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Study of Electron Impact Ionization Cross-Sections of Nitrogen Molecule by Inelastic Collision

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ABSTRACT

In this article, the calculation of ionization cross-section of N_2 molecule by electron impact is reviewed. The work on ionization cross-sections from threshold to high (10 KeV) incident electron energies are calculated and their applications are discussed. To find exact values of total ionization cross-sections for the N_2 molecule, a semi-empirical approach of Jain and Khare (1976) is adopted which is a modification to eliminate the error factors, and then it is compared with the existing experimental and/or theoretical data which gives satisfactory results

KEYWORDS Cross-section, Electron impact, Partial and total ionization.

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INTRODUCTION

Nitrogen is the largely important chemical element present in our earth's atmosphere. Nitrogen has the application in auroral and ionospheric phenomena taking place in the uppermost atmosphere of earth, in electrical discharges, etc. The symbol for the nitrogen element is 'N' and its atomic number is '7'. Nitrogen has two stable isotopes N^{14} and N^{15}. Nitrogen in its elemental form is an odorless, colorless, tasteless, and inert diatomic gas at standard conditions. Out of the total volume of the earth's atmosphere Nitrogen constitutes 78.09%, these are some of the properties of nitrogen due to which it becomes an important element. The data obtained on electron impact ionization of the molecular Nitrogen is of utmost importance in the field of astrophysics, atmospheric physic, and related applications such as space vehicle re-entry and many more.

The ionization process is the process in which targeting an incident particle on a bounding electron of the atom becomes free. This happens due to the transfer of energy from the incident particle to the bound electron when it exceeds electron binding energy. The data relating to the total electron impact ionization cross-section and the partial ionization cross-section of different molecules (fragmented ions) has a wide range of importance. These data can be of great use in the fields of collision theory, plasma physics, radiation chemistry, etc. The studies of electron impact ionization fall into two general classes, the first class to find the TICS "total ionization cross-section" and the second class to find the partial ionization cross-section. The findings of the total ionization cross-sections are a much simpler task and the agreement between the results is moderately satisfactory. The most comprehensive result of this class in starting is given by Rapp and Englander Golden in the year 1965 [1]. They experimentally find total ionization cross-section and partial ionization cross-section for N_2 in the very much limited energy range, it is mainly from threshold to 1000eV. The results of PICS are in disagreement, this is due to the reason it is very difficult to collect the fragments of the ions as they often formed with kinetic energy, thus ensuring the complete collection of fragments ions is a very difficult task due to which disparities occur in the estimation of PICS "Partial ionization cross-section".

Later on, in 1970 Khare and Padalia (1970) use the semi-empirical approach to give the total ionization cross-sections for the He, N_2, H_2, and O_2 molecules [2] from threshold to high incident electron energy. Opal et al. (1972), [3] investigate the total and differential ionization cross-section (50-2000 eV) of different atomic and molecular gaseous by experimentally using the crossed-beam analyzer. In 1992, Jain and Baluja (1992) [4] determine the elastic and inelastic cross-sections for N_2 (10 eV to 5000 eV) and other molecules using a complex optical potential methodology. In 1997, Saksena V. et al. improved the formula and repeated the calculation by using OOS (optical oscillator strength) instead of GOS (generalized oscillator strength) [5]. In 1995, Straub et al. (1995) [6] the absolute partial cross-section for N_2, H_2, and O_2 molecules was determined experimentally by the use of a time-of-flight mass spectrometer from threshold to 1000 eV. Brook et al. (1978) [7] also used the crossed beam method for the Nitrogen which was found to be in good agreement with data which is obtained from earlier crossed beams experiments that make use of the thermal energy atoms beams but the data recorded has a low value in magnitude at lower energies as compared to Rapp and Briglia (1965). Rapp and Briglia (1965) use the technique which is known as the static gas target technique. Then with the advancement in technology, the detection of the ionic fragments formed during partial ionization cross-section becomes easy and also the detection of the dissociation channels becomes possible by using an ion imaging mass spectrometer.

