ABSOLUTE ELECTRON IMPACT IONIZATION CROSS SECTIONS OF OXYGEN ATOM

Ravinder Sharma[1,2]*, S.P.Sharma [1]

[1]Department of Chemistry, Baba Mast Nath University, Rohtak ,

[2]Department of Biomedical Engineering, DCRUST, Murthal, Sonepat (HR)

ABSTRACT

Absolute electron impact ionization cross section of Oxygen atom is determined from threshold to high energy (10 KeV) by by means of modified Jain-Khare semi-empirical approach. In this literature the absolute ionization cross section data have compared with obtainable experimental data and theoretical data. It is found that the current results are in better account for the ionization cross sections up to higher energy. Presently there is no theoretical or experimental available data for SDCS and DDCS for oxygen atom. We have also calculated the single and double differential cross sections of oxygen atom.

KEYWORDS

Absolute Ionization Cross Section, Electron impact ionization, Single and double differential cross section.

I. INTRODUCTION

Oxygen is an interesting atom to study. However, many works have been done on oxygen atom . Some have evaluated the partial and absolute total ionization cross section of Oxygen atom experimentally from threshold to intermediate energy and some others intermediate to higher energy. There are many applications of electron impact ionization cross sections in the field of plasma processes, vacuum technology, ionosphere, gas discharges, in biomedical research as well as in basic theory of atomic and molecular collisions and others [28]. As in biomedical research the electron impact ionization cross sections of oxygen atom plays an important role in the study of radiological effects due to Auger electrons [1-3]

Since 1940s, many works on experimental and theoretical electron impact ionization cross sections have been done for oxygen atom and to find out the results more accurately the collision methods are improved time to time [4-29]. There are various theoretical formalism to determine the partial and total ionization cross sections [33]. For better accuracy, we use the modified Jain-Khare semi-empirical approach [32,34-36] to determine absolute and differential ionization cross section of oxygen atom.

II. THEORETICAL METHODOLOGY

The partial and total ionization cross section is determined via modified Jain-Khare approach. We have developed the MATLAB programming codes for the calculation of huge numeral of molecular ionization cross sections. This gives ionization cross section to the production of an ith type of ion in the ionization of an atom by an incident electron of energy E solving the following given equations [34].

$$Q_iE = \frac{4\pi a_0^2 R}{E}\left[\frac{E}{E-Ii}\left(Mi^2 - \frac{R}{E} Si\right) ln[1 + Ci(E-Ii)] + \frac{R(E-Ii)}{E} Si \times \int_0^{(E-Ii)/2} \frac{1}{\varepsilon^3 + \varepsilon_0^3}\left(\varepsilon - \frac{\varepsilon^2}{(E-\varepsilon)} + \frac{\varepsilon^3}{(E-\varepsilon)^2}\right) d\varepsilon\right]$$

----------- Eq. (1)

Where

$$Mi^2 = \int_{Ii}^{(E+Ii)} \frac{R}{w}\frac{dfi(w,0)}{dw} dw$$

----------- Eq. (2)

$$Si = \int_{Ii}^{(E+Ii)} \frac{dfi(w,0)}{dw} dw$$

----------- Eq. (3)

$$C_{i=}\ C_T \exp\left[n\left(\frac{\sum_{i>1} Mi^2 \ln Si}{\sum_{i>1} Mi^2} - \ln Si\right)\right]$$

----------- Eq. (4)

Where

W= energy loss suffered by the incident electron.

I_i = Ionization Potential.

a_0= Bohr radius,

ε_0= Mixing parameter,

C_i= collision parameter,

S_i= number of ionizable electrons and

R= Rydberg energy respectively.

And oscillator strength df_i/dw is the key parameter. We have not found the experimental values of oscillator strength. The oscillator strength is directly proportional to the photoionization cross section [35]. So, we use this relationship to determine the oscillator strength (df_i/dw) at given photon energy [30-31,39] by solving the equation (4).

$$df_i/dw=9.112*10^{16}\, Qp_i\, eV^{-1}$$ ----------- Eq. (5)

Where,

Qp_i is the photoionization cross section (in cm^2)

For calculating the electron impact ionization cross section of oxygen atom, we have used the photoionization data [37] which gives oscillator strengths for this atom. This data of photoionization is available upto 1500 eV. Thus, for higher energies, the same data have been extrapolated by the TRK sum rule, within 10% error bars [40-42]. The ionization potential for oxygen atom is 13.6 eV [38]. The value of the collision parameter and mixing parameter are (C_i= 0.02130) and (ε_0=90) respectively.

