RESEARCH ARTICLE

Scattering of $e^\pm$ from N_2 in the energy range 1 eV–10 keV

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ABSTRACT

The differential, integrated elastic, inelastic, total, momentum transfer, viscosity, and ionisation cross sections for electron and positron scattering from the homonuclear diatomic nitrogen molecule over an incident energy range of 1 eV–10 keV are calculated using the additivity rule. Dirac partial wave analysis is employed to calculate the cross sections of the constituent atoms of molecules, using a complex optical model potential (OPM). Comparison of our results of the additivity rule with the available experimental data and other theoretical predictions is presented. Our findings produce reasonable results in intermediate and high energies.

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1. Introduction

Nitrogen is one of the most fundamental molecules and most abundant constituent of Earth's atmosphere. Scatterings of electrons and positrons from nitrogen molecules have a special role in ionospheric and auroral phenomena in the Earth's upper atmosphere. These scattering cross sections also have applications in low-temperature processing plasmas, fusion edge plasmas, gas discharges, planetary, stellar, and cometary atmospheres, radiation physics, mass spectrometry, material-processing applications, manufacturing semiconductor devices and modelling of various laser systems [1–4].

The multicentre nature, the lack of centre of symmetry and nuclear motion of the $e^\pm$ -molecule scattering feature its noticeable differences from the $e^\pm$ -atom scattering [5]. Many approximated theoretical methods have been proposed to explain $e^\pm$ -molecule scattering data. Among them, the additivity (AR) is a relatively simple but effective one. In AR, the anisotropic nature of molecular scattering, originated from the projectile scattering off the electric multipoles of molecules, is ignored as it does not play a significant role in shaping up cross sections at intermediate and high-energies [6]. This work uses this easy-to-use AR to study the scattering of electron

and positron from nitrogen molecule in which molecular cross sections are expressed as the sum of those of the constituent atoms. The molecular scattering problem is thus reduced to an atomic scattering problem.

The spin-polarisation during the scattering of electron and positron requires the inclusion of spin-orbit interaction term in the Schrödinger equation. On the other hand, this term is simply incorporated in Dirac's relativistic equation. McEacharan and Stauffer [7] carried out relativistic calculations on the momentum transfer cross section, scattering length and differential cross sections at low energies for the electron-argon scattering. The results produced an excellent agreement with experiments and showed an improvement over the non-relativistic analysis. Encouraged by the above facts, we adopt Dirac partial wave analysis, with complex atomic OPM, to calculate differential cross section (DCS), integrated elastic cross section (IECS), momentum transfer cross section (MTCS), viscosity cross section (VCS), inelastic cross section (INCS), total cross section (TCS) and total ionisation cross section (TICS) for the scattering of electron and positron from nitrogen atom. Then sums of these cross sections of the individual atoms are taken to produce corresponding molecular cross sections. These cross sections obtained in this simplistic way of AR are used for modelling codes for various applications as stated above.

In the optical potential method, the non-local optical potential is approximated by a local complex potential to avoid arduous and lengthy computation. The complex electron-atom OPM has both real and imaginary parts. At energies below inelastic scattering thresholds, scattering phenomena can be well represented by the real part, which consists of static, exchange and correlation-polarisation potentials. The electrostatic potential is determined by electronic and nuclear charge distribution of the free atoms. Rearrangement collisions between the projectile electron and bound electrons are handled by replacing the non-local exchange interaction with the approximate local exchange potential. The correlation-polarisation potential accounts the polarisation of the target charge distribution under the action of projectile's electric field. Above inelastic scattering thresholds, a loss of projectile flux occurs from elastic channel to inelastic channel. This loss is described by the semi-relativistic negative imaginary potential.

Positronium formation, the short-lived exotic hydrogen like an atom, takes place at low and intermediate energies as a result of interaction of the positron with the bound electrons of the target [8]. The coupled channel, quantum electrodynamics, R-matrix and many-body theories are used to treat this cumbersome theory. Annihilation occurs from direct interaction of the positron

with the bound electrons and also from the excited state of the positronium. Our method lacks the option for the treatment of the positronium formation and annihilation.

