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Partial ionization cross sections of Silicon by Electron impact Ionization process

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Abstract

Abstract: Electron-impact single-ionization cross sections of Si by electron impact have been solved theoretically for the full range of kinematics and collision geometries of practical interest by S.P. Khare theoretical model. The corresponding partial and total ionization cross sections have also been derived in the energy range varying from ionization thresholds to 6000 eV. Comparison of the evaluated partial and total ionization cross sections is made with the experimental and theoretical data wherever available. **Objective:**Our objective is to find the partial and total ionization cross sections Silicon atom and its fragmentation ion at different energy levels and analysis of results with other available data. **Method:** In this present work we have measured partial ionization cross sections of Silicon atom using semi-empirical formalism of Jain & Khare due to electron impact at incident electron energy from ionization threshold to 6000 eV. **Findings:** Comparison of the evaluated partial and total ionization cross sections is made with the experimental and theoretical data wherever available. A good agreement is observed when we compared our data for electron impact ionization cross section for Silicon and its fragment ions. Also some disagreement is found between our data and other available data. Our results are higher for Si^{2+}, Si^{4+}, Si^{5+} and Si^{6+} fragment ions. For Silicon atom, good agreement between theory and experiment is achieved. **Novelty:** The total ionization cross-sections by electron impact of atoms are required in the study of plasma diagnostics, astrophysical and fusion applications, radiation physics, mass spectrometry, ionization in gas discharge, modeling of fusion plasmas, modeling of radiation effects for both materials & medical research and astronomy. We have calculated partial and total ionization cross section for higher energy range i.e from threshold to 6000 eV, which have not been done by other researchers.

Keywords: Ionization; cross section; electron impact

1 Introduction

The electron-impact ionization cross section is one of the fundamental properties of atoms and molecules not only for its intrinsic importance in atomic collision theory, but also for a wide scope of uses, for example, fusion plasma diagnostics, modeling of semiconductor etching in plasma reactors, radiation effects on materials and astrophysics. Numerous theoretical and experimental results on electron-impact ionization of different molecules have been published since the 1930s. Although most experimental results on the total ionization cross section (TICS) are in phenomenal concurrence with one another, singly differential cross sections (SDCS) on the energy distribution of ejected electrons are still discordant. The experimental SDCS is normally acquired by incorporating measured angular distribution of ejected electrons, a procedure that entails significant uncertainties in estimating the forward and backward angle cross sections outside the range of direct measurements.

Kinematically complete experiments on single ionization of atoms, so-called (e,2e) experiments, measure the momentum vectors of all final-state continuum particles (the scattered and ejected electrons as well as the recoil ion) and hence triple-differential cross sections (TDCSs) are determined. Thereby (e,2e) studies serve as a powerful method for the investigation of the dynamics of quantum mechanical few body interactions. Considerable progress in the experimental determination of cross sections for atomic and molecular targets has been achieved in the past decade. TDCSs have been extensively studied experimentally and theoretically for a broad range of targets and kinematic conditions[1,2]. The most regularly studied experimental collision geometry is the so-called coplanar geometry in which both final-state electrons move in the plane that also contains the incoming projectile momentum. As of late, the hypothesis has gained colossal ground in portraying the collision dynamics. The agreement between theoretical predictions and experiment has been constantly improving, especially for the fundamental target of atomic hydrogen, which is claimed to have been numerically solved with non-perturbative approaches such as (i) exterior complex scaling (ECS)[3,4], (ii) convergent close coupling (CCC)[5], and (iii) time-dependent close coupling (TDCC)[6]. As the next step, the process of electron-helium scattering has also been described very well in both CCC and TDCC calculations. To date, the convergent close-coupled (CCC), methodology for a general discussion of this method has provided the best correlation of scattering theory with experimental results[7]. However, this method is computationally intensive and is currently limited to the valence shell of atoms containing only one or two valence electrons. M.Baetrschy's work has described the exterior complex scaling (ECS) method, which requires massively parallel supercomputing to solve the three-body problem without significant approximation. This has provided very accurate theoretical results for hydrogen at low incident energies, but will require significant advances in computing technology before it can be applied to larger atoms[8].