In this literature, we have calculated the absolute ionization cross section over the secondary electron energy varying from 0 to (E-I)/2 using equations (1). Because the results are more accurate and precise at this energy using equation (1). If we varying secondary electron energy from 0 to (E-I), then results at low incident energy are more as compared experimental and all other theoretical data. We have calculated the single and double differential ionization cross section using the equation (6) and (7) which are given below [34].

$$Q_{i(E,W)}=\frac{4\pi\, a_0^2 R}{E}\left[\left(1-\frac{\varepsilon}{E-Ii}\right)\left(\frac{R}{W}\right)\times\frac{dfi(w,0)}{dw}\, ln[1+Ci(E-Ii)]+\frac{R}{E}\, Si \times\frac{(E-Ii)}{\varepsilon^3+\varepsilon_0^3}\left(\varepsilon-\frac{\varepsilon^2}{(E-\varepsilon)}+\frac{\varepsilon^3}{(E-\varepsilon)^2}\right)\right]$$

----------- Eq. (6)

$$Q_{i\,(E,W,\theta)}=\frac{4\pi\, a_0^2 R^2}{E}\left[\frac{8R^2Z^2}{W^3}\left(1-\frac{\varepsilon}{E-Ii}\right)\sqrt{\left(1-\frac{W}{E}\right)}\times\sin\theta\,\frac{dfi(w,0)}{dw}\, ln[1+Ci(E-Ii)]+Si\times\frac{(E-Ii)}{E}\times\frac{1}{\varepsilon^3+\varepsilon_0^3}\left(\varepsilon-\frac{\varepsilon^2}{(E-\varepsilon)}+\frac{\varepsilon^3}{(E-\varepsilon)^2}\right)(\sin\theta)/2\right]$$

----------- Eq. (7)

III. RESULTS AND DISCUSSION

In this literature, we have calculated the absolute ionization cross section of oxygen atom via the modified Jain-Khare semi-empirical approach using Equations (1) to (5) with the help of MATLAB programming codes. The calculated ionization cross section from 25 eV to 10,000 eV of incident electron energy which is tabulated in Table 1 and presented graphically in Fig. 1. We have compared the total ionization cross sections with theoretical and experimental data [20, 26, 29] also shown in Fig.1. All these are in good agreement from threshold up to high energy.

Table 1

Present Result for Absolute total Ionization cross-section of Oxygen Atom (10^{-16} cm^2)

Energy (eV)	TICS	Energy (eV)	TICS	Energy (eV)	TICS
25	0.0426	450	1.0416	2600	0.3320
30	0.3397	460	1.0297	2700	0.3226
35	0.5758	470	1.0181	2800	0.3138
40	0.7643	480	1.0067	2900	0.3055
45	0.9153	490	0.9956	3000	0.2976
50	1.0366	500	0.9847	3100	0.2902
55	1.1344	520	0.9637	3200	0.2832
60	1.2134	540	0.9448	3300	0.2765
65	1.2771	560	0.9272	3400	0.2702
70	1.3286	580	0.9102	3500	0.2642
75	1.3700	600	0.8940	3600	0.2585
80	1.4033	620	0.8783	3700	0.2530
85	1.4299	640	0.8631	3800	0.2478
90	1.4509	660	0.8485	3900	0.2428
95	1.4674	680	0.8343	4000	0.2380
100	1.4800	700	0.8207	4100	0.2334
110	1.4961	720	0.8075	4200	0.2290
120	1.5031	740	0.7947	4300	0.2248
130	1.5035	760	0.7824	4400	0.2208
140	1.4992	780	0.7704	4500	0.2169

150	1.4913	800	0.7589	4600	0.2131
160	1.4808	850	0.7310	4700	0.2095
170	1.4684	900	0.7047	4800	0.2060
180	1.4544	950	0.6804	4900	0.2027
190	1.4394	1000	0.6578	5000	0.1994
200	1.4236	1050	0.6368	5200	0.1933
210	1.4073	1100	0.6173	5400	0.1875
220	1.3905	1150	0.5990	5600	0.1822
230	1.3735	1200	0.5818	5800	0.1771
240	1.3564	1250	0.5657	6000	0.1723
250	1.3392	1300	0.5505	6200	0.1678
260	1.3221	1350	0.5362	6400	0.1636
270	1.3050	1400	0.5227	6600	0.1595
280	1.2882	1450	0.5099	6800	0.1557
290	1.2715	1500	0.4978	7000	0.1521
300	1.2551	1550	0.4863	7200	0.1487
310	1.2389	1600	0.4754	7400	0.1454
320	1.2229	1650	0.4650	7600	0.1423
330	1.2071	1700	0.4551	7800	0.1393
340	1.1917	1750	0.4456	8000	0.1364
350	1.1765	1800	0.4366	8200	0.1337
360	1.1616	1850	0.4279	8400	0.1311
370	1.1471	1900	0.4196	8600	0.1286
380	1.1328	1950	0.4117	8800	0.1262
390	1.1189	2000	0.4041	9000	0.1239
400	1.1053	2100	0.3898	9200	0.1216
410	1.0920	2200	0.3765	9400	0.1195
420	1.0789	2300	0.3642	9600	0.1174

