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Total cross sections for electron scattering from CF_4, C_2F_4, C_2F_6, C_3F_8 in the energy range from 100 eV to 5000 eV

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Abstract. The additivity rule for electron scattering from molecule has been revised by considering the difference between the free atom and the corresponding bound atom in the molecule. The total cross sections for electron scattering from plasma etching molecules CF_4, C_2F_4, C_2F_6 and C_3F_8 have been calculated in the energy range from 100 eV to 5000 eV with the revised additivity rule. The present calculations are compared with the original additivity rule results and the existing experimental data. A better agreement between the present results and the experimental data is obtained.

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Key words: total cross section, electron scattering, the revised additivity rule.

1 Introduction

Accurate total cross sections for electron scattering from CF_4, C_2F_4, C_2F_6 and C_3F_8 for a wide electron energy range are required in many applied science and semiconductor plasma industry, because these molecules are indispensable in the plasma etching process [1,2]. These cross sections are needed in developing and detecting the models in theory for understanding the interaction process between the incident electrons and molecules over a wide energy rage [3]. To our knowledge, the total cross sections for these molecules are scarce especially above 2000 eV. For CF_4, five groups: Manero *et al* [4], Zecca *et al* [5], Sueoka *et al* [6], Szmytkowski *et al* [7], Ariyasinghe *et al* [3] have measured the total cross sections for electron scattering. For C_2F_4, Szmytkowski *et al.* measured the total cross sections below 370 eV [8]. Szmytkowski *et al.* measured the total cross sections for C_2F_6 below 250 eV [9]. Nishimura *et al.* [10] and Ariyasinghe *et al.* [3] measured the total

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cross sections for C_2F_6 below 3000 eV and 1500 eV, respectively. For C_3F_8, two groups, Nishimura *et al.* [10] and Tanaka *et al.* [11], measured the total cross sections below 3000 eV and 600 eV, respectively.

In theory, many approximation methods have been proposed and developed. Among them, the additivity rule is a relatively simple but effective one [12-14]. In the additivity rule method, the total cross section for a molecule is the sum of the total cross sections for the constituent atoms, so the molecular scattering is reduced to atomic scattering. It is successful for smaller molecules at high enough energies. However, for larger molecules, the additivity rule results are not encouraging. Considering the difference between the free atom and the corresponding bond atom in a molecule, the additivity rule method is revised. By the revised additivity rule method, the total cross sections for electron scattering from CF_4, C_2F_4, C_2F_6 and C_3F_8 for a wide electron energy range from 100 eV to 5000 eV are calculated and compared with the available experimental and theoretical data.

2 Theoretical model

In the original additivity rule model [13], molecule orbits can be described by the sum of the valence orbits of all atoms present in the molecule. As a result, the total cross section of electron-molecule scattering is written as the sum of the total cross sections of atoms. Thus the total cross section Q_T for molecule is given by

$$Q_T = \frac{4\pi}{k} Im f_M(\theta=0) = \frac{4\pi}{k} Im \sum_{j=1}^{N} f_j(\theta=0) = \sum_{j=1}^{N} q_T^j(E). \tag{1}$$

Where q_T^j and f_j are the total cross section due to the jth atom of the molecule and the complex scattering amplitude for constituent atoms of the molecule, respectively. The q_T^j of Eq. (1) for the jth atom is obtained by the method of partial waves:

$$q_T^j = \frac{\pi}{k^2} \sum_{l=0}^{l_{\max}} (2l+1)[\left|1-s_l^j\right|^2 + (1-\left|s_l^j\right|^2)]. \tag{2}$$

Where s_l^j is the lth complex scattering matrix element of the jth atom, which is related to the partial wave phase shift as $s_l^j = \exp(2i\delta_{lJ})$. The limit $l_{\max}$ is taken, which is enough to generate the higher partial-wave contributions until a convergence of less than 0.5% is achieved in the total cross section calculation. To obtain s_l^j we solve the following radial equation

$$(\frac{d^2}{dr^2} + k^2 - 2V_{opt} - \frac{l(l+1)}{r^2}) u_l(r) = 0. \tag{3}$$

Under the boundary condition

$$u_l(kr) \sim kr[j_l(kr) - in_l(kr)] + s_l kr[j_l(kr) + in_l(kr)]. \tag{4}$$

Where j_l and n_l are spherical Bessel and Neumann functions separately. The atom is replaced by the complex optical potential

