ELECTRON INTERACTIONS WITH SF_6

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ABSTRACT

We have comprehensively reviewed and critically assessed the state of knowledge on electron-interaction cross sections and electron-swarm parameters in SF_6. In this paper are presented our: (1) assessed data for the total electron scattering, elastic integral, elastic momentum, total ionization, and dissociative and nondissociative electron attachment cross sections; (2) deduced cross sections for the total vibrational excitation and total dissociation into neutrals; and (3) assessed data for the coefficients of electron-impact ionization, effective ionization, electron attachment, electron drift, and electron diffusion.

INTRODUCTION

The data presented in this paper are based on a comprehensive work we have conducted on electron interactions with SF_6 [1]. This work is part of our program to review, critically assess, and recommend data on electron collisions with plasma processing gases. The procedure that has been followed for assessing and recommending or suggesting the data in this paper is the same as in the previous papers in this series [2-4]. Only the assessed values of the cross sections and transport coefficients are presented in this paper. The complete sets of data, their origins, and their assessment are given in Ref. [1].

It is hoped that the abbreviated data presented here and the extended data and their discussion in Ref. [1] are useful in the modeling of gas discharges and plasma reactors employing the SF_6 gas.

ASSESSED CROSS SECTIONS

In Fig. 1 are shown the assessed total electron scattering cross section [$\sigma_{sc,t}$ (ε)], elastic integral electron scattering cross section [$\sigma_{e,int}$ (ε)],

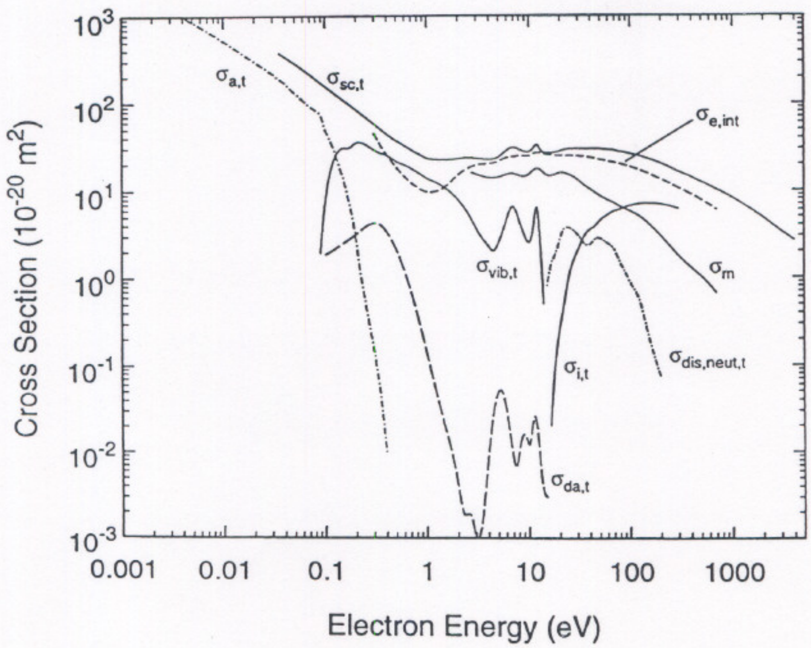

Fig. 1. Recommended or suggested values for the cross sections $\sigma_{sc,t}$ (ε), $\sigma_{e,int}$ (ε), σ_m (ε), $\sigma_{i,t}$ (ε), $\sigma_{a,t}$ (ε), and $\sigma_{da,t}$ (ε) for SF_6, and the deduced cross sections $\sigma_{vib,t}$ (ε) and $\sigma_{dis,neut,t}$ (ε).

momentum transfer (elastic) electron scattering cross section [$\sigma_m(\varepsilon)$], total ionization cross section [$\sigma_{i,t}(\varepsilon)$], electron attachment cross section for the formation of SF_6^- [$\sigma_{a,t}(\varepsilon)$], and total dissociative electron attachment cross section [$\sigma_{da,t}(\varepsilon)$]. The last cross section has been determined by summing the assessed cross sections for the major fragment negative ions formed by dissociative electron attachment to SF_6, namely those for SF_5^-, SF_4^-, SF_3^-, SF_2^-, F_2^-, and F^- shown in Fig. 2.

DEDUCED CROSS SECTIONS

Presently, there are no absolute data on the total cross section, $\sigma_{vib,t}(\varepsilon)$, for electron-impact vibrational excitation of the SF_6 molecule, or the total cross section, $\sigma_{dis,neut,t}(\varepsilon)$, for electron-impact dissociation of SF_6 into neutral fragments. In the absence of direct measurements of the cross sections for these two important processes, we used the assessed cross sections in Fig. 1 and deduced values for these two cross sections which as shown in Fig. 3.