430	1.0662	2400	0.3527	9800	0.1155
440	1.0538	2500	0.3420	10000	0.1136

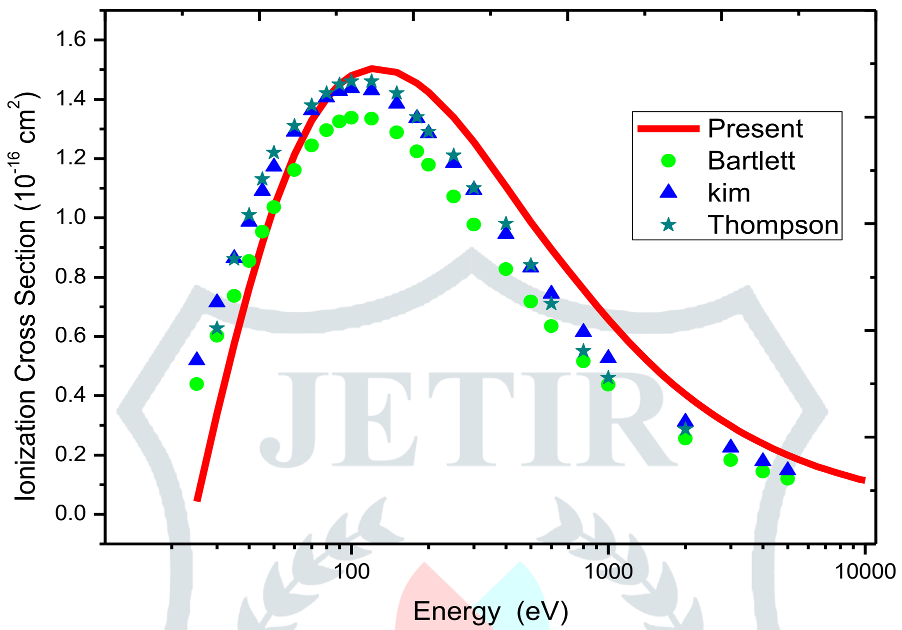

Fig.1: Oxygen Atom absolute total ionization cross section in Å^2. Solid line, Present result; Triangle, Kim et al.[20];Circle, Bartlett et al. [29]; and star, Thompson et al. [26].

The results are evaluated for SDCS as a function of W (loss of energy) at fixed incident electron energy 100 eV, 200 eV and 500 eV are given in table 2 and shown in Fig. 2-4 respectively.

Table 2

Single differential ionization cross-section of Oxygen atom by electron impact at fixed electron energy E=100 eV, 200 eV and 500 eV with respect to secondary electron energy

W (eV)	E=100 eV	E=200 eV	E=500 eV
20	3.09E-17	2.48E-17	1.53E-17
25	2.18E-17	1.81E-17	1.14E-17
30	1.53E-17	1.32E-17	8.47E-18
35	1.18E-17	1.06E-17	6.92E-18
40	8.53E-18	8.06E-18	5.36E-18

45	6.21E-18	6.18E-18	4.19E-18
50	4.54E-18	4.77E-18	3.29E-18
55	3.33E-18	3.70E-18	2.61E-18
60	2.49E-18	2.91E-18	2.09E-18
65	1.91E-18	2.30E-18	1.68E-18
70	1.56E-18	1.84E-18	1.37E-18
75	1.43E-18	1.49E-18	1.13E-18
80	1.55E-18	1.22E-18	9.39E-19
85	2.02E-18	1.01E-18	7.88E-19
90	3.15E-18	8.45E-19	6.68E-19
95	5.69E-18	7.18E-19	5.71E-19
100	1.22E-17	6.19E-19	4.91E-19
120		4.15E-19	2.86E-19
140		4.38E-19	1.80E-19
160		7.72E-19	1.20E-19
180		2.18E-18	8.40E-20
200		1.53E-17	6.15E-20
250			3.55E-20
300			3.08E-20
350			4.29E-20
400			9.02E-20
450			3.16E-19
500			7.69E-18