The electron impact ionization (EII) cross section is the sum of direct ionization (DI) channels and various auto ionizing channels. An important auto ionization channel is collisional excitation to a state which then auto ionizes, a process commonly referred to as excitation auto ionization (EA). The vast majority of theoretical calculations for these systems have been performed using a distorted wave (DW) approach. Laboratory studies, though, have largely been limited to single pass experiments using ions beams contaminated by a typically unknown metastable fraction. Experimental works for all other sequences is typically undermined by unknown metastable fractions.

The cross sections for a variety of collision processes such as excitation, dissociation, ionization or photon emission must be known with right correctness for such applications, modeling and diagnostics. Also, diverse features, such as energy distributions and angular (spatial) distributions, of products, ions, atoms, molecules or photons, are key parameters necessary in understanding electron-molecule or electron-molecular-ion collisions and also in modeling of molecule-related phenomena such as plasma behavior. For example, the energy distributions of atomic hydrogen produced through dissociative processes are significant in determining the mean free path for ionization in media such as plasmas. Electron impact ionization of atoms and molecules is of primary importance in mass spectrometry, plasma processes, and atmospheric science[9–13].

2 Theory

The BEB model is a simplified version of the more detailed binary-encounter-dipole (BED) model of Kim and P M Stone[14]. The BED model combines a modified form of the Mott cross section[15] with the Bethe theory[16]. 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 Khare Model, the ionization cross section by

$$\sigma_T = \sigma_{PCC} + \sigma_{PMC} + \sigma_t \tag{1}$$

Where the Bethe cross section

$$\sigma_{PCC} = \frac{SI_r^2}{(t+f)} \int_{I_r}^{E_e} \frac{1}{\phi^3} \ln\left(\frac{\phi}{U_-}\right) d\phi \tag{2}$$

Where ϕ denotes the energy loss and U_ denotes the recoil energy.

Mott cross section due to traverse interaction is

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

The cross section due to transverse interaction is

$$\sigma_t = \frac{SI_r^2}{\mathrm{NR}(t+f)} M^2 \left(\ln\left(1-\delta^2\right) + \delta^2\right) \tag{4}$$

Where R is Rydberg energy, N is number of electrons and δ is the ratio of the incident velocity and the velocity of light. The relation between M^2 (total dipole matrix squared for the ionization) and Bethe collision parameter (b_{nl}) is given by

$$b_{nl} = \frac{I_r M^2}{z_{nl} R} \tag{5}$$

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

$$\sigma_t = -\frac{Sb_{nl}}{(t+p)} \left(\ln\left(1-\delta^2\right) + \delta^2\right) \tag{6}$$

With continuum optical oscillator strength (COOS) d f /d ω=N I /ω^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

$$b_{nl} = \chi j^{-\alpha} \tag{7}$$

Where j = I / I_s , $I_s = Z_s^2 R$, Z_s = Z-s is the effective atomic number and the Khare parameters are χ = 0.285 and α = 1.70.

The recoil energy U_- is given by

$$U_- = 0.5mc^2 \left(\left(E_r\left(E_r - \phi\right)\right)^{\frac{1}{2}} - \left(\left(E_r - \phi\right)\left(E_r - \phi + 2mc^2\right)\right)^{\frac{1}{2}} \right)^2 \tag{8}$$

From equation (8) ϕ<< E due to the assumption of that a large contribution to the integral comes from the small values of ϕ.

$$U_- = \frac{\phi^2}{4} \left(\frac{1}{2}mc^2 + \frac{1}{E_e}\right) \tag{9}$$

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

$$\sigma_{PCC} = \left(\frac{S}{t+p}\right) \times \left(0.4431\left(1 - \frac{1}{t^2}\right) - 0.5\ln\left(\frac{1}{t} + \frac{I_r}{2mc^2}\right) + \frac{1}{2t^2} \ln\left(1 + \frac{E_e}{2mc^2}\right)\right) \tag{10}$$

Where I is threshold ionization and s is screening parameter After putting the values of σ_{PMC} , σ_t and σ_{PCC} from Eqs. (3), (6) and (10) into Eq. (1), the ionization cross sections are obtained for atom.

