cross-section values for Chromium

Electron Energy Ionization-cross section (10^{-16} cm^2) (eV) Fragmented ions											
eV	Cr^+	Cr^{2+}	Cr^{3+}	Cr^{4+}	Cr^{5+}	Cr^{6+}	Cr^{7+}	Cr^{8+}	Cr^{9+}	Cr^{10+}	Total
11	0.868445										0.868445
12	1.10668										1.10668
14	1.52196										1.52196
16	1.85474										1.85474
18	2.11598	0.354223									2.470203
20	2.31908	0.601481									2.920561
25	2.64542	0.835875									3.481295
30	2.80716	0.991775									3.798935
40	2.89146	1.20836	0.417993								4.517813
50	2.84001	1.33413	0.580658	0.053102							4.8079
100	2.3102	1.42099	0.873352	0.532794	0.303047	0.115467					5.55585
150	1.91016	1.30944	0.919747	0.647209	0.450241	0.307205					5.544002
200	1.63509	1.19401	0.90771	0.697326	0.532874	0.402576	0.130396	0.058521			5.558503
300	1.28271	1.00689	0.839004	0.717954	0.617476	0.52637	0.261407	0.199326	0.203695	0.122821	5.777653
400	1.06413	0.868895	0.760324	0.689939	0.634141	0.581091	0.372871	0.315165	0.326589	0.241133	5.854278
500	0.914036	0.764904	0.689229	0.647349	0.618433	0.591256	0.447103	0.405753	0.431532	0.353583	5.863178
900	0.597933	0.524017	0.49669	0.493715	0.501836	0.512685	0.499547	0.503044	0.565842	0.544599	5.239908
1000	0.552461	0.487152	0.464624	0.464833	0.475741	0.48959	0.490205	0.498712	0.564265	0.551539	5.039122
1400	0.42701	0.382799	0.370876	0.376998	0.392246	0.410692	0.438928	0.45746	0.524279	0.531114	4.312402
1600	0.384787	0.346851	0.337663	0.344822	0.360466	0.379284	0.413063	0.433448	0.498454	0.510121	4.008959
2000	0.322646	0.293165	0.287328	0.295286	0.310544	0.32881	0.367134	0.38871	0.44874	0.465486	3.507849
2500	0.269903	0.246914	0.243319	0.251158	0.265324	0.282212	0.321003	0.34207	0.39584	0.414734	3.032477
3000	0.232899	0.214092	0.211724	0.219158	0.232091	0.247547	0.28479	0.304654	0.352897	0.372161	2.672013
3400	0.210311	0.193913	0.192174	0.199232	0.211276	0.225615	0.2612	0.280052	0.324429	0.343389	2.441591
4000	0.184068	0.170319	0.169133	0.175613	0.186495	0.199435	0.232413	0.249675	0.289342	0.307409	2.163902
4500	0.16702	0.154908	0.154066	0.160089	0.170119	0.182056	0.212972	0.229077	0.265371	0.282566	1.978244
5000	0.153054	0.142228	0.141618	0.147255	0.156566	0.167633	0.196597	0.211658	0.24515	0.261536	1.823295
5500	0.141381	0.13161	0.131161	0.136454	0.145107	0.155396	0.182637	0.1968	0.227857	0.243419	1.691822
6000	0.131477	0.122559	0.122236	0.12721	0.135323	0.144952	0.170607	0.183849	0.212899	0.227667	1.578779

Figure 1 shows our partial ionization cross-sections for Cr^+ in the energy range from threshold to 6000 eV, together with the earlier results of K F Mann et al., Our results at lower energies are quite similar with K F Mann et al., both in terms of absolute cross section values and cross section shape.