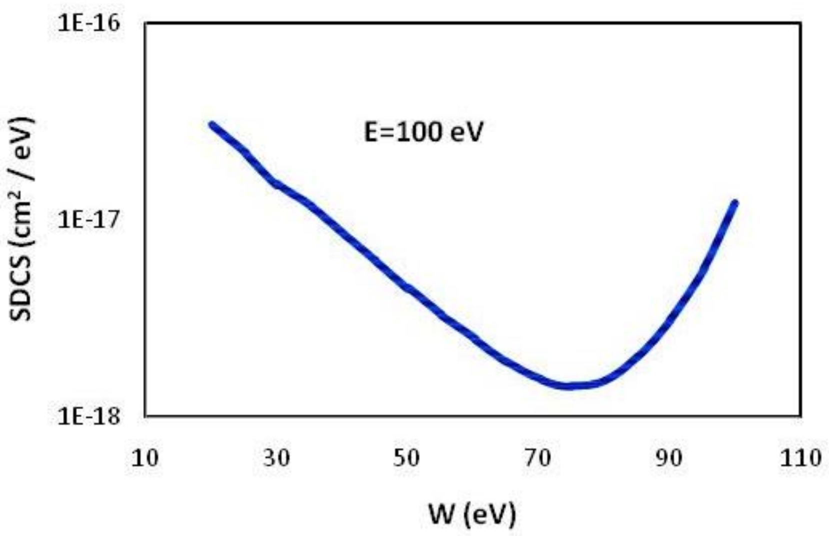

Fig.2: Single differential cross section (SDCS) of Oxygen Atom at fixed incident electron energy 100 eV.

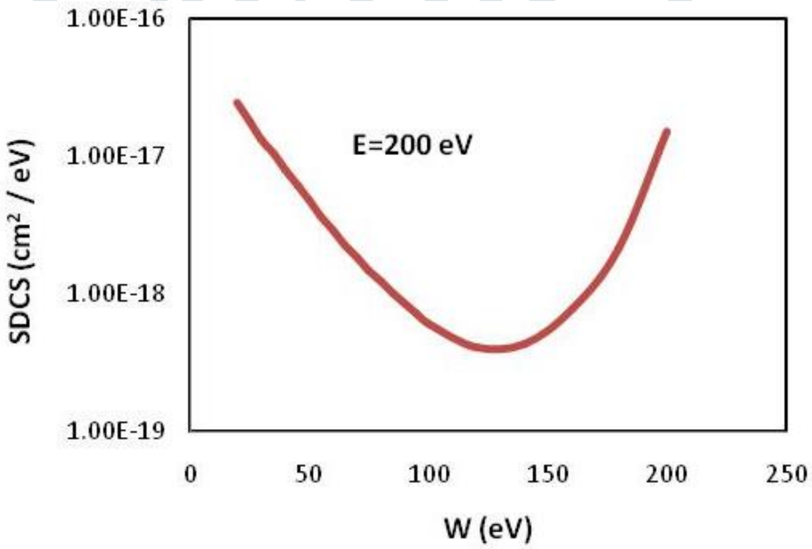

Fig.3: Single differential cross section (SDCS) of Oxygen Atom at fixed incident electron energy 200 eV.

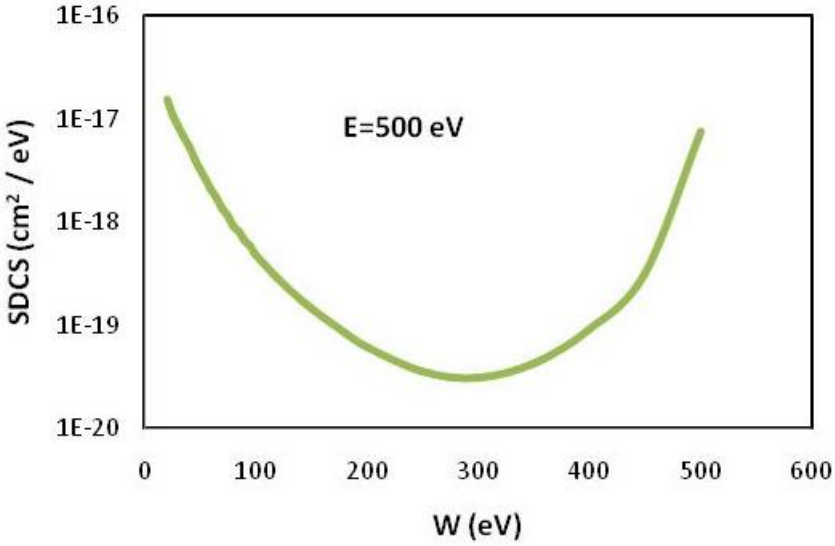

Fig.4: Single differential cross section (SDCS) of Oxygen Atom at fixed incident electron energy 500 eV.