3 Result and Discussion

The values of all seven calculated partial ionization cross-sections (Si^+ to Si^{7+}) for Silicon 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 Silicon atom is also given in Table 1.

Table 1. Partial ionization cross-section values for Si (Silicon)

Energy	Si^{+}	Si^{2+}	Si^{3+}	Si^{4+}	Si^{5+}	Si^{6+}	Si^{7+}	Total
10	0.121945							0.121945
15	1.14927							1.14927
20	1.84341	0.645443						2.488853
25	2.24732	0.903957						3.151277
30	2.47352	1.08522						3.55874
35	2.59393	1.22604	0.131717					3.951687
40	2.64966	1.33276	0.370117					4.352537
45	2.66601	1.41213	0.478961					4.557101
50	2.65701	1.46935	0.554393	0.217886				4.898639
55	2.63281	1.51008	0.612689	0.316858				5.072437
60	2.59828	1.53729	0.660307	0.382944				5.178821
65	2.55832	1.55505	0.699842	0.433924				5.247136
70	2.51428	1.56447	0.733515	0.47594				5.288205
75	2.46904	1.56867	0.761771	0.511554				5.311035
80	2.42245	1.56755	0.786262	0.542667				5.318929
85	2.37659	1.56373	0.806633	0.569714				5.316667
90	2.33059	1.55637	0.824567	0.593991				5.305518
95	2.28617	1.54784	0.839186	0.615151				5.288347
100	2.24214	1.5368	0.852312	0.634518				5.26577
150	1.87559	1.40015	0.905534	0.745349				4.926623
170	1.76116	1.3448	0.906896	0.765956	0.020217			4.799029
175	1.73519	1.33192	0.905623	0.769166	0.040283			4.782182
200	1.61538	1.26748	0.899522	0.783722	0.096679			4.662783
250	1.42339	1.15473	0.873282	0.790909	0.156453	0.084314	0.010927	4.494004
300	1.27551	1.05964	0.838674	0.780865	0.209147	0.131583	0.073275	4.368694
350	1.15778	0.978938	0.801166	0.761121	0.264336	0.181229	0.113973	4.258543
400	1.06162	0.909876	0.763737	0.73656	0.316117	0.235216	0.160079	4.183205
500	0.913616	0.798387	0.694284	0.683373	0.393843	0.332315	0.261545	4.077363
600	0.80463	0.712545	0.634311	0.632497	0.437896	0.398767	0.34495	3.965596
650	0.760136	0.676647	0.607769	0.608926	0.450651	0.421389	0.376518	3.902036
700	0.720737	0.644481	0.583304	0.586763	0.459004	0.438469	0.401966	3.834724
750	0.685582	0.615472	0.560736	0.566001	0.463866	0.451007	0.422169	3.764833
800	0.653998	0.589156	0.539844	0.546539	0.466106	0.459855	0.437933	3.693431
850	0.625449	0.565198	0.520543	0.528289	0.466286	0.465788	0.450016	3.621569
900	0.59951	0.543277	0.502613	0.511216	0.464886	0.469375	0.459079	3.549956
950	0.575834	0.523135	0.485924	0.495202	0.462272	0.471068	0.465636	3.479071
1000	0.554112	0.504563	0.47037	0.480169	0.458774	0.471266	0.470071	3.409325
1100	0.515648	0.471431	0.442205	0.452738	0.449807	0.468281	0.474268	3.274378
1200	0.482593	0.442721	0.417433	0.428373	0.439294	0.462243	0.47376	3.146417
1300	0.453867	0.417576	0.395458	0.406598	0.428012	0.45427	0.470124	3.025905
1400	0.428637	0.395374	0.375864	0.387029	0.416442	0.445165	0.464414	2.912925
1500	0.406285	0.375618	0.358222	0.369377	0.404867	0.435402	0.457304	2.807075
1600	0.386341	0.357862	0.342281	0.353333	0.393526	0.425357	0.449313	2.708013
1700	0.368407	0.34188	0.327794	0.338712	0.382486	0.415232	0.440769	2.61528
1800	0.352206	0.327377	0.314588	0.325353	0.371802	0.405203	0.431958	2.528487
1900	0.337488	0.31416	0.302483	0.313035	0.361566	0.395385	0.423025	2.447142
2000	0.32404	0.302031	0.291354	0.301716	0.351761	0.385779	0.414098	2.370779
2500	0.271115	0.254036	0.246719	0.256076	0.308917	0.342313	0.371824	2.051
3000	0.233962	0.220044	0.214699	0.223086	0.274872	0.306505	0.335413	1.808581
3500	0.206337	0.194606	0.190497	0.198091	0.247536	0.277143	0.304722	1.618932
4000	0.184914	0.174784	0.171523	0.178404	0.225181	0.252828	0.278886	1.46652
4500	0.167786	0.158883	0.156206	0.162519	0.206606	0.232414	0.256963	1.341377
5000	0.156356	0.148239	0.145903	0.151835	0.193818	0.218274	0.241824	1.256249
5500	0.142029	0.134859	0.132947	0.138369	0.177509	0.200187	0.222066	1.147966