The cross sections $\sigma_{vib,t}(\varepsilon)$ and $\sigma_{dis,neut,t}(\varepsilon)$ have been determined as follows: We began by estimating the total vibrational excitation cross section, $\sigma_{vib,t}(\varepsilon)$, below 1 eV from vibrational energy-loss measurements made by Randell *et al.* [5] and by Rohr [6,7] using a crossed-beam apparatus. In particular, Randell *et al.* measured the relative total elastic electron scattering cross section, $\sigma_{e,t}(\varepsilon)$ and the relative cross section for vibrational excitation of υ_1, υ_3, $2\upsilon_1$, and $\upsilon_1 + \upsilon_3$ using 0.05 eV to 1 eV incident-energy electrons and at a fixed scattering angle of 90°. In addition, the vibrational energy-loss measurements of both Randell *et al.* [5] and Rohr [6] showed that the major contribution to the vibrational excitation of SF_6 by electron impact below ~ 3 eV comes from υ_1 (indirect excitation via the SF_6^{-*} resonances) and υ_3 (direct excitation via the dipole interaction) vibrations and their combinational excitations. In view of these findings, we have added the relative vibrational excitation cross sections of Randell *et al.* for υ_1, υ_3, $2\upsilon_1$, and $\upsilon_1 + \upsilon_3$ and considered their sum to represent the total vibrational excitation cross section, $\sigma_{vib,t}(\varepsilon)$, relative to their total elastic electron scattering cross section. We, then, normalized the relative total elastic electron scattering cross section of Randell *et al.* at 1 eV to the value of $\sigma_{e,int}(\varepsilon)$ given by Rohr [7] for this energy, and thus put $\sigma_{vib,t}(\varepsilon)$ on an absolute scale. The values of $\sigma_{vib,t}(\varepsilon)$ determined this way are shown in Fig. 3a by the closed circles.

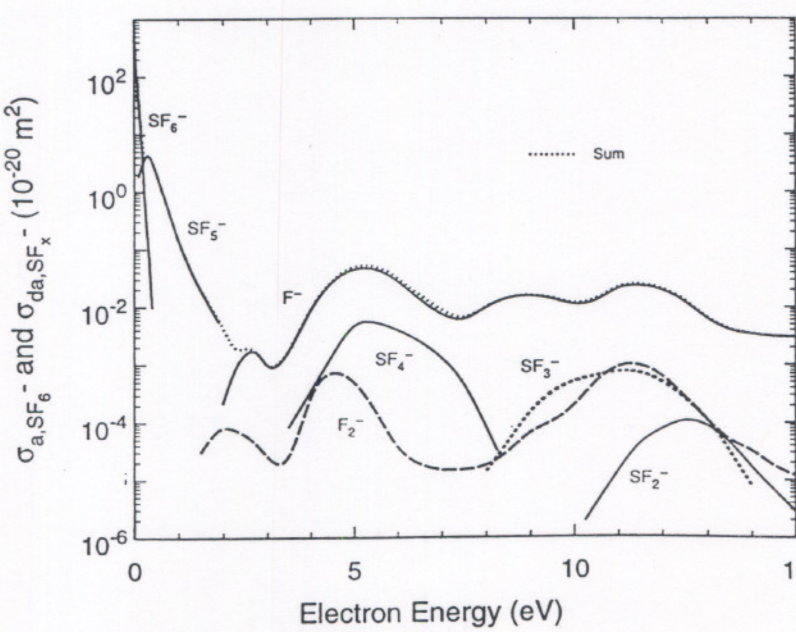

Fig. 2. Cross sections for the formation of SF_6^-, and the fragment anions SF_5^-, SF_4^-, SF_3^-, SF_2^-, F_2^-, and F^-. The sum of the cross sections for all negative ion fragments is indicated in the figure by the dotted line and represents the total dissociative electron attachment cross section $\sigma_{da,t}(\varepsilon)$.