DDCS is evaluated as a function of secondary electron energy and with respect to the fixed incident angles 30̊, 60̊ and 90̊ of an electron at the fixed incident electron energies 100 eV, 200 eV and 500 eV are represented in figure 5 to 7and their respective tables are given from tables 3 to 5.

Table 3

Double differential ionization cross-section of Oxygen Atom at E=100 eV with respect to secondary electron energy at fixed angles 30̊, 60̊ and 90̊.

W (eV)	θ, 30̊	θ, 60̊	θ, 90̊
20	5.11E-17	8.85E-17	1.02E-16
25	2.23E-17	3.87E-17	4.46E-17
30	1.05E-17	1.82E-17	2.10E-17
35	5.69E-18	9.86E-18	1.14E-17
40	3.04E-18	5.27E-18	6.08E-18
45	1.68E-18	2.91E-18	3.36E-18
50	9.57E-19	1.66E-18	1.91E-18
55	5.67E-19	9.81E-19	1.13E-18
60	3.56E-19	6.17E-19	7.12E-19

65	2.49E-19	4.32E-19	4.99E-19
70	2.09E-19	3.62E-19	4.18E-19
75	2.21E-19	3.83E-19	4.42E-19
80	2.90E-19	5.01E-19	5.79E-19
85	4.41E-19	7.64E-19	8.83E-19
90	7.48E-19	1.30E-18	1.50E-18
95	1.41E-18	2.43E-18	2.81E-18
100	3.05E-18	5.29E-18	6.11E-18

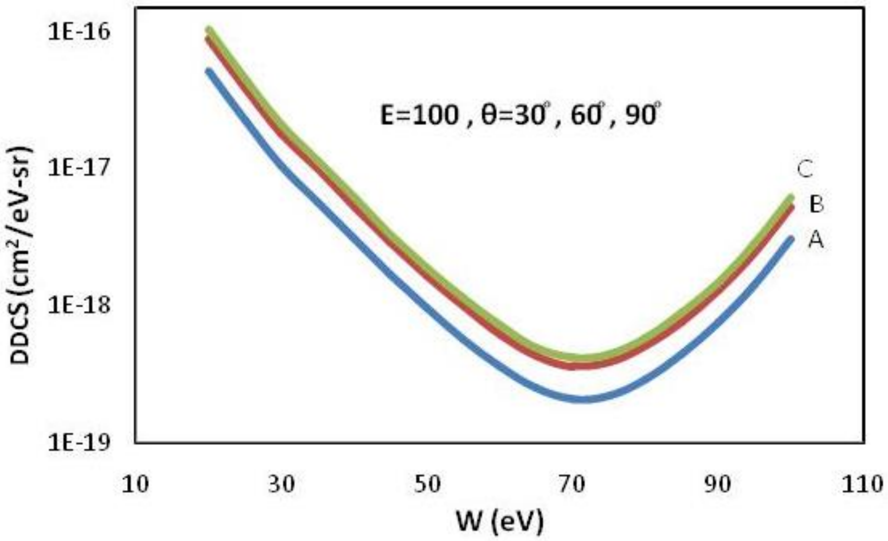

Fig.5: DDCS of Oxygen Atom at fixed incident electron energy 100 eV

with fixed incident angle A, 30°; B, 60°; C, 90°.

Table 4

Double differential ionization cross-section of Oxygen Atom at E=200 eV with respect to secondary electron energy at fixed angles 30°, 60° and 90°

W (eV)	θ, 30°	θ, 60°	θ, 90°
20	4.34E-17	7.52E-17	8.68E-17
25	2.00E-17	3.47E-17	4.00E-17

30	9.98E-18	1.73E-17	2.00E-17
35	5.78E-18	1.00E-17	1.16E-17
40	3.32E-18	5.75E-18	6.63E-18
45	1.98E-18	3.43E-18	3.96E-18
50	1.22E-18	2.11E-18	2.44E-18
55	7.77E-19	1.35E-18	1.55E-18
60	5.11E-19	8.86E-19	1.02E-18
65	3.47E-19	6.02E-19	6.95E-19
70	2.44E-19	4.23E-19	4.89E-19
75	1.78E-19	3.09E-19	3.57E-19
80	1.35E-19	2.35E-19	2.71E-19
85	1.07E-19	1.85E-19	2.14E-19
90	8.79E-20	1.52E-19	1.76E-19
95	7.51E-20	1.30E-19	1.50E-19
100	6.67E-20	1.16E-19	1.33E-19
120	6.02E-20	1.04E-19	1.20E-19
140	8.86E-20	1.53E-19	1.77E-19
160	1.84E-19	3.18E-19	3.67E-19
180	5.42E-19	9.39E-19	1.08E-18
200	3.83E-18	6.63E-18	7.65E-18