$$V_{opt} = V_s(r) + V_e(r) + V_p(r) + iV_a(r). \tag{5}$$

It incorporates all the important physical effects. Presently the static potential $V_s(r)$ for electron-atom system is calculated from the well-known Hartree-Fock atomic wave functions [15]. Exchange potential $V_e(r)$ provides a semi-classical energy-dependent form of Riley *et al.* [16]. Zhang *et al.* [17] gives a smooth form at all r for polarization potential. The imaginary part of the optical potential $V_a(r)$ is the absorption potential, which represents approximately the combined effect of all the inelastic channels. The absorption potential of Jiang *et al.* [18] is adopted. The optical potential is dependent on the atomic charge density $\rho_0(r)$.

From the above equations, we can see that the original additivity rule model does not differentiate between the free atom and the bound atom in the molecule. Considering this, we present

$$\rho(r) = f \cdot \rho_0(r). \tag{6}$$

Here, $\rho(r)$ is the charge density of the bound atom in the molecule and $\rho(r)$ is the charge density of the corresponding free atom. f is a revised factor for a bound atom in the molecule which depends on the molecular structure.

$$f = 1 - \frac{R}{R+d}\frac{N-Z}{N}. \tag{7}$$

Where, d is the bond length between two bound atoms in the molecule and R is the sum of the radius of the corresponding two free atoms. Z is the number of electron in the atom and N is the sum of the number of electron of the two atoms which form the chemical bond.

3 Results and discussion

By use of the revised additivity rule considering the difference between the free atom and the bond atom in a molecule, the total cross sections for electron scattering from plasma etching molecules CF_4, C_2F_4, C_2F_6 and C_3F_8 have been calculated in the energy range from 100 eV to 5000 eV. The present results along with the available other data are compared shown in Figs. 1-4.

Fig. 1 shows the variations of the total cross sections for CF_4 at energies from 100 eV to 5000 eV. The present results are in good agreement with the experimental data in the whole energy range, while the original additivity rule results are much higher than the experimental data below 2000 eV. For example, the difference between the present result and the datum of Zecca *et al* is only 6.18%, while the difference between the original additivity rule result and the experimental datum of Zecca *et al.* [5] reaches 26.28% at 400 eV.

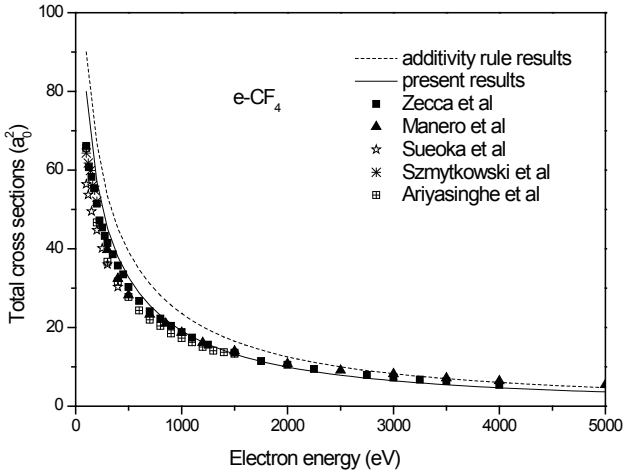

Figure 1: Total cross sections for electron scattering from CF_4. Solid line: present results, dash line: additivity rule results. Experimental data: Zecca *et al* [5], Manero *et al* [4], Sueoka *et al* [6], Szmytkowski *et al* [7], Ariyasinghe *et al* [3].

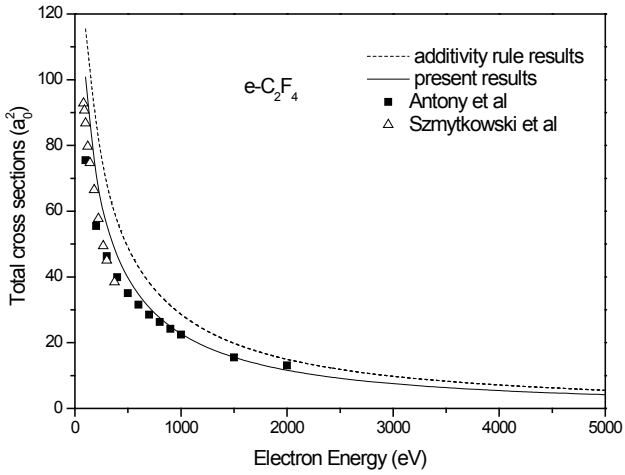

Figure 2: Total cross sections for electron scattering from C_2F_4. Solid line: present results, dash line: additivity rule results. Theoretical data: Antony *et al* [19]. Experimental data: Szmytkowski *et al* [8].