The elastic scattering of electrons from N_2 has been studied extensively by both experimental and theoretical methods. Using a crossed-beam method Shyn and Carignan [9] measured DCS, IECS and MTCS over the energy range 1.5–400 eV. Srivastava *et al.* [10] published the measurements on DCS, IECS and MTCS (5–75 eV) using the cross interaction of electron and N_2 gas beams. DCS and IECS (20–800 eV) were measured by DuBois and Rudd [11] for electrons scattered between 2° and 150° by the static gas target of nitrogen. Jansen *et al.* [12] used an electron spectrometer and measured DCS and IECS over the energy range 100–3000 eV. DCS (300–500 eV) measurements have also been reported by Bromberg *et al.* [13]. Nickel *et al.* [14] measured DCS (20–100 eV) using a relative flow technique. TCS data for electron scattering have been published by Blaauw *et al.* [15], Aberth *et al.* [16], Dalba *et al.* [17] and Garcia *et al.* [18] and for positron scattering by Charlton *et al.* [19] and Sueoka and Mori [20]. TCS data for both electron and positron scattering have been measured by Hoffman *et al.* [21]. IECS measurements have been reported by Finn and Doering [22]. Furthermore, Itikawa [4], Shyn and Carignan [9] and Srivastava *et al.* [10] reported data on IECS and MTCS. Straub [23], Tate and Smith [24], Schram *et al.* [25] and Rapp and Golden [26] have published INCS data for electron and Bluhme *et al.* [27] and Marler and Surko [28] for positron.

There are theoretical studies on $e^\pm$ scattering from nitrogen molecule in the literature. Lee and Iga [29] used a complex optical potential derived from a fully molecular wavefunction within the framework of the Schwinger variational iterative method combined with the distorted-wave approximation to calculate DCS, IECS and MTCS for $e^- - N_2$ scattering in the energy range 20–800 eV. Jain *et al.* [3] investigated the elastic scattering of $e^- - N_2$ in a two potential coherent approach to calculate DCS, IECS and MTCS (50–800 eV). Using a realistic effective interaction potential as a function of molecular orientation and internuclear distance, Maynard *et al.* [30] calculated DCS (30–75 eV) for the elastic scattering of $e^- - N_2$ by solving close-coupling equations. Jain and Baluja [31] reported calculations on TCS (10–5000 eV) by calculating the complex optical potential for the $e^\pm - N_2$ collision system from the corresponding molecular wave function at the Hartree-Fock level. Blanco and Garcia [32] published their calculations on DCS, TCS and IECS (10–10,000 eV) for $e^- - N_2$ scattering using the independent atom model (IAM). Wedde and Strand [33] reported calculations on DCS (20–90 eV)

using the phase-amplitude method. Phelps and Pitchford [34] calculated IECS, INCS, MTCS, TICS and TCS for electron energies from 0.003 to 10 keV with use of the multiterm spherical-harmonic expansion solution of the Boltzmann equation. For positron scattering, Sun *et al.* [6] published additivity calculations on TCS (10–800 eV). Kothari and Joshipura [35] employed complex scattering potential to calculate TCS and IECS (15–2000 eV). Gillespie and Thompson [36] reported calculations on IECS and MTCS (~ 1 –13.6 eV) in terms of fixed molecule S matrix elements.

The present work uses the AR model for the projectile- N_2 scattering. Our calculations employ a different combination of the components of the complex optical potential, and produce results for scattering observables, not all treated in a single fold so far. The work also covers a broader energy domain than most of the aforesaid review works. Moreover, our method is easy to implement and so suitable for fast generation of cross-sections desirable for modelling various processes involved in science and technologies.

The organisation of the paper is as follows. In Section 2, the outline of the theory is discussed. In Section 3, results of our theory and comparison with other theories are given. In Section 4, we have drawn conclusion on our results.

2. Outline of the theory

2.1. The interaction potential

The complex optical potential used for the electron atom or molecule scattering calculations has the following form [37]:

$$V(r) = V_{st}(r) + V_{ex}(r) + V_{cp}(r) - iW_{abs}(r). \quad (1)$$

Here, $V_{st}(r)$, $V_{ex}(r)$ and $V_{cp}(r)$, the components of the real part of OPM, represent the static, exchange and correlation–polarisation potentials, respectively, and the imaginary part, W_{abs} represents the absorption potential. For positron, V_{ex} in $V(r)$ is omitted as exchange does not arise due to distinguishability of the projectile positron and bound electrons.

