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Differential, elastic integral and moment transfer cross sections for electron scattering from N_2 at intermediate- and high-energies*

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A complex optical model potential modified by incorporating the concept of bonded atom, with the overlapping effect of electron clouds between two atoms in a molecule taken into consideration, is firstly employed to calculate the differential cross sections, elastic integral cross sections, and moment transfer cross sections for electron scattering from molecular nitrogen over the energy range 300–1000eV by using additivity rule model at Hartree–Fock level. The bonded-atom concept is used in the study of the complex optical model potential composed of static, exchange, correlation polarization and absorption contributions. The calculated quantitative molecular differential cross sections, elastic integral cross sections, and moment transfer cross sections are compared with the experimental and theoretical ones wherever available, and they are found to be in good agreement with each other. It is shown that the additivity rule model together with the complex optical model potential modified by incorporating the concept of bonded atom is completely suitable for the calculations of differential cross section, elastic integral cross section and moment transfer cross section over the intermediate- and high-energy ranges.

Keywords: electron scattering, additivity rule, differential cross section, elastic integral cross section, moment transfer cross section
PACC: 3410, 3440, 3480

1. Introduction

In recent years, there has been an increasing interest in the calculation of differential cross sections (DCSs), elastic integral cross sections (ICSs), and moment transfer cross sections (MTCSs) for electron scattering from molecules. The reason is twofold. Firstly, the availability of new DCS, ICS and MTCS measurements (especially at higher incident energies) enables a fairly detailed comparison between calculations and measurements. Secondly, DCS, ICS and MTCS are increasingly demanded, since these theories over the wide energy and angular ranges can be used in many fields, such as plasma-assisted material processing, laser, atmospheric science and aeronautical fields, etc.

However, it is well known that the problem of electron–molecule scattering is more complicated than that of the corresponding electron–atom scattering, which is due to the multicentre nature, the lack of symmetric centre (in the case of polyatomic and hetero-nuclear molecules) and its nuclear motion. Hence, for electron–molecule scattering, many different approaches have been proposed.[1−3] Here, over the intermediate- and high-energy ranges, almost all inelastic channels (rotational, vibrational, electronic excitation and ionization process, etc) are open, so it is difficult to obtain the wavefunction of a molecule. Thus, it is almost impossible to carry out the calculation of conventional close-coupling for electron–molecule scattering. It is therefore unsurprising that many previous calculations on the DCS, ICS and MTCS for electron–molecule scattering are limited to a low-energy region.

Recently, a fairly simple approach, namely the

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additivity rule (AR) model, where a molecular cross section is an incoherent sum of the cross sections of the constituent atoms, was employed successfully by Raj[4] to obtain the total cross section (the momentum transfer cross section, the elastic integral cross section) for electron scattering by a sample of four molecules (O_2, CO, CO_2 and CF_4) at 100–500eV. Lately, Joshipura and Patel[5] employed the AR model and the complex optical model potential to obtain the total cross section for electron scattering from molecules (O_2, N_2, CO and CO_2) at 100–1000eV. Very recently, considering two different shielding effects, Sun *et al*[6] also used the AR model and the complex optical model potential to calculate the total cross section for electron scattering from molecules (C_2H_2, C_2H_4, C_2H_6, and C_3H_8) at 10–2000eV. Though many other authors[2,4] gave the DCSs for electron scattering by molecules through the use of the AR model and complex optical model potential below 1000eV, there exist large differences between calculations and measurements.

In this paper, the complex optical model potential, which takes into account the overlapping effect of electron clouds between two atoms in a molecule, is firstly employed to calculate the DCSs, ICSs and MTCSs for electron scattering from the molecular nitrogen at intermediate and high energies. In the next section, we describe in detail the modified potential and the AR model. In Section 3, we present the calculations and discussion for the DCS, ICS and MTCS of the molecular nitrogen and compare them with the available measurements. Concluding remarks are made in Section 4. Atomic units are used throughout this paper unless otherwise specified.