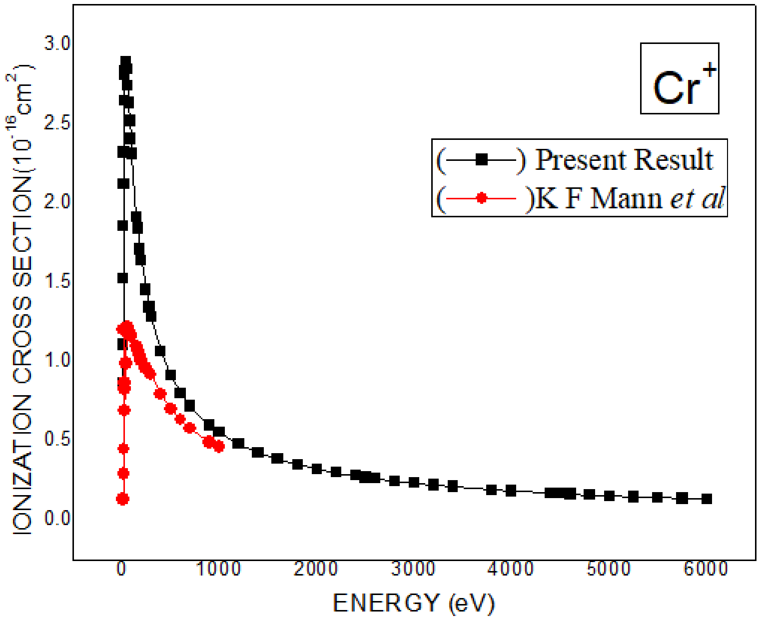

Fig 1. Cr^{+}(Present result & comparison with K F Mann et al.).

In Figures 2 and 3, we report the cross sections for the production of Cr^{2+} and Cr^{3+} ions through electron impact from threshold to 4000 eV. Maximum value of ionization cross section for Cr^{2+} ion calculated to be 1.19 at 200 eV and for Cr^{3+} ion calculated to be 0 .919 at 150 eV.