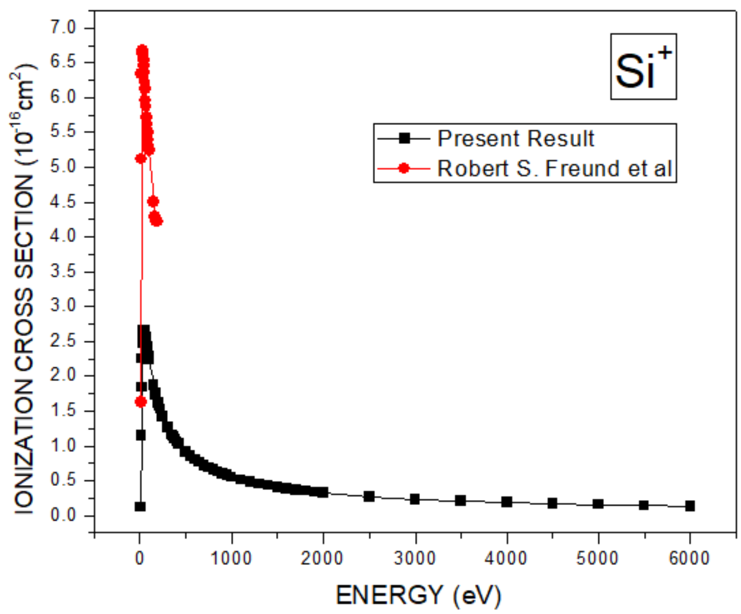

Fig 1. Si^{+} (Present Result & comparison with Robert S. Freund et al.)

Figures 1 and 2 shows our partial ionization cross-sections for Si^{+} in the energy range from threshold to 6000 eV, collectively with the earlier results of Robert S. Freund et al. [17]. Our results at lower energies are quite similar to Robert S. Freund et al., both in terms of absolute cross section values and cross section shape. However, at higher range of energy for Si^{+} ion, our calculated ionization cross section value is found to be lowered and in the case of Si^{2+} ion is found to be higher in comparison with the reported results of Robert S. Freund et al.

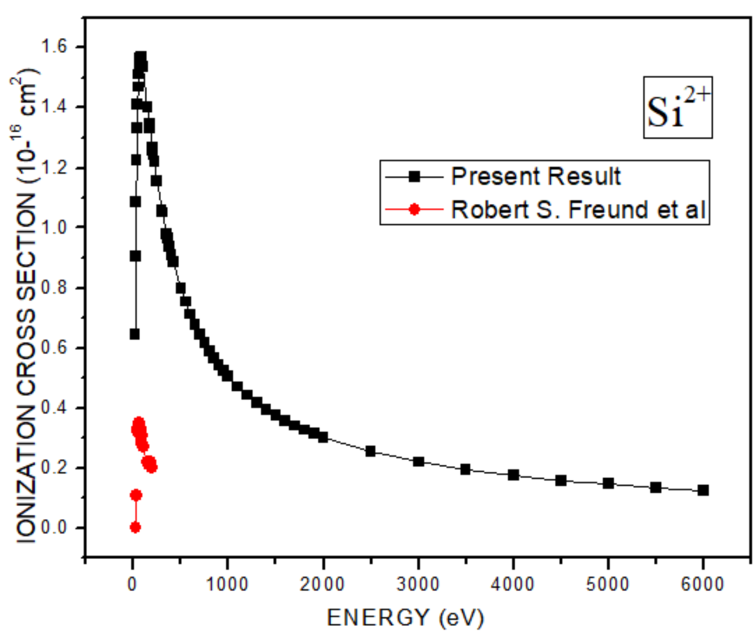

Fig 2. Si^{2+} (Present Result & comparison with Robert S. Freund et al.)