The static potential arises from the electrostatic interaction between the projectile and the target charge distribution. Within the static-field approximation, this potential is accurately determined by the nuclear and electronic charge distributions. Fermi nuclear charge distribution and analytical electron density, for neutral atom, given by Koga [38] are used in the present calculations.

Rearrangement collisions between the incident electron and target electrons arise from the antisymmetrisation of the wavefunction of the whole projectile-target system with respect to electrons. These collisions lead to a set of coupled integro-differential equations. Therefore, this interaction potential is non-local and short range by nature and a unique feature of electron scattering [39]. An approximate local potential is used to replace this non-local potential for an easy but accurate solution of Dirac equation, as the exchange potential is negligible at high energies [40]. In the present work, we use the semi-classical exchange potential of Furness and McCarthy [41] obtained from the non-local exchange interaction using the WKB like wave function. This exchange potential is given as

$$V_{ex}(r) = \frac{1}{2} [E_i - V_{st}(r)] - \frac{1}{2} \{ [E_i - V_{st}(r)]^2 + 4\pi a_0 e^4 \rho_e(r) \}^{1/2}. \quad (2)$$

Here, E_i is the impact energy of the electron and a_0 is the Bohr radius.

The incident projectile, electron or positron, causes polarisation and thereby induces electric dipole moment of the target atom or molecule. The interaction of the projectile with this induced dipole moment is described by the correlation–polarisation potential (CPP). The asymptotic behaviour of CPP is the same for both electron and positron and is given by the Buckingham as

$$V_{cp,B}(r) = -\frac{\alpha_d e^2}{2(r^2 + d^2)^2}, \quad (3)$$

where α_d is the dipole polarisability of the target atom and d is the phenomenological cut-off parameter which is introduced to avoid singularity at the $r = 0$. Mittleman and Watson [42] suggested

$$d^4 = \frac{1}{2} \alpha_d a_0 Z^{-1/3} b_{pol}^2. \quad (4)$$

Here, b_{pol} is an adjustable energy dependent parameter. Considering the fact that the magnitude of the polarisation effects decreases as the projectile energy increases, Seltzer [37] suggested the following empirical formula:

$$b_{pol}^2 = \max\{(E - 50 \text{ eV})/(16 \text{ eV}), 1\}. \quad (5)$$

For a small value of r , the distortion of the target charge cloud becomes different for different projectiles and the correlation interaction becomes more complex. During the penetration of projectile electron through the bulk of the target, a Coulomb hole is formed surrounding that electron from which bound electrons get repelled. In

local density approximation (LDA), the short range correlation potential is calculated as the functional derivative of the free electron gas (FEG) correlation energy with respect to local atomic electron density ρ [43]. It is convenient to introduce the density parameter

$$r_s \equiv \frac{1}{a_0} \left[\frac{3}{4\pi\rho_e(r)} \right]^{\frac{1}{3}}. \quad (6)$$

For electrons, Perdew and Zunger [44] gave the following parameterisation for the following correlation potential:

$$V_{co}^{(-)}(r) = -\frac{e^2}{a_0} (0.0311 \ln(r_s) - 0.0584 + 0.00133r_s \ln(r_s) - 0.0084r_s), \quad \text{for } r_s < 1 \quad (7)$$

and

$$V_{co}(r) = -\frac{e^2}{a_0} \beta_0 \frac{1 + (7/6)\beta_1 r_s^{\frac{1}{2}} + (4/3)\beta_2 r_s}{(1 + \beta_1 r_s^{\frac{1}{2}} + \beta_2 r_s)^2} \quad \text{for } r_s \geq 1. \quad (8)$$

Here, $\beta_0 = 0.1423$, $\beta_1 = 1.0529$ and $\beta_2 = 0.3334$.

For positrons, the correlation potential, as given by Jain [45], is

$$V_{co}^{(+)}(r) = \frac{e^2}{2a_0} \{-1.82r_s^{-1/2} + [0.051 \ln(r_s) - 0.115] \times \ln(r_s) + 1.167\}, \quad \text{for } r_s < 0.302, \quad (9)$$

$$V_{co}^{(+)}(r) = \frac{e^2}{2a_0} [-0.92305 - 0.09098r_s^{-2}] \quad \text{for } 0.302 \leq r_s < 0.56, \quad (10)$$

and

$$V_{co}^{(+)}(r) = \frac{e^2}{2a_0} \left[-\frac{8.7674}{(r_s + 2.5)^3} + \frac{-13.151 + 0.9552r_s}{(r_s + 2.5)^2} + \frac{2.8655}{(r_s + 2.5)} - 0.6298 \right] \quad \text{for } 0.56 \leq r_s < 8.0. \quad (11)$$

For the asymptotic region, $8.0 \leq r_s \leq \infty$, the polarisation potential is accurately given by the Buckingham potential.

