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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

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