In Figures 3, 4 and 5, we report the cross sections for the production of Si^{3+} , Si^{4+} and Si^{5+} ions through electron impact from threshold to 6000 eV. Si^{3+} has been compared with the results of D.H.Crandall et al. which has been found in good agreement in terms of shape and cross section values. The results of Si^{4+} and Si^{5+} compared with the results of J.S.Thompson et al. Good agreement has been observed in shape and cross section values especially at higher energy in Si^{4+} and Si^{5+}.

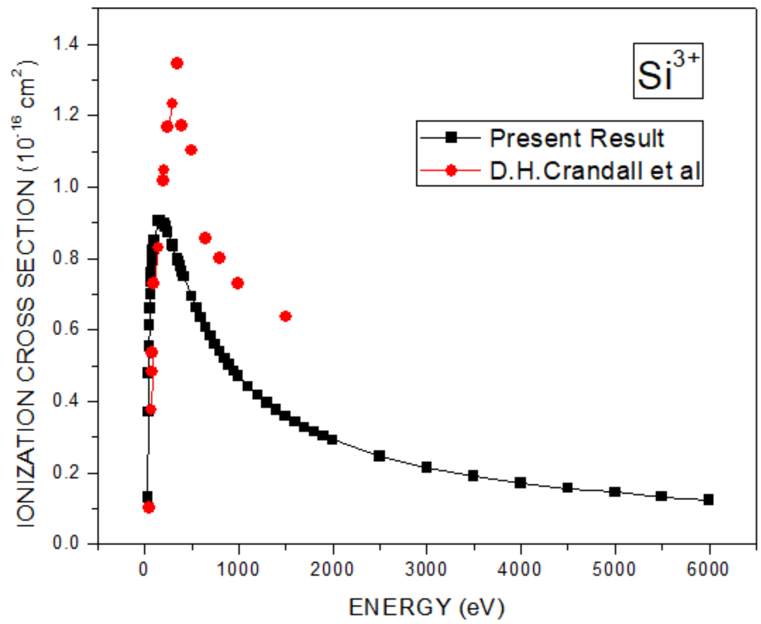

Fig 3. Si^{3+} (Present Result & comparison with D.H.Crandall et al.)

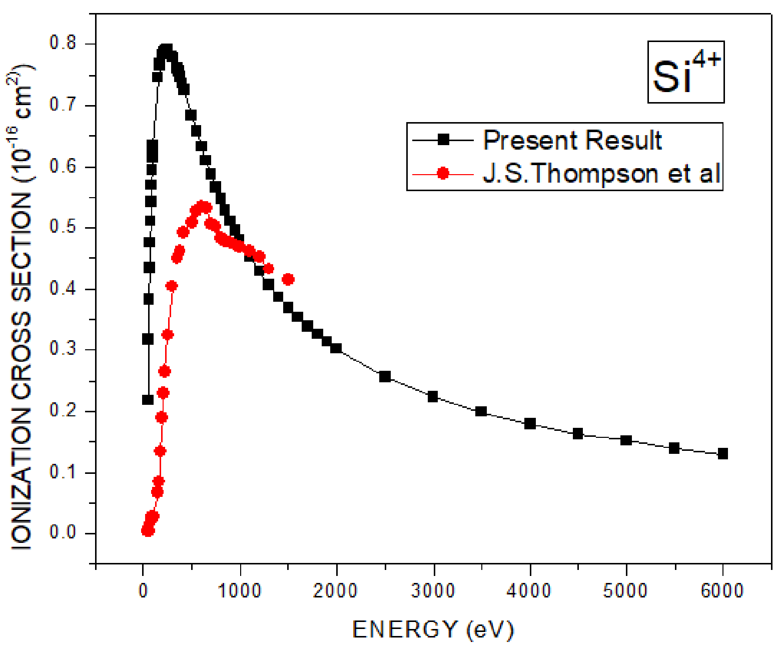

Fig 4. Si^{4+} (Present Result & comparison with J.S.Thompson et al.)