The global correlation–polarisation potential is determined by combining the long range Buckingham potential with the short range LDA correlation potential as follows [37]:

$$V_{cp}^{\pm}(r) \equiv \begin{cases} \max\{V_{co}^{\pm}(r), V_{cp,B}(r)\} & \text{if } r < r_{cp}, \\ V_{cp,B}(r) & \text{if } r \geq r_{cp}. \end{cases} \quad (12)$$

Here, r_{cp} is the outer radius at which $V_{co}(r)$ and $V_{pol}(r)$ cross first.

Excitations of the target occur when the energy lost by the projectile is greater than the first inelastic threshold. This causes a loss of flux from elastic channels to inelastic channels. This loss can be described by the semi-relativistic absorption potential [46]

$$W_{abs}(r) \equiv \sqrt{\frac{2(E_L + m_e c^2)^2}{m_e c^2 (E_L + 2m_e c^2)}} \times A_{abs} \frac{\hbar}{2} [\nu_L \rho_e(r) \sigma_{bc}(E_L, \rho_e, \epsilon_1)]. \quad (13)$$

Here, m_e is the mass of the electron, ν_L is the local velocity of the projectile electron with which it interacts with the bound electrons. It appears as if it were moving within a homogeneous electrons gas of density $\rho_e(r)$ with $\nu_L = \sqrt{2E_L/m_e}$ corresponding to the local kinetic energy $E_L(r) = E - V_{st}(r) - V_{ex}(r)$. The quantity $\sigma_{bc}(E_L, \rho_e, \epsilon_1)$ is the cross section for collisions involving energy transfer greater than the first excitation energy ϵ_1 of the target molecule [37]. The expression (13) are based on some approximations. This semi-relativistic correction is not very significant for light atom like nitrogen. In the present calculations, the value of the empirical parameter A_{abs} is taken as 2.7 for electron and 2 for positron to fit the corresponding experimental data. A_{abs} is an adjustable parameter and its value depends on the projectile-target combination.

2.2. Partial wave analysis

The scattering of electrons and positrons by a central field $V(r)$ is completely described by the direct and spin flip scattering amplitudes, given by [47,48]

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \{(\ell + 1) [\exp(2i\delta_{\kappa=-\ell-1}) - 1] + \ell [\exp(2i\delta_{\kappa=\ell}) - 1]\} P_{\ell}(\cos\theta) \quad (14)$$

and

$$g(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} [\exp(2i\delta_{\kappa=\ell}) - \exp(2i\delta_{\kappa=-\ell-1})] \times P_{\ell}^1(\cos\theta), \quad (15)$$

respectively. Here, k is the relativistic wave number of the projectile which is related to the kinetic energy E_i by

$$(c\hbar k)^2 = E_i(E_i + 2m_e c^2). \quad (16)$$

$P_{\ell}(\cos\theta)$ and $P_{\ell}^1(\cos\theta)$ are the Legendre polynomials and associated Legendre functions, respectively. κ is relativistic quantum number defined as $\kappa = (\ell - j)(2j + 1)$,

where j and ℓ are the total and orbital angular momentum quantum numbers that are both determined by the value of κ as $j = |\kappa| - 1/2$, $\ell = j + \kappa/(2|\kappa|)$. The radial parts of the large and small components of the scattering wave function, $P_{E\kappa}(r)$ and $Q_{E\kappa}(r)$, respectively, satisfy the following set of coupled differential Equations [49]

$$\frac{dP_{E\kappa}}{dr} = -\frac{\kappa}{r}P_{E\kappa}(r) + \frac{E_i - V + 2m_e c^2}{c\hbar}Q_{E\kappa}(r) \quad (17)$$

and

$$\frac{dQ_{E\kappa}}{dr} = -\frac{E_i - V}{c\hbar}P_{E\kappa}(r) + \frac{\kappa}{r}Q_{E\kappa}(r). \quad (18)$$

