The electron impact ionization cross sections of Nitrogen from threshold to 10 MeV.

Pramod Kumar[1], Kiran Pal[2*], Amrita[2], Yogesh Kumar[2], Manoj Kumar[3]

1. Department of Physics, Vardhaman College, Bijnor-246701, India.
2. Department of Physics, D.A.V. College, Muzaffarnagar-251001, India.
3. Department of Physics, Meerut College, Meerut-250001, India.

Corresponding Author: Kiran Pal

***Abstract*: In present article, we have calculated the electron impact ionization cross section for Nitrogen molecule (N_2) from ionization threshold to 10 MeV. The modified Khare model has been employed. We have only one experimental data set at relativistic energies which is measured by Reike and Prepejchal in terms of two collision parameters C_{RP} and M^2 to compare our calculated results. The collision parameters C_{RP} and M^2 also have been calculated. The calculations are compared with available previous experimental data as well as theoretical results. A remarkable agreement is found among the present results, other previous calculations and experimental data.**

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***Keywords*: Collision, Cross sections, Electron impact ionization, Nitrogen**.

Introduction:

The ionization of atoms and molecules by electron impact has an importance in various research areas such as atmospheric physics, astrophysics, radiation physics etc. The ionization cross sections due to electron are important to understand the basic collision mechanism and in wide range of experimental applications, for instance the modelling of semi-conduction manufacturing by plasma processing needs ionization cross sections of molecules used as the ideal gas. The ionization cross sections are also needed Nitrogen molecule (N_2) is detected in atmosphere of Titan, Saturn's largest satellite. Where cosmic rays strike on these molecules and ionized them. Thus ionization cross section play important role to understand fundamental process of ionization. Nitrogen is the most abundant molecule of the earth's atmosphere. Collision of electron with Nitrogen molecules plays an important role in ionosphere and auroral phenomena in the atmosphere of the earth. Furthermore, Nitrogen plasma is used in treatment of spin diseases. There is the important process in electric discharges involving atmospheric gases. There discharges make a basic technique in the fields of gaseous electrons and plasma processing. [1-5].Recently, Shen et al. [6] have reported the total ionization cross sections for N_2 in gas phase by electron impact in a wide energy range (250-8000 eV). They have employed ion imaging mass spectrometer. In 2006, Itikawa [7] reviewed the experimental data of Nitrogen molecule, those recommended by Lindsay and Mangan [8]. Straub et al. [9] measured the experimental data for ionization cross section of Nitrogen molecule due to electron impact. They have used time of flight mass spectrometer with a position sensitive detector to collect the all energetic fragments ions. They claimed 3.5% in their experimental studies. Rapp and Englander-Golden [10] have reported the total ionization cross section of N_2 molecule from threshold to 1 keV by using ionization tube from threshold to1 keV. We have also an old experimental data those measured by Schram et al. [11] Nitrogen molecule for incident energy range 0.6-20 keV. We have only one experimental data at relativistic energies (0.1-2.7 MeV) those measured by Rieke and Prepejchal [12]. They measured the cross sections in term of two collision parameters C_{RP} and M^2.

Theory

In 2019, Kumar et al. [13] have modified Khare-BEB model [14]. They simplified the Bethe cross section of Khare-BEB model. In this modified model, the ionization cross section due to electron impact for jth molecular orbital is given by

$$\sigma_{jT} = \sigma_{jM} + \sigma_{jB} + \sigma_{tj} \qquad (1)$$

Where Mott cross section, σ_{jM} is given by

$$\sigma_{jM} = \frac{AN}{[E+I+U]I} \times \left[1 - \frac{2}{t+1} + \frac{t-1}{2t^2} + \frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)} - \frac{t+1}{t^2}\ln\left(\frac{t+1}{2}\right) \right] \qquad (2)$$

where $t = E/I$, $E = \frac{1}{2}mc^2\left[1 - \frac{1}{1+\frac{T}{mc^2}}\right]$, $A = 4\pi a_0^2 R^2$. The notations U, a_0, I, N, T, m, c and R stand for the average kinetic energy of bound electron, the first Bohr radius, the ionization energy, the occupation number of molecular orbital, the kinetic energy of the incident electron, rest mass of electron, velocity of light and Rydberg energy respectively. The Bethe cross-section σ_{jB} is given by

$$\sigma_{jB} = \frac{AN}{2[E+I+U]I}\left[\frac{1}{2}\left(1-\frac{1}{t^2}\right)-X\right] \qquad (3)$$