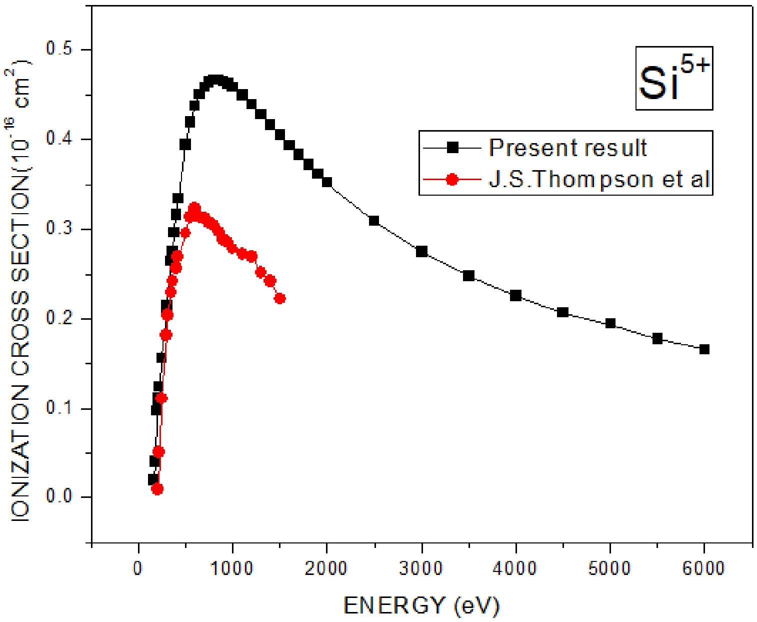

Fig 5. Si^{5+} (Present Result & comparison with J.S.Thompson et al.)

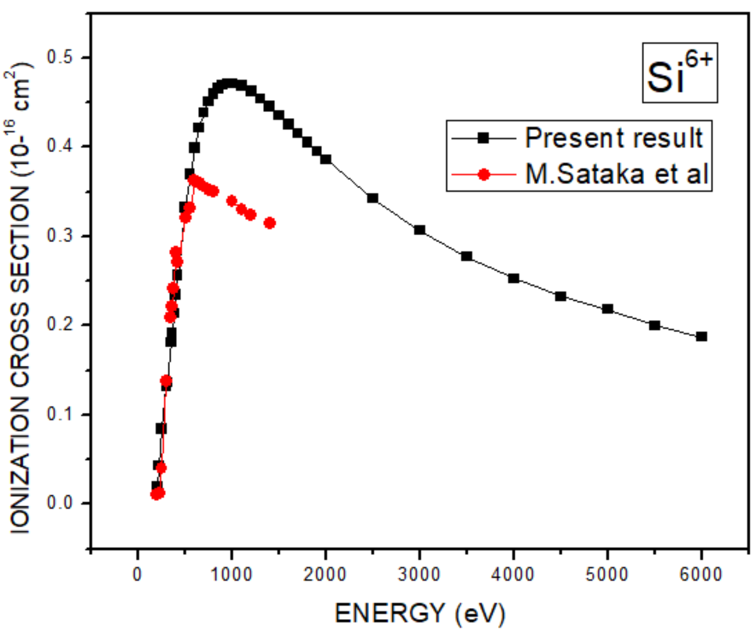

Fig 6. Si^{6+} (Present Result & comparison with M.Sataka et al.)

In Figures 6 and 7, we report the cross sections for the production of Si^{6+} and Si^{7+} ions through electron impact from threshold to 6000 eV. Comparison for these ions has been done with the results of M.Sataka et al. Cross section shape is found to be in good agreement in both ions. Cross section value at intermediate energy range is found to be excellent for Si^{6+} and Si^{7+} as compared with M.Sataka et al.