Various scattering cross sections are determined from the asymptotic form of the large component $P_{E\kappa}(r)$ of the scattering wave function which can be expressed in terms of the complex phase-shift δ_κ as

$$P_{E\kappa}(r) \simeq \sin\left(kr - \ell\frac{\pi}{2} + \delta_\kappa\right). \quad (19)$$

Here, k is the wave number of the electron. Equations (17) and (18) satisfying the asymptotic condition (19) are solved numerically using the subroutine package RADIAL [50]. Once the phase shifts and the scattering amplitudes for the constituent atoms are determined, the corresponding projectile-atom DCS is obtained as

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2. \quad (20)$$

The total integrated elastic σ_{el} , the momentum transfer σ_m and viscosity σ_v cross sections for the projectile-atom scattering are expressed in terms of the scattering amplitudes $f(\theta)$ and $g(\theta)$ as

$$\sigma_{el} = \int \frac{d\sigma}{d\Omega} d\Omega = 2\pi \int_0^\pi (|f(\theta)|^2 + |g(\theta)|^2) \sin(\theta) d\theta, \quad (21)$$

$$\sigma_m = 2\pi \int_0^\pi (1 - \cos\theta)(|f(\theta)|^2 + |g(\theta)|^2) \sin(\theta) d\theta, \quad (22)$$

$$\sigma_v = 3\pi \int_0^\pi [1 - (\cos\theta)^2](|f(\theta)|^2 + |g(\theta)|^2) \sin(\theta) d\theta. \quad (23)$$

The corresponding lepton-atom total cross section (TCS) σ_{tot} , sum of the total elastic (σ_{el}) and absorption cross section (σ_{inel}), is obtained by the following relation:

$$\sigma_{tot} = \frac{4\pi}{k} \text{Im}f(0), \quad (24)$$

where Im denotes the imaginary part of the expression that follows and $f(0)$ stands for the scattering amplitude in the forward direction.

The molecular cross sections are obtained using the AR method by simply adding the cross sections of the individual atoms that make up the molecule

$$\sigma = \sum_i^2 \sigma_i, \quad (25)$$

where σ_i s stand for DCS, integrated elastic, momentum transfer, viscosity and total cross sections.

In the independent atom approximation (IAM), the direct and spin flip scattering amplitudes to describe the scattering from a molecule with a given orientation are given by [48]

$$F(\theta) = \sum_i \exp(i\mathbf{q}\cdot\mathbf{r}_i) f_i(\theta) \\ \text{and} \\ G(\theta) = \sum_i \exp(i\mathbf{q}\cdot\mathbf{r}_i) g_i(\theta), \quad (26)$$

where $\hbar\mathbf{q}$ is the momentum transfer, $\mathbf{r}_i$ is the position vector of the nucleus of the i th atom, relative to an arbitrary origin. The corresponding DCS is obtained by averaging the orientations of all the randomly oriented molecules as

$$\frac{d\sigma}{d\Omega} = \langle |F(\theta)|^2 + |G(\theta)|^2 \rangle \\ = \sum_{ij} \frac{\sin(qr_{ij})}{qr_{ij}} [f_i(\theta)f_j^*(\theta) + g_i(\theta)g_j^*(\theta)]. \quad (27)$$

Total inelastic cross section σ_{inel} and Ionisation cross section σ_{ion} satisfy the following relation:

$$\sigma_{inel} \geq \sigma_{ion} \quad (28)$$

as the former itself is partitioned into excitation and ionisation cross section. σ_{ion} can be calculated from the following energy dependent ratio as is done in [51,52]:

$$R(E_i) = \frac{\sigma_{ion}(E_i)}{\sigma_{inel}(E_i)}. \quad (29)$$

The ratio $R(E_i)$ is a continuous function of energy. For $E_i > I$ (ionisation potential), this function is fitted to the equation

$$R(E_i) = 1 - A \left[\frac{B}{U + C} + \frac{\ln U}{U} \right], \quad (30)$$

where $U = E_i/I$ is the reduced energy. The adjustable parameters A , B and C are determined using the following conditions:

$$R(E_i) = \begin{cases} 0 & \text{for } E_i \leq I, \\ R_p & \text{for } E_i = E_p, \\ R_F & \text{for } E_i \geq E_F > E_p. \end{cases} \quad (31)$$