2. Theory and method

With the AR model, the DCS, ICS and MTCS for a molecule containing N atoms averaged over all the orientations of the rotating molecule are given by

$$I(\theta) = \sum_{i=1}^{N} |f_i(\theta)|^2, \tag{1}$$

$$Q_{\rm I}(E) = 2\pi \int_0^{\pi} I(\theta) \sin\theta {\rm d}\theta, \tag{2}$$

$$Q_{\rm M}(E) = 2\pi \int_0^{\pi} I(\theta)(1-\cos\theta) \sin\theta {\rm d}\theta, \tag{3}$$

where $I(\theta)$ is the DCS for the molecule, θ is the scattering angle, $f_i(\theta)$ is the scattering amplitude of the ith atom constituting the molecule, $Q_{\rm I}(E)$ and $Q_{\rm M}(E)$ are ICS and MTCS of the molecule, respectively. From Eq.(1), we easily see that the atomic scattering amplitudes referred to a single centre are added incoherently. So, no molecular geometry is involved in the AR model of the DCS. Thus, a molecular scattering problem is reduced to an atomic problem which is easier to handle.

The scattering amplitude of the ith atom in terms of partial waves is given by

$$f_i(\theta) = \frac{1}{2{\rm i}k} \cdot \sum_l (2l+1)(S_l - 1) P_l(\cos\theta), \tag{4}$$

where S_l is the complex scattering matrix and can be obtained by solving the following radial equation:

$$\left(\frac{{\rm d}^2}{{\rm d}r^2} + k^2 - V_{\rm opt} - \frac{l(l+1)}{r^2} \right) u_l(r) = 0 \tag{5}$$

under the boundary condition ($r \sim \infty$)

$$u_l(kr) \sim kr[j_l(kr) - {\rm i}n_l(kr)] + S_l kr[j_l(kr) + {\rm i}n_l(kr)]. \tag{6}$$

Here j_l and n_l are spherical Bessel and Neumann functions, respectively. The limit l is taken to be large enough to make the higher partial-wave contributions until a convergence less than 0.5% is achieved again in the DCS, ICS and MTCS. $V_{\rm opt}$ is the appropriate complex optical potential which includes all the important physical effects.

In the present study, the $V_{\rm opt}$ of the atom in a molecule is given by

$$V_{\rm opt}(r) = V_{\rm s}(r) + V_{\rm p}(r) + V_{\rm e}(r) + {\rm i}V_{\rm a}(r). \tag{7}$$

The static potential $V_{\rm s}(r)$ for e–atom scattering is calculated by using the atomic charge density determined from the well-known Hartree–Fock atomic wavefunction.[7] The exchange potential $V_{\rm e}(r)$ provides a semiclassical energy-dependent form presented by Riley and Truhlar.[8] The polarization potential $V_{\rm p}(r)$ is given by our group,[9] which has a correct asymptotic form $-\alpha/2r^4$ at a large r. The absorption potential $V_\alpha(r)$ represents the combined effect of all the inelastic channels and is given by Staszewska *et al.*[10]

In the previous study, the AR model of the DCS did not consider the formation of the chemical bond and overlapping effect of electron clouds between two atoms in a molecule. So, the errors in calculations are large.

Here, we introduce the concept of bonded atom and take into consideration the overlapping effect of

electron clouds between two atoms. That is to say, the atom in molecules is different from the one in a free state. Thus, electron charge density $\rho(r)$ must be rewritten as the following form:

$$\rho'(r) = f \cdot \rho(r), \tag{8}$$

$$f = 1 - \frac{d}{R} \cdot \frac{Z}{N}, \tag{9}$$

where f is a structural factor, d and R are the bond length and the sum of the radii of the two atoms respectively, and Z and N are the electron number of the outmost shell and the total electron number of the atom, respectively. So, Eq.(7) can be rewritten as

$$V_{\rm opt}(r) = f \cdot V_{\rm s}(r) + V_{\rm p}(r) + V_{\rm e}(r) + {\rm i}f \cdot V_{\rm a}(r). \tag{10}$$

According to the concept of the bonded atom mentioned above, the DCSs for the same atoms in different molecules may be different, which is because the overlapping effect of the electron clouds for the same atoms in different molecules may be different.