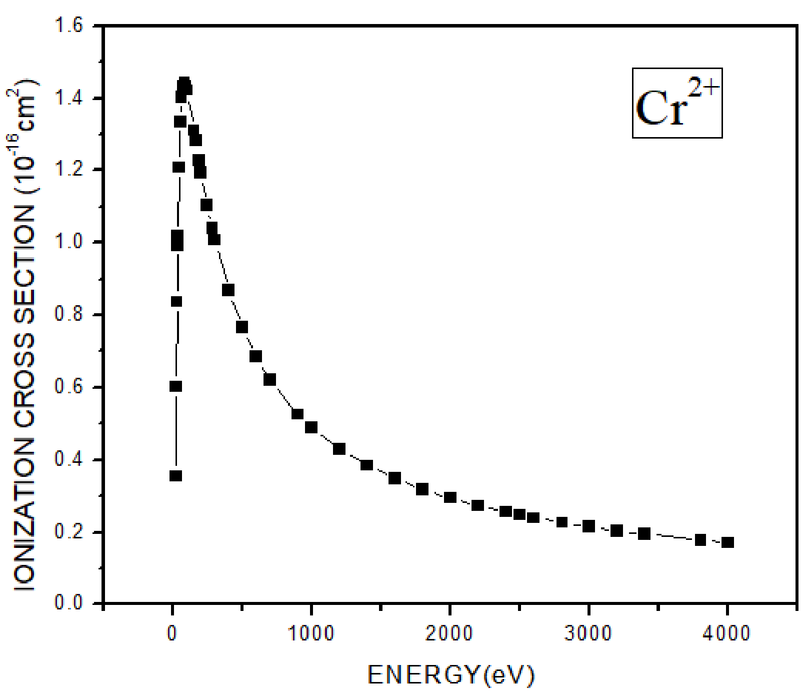

Fig 2. Present result of Cr^{2+}

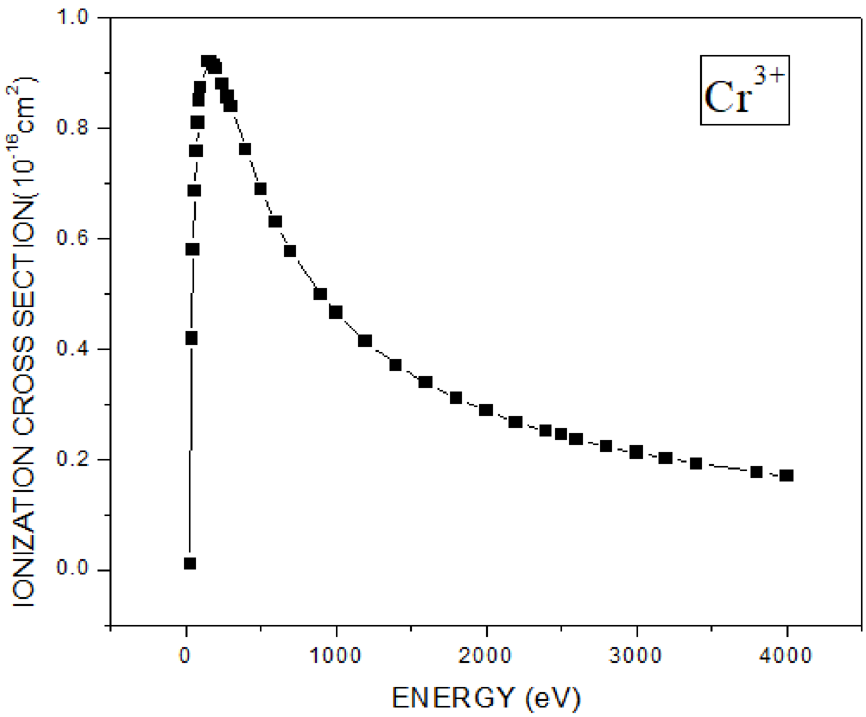

Fig 3. Present result of Cr^{3+}

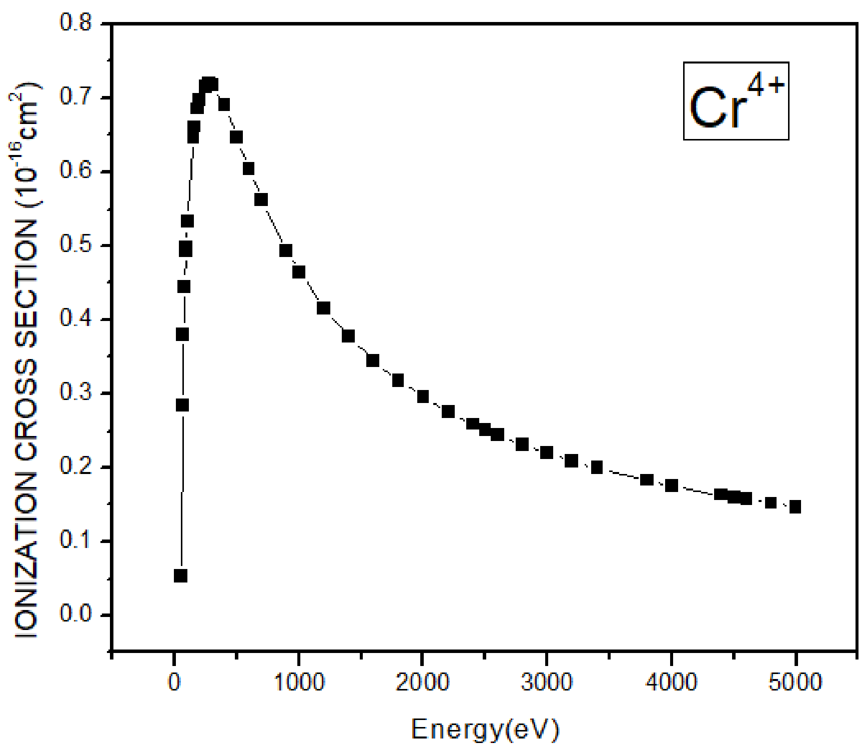

Fig 4. Present result of Cr^{4+}

In Figures 4 and 5, we report the cross sections for the production of Cr^{4+} and Cr^{5+} ions through electron impact from threshold to 5000 eV. At higher values of energy decrement in the values of ionization cross section peak has been observed for both Cr^{4+} and Cr^{5+} in comparison to Cr^{2+} and Cr^{3+}.