First of the above three expressions in (31) suggests that no ionisation takes place below the ionisation threshold, the ionisation potential of the atom. Here, R_p is the

value of R at $E_i = E_p$ with E_p being the incident energy at which the maximum absorption occurs. The present study observes the maximum absorption at $E_p = 60$ eV

Figure 1. DCS (a_0^2/Sr) for the elastic scattering of electrons from nitrogen at energies 15, 20, 30, 40, 50 and 60 eV. Theoretical: Present Work, Additivity Rule; IAM, Independent Atom Approximation; WE, Additivity Rule Without Exchange; Lee and Iga [29], Maynard *et al.* [30], Jain *et al.* [3] and Wedde and Strand [33]. Experimental: Shyn and Carignan [9], Srivastava *et al.* [10], Nickel *et al.* [14] and DuBois and Rudd [11].

for electron scattering and at $E_p = 25$ eV for positron scattering. In line with the discussion in references [51–53], we choose the values $R_p = 0.65$ for electron and $R_p = 0.85$ for positron. At impact energies $E_i \geq E_F$, well beyond the peak position E_p , the value of R increases to R_F (very close to 1). However, it has been observed that maximum ionisation ($R(E_i) = 1$) does not occur even at high energies. This implies that $R(E_i)$ should be less than one. Here, we choose $R_F \approx 0.8$ at $E_F = 200$ eV for

electron and $R_F \approx 0.85$ at $E_F = 300$ eV positron scattering to get the optimum fit to the available experimental data. The values of the parameter parameter A , B and C are obtained from the numerical solution of the three non-linear equations (31) using a FORTRAN program. The values of the parameters A , B and C are, respectively, found to be -1.172 , -7.714 and 8.037 for electron scattering; -2.447 , -8.274 and 19.245 for positron scattering.

Figure 2. DCS for the same as in Figure 1 at energies 70, 75, 100, 150, 200 and 250 eV. Theoretical: References in Figure 1 and Blanco and Garcia [32]. Experimental: References in Figure 1 and Jansen *et al.* [12] and Shyn *et al.* [54].

3. Results and discussions

In this paper, the ELSEPA code [46] is used to calculate the scattering cross sections of electrons and positrons by nitrogen molecule. DCSs for electron scattering calculated over a wide range of energy (15 eV–10 keV) are compared with the experimental data [9–12] and the theoretical calculations [3,29,30,32]. DCSs for positron scattering are calculated over the energy range 10 eV–10 keV.

TCSs, VICs, IECs, INCs, MTCs and TICSs for both electron and positron scattering are calculated over the energy range 1 eV–10 keV.

In Figure 1(a–f), we present our DCS calculations at energies 15, 20, 30, 40, 50 and 60 eV. At energies 15 and 20 eV, our results show noticeable disagreement with the experiments [9–11,14], but agree with the number of minima with a shift in position. This result indicates that the AR rule does not work well at these low energies due

Figure 3. DCS for the same as in Figure 1 at energies 300, 350, 400, 500, 600 and 750 eV. Theoretical: References in Figure 2 and Lee and Iga [29]. Experimental: References in Figure 2 and Bromberg [13].

to the structure effect of the molecule. At 15 eV, the variation of DCS is shown with and without exchange (WE). It is seen that the inclusion of exchange decreases the cross section at lower angles and raises the deep of DCS. Our DCS calculations at 30 eV show a fair agreement with the experimental data of Shyn and Carignan [9], Srivastava [10] and Nickel *et al.* [14]. Our model produces a deep minimum at $\sim 100^\circ$ while the measured minimum is witnessed at $\sim 95^\circ$. Calculations of Maynard *et al.* produced a less deeper minimum, but shifted towards higher angles by $\sim 35^\circ$. Moreover, their calculations failed to

reproduce higher angle DCS data. At 40 eV, our model shows reasonable agreement with the experimental data [9,10,14] except at the minimum. This might be due to the deformation of the molecule causing the higher density of charges near the nuclei and lesser charges in the outer region, thereby lessening of DCS value at the minimum formed due to interference of waves from the bound electrons. At energy 50 eV, our calculations and those of Jain *et al.* [3] show quite reasonable agreement with the experimental data [9–11,14] and appear competitive to those of Maynard *et al.* [30]. The curve for 50 eV

Figure 4. DCS for the same as in Figure 1 at energies 800, 900, 1000, 2000, 3000, 5000, 7000 and 1000 eV. References: Available in Figure 3.

shows the increase of DCS almost over the whole angular domain with the inclusion of the exchange term. At 60 eV, our calculations show good agreement with the experimental observations [10,14] with slight underestimation at higher angles.