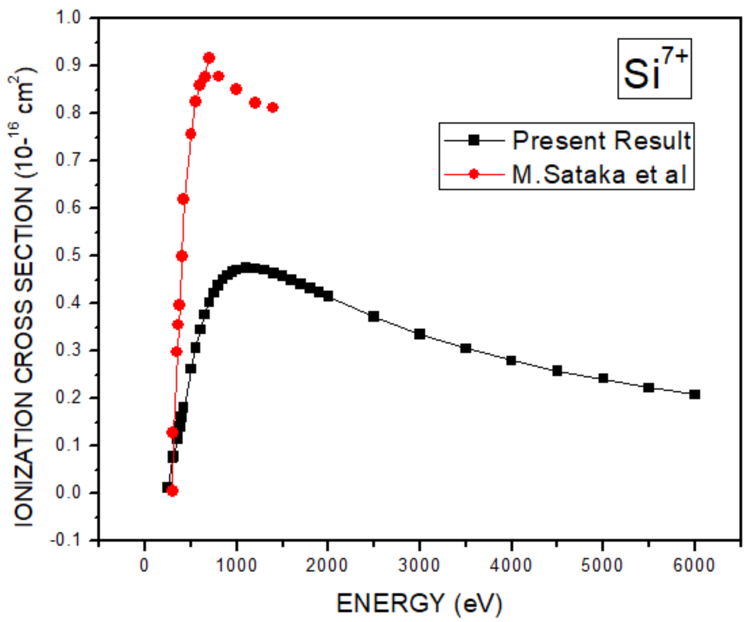

Fig 7. Si^{7+} (Present Result & comparison with M.Sataka et al.)

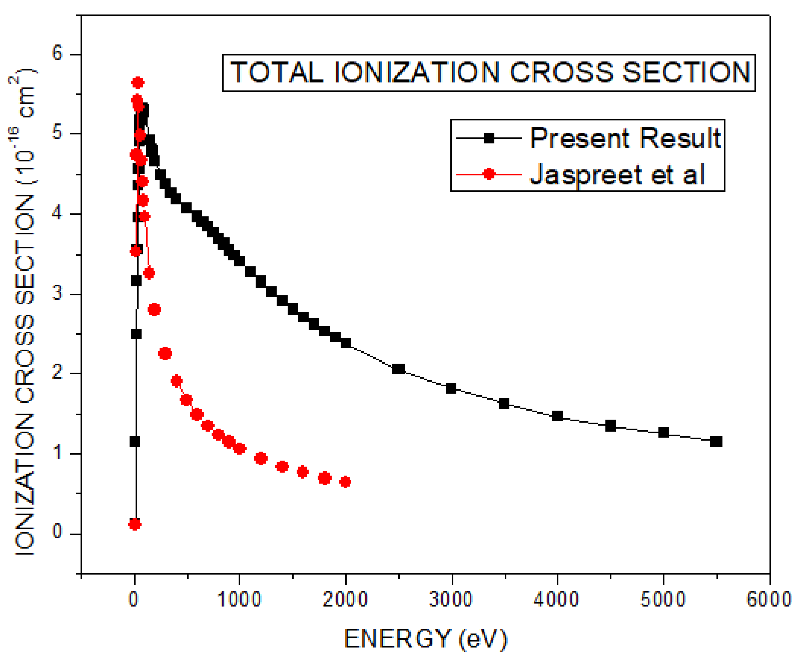

Fig 8. TICS of Si (Present Result & comparison with Jaspreet et al.)

4 Conclusion

We conclude that ionization cross-section of Si (Silicon) is calculated, there is a good comparison between our results and Robert S. Freund et al., D.H.Crandall et al., J.S. Thompson et al., M. Sataka et al. and Jaspreet et al.

According to the availability of data we can estimate partial ionization cross-section and total of Si (Silicon) at energies up to 6000 eV. There is a difference in our values for cross section with the earlier measurements of J.S. Thompson et al., M. Sataka et al. Such difference between the measurements is very difficult to explain. The Present determinations also provide information regarding the total ionization cross section. Present results are compared with available data Jaspreet et al. and overall good adaptation is observed[(17–21)].

The most recent total cross section of Si (Silicon) measurements are in good acceptance with those cross section measurements as reported in the presented work.

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