The value of parameter R in molecular nitrogen is achieved by using the atomic charge density determined from the well known Hartree–Fock atomic wavefunction.[7]

3. Results and discussion

Employing the AR model along with the modified optical potential, we calculate the DCSs, ICSs and MTCSs of electrons scattering from molecular nitrogen at 300, 400, 500, 800 and 1000eV. Our results together with the available measurements[11–16] and other calculations[2] are shown in Figs.1–5 and Table 1.

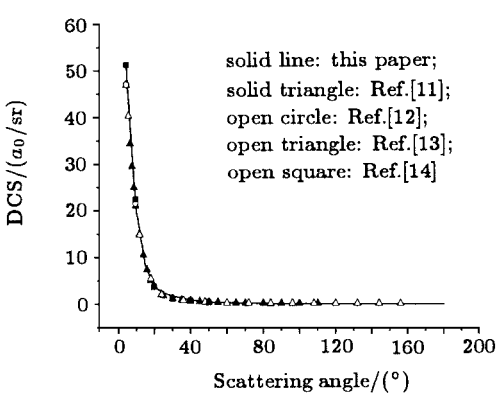


Fig.1. Differential cross sections for e–N_2 scattering at 300eV.

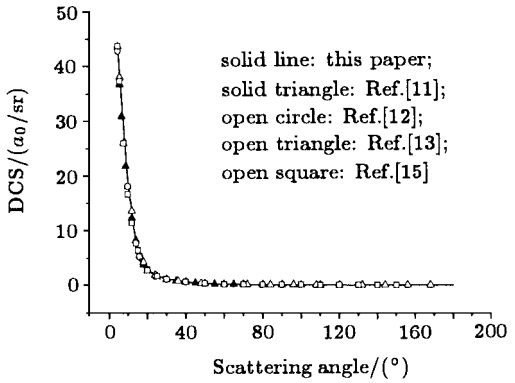


Fig.2. Differential cross sections for e–N_2 scattering at 400eV.

From Figs.1 and 2, we can easily see that the present DCS results are in good agreement with the available measurements,[11–15] and the largest discrepancy is about 15% at 300eV. These prove that the complex optical model potential modified by incorporating the concept of bonded atom is completely suitable for the DCS calculations.

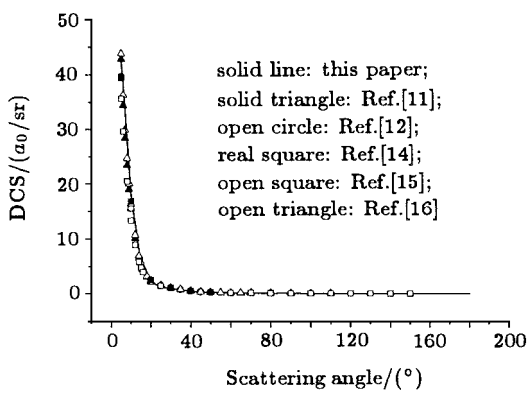


Fig.3. Differential cross sections for e–N_2 scattering at 500eV.

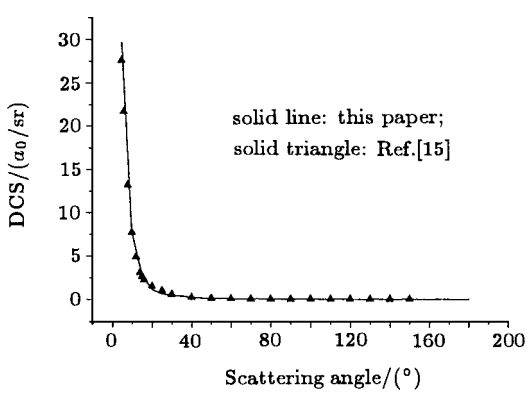


Fig.4. Differential cross sections for e–N_2 scattering at 800eV.

