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The evaluation and estimation of electron collision cross section set
電子衝突断面積セットの評価・推定

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The evaluation and estimation method of electron collision cross section set using “the electron swarm method” is introduced, and estimated electron collision cross section set of SiF_4 using the swarm method and electron transport coefficients form the cross section set are described. The cross section set consists of a momentum transfer, three kinds of electron attachment, a direct and eleven kinds of dissociative ionisation, four kinds of neutral dissociation, and four kinds of vibrational excitation cross sections. The values of calculated drift velocity and effective ionisation coefficient are in good agreement with measured data.

1. Introduction

Gas discharge plasma has a wide variety of applications, such as plasma process for semiconductor fabrication, new material invention, gas cleaning, medical application, etc., and to control the plasma as desired, detailed understanding of the plasma characteristics is essential. Plasma simulation provides us the precise behavior of species in the plasma, and the improvement of computer performance and the development of simulation technique have been done, so that the plasma simulation has attracted attention as useful tool to understand plasma characteristics.

In the plasma simulation, the continuity equations are often used for describing the behaviour of species with rate equations for chemical reactions. Thus, the accuracy and validity of the plasma simulation depend on those of parameters used in the equations, as well as those of modelling and simulation method. Electrons have the highest mobility and activity in the plasma, and those are responsible for the production of species in the plasma; therefore, the behaviour of the electrons needs to be described accurately for reliable plasma simulation. However, discharge parameters are not necessarily used with close examination. Further, the parameters are still calculated from electron collision cross section, which is the most fundamental data describing electron behaviour in gases, by two-term Boltzmann equation analysis, though the validity of the analysis is found to be limited.

In this work, the electron swarm method to evaluate and estimate collision cross sections for gases is mentioned, and then the results of evaluation and estimation of collision cross section set for SiF_4 are described.

2. Electron swarm method

Fig.1 shows the flow of electron swarm method. An initial set of cross sections is assembled using partial cross sections obtained by theoretical calculation, measurement, and also by estimation. Transport coefficients, such as drift velocity, ionisation coefficients, etc., are calculated from the initial set, those are compared with measured data, and then the initial set is modified. This procedure is repeated until calculated coefficients agree well with measured coefficients. To increase the accuracy and validity of estimated cross section set by this method, accurate calculation methods such as multi-term Boltzmann equation analysis and Monte Carlo simulation must be used, as well as the usage of accurately measured data.

Proper comparison between calculated and measured coefficients is another issue. Methods and definitions to measure the coefficients are not necessarily equal to those considered in the

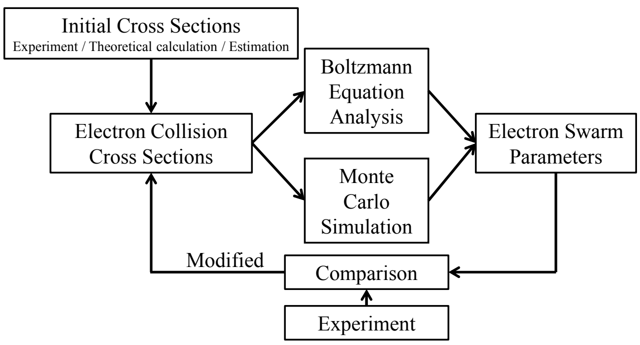

Fig. 1. Electron swarm method.

calculation methods mentioned above; therefore, correspondence between calculated and measured coefficients needs to be examined using refs. [1] and [2].

3. Calculation Method and Conditions

The behaviour of electrons is traced using Monte Carlo method in free space under a uniform electric field. Initial energy distribution of electrons is assumed to be the Maxwell-Boltzmann distribution with a mean energy of 1.0 eV, representing photoelectron emitted from a metal cathode. The collision between an electron and a gas molecule is only considered, and the collision between an electron and a fragment produced from gas molecules is not considered. The gas number density N sets $3.535 \times 10^{16}\ \mathrm{cm}^{-3}$ at 1 Torr and at 0 ℃. The definition of transport coefficients and sampling methods are shown in ref. [3].