Where the term X is given by

$$X = 2ln\left(\sqrt{t}-\sqrt{(t-1)}\right)+\frac{1}{2t^2}\left\{\begin{array}{c} 1-\frac{1}{2}\left(\frac{t}{t-\sqrt{t(t-1)}}\right)^2 \\ +\frac{1}{2}\left(\frac{t}{t+\sqrt{t(t-1)}}\right)-\left(\frac{t}{t-\sqrt{t(t-1)}}\right) \\ -\frac{3}{4}ln\left(\frac{t+\sqrt{t(t-1)}}{t-\sqrt{t(t-1)}}\right) \end{array}\right\}$$

The cross section due to the transverse interaction is

$$\sigma_{tj} = -\frac{4\pi a_0^2 R}{E} M_j^2[\ln(1-\beta^2)+\beta^2] \quad (4)$$

where β is the ratio of the incident velocity v and the velocity of light c, M_j^2 represents the total dipole matrix squared measured in units of a_0^2 and given by

$$M_j^2 = \int_{I_j}^{E} \frac{R}{w}\frac{df_j(w,0)}{dw}dw \qquad (5)$$

Where $\frac{df_j(w,0)}{dw}$ is the continuum optical oscillator strength (COOS) per unit energy range and given by

$$\frac{df_j(w,0)}{dw} = \frac{NI_j}{w^2} \qquad (6)$$

The expression of collision parameter for j[th] molecular orbit C_{jRP} is given by

$$C_{jRP} = \frac{RE}{A}\sum_{j}(\sigma_{jB}+\sigma_{jM}) - {M_j}^2 ln\beta^2 \quad (7)$$

Results and discussion

Equation (1) along with equations (2 –4) have been used to evaluate total ionization cross section due to electron impact of Nitrogen molecule. We have calculated the cross sections by using Kim BEB method [15] to compare our calculations. The collision parameters of N_2 molecule are calculated by using equations (5) and (7). The required molecular parameters binding energies I, kinetic energies of bound electrons U and occupation numbers N are taken from reference [16].

The present calculated cross sections along with other previous data for Nitrogen molecule from threshold to 10 keV have been shown in figure (1). Our results are in good agreement with the experimental data those measured by Struab et al. [9] within 6% except at near threshold. At near threshold (E < 50 eV) our calculations are slightly greater than the experimental results, present cross sections are in good agreement with experimental data of Rapp et al. [10] for 20 eV < E< 100 eV within 9%. However, beyond this range our calculations under estimate the experimental results. A good agreement is found between excremental results of Itikawa [7] and present calculations within 4% for E > 70 eV, While for E < 70 eV, present results are slightly greater than the experimental data. Our calculations are also in good agreement with the experimental data those measured by Shen et al. [6] and Schram et al. [11] for whole range of energy studied by them.