Theoretical approaches used classical computation for the electron impact ionization for almost a century. Thomson (1912) derived an equation based on which diverse models have been developed [8]. The further development embraced the progress of an examination by Bethe. Several non-perturbative methods that are used to calculate the ionization cross-sections of atoms/atomic ions in the last three decades show very good agreement with each other and with experimental results. Margreiter et al. (1990) [9] determine the electron impact ionization cross-section applying the newly developed semi-classical formula from threshold to a high value of 200 eV energy. After that, this semi-classical formula was updated by Deutsch et al. (2000) [10] and calculated 31 molecules from low to high incident electron energy including the N_2 molecule, and comparison showed good agreements. The various theoretical methods to calculate partial and total ionization cross-section include the methods of Partial Wave Approximation, Ab-Initio electrostatic method, R-matrix method, close-coupling method, coupled Integral-differential equation, Binary Encounter Bethe method, Born-Oppenheimer approximation, the formalism of Kim and Rudd, the method involving Plane-wave born approximation, and semi-empirical methods. The close coupling and R-matrix yield results for a wide range of incident energies. The other theoretical method used by Joshipura (1993) [11] is the Complex Optical Potential approach. He adopted an additivity rule and work at high energy levels. G. Garcia et al. (1997), [12] theoretically evaluate the N_2 molecule scattering from 1 to 10 KeV using the method of Born-Bethe approximation. The total interaction with the target of the incident electron in this method is shown by the local, complex optical potential which is dependent on energy. Kothari and Joshipura (2011) [13] finds the total ionization cross-section of N_2 molecule by positron impact CSP-ic "Complex Scattering Potential-ionization contribution" method between the energy range 15 eV to 2000 eV. Besides this, Singh et al. (2016) [14] also estimate the positive scattering cross-section for Carbon, Nitrogen, Oxygen, and diatomic molecules that is C_2, N_2, and O_2 from 1eV to 5000 eV using SCOP "Spherical Complex Optical Potential" formalism. Shen et al. (2018) [15] also work on the partial and the total ionization cross-sections for gas-phase N_2 molecule by using the experimental electron impact method in a wide energy range from 250eV to 8000eV by ion imaging mass spectrometer. Stefan E. Huber et al. (2019) [16] estimate the partial and total ionization cross-section of the diatomic molecules which are fusion–relevant including N_2 molecule from threshold to10 KeV energy using BEB and DM formalism and also compared available data which gives a better agreement. So, there are many theoretical and experimental investigations for calculating the ionization cross-section of N_2 molecules. There is so abundant work done on this molecule, that it is difficult to include all the previous findings of the N_2 molecule. For this work, many techniques are used for better results. Hence, many improvements are there over earlier work. Because of the experimental difficulties the finding of the quantitative understanding of the electron impact ionization cross-sections of Nitrogen molecules is not sufficient for its applications. It became more interesting to review the total electron impact ionization cross-section of gaseous molecular Nitrogen. So, the ionization cross-section for N_2 is determined by using modified Jaina and Khere (1976) formalism which gives more accurate results than another comparison.

THEORETICAL METHODOLOGY

To investigate the total and partial electron impact ionization, we have applied the theoretical modified Jain and Khare methodology. In 1976 Khare *et al.* [17] provided this formula and improved it from time to time. In his, work Khare combined the Mott and Bethe theories, which describe ionization cross-section at high and low impact parameters respectively. They used the Inokuti formalism to determine an SDICS "single differential ionization cross-section" having the combination of the Mott cross-section and Bethe cross-section (Khare and Meath, 1987) [18] that is collectively shown in equation 1.

$$Q_i(E,\in)=\frac{4\pi.a_0^2R^2}{E}\left[\left(1-\frac{\in}{E-I_i}\right)\frac{R}{W}\frac{df_i(W,0)}{dW}.\ln[1+C_i(E-I_i)]+\frac{R}{E}S_i\frac{(E-I_i)}{(\in^3+\in_0^3)}\left(\in-\frac{\in^2}{(E-\in)}+\frac{\in^3}{(E-\in)^2}\right)\right] \quad \text{.......(1)}$$

The secondary electron(s) energies (ε) vary from minimum (zero) to maximum (incident electron energy E). In the calculations of the SDCS for the production of an i^{th} type of ion, we have replaced W with $(\varepsilon+I_i)$, the loss of energy suffered by the primary electron is from I_i to maximum i.e. E [19-26], that given in equation 2.