4. Collision cross section set and transport coefficient of SiF_4

Figs. 2 (a) and (b) show the sets of electron collision cross sections for SiF_4, respectively reported by Nagpal *et al.*[3] and estimated here. Nagpal's set consists of a momentum transfer q_m, three kinds of vibrational excitation q_{vib}, an electron attachment q_a, two kinds of dissociation q_{nd} and an ionisation q_i cross section. Present set consists of q_m, three kinds of q_a, a direct and eleven kinds of dissociative q_i, four kinds of q_{nd} and four kinds of q_{vib}. Direct and dissociative ionisation cross sections are follow the measured data by Basner [5], and partial cross sections are SiF_3^+, SiF_2^+, SiF^+, Si^+, F^+, SiF_3^{2+}, SiF_2^{2+}, Si^{2+}, F^{2+} and Si^{3+}. The shapes of partial cross sections for q_a and q_{nd} follow those of Iga et al.[6] and Nakano *et al.*[7], but the magnitude of q_a and q_{nd} is multiplied by 1.5 and 7, respectively. For q_{vib}, four modes of vibration, namely, degeneracy bending (deformation) vibration υ_1, triple degeneracy bending vibration υ_2, symmetric stretching vibration υ_3 and triple degeneracy stretching vibration υ_4, are considered according to the results of beam measurement by Kato *et al.* [8]. Further, differential cross section (DCS) of q_{vib} suggests the presence of resonance structure around 7 eV, so that the shape of q_{vib} in the present set is estimated with considering resonance feature around 7 eV and values of cross sections at resonance, calculated by the integration of the DCS over scattering angle. The shape of q_m is estimated using measured data by Kato *et al.*[8].

Figs.3 (a) and (b) show effective ionisation coefficient and electron drift velocity as functions of E/N, together with those measured by pulsed experiment [9]. These transport coefficients calculated from the present cross section set agree excellently with measured coefficients in wide range of E/N. Particularly, the distinctive behaviour of drift velocity, namely, negative differential conductivity, appearing around 40 Td, can be presented by the calculated data from present cross section set. This leads the validity of estimated cross section set in this work.

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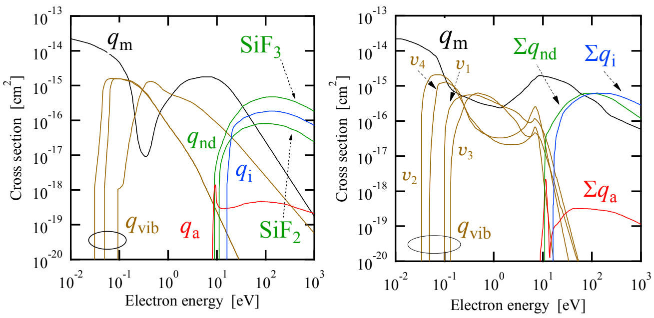
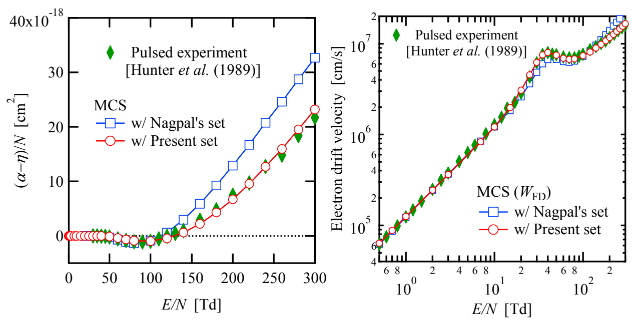


(a) (b)

Fig.2 Electron collision cross section sets of SiF_4. (a) Nagpal *et al.* and (b) present.



(a) (b)

Fig.3 (a) effective ionisation coefiicient and (b) electron drift velocities, as functions of E/N.