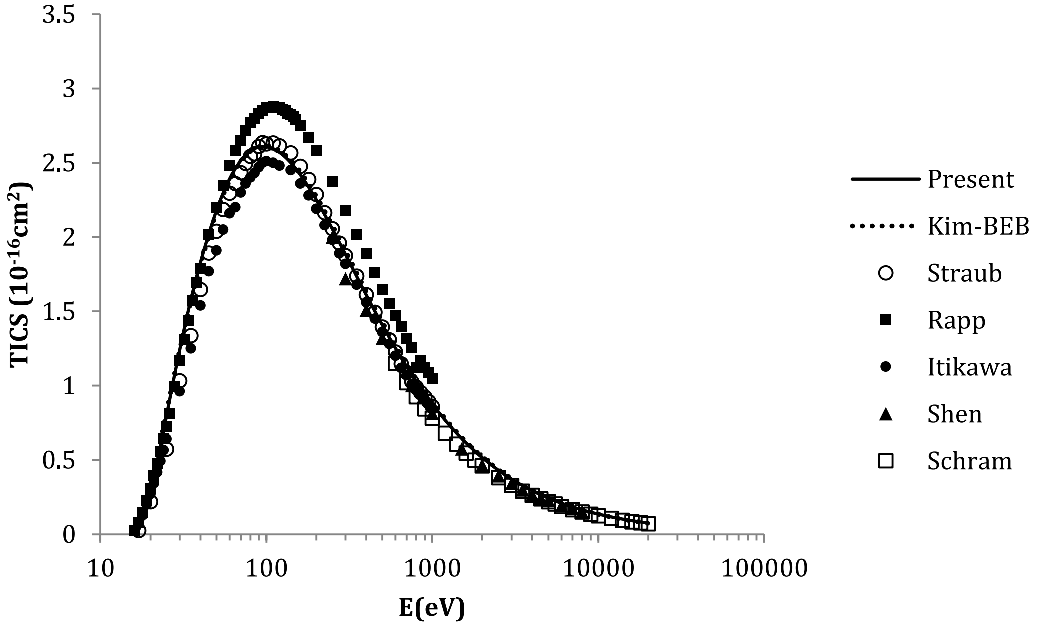

Fig.1 Total ionization cross sections (TICS) for Nitrogen molecule in 10^{-16} cm^2. Solid line and dotted line represent present results and Kim-BEB calculations respectively. Open circles, filled rectangles, filled circles, filled triangles and open rectangles represent the experimental results of Straub et al., Rapp & Englander-Golden, Itikawa, Shen et al. and Schram et al. respectively.

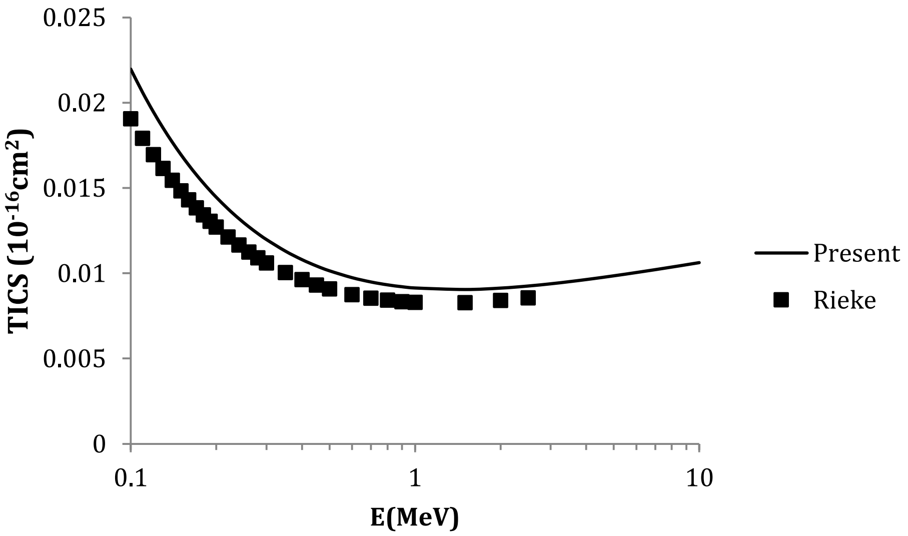

Fig. 2 This figure shows the present total ionization cross sections along with experimental data of Reike and Prepejchal for Nitrogen molecule in energy range (0.1-10MeV) in 10^{-16} cm^2

The figures (2) shows the total ionization cross sections due to electron impact for Nitrogen molecules are shown respectively. In this figure we have compared the present calculation with the experimental results those measured by Reike and Prepejchal [12]. Our theoretical results are greater than experimental data but difference is not large.

In table (1), the present theoretical collision parameters along with experimental data are represented.

Molecules	C_{RP} (at 1MeV)	C_{RP} (at 10MeV)	C_{RP} (at 100MeV)	C_{RP} (Exp. Rieke)	Present M_j^2	M_j^2 (Exp.Rieke)	M_j^2 (Exp.Schram)
Nitrogen	39.05	38.88	38.88	34.84	3.44	3.74	3.85

Table1 Present calculated values of collision parameter C_{RP} and M_j^2 (in unit of a_0^2) are shown along with the experimental values given by Rieke and Prepejchal [12]. The values of C_{RP} are calculated at incident energies 1MeV, 10MeV and 100 MeV using equation (7).

On increasing the kinetic energy of incident electron calculated value remains nearly constant, which is according to expectation? The calculated value of C_{RP} is greater that the experimental value by 11.6 %, however present value of dipole matrix squared M_j^2 is lower than the experimental value of Reike and Prapejchal [8] by 8% and experimental value of Schram et al [11] by 10.42 but the difference between values of theoretical and experimental results of collision parameters are also not large. Hence a remarkable agreement is found between calculated results and experimental data.

Conclusion:

Khare-BEB model is used to calculate the ionization cross action of nitrogen from ionization threshold to 10 MeV. The present cross sections are found in the good agreement with available experimental data over most of incident energy range. The calculated values of parameters are also found in good agreement with the experimental values.

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