$$Q_i(E,W)=\frac{4\pi.a_0^2R^2}{E}\left[\left(1-\frac{\in}{E-I_i}\right)\frac{R}{W}\frac{df_i(W,0)}{dW}.\ln[1+C_i(E-I_i)]+\right.$$
$$\left.\frac{R}{E}S_i\frac{(E-I_i)}{(\in^3+\in_0^3)}\left(\in-\frac{\in^2}{(E-\in)}+\frac{\in^3}{(E-\in)^2}\right)\right] \quad \ldots\ldots(2)$$

The total single differential cross-section can be calculated by the summation of all i[th] type cross-sections i.e.

$$Q_i^T(E,W)=\sum_i Q_i(E,W) \quad \ldots..(3)$$

The integral cross-section i.e. the partial ionization cross-section is produced by the integral of equation (2) given the energy loss "W" from the ionization threshold to the maximum E.

$$Q_i(E)=\frac{4\pi a_0^2R}{E}\left[\frac{E}{(E-I_i)\left(1+\frac{I_i}{E}\right)}\left(M_i^2-\frac{R}{W}S_i\right)\ln[1+C_i(E-I_i)]+\right.$$
$$\left.\int_{I_i}^{E}\frac{R}{E}S_i\frac{(E-I_i)}{(\in_0^3+\in^3)}\left[\in-\frac{\in^2}{(E-\in)}+\frac{\in^3}{(E-\in)^2}\right]\right]dW \quad \ldots.(4)$$

The total ionization cross-section is given as

$$Q_i^T(E)=\sum_i Q_i(E) \quad \ldots..(5)$$

For the evaluation of ionization rate coefficients, we use Maxwell-Boltzmann distribution **[27-32]** as a function of temperature concerning the different types of cross-sections i.e.

$$R_i(E)=\int_{-\infty}^{+\infty}4\pi\left(\frac{1}{2\pi mkT}\right)^{\frac{3}{2}}me^{-E/kT}Q_i(E)EdE \quad \ldots..(6)$$

Where, T, k, and m are the absolute temperature, Boltzmann constant, and mass of the electron, respectively.

RESULTS AND DISCUSSION

We determine the total ionization cross-section of the Nitrogen Molecule by electron impact using modified Jain-Khere formulism from threshold up to high energy. The most important factor in the findings of the ionization cross-sections is the oscillator strength which is taken from Chain et al. (1993) **[33]** ranges from 13 to 40eV for N_2 molecule and higher energy oscillator strength is extrapolated up to desired energy loss using TRK sum rule. The Ionization potential has been taken for N_2 is 15.58 eV [4, 13, 14, 16]. The energy parameter and Collision parameters measured for the N_2 molecule are 50 eV and 0.02249 respectively. MATLAB codes have been developed to solve the above equations [24] and the calculated results are tabulated in Table 1 and graphically represented in Figure 1. We compared our results with National Institute of Standards and Technology (NIST) laboratory data [34] and one more theoretical data [4]. We also compared our results with available experimental data [1, 3, 6] which shows very good agreements and graphically are shown in Figure 2.

Table 1: Total Ionization Cross-Sections (10^{-16}cm^2) of N_2 molecule

Energy (eV)	TICS	Energy (eV)	TICS
20	0.089	250	2.699
22	0.103	300	2.493
24	0.136	350	2.312
26	0.152	400	2.153
28	0.424	450	2.015
30	0.665	500	1.895
32	0.880	550	1.788
34	1.091	600	1.694
36	1.276	650	1.610
38	1.440	700	1.534
40	1.585	750	1.466
45	1.884	800	1.404
50	2.112	850	1.348
60	2.360	900	1.296
65	2.526	950	1.249
70	2.660	1000	1.205
75	2.768	1100	1.126
80	2.855	1200	1.058
85	2.927	1300	0.999
90	2.983	1400	0.946
95	3.029	1500	0.899
100	3.064	1600	0.857
105	3.091	1700	0.819
110	3.110	1800	0.785
115	3.124	1900	0.754
120	3.132	2000	0.725
125	3.135	2100	0.698
130	3.134	2200	0.674
135	3.131	2300	0.651
140	3.124	2400	0.630
145	3.114	2500	0.611
150	3.103	2600	0.592
155	3.089	2700	0.575
160	3.074	2800	0.559
170	3.040	3000	0.530
180	3.002	4000	0.421
190	2.961	5000	0.352
200	2.918	6000	0.303
210	2.874	7000	0.267
220	2.830	8000	0.239
230	2.786	9000	0.217
240	2.742	10000	0.199