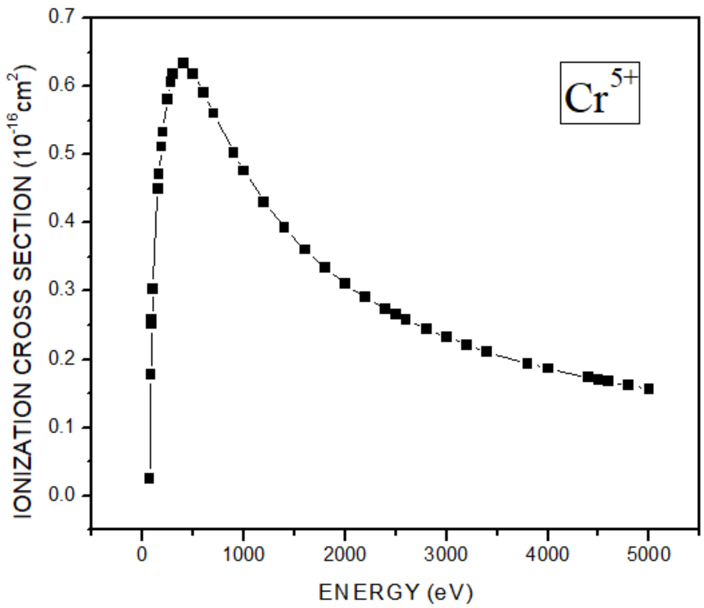

Fig 5. Present result of Cr^{5+}.

Figures 6, 7 and 8 shows our partial ionization cross-sections for Cr6+, Cr^{7+} and Cr^{8+} in the energy range from threshold to 6000 eV, together with the earlier results of M Sataka et al., Our results at lower energies are quite similar with M Sataka et al., both in terms of absolute cross section values and cross section shape. But our cross-section values are lower for Cr^{6+}, higher for Cr^{7+} and Cr^{8+} as reported by M Sataka et al. However, a good agreement in shapes has been observed for these ions.

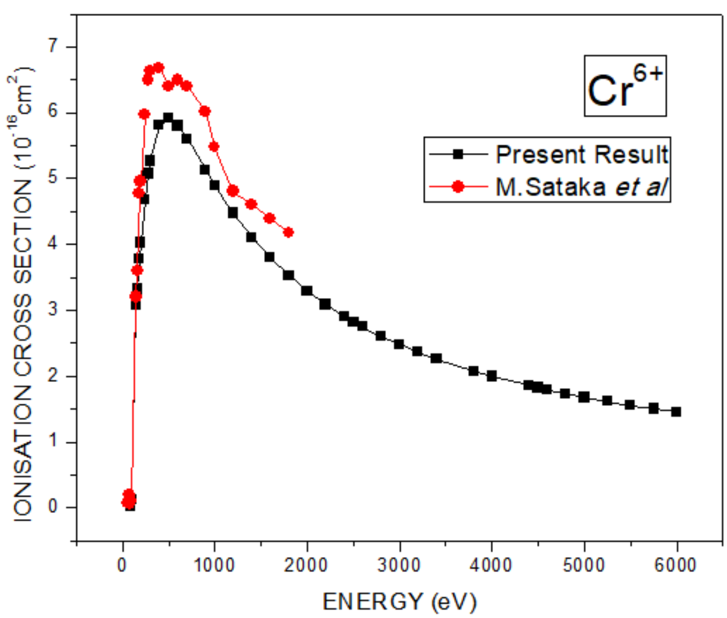

Fig 6. Cr^{6+}(Present result & comparison with M. Sataka et al.).