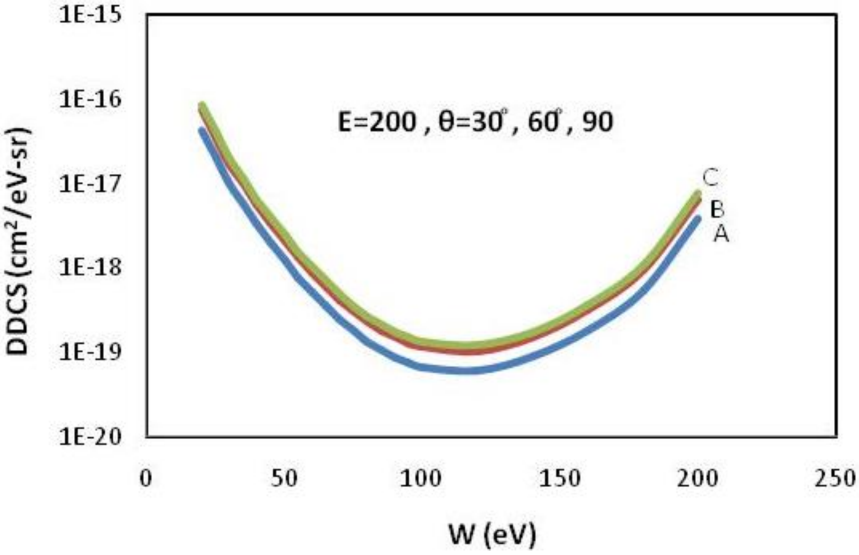

Fig.6: DDCS of Oxygen Atom at fixed incident electron energy 200 eV with fixed incident angle A, 30̊; B, 60̊; C, 90̊.

Table 5
Double differential ionization cross-section of Oxygen Atom at E=500 eV with respect to secondary electron energy at fixed angles 30̊, 60̊ and 90̊

W (eV)	θ, 30̊	θ, 60̊	θ, 90̊
20	2.78E-17	4.81E-17	5.55E-17
25	1.32E-17	2.28E-17	2.63E-17
30	6.74E-18	1.17E-17	1.35E-17
35	4.01E-18	6.95E-18	8.03E-18
40	2.37E-18	4.10E-18	4.74E-18
45	1.45E-18	2.52E-18	2.91E-18
50	9.23E-19	1.60E-18	1.85E-18
55	6.04E-19	1.05E-18	1.21E-18
60	4.07E-19	7.05E-19	8.13E-19
65	2.82E-19	4.88E-19	5.64E-19
70	2.01E-19	3.48E-19	4.02E-19
75	1.48E-19	2.56E-19	2.95E-19

80	1.12E-19	1.93E-19	2.23E-19
85	8.65E-20	1.50E-19	1.73E-19
90	6.89E-20	1.19E-19	1.38E-19
95	5.61E-20	9.72E-20	1.12E-19
100	4.67E-20	8.09E-20	9.34E-20
120	2.61E-20	4.53E-20	5.23E-20
140	1.72E-20	2.98E-20	3.44E-20
160	1.24E-20	2.15E-20	2.48E-20
180	9.51E-21	1.65E-20	1.90E-20
200	7.69E-21	1.33E-20	1.54E-20
250	5.77E-21	9.99E-21	1.15E-20
300	6.36E-21	1.10E-20	1.27E-20
350	1.01E-20	1.75E-20	2.02E-20
400	2.23E-20	3.86E-20	4.46E-20
450	7.89E-20	1.37E-19	1.58E-19
500	1.92E-18	3.33E-18	3.84E-18