In Figure 2(a–f), we present our DCS calculations for electron scattering at 70, 75, 90, 100, 150 and 200 eV and compare with the experimental data [9–12,14] and theoretical calculations [3,30,32,33]. Our calculations show quite good agreement with the experimental

measurements. However, our results at the energy 75 eV disagree with those of Maynard *et al.* [30] at higher angles. DCS at 150 eV shows a slight increase of cross section values over those obtained without the exchange term. In Figures 3 and 4, we compare our results with the available measurements [9,11–13] and theoretical calculations [3,29,32]. We see the very close agreement of our DCS results with the experimental and other theoretical data. Beyond 200 eV, no extremum is observed, signifying that no destructive interference of

Figure 5. DCS for the elastic scattering of positrons from nitrogen at (a) 10, 20 and 30 eV, (b) 40, 60 and 80 eV, (c) 100, 300 and 500 eV, (d) 700, 900 and 1000 eV, (e) 2000, 3000 and 5000 eV and (f) 7000, 9000 and 10000 eV.

Figure 6. Variation of DCS with energy for the scattering of electrons from nitrogen.

Figure 7. Variation of DCS with energy for the scattering of positrons from nitrogen.

waves emitted from the bound electrons occurs due to the increased number angular momentum waves. At and beyond 350 eV, the exchange effect is almost negligible. This study reveals that the exchange effect decreases with the increase of energy, signifying that the latter effect depends upon the interaction time. At energies 15, 60, 70, 250, 500, 600, 900 and 3000 eV, we calculate the DCSs in the framework of ‘Independent Atom Approximation’ (IAM) [46,55,56] including the interference terms and compare with results obtained from the AR model. The comparison shows that both the results are comparable to one another with the observation that, at some energies, IAM performs better, and at other energies, poorer than the AR model. As the calculation using IAM requires

more parameters than the AR model, but the overall outputs are almost the same, we prefer the easy-to-use AR model. Although no experimental data for the DCS of $e^+ - N_2$ elastic scattering is found in literature, the performance of our DCS results for electron scattering encourages us to calculate DCS for $e^+ - N_2$ (Figure 5) for prospective researchers to compare with and to examine the points of differences in the scatterings of the above two projectiles differing in the sign of charge. In Figures 6 and 7, we present the energy variation of DCS for electron and positron, respectively. Monotonic behaviour is observed in DCS at high energies, which might be due to the short interaction time of the projectile.

In Figure 8, we depict TCS, VICS, IECS, INCS, MTCS and TICS for the scattering of the electron from nitrogen molecule. In Figure 8(a), our calculated TCSs show quite good agreement with the experimental data [4,15–18,21] at energies above 10 eV. Below 10 eV, our calculations and those of Blanco and Garcia [32] and Jain *et al.* [31] over-estimated TCSs. Calculations of Phelps and Pitchford [34] showed good agreement with the experimental data. The significant disagreements of the above theoretical calculations with the experimental data are due to the neglect of multicentre scattering and valence-bond effect in the AR. Moreover, close-packed molecules are not fully transparent to electrons and positrons for low energy owing to large de Broglie wavelength compared to the bond length. Inner atoms of the molecule are screened by the outer atoms which do not contribute to the scattering, thereby causing the lessening of the cross-section. In Figures 8(b, c), we present IECS and MTCS, respectively, along with the experimental data [4,9–12,22,34] and theoretical calculations [29,31,32]. In both cases, our calculations show good agreement with the experimental observations above 10 eV. The slight disagreement between the theories and experiments stems from the structure effect as mentioned earlier. A good agreement of the AR rule with the experiments is due to the fact that the de Broglie wavelength of an incident of projectile gradually decreases with the increase of energy compared to the bond length of the molecule. So the valence-bond and screening effects accordingly become less upon the scattering observables. This fact lies at the root of the good functioning of AR Rule and optical model. In Figure 8(d), we present VICS for future reference. We compare our INCS calculations (Figure 8(e)) with the inelastic data obtained from the subtraction of IECS data [12] from the TCS data [15,21,32] of corresponding energies and we find good agreement. We also compare our INCS results with the calculations of Jain and Baluja [31]. Both calculations agree with each other above ~ 100 eV, but below this range they agree in the pattern but differ in magnitudes by up to $\sim 58\%$. In Figure 8(f), we