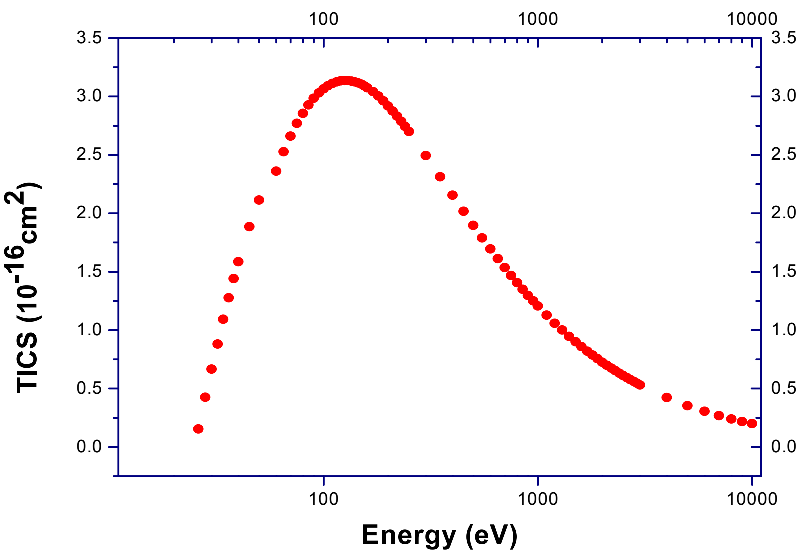

Figure 1: Total Ionization Cross-Section of N_2.

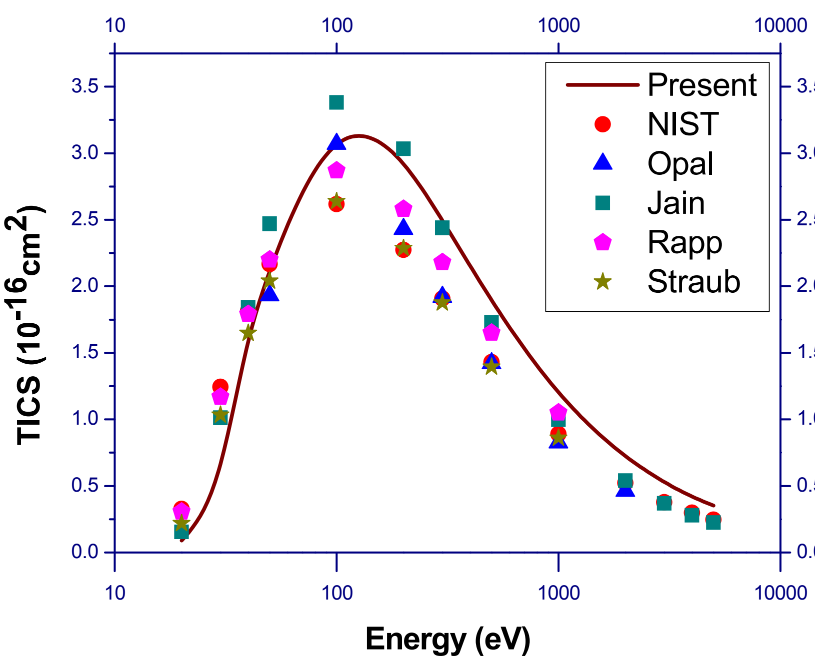

Figure 2: Comparison of N_2TICS: Solid line, Present result; Pentagon, Donald Rapp [1]; Triangle, C.B. Opal [3]; Squire, Ashok Jain[4]; Star, H.C. Straub [6]; Solid dot, NIST [34]

CONCLUSIONS

Satyendra Pal et al. (2020) determine both the single and double differential ionization cross-section for N_2 and O_2 molecules [25]. But the data for the Absolute ionization cross-section of these molecules are not available by using the modified Jain and Khere method. Here we have calculated the total ionization cross-section of the N_2 molecule using this approach. Comparing the results with theoretical and experimental data gives a good agreement. It is observed that at the low ionization energy, all the graphs show the peak whereas with the increase in the ionization energy the curve shows the decrease.

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