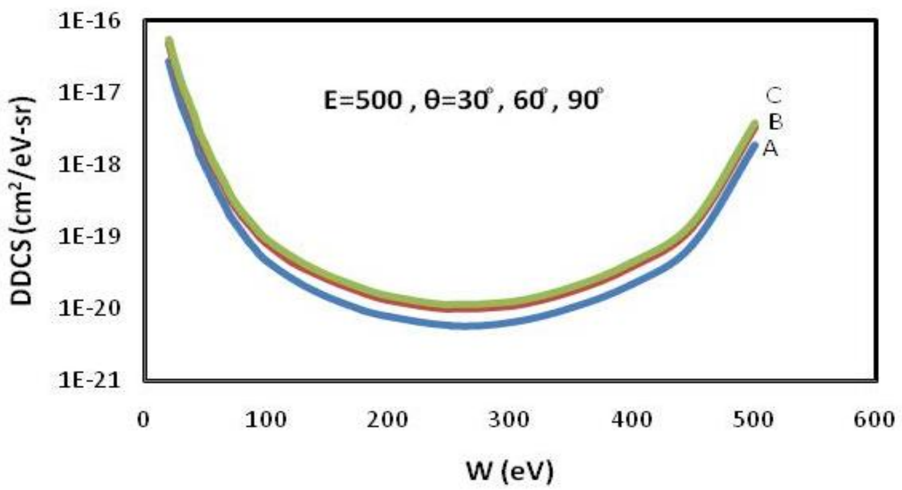

Fig.7: DDCS of Oxygen Atom at fixed incident electron energy

500 eV with fixed incident angle A, 30°; B, 60°; C, 90°.

We have also determined the angular behavior of DDCS at fixed incident electron energies 100, 200, and 500 eV with fixed secondary electron energies 10 eV and 20 eV by altering scattering angle from 0° to 180° are also given in figure 8-10 and tabulated in table 6.

Table 6

Double differential ionization cross-section of Oxygen Atom at E=100 eV, 200 eV and 500 eV with respect to angle θ at constant secondary electron energy ε=10 eV and 20 eV.

Angle θ	E=100 eV		E=200 eV		E=500 eV	
	ε=10 eV	ε=20 eV	ε=10 eV	ε=20 eV	ε=10 eV	ε=20 eV
20	1.87E-17	4.54E-18	1.65E-17	4.53E-18	1.07E-17	3.12E-18
30	2.73E-17	6.63E-18	2.41E-17	6.62E-18	1.57E-17	4.56E-18
40	3.51E-17	8.53E-18	3.10E-17	8.5E-18	2.02E-17	5.86E-18
50	4.18E-17	1.02E-17	3.69E-17	1.01E-17	2.41E-17	6.98E-18
60	4.72E-17	1.15E-17	4.17E-17	1.15E-17	2.72E-17	7.89E-18
70	5.13E-17	1.25E-17	4.53E-17	1.24E-17	2.95E-17	8.56E-18
80	5.37E-17	1.31E-17	4.74E-17	1.30E-17	3.09E-17	8.97E-18
90	5.46E-17	1.33E-17	4.82E-17	1.32E-17	3.14E-17	9.11E-18
100	5.37E-17	1.31E-17	4.74E-17	1.30E-17	3.09E-17	8.97E-18
110	5.13E-17	1.25E-17	4.53E-17	1.24E-17	2.95E-17	8.56E-18
120	4.72E-17	1.15E-17	4.17E-17	1.15E-17	2.72E-17	7.89E-18
130	4.18E-17	1.02E-17	3.69E-17	1.01E-17	2.41E-17	6.98E-18
140	3.51E-17	8.53E-18	3.10E-17	8.50E-18	2.02E-17	5.86E-18
150	2.73E-17	6.63E-18	2.41E-17	6.62E-18	1.57E-17	4.56E-18
160	1.87E-17	4.54E-18	1.65E-17	4.53E-18	1.07E-17	3.12E-18

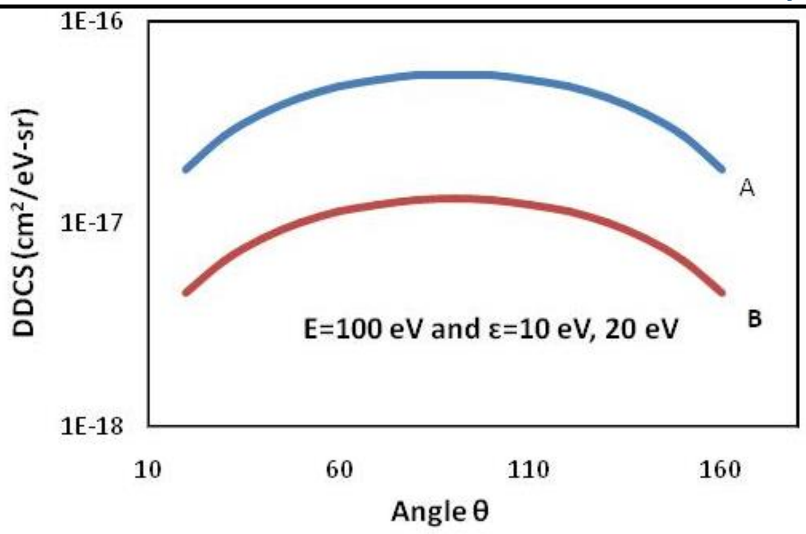

Fig.8: DDCS of Oxygen Atom at fixed incident electron energy 100 eV with fixed secondary electron energy A, 10 eV; and B, 20 eV.