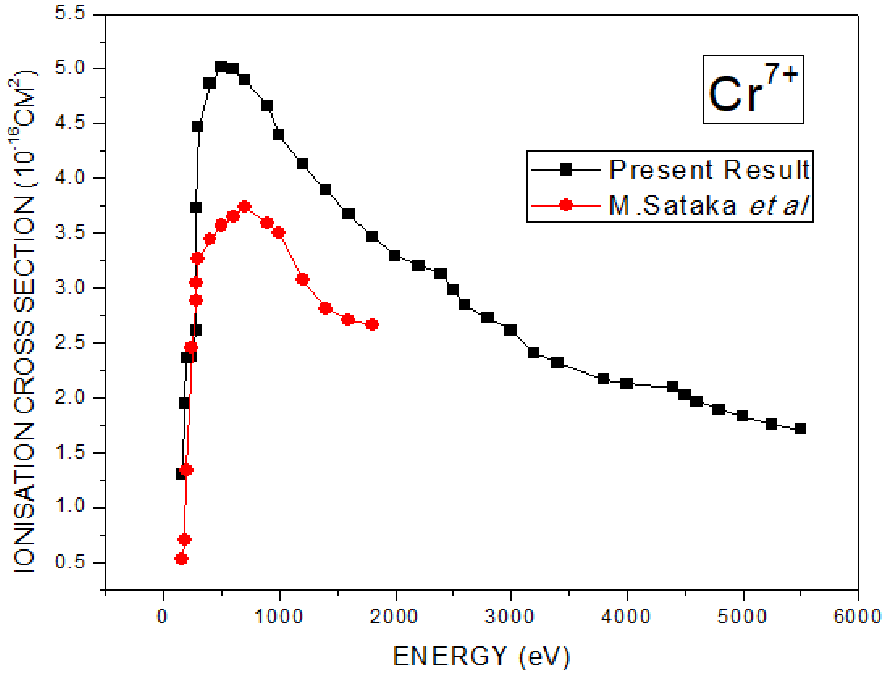

Fig 7. Cr^{7+}(Present Result & comparison with M.Sataka et al).

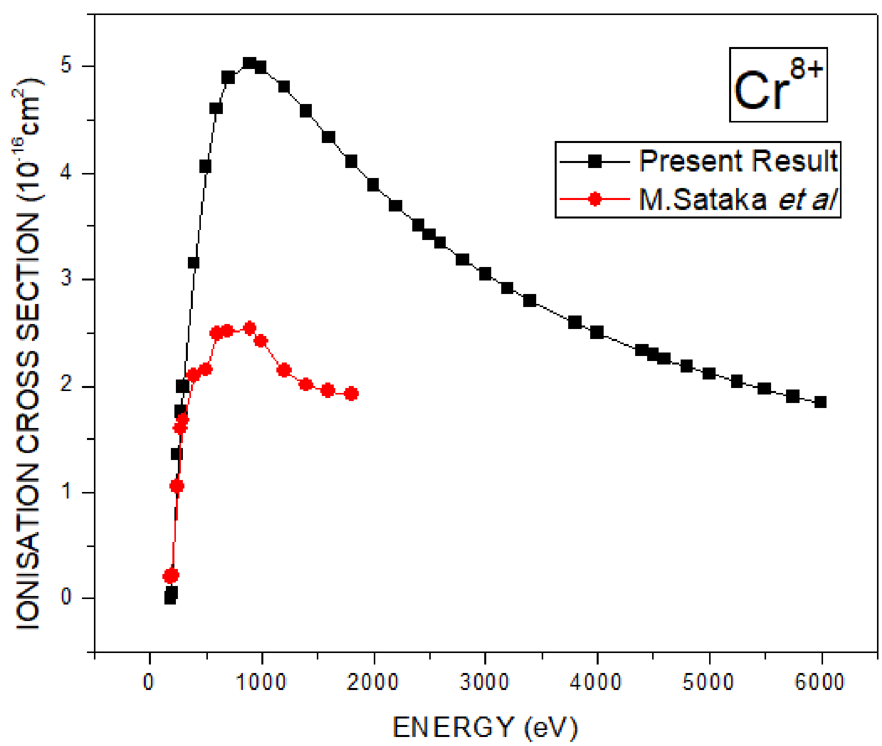

Fig 8. Cr^{8+}(Present Result & comparison with M. Sataka et al).