present TICSs for electron scattering and compare with the experimental observations of [23–26] and theoretical calculations of Phelps and Pitchford [34]. We see a reasonable agreement of our calculations with one or another set of experimental data beyond the peak region, but noticeable disagreement is found at lower energies. Our calculations overestimated the TICSs below 100 eV and produce maximum at ~ 80 eV in contrast to the experimental maximum at ~ 100 eV. The predictions of Phelps and Pitchford [34] show good agreement with the

experimental data. This result indicates that the present easy-to-implement method does not work well at low energies for the production of TICS. So the shape resonance cannot be explained by this procedure. The shape resonance can be explained in the frame works of R-matrix, and multi-channel formalism.

In Figure 9(a–f), we present TCS, VICS, IECS, INCS, MTCS and TICS for the scattering of the positron from N_2 . We see quite good agreement between our calculations of TCSs and the experimental data [19–21].

Figure 8. (a) TCS, (b) VICS, (c) IECS, (d) INCS, (e) MTCS and (f) TICS for the scattering of electrons from nitrogen. Theoretical: [29,31,32]. Experimental: [4,9–12,15–18,21–26].

Figure 9. (a) TCS, (b) VICS, (c) IECS, (d) INCS, (e) MTCS and (f) TICS for the scattering of positrons from nitrogen. Theoretical: [6,31,35,36]. Experimental: [19–21,27,28].

Our calculations perform better than the calculations of Sun *et al.* [6] and Jain and Baluja [31] between ~ 10 and 100 eV. Kothari and Joshipura [35] underestimated TCSs by approximately 70%. No experimental data are available in the literature for IECS, MTCS, VICS and INCS for positron scattering. We calculate these observables for future researchers to compare with. Our calculations disagree with the calculations of Kothari and Joshipura [35] and Gillespie and Thompson

[36]. MTCS calculations also show similar disagreement between the calculations of ours and Kothari and Joshipura [35]. In Figure 9(f), we compare our TICS calculations with the experimental data [27,28] and the theoretical calculations [35]. Our results show a reasonable agreement with the data of Marler and Surko [28]. Two data sets show noticeable differences with one another and our calculations in and around the peak region.

4. Conclusion

This work used the easy-to-use AR approach to describe the scattering of electron and positron from nitrogen molecule. Individual projectile-atom cross sections are calculated by OPM method using the free density of the atom and then the additivity rule is used to calculate the molecular cross sections for electron and positron scattering from nitrogen molecule. The results are compared with the available experimental data and other theoretical calculations. Our calculations agree quite reasonably with the experimental data in intermediate and high energies and show a mix of agreements and disagreements with other calculations. Our results show monotonic behaviour with the increase of energy. The monotonic pattern in DCS starts at much lower energy for positron scattering than for electron scattering. The monotonic behaviour of DCSs at high energies might be due to the contributions of the scattered waves of the greater number of angular momentum states causing incoherent interference and absence of resonances at high energies. This work also reveals that positron-target interaction is weaker than the electron-target interaction, leading to the lesser values of the scattering observables in positron scattering than those in the electron scattering. It is also apparent that the exchange term in the optical potential does play a role at low and intermediate energies. This exchange effect decreases with the increase of energy and becomes negligible at high energy, i.e. decrease of interaction time. The discrepancies of our results with the available experimental data at low energies is due to the molecular structure effect, not adequately included in our AR method. Finally, it is concluded that the values of different cross sections obtained by the use of the AR approach are in reasonable agreement with the available experimental data. Hence, without involving molecular symmetry, a fairly simple additivity approach may provide a satisfactory description of projectile-diatomic molecular scattering. Applicability of this theoretical approach to other molecules should be explored to provide a rigid theoretical validity.

Disclosure statement

No potential conflict of interest was reported by the authors.

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