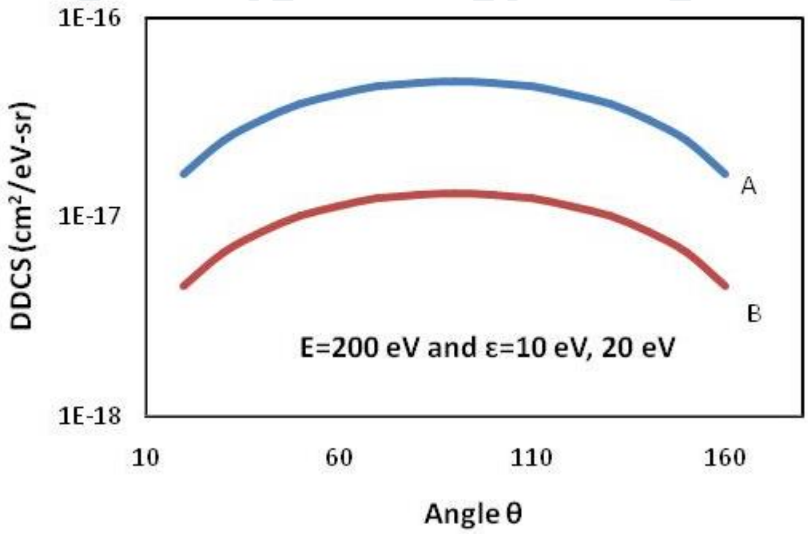

Fig.9: DDCS of Oxygen Atom at fixed incident electron energy 200 eV with fixed secondary electron energy A, 10 eV; and B, 20 eV

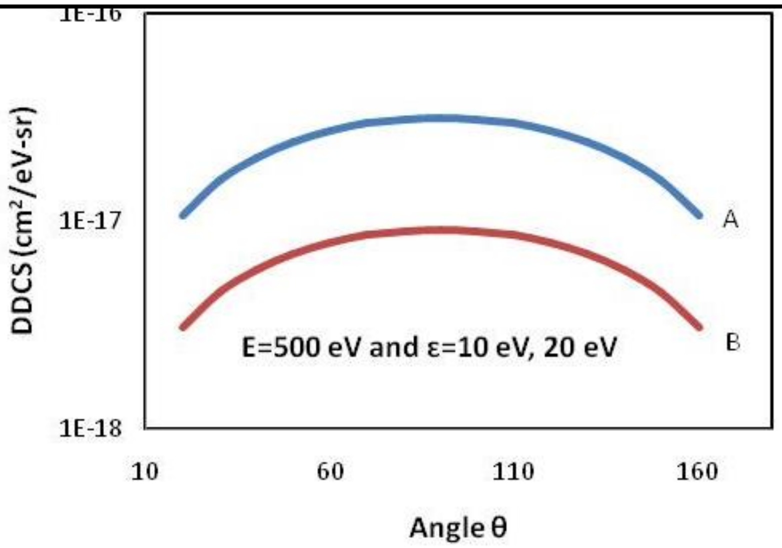

Fig.10: DDCS of Oxygen Atom at fixed incident electron energy 500 eV

with fixed secondary electron energy A, 10 eV; and B, 20 eV.

IV. CONCLUSION

We have calculated the absolute total ionization cross section of oxygen atom via modified Jain-Khare formalism and compared with theoretical and experimental data from threshold energy to high energy [20, 26, 29]. Its in satisfactory agreement with compared data curves. The SDCS are also determined. These comparisons have a very good agreement with each other. Thus, from the compared data and graph, we can say that the results are very reliable in strength and shape and establish that present method and developed programming can produce reliable cross sections even for complex atoms also. Here, the DDCS is determined as a function of secondary electron energy and the incident angle of an electron at the fixed incident electron energies 100 eV, 200 eV and 500 eV, with respect to the fixed angles 30°, 60° and 90° and also calculated the DDCS with respect to the incident electron angle 0° -180°. To the best of my knowledge, no other experimental and/or theoretical data for single and double differential cross sections are available for comparison, till now. However, the qualitative behavior of the cross sections is the same as for other atoms. Thus, it is believed that the present data is reliable and could be used in the plasma process and other modeling systems.

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