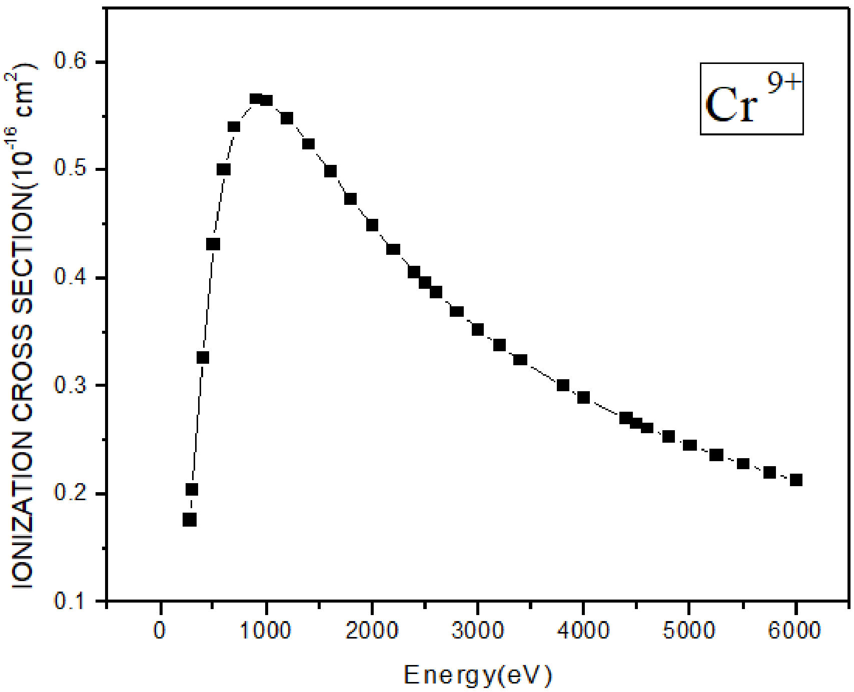

Fig 9. Present result of Cr^{9+}.

In Figures 9 and 10 ionization cross section for Cr^{9+} and Cr^{10+} ions have been shown. A discrepancy has been seen in case of Cr^{10+} ion in the values of ionization cross section around 6000 eV, our cross section values are lower than the reported results of M. Sataka et al. but still the shape of cross section is in good agreement even at higher range of energy.

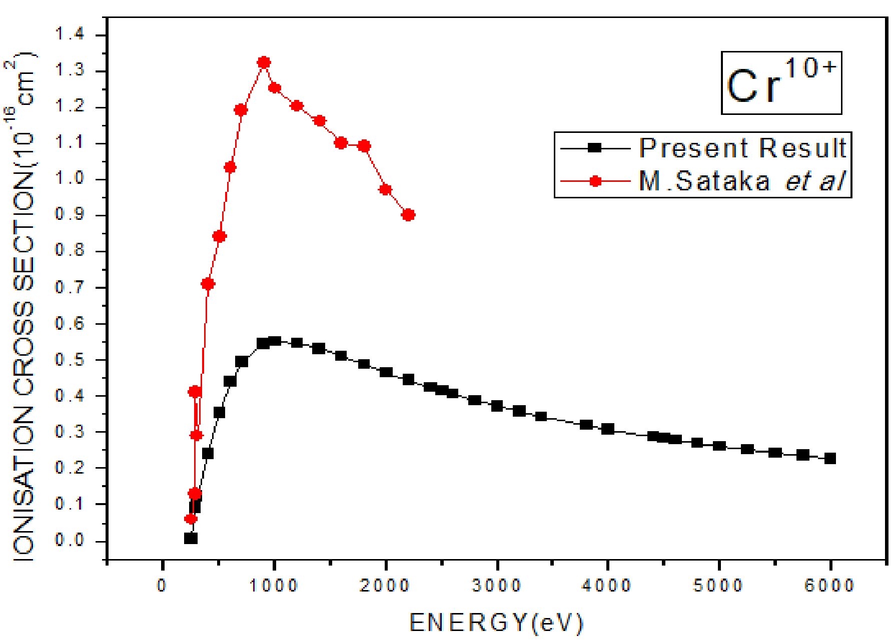

Fig 10. Cr^{10+}(Present result & comparison with M. Sataka et al.).