It may be noted that the present DCS results are higher than the measurements in Fig.1 and the discrepancies mainly exist at small angles from 15° to

30°, which may be attributed to the multiple scattering and the valence distortion which have been neglected in the present study. At lower incident energies, the de Brogile wavelength associated with the incident particle will become comparable to the internuclear distance which will increase the possibility of multiple scattering. It is expected that the inclusion of multiple scattering effects at lower energies will reduce the DCS values by a significant amount.[17] The likely effect of the valence bond distortion is also to reduce the DCS values at lower energies.[18] Further work to investigate the quantitative results of multiple scattering effects on DCS is under way.

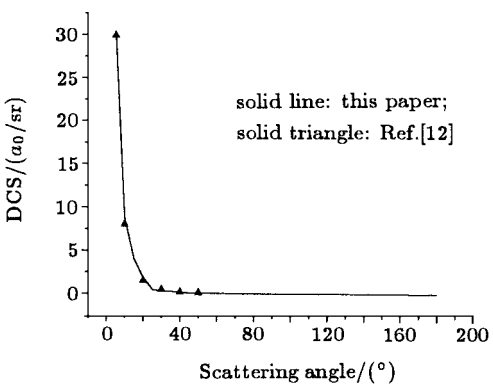


Fig.5. Differential cross sections for e–N_2 scattering at 1000eV.

From Figs.3–5, we also see that the present DCS results are in agreement with all the measurements[11,12,14–16] at all angles. These fully prove that the AR model together with the complex optical model potential modified by incorporating the concept of bonded atom is completely suitable for the DCS calculations of e–N_2 scattering, though we do not consider multiple scattering and valence distortion in the present study.

Table 1 shows that the present ICS results are slightly lower than the theoretical results obtained by Lee and Iga[2] at 300–800eV and accord well with them[2] as the incident electron energy increases. For example, at 300eV, the present ICS result is only about 7.6% lower than the calculations.[2] At 400eV, the present ICS result is only 1.2% higher than the measurement.[15] For MTCS results, the discrepancies between the present calculations and the theoretical results presented by Lee and Iga[2] or the measurements given by DuBois and Rudd[15] are within 7.0%. Thus, they are in good agreement with each other. Though there are no measurements about ICS and MTCS at 1000eV, from the good agreement between our calculations and the available measurements at 300, 400, 500, 700 and 800eV, we can deduce that our results at 1000eV must be reliable, too.

Obviously, the present results are shown to be in good agreement with the measurements[11–16] and other calculations[2] as shown in Figs.1–5 and Table 1 over the whole energy range. From the above calculations, we may consider this approach as a successful attempt at using the AR model to convert a molecular scattering problem into an atomic scattering problem which is easier to handle, in particular at higher energies. Though this method cannot provide very accurate calculations, the present results are comparable with the available measurements and calculations qualitatively. They can predict the outcome of experimental research, particularly for these molecules of which the wavefunctions are not available at present. We hope that the AR model can encourage more experimental work and theoretical calculations of DCS, ICS and MTCS over the intermediate and high energy range in the near future.

Table 1. ICSs and MTCSs for e-N_2 scattering.

source	energy					
	300	400	500	700	800	1000
ICS						
This paper	10.05	7.86	7.03	6.12	4.32	3.25
Ref.[2]	10.88	7.92	7.46	6.21	4.73	–
Ref.[15]	–	7.77	6.22	–	3.87	–
MTCS						
This paper	1.91	1.30	0.88	0.71	0.498	0.359
Ref.[2]	1.83	1.29	0.89	0.72	0.51	–
Ref.[13]	1.79	1.31	–	–	–	–

4. Conclusions

By using the AR model which ignores molecular geometry, a molecular scattering problem is reduced to an atomic scattering problem which is easier to handle. In this paper, we have employed the AR model and the modified optical potential to obtain quite encouraging results for the DCSs, ICSs and MTCSs of e–N_2 scattering system. As further research, we will employ the AR model and the modified optical potential to calculate more DCSs, ICSs and MTCSs for electrons scattered by molecules, so that we can check to what extent calculations and measurements are in agreement with each other.

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