In Fig. 2, the present results for C_2F_4 are compared with the experimental data and the original additivity rule results. From Fig. 2, we can see that the present results are in better agreement with the available experimental data than the original additivity rule results. For example, the original additivity rule result deviates from the experimental data of Szmytkowski *et al* [8] by 49.18%, while the present result deviates only by 23.98% at 300 eV. Above 400 eV, there are no experimental data, so the present results are compared with the theoretical data of Antony *et al* [19]. The difference between the present results and the theoretical data is only 4.95%, while the difference for the original additivity rule results is 30.75% at 800 eV.

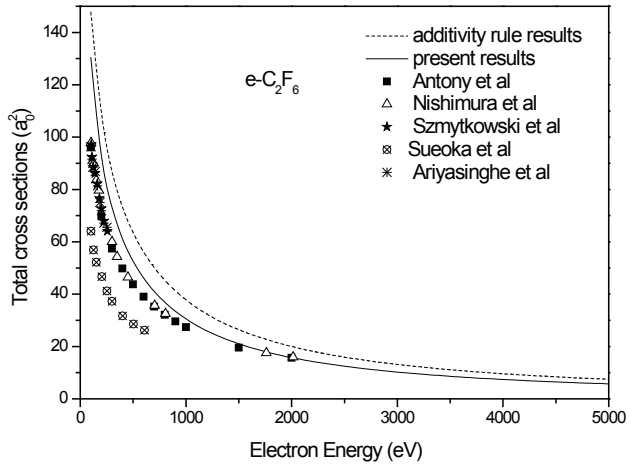

Figure 3: Total cross sections for electron scattering from C_2F_6. Solid line: present results, dash line: additivity rule results. Theoretical data: Antony *et al* [19]. Experimental data: Nishimura *et al* [10], Szmytkowski *et al* [9], Sueoka *et al* [20], Ariyasinghe *et al* [3].

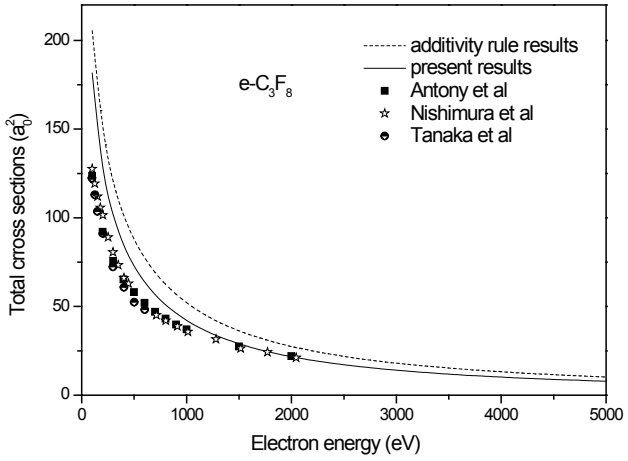

Figure 4: Total cross sections for electron scattering from C_3F_8. Solid line: present results, dash line: additivity rule results. Theoretical data: Antony *et al* [19]. Experimental data: Nishimura *et al* [10], Tanaka *et al* [11].

The present calculations are compared with the available experimental and theoretical data in Fig. 3 for C_2F_6. From Fig. 3, we can see that experimental and our theoretical curves resemble well each other. For example, the original additivity rule result deviates from the experimental datum of Nishimura *et al* [10] by 39.46%, while the present result only deviates by 13.51% at 800 eV. We also notice that the results of Sueoka *et al* [20] deviate much away from the other results.

Fig. 4 shows the total cross sections of the present calculations for C_3F_8 together with the experimental data of Nishimura *et al* [10] and Tanaka *et al* [11]. From Fig. 4, we can see that the present results give a better agreement with the experimental data than the original additivity rule results.

4 Conclusion

Considering the difference between the free atom and the bound atom in the molecule, the original additivity rule has been revised. With the revised additivity rule, the total cross sections for electron scattering from plasma etching molecules CF_4, C_2F_4, C_2F_6 and C_3F_8 have been calculated in the energy range from 100 eV to 5000 eV. The present results are compared with the available data and the original additivity rule results. From these comparisons, we can see that the revised additivity rule is more successful than the original additivity rule.

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