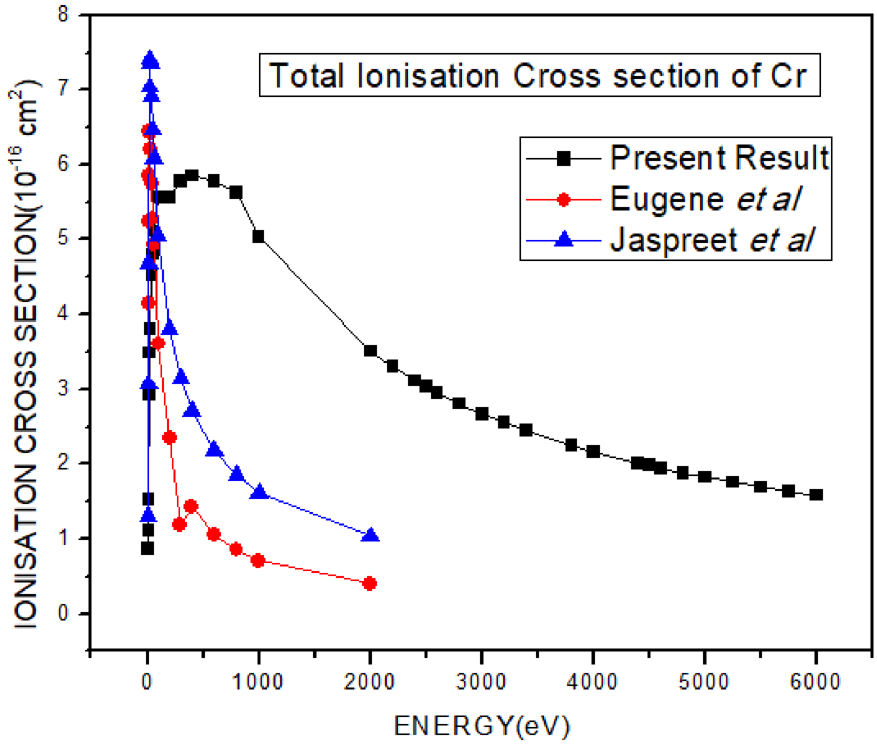

Fig 11. TICS of Chromium (Present result & comparison with Eugene et al. and Jaspreet et al.).

In the case of Cr cross section, the data we have calculated appears to consistently higher than the other measured results reported by K F Mann et al., M. Sataka et al., Jaspreet kaur et al. and M Alfaz Uddin et al.

Figure 11 TICS for Cr shows good agreement as before in stipulations of the electron impact cross section shapes, but our values for the same are some lower than the values reported by Eugene et al. and Jaspreet et al. We have calculated in this work absolute single electron impact ionization cross section for chromium, which we achieved by addition of all measured partial electron impact ionization cross sections for same energy range. Electron impact ionization cross sections values are given in Table 1.

4 Conclusion

Of the three theories used to calculate electron impact ionization cross sections for chromium and their fragmented ion, the SP Khare model gives the best all round agreement with the available measured data. In this work we calculated electron impact ionization cross sections (partial/total) for chromium atom using semi-empirical model developed by Jain & Khare. The present study investigates partial and total electron impact ionization cross sections (EIICS) for chromium from threshold to 6000 eV. We have compared our data for electron impact ionization cross section with the available experimental and theoretical records of K F Mann et al., M. Sataka et al., Eugene et al., Jaspreet Kaur et al. and M Alfaz Uddin et al. A good agreement is observed when we compared our data for electron impact ionization cross section and the records of M. Sataka et al for Cr6+, Cr^{7+}, Cr^{8+} and Cr^{10+} fragment ions. We found there is some disagreement between our data and the data of K F Mann et al., M. Sataka et al., Eugene et al., Jaspreet Kaur et al. and M Alfaz Uddin et al.for Chromium. Our results are higher for Cr^{7+}, Cr^{8+} fragment ions[(18–24)].

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