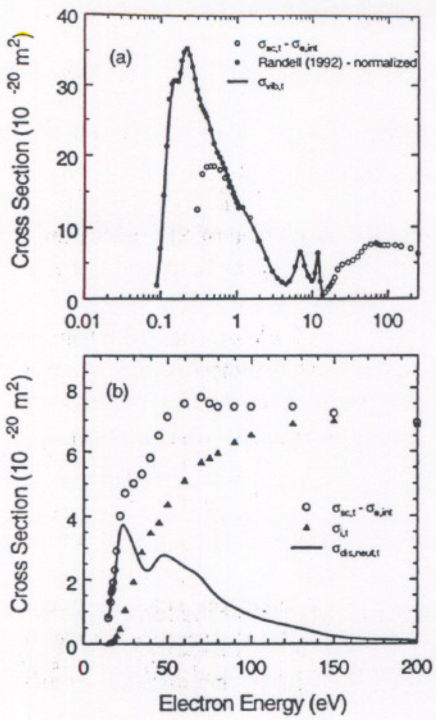

Fig. 3. (a) Deduced total vibrational excitation cross section, $\sigma_{vib,t}$ (ε), for SF_6: (•) Randell *et al.* [5] normalized as discussed in text; (∘) difference, $\sigma_{sc,t}$ (ε) - $\sigma_{e,int}$ (ε), of the recommended values for $\sigma_{sc,t}$ (ε) and $\sigma_{e,int}$ (ε); (—) suggested values of $\sigma_{vib,t}$ (ε). (b) Deduced cross section, $\sigma_{dis,neut,t}$ (ε), for the total dissociation of SF_6 into neutrals: (∘) $\sigma_{sc,t}$ (ε) - $\sigma_{e,int}$ (ε); (▴) $\sigma_{i,t}$ (ε); (—) $\sigma_{dis,neut,t}(\varepsilon) = [\sigma_{sc,t}(\varepsilon) - \sigma_{e,int}(\varepsilon)] - \sigma_{i,t}(\varepsilon)$.

Confirmation of these deduced values of $\sigma_{vib,t}$ (ε) and extension to higher electron energies has been accomplished by observing that at energies above ~ 1 eV – where the total electron attachment cross section of SF_6 is very much smaller than the total electron scattering cross section (Fig. 1) – and below the region of significant electronic excitation, the cross section $\sigma_{vib,t}$ (ε) ia given by the difference $\sigma_{sc,t}$ (ε) - $\sigma_{e,int}$ (ε), *viz.*,

$$\begin{aligned}\sigma_{vib,t}(\varepsilon) &= \sigma_{sc,t}(\varepsilon) - \sigma_{e,int}(\varepsilon) - \sigma_{a,t}(\varepsilon)\\ &\approx \sigma_{sc,t}(\varepsilon) - \sigma_{e,int}(\varepsilon).\end{aligned}$$

Using the assessed values of $\sigma_{sc,t}$ (ε) and $\sigma_{e,int}$ (ε) determined in this work (Fig. 1), we obtained the difference $\sigma_{sc,t}$ (ε) - $\sigma_{e,int}$ (ε) which is shown in Fig. 3a by the open circles. It is encouraging to see the agreement of the two determinations of $\sigma_{vib,t}$ (ε) in the energy range from ~0.5 eV to 1 eV. However, the two sets of values differ at energies below ~0.5 eV, indicating possible errors in the various cross sections employed at these energies. Nonetheless, in the absence of direct measurements of $\sigma_{vib,t}$ (ε), we take the difference $\sigma_{sc,t}$ (ε) - $\sigma_{e,int}$ (ε) to be a measure of $\sigma_{vib,t}$ (ε) between ~0. 5 eV and ~15 eV. The solid line in Fig. 3a represents our currently suggested values for the total vibrational cross section, $\sigma_{vib,t}$ (ε), for SF_6 using our deduced cross sections as just described.

Above about 20 eV where $\sigma_{vib,t}$ (ε) is small, the difference $\sigma_{sc,t}$ (ε) - $\sigma_{e,int}$ (ε) can be used to deduce a value for the total cross section, $\sigma_{dis,neut,t}$ (ε), for electron-impact dissociation of SF_6 into neutral fragments, namely via the relation

$$\sigma_{dis,neut,t}(\varepsilon) = [\sigma_{sc,t}(\varepsilon) - \sigma_{e,int}(\varepsilon)] - \sigma_{i,t}(\varepsilon).$$

The quantities $\sigma_{sc,t}$ (ε), $\sigma_{e,int}$ (ε), and $\sigma_{i,t}$ (ε) (our recommended cross section for the total ionization cross section shown in Fig. 1), along with their difference, $\sigma_{dis,neut,t}$ (ε), are shown in Fig. 3b.

ASSESSED COEFFICIENTS

Assessed values of the density-reduced electron-impact ionization coefficient [α/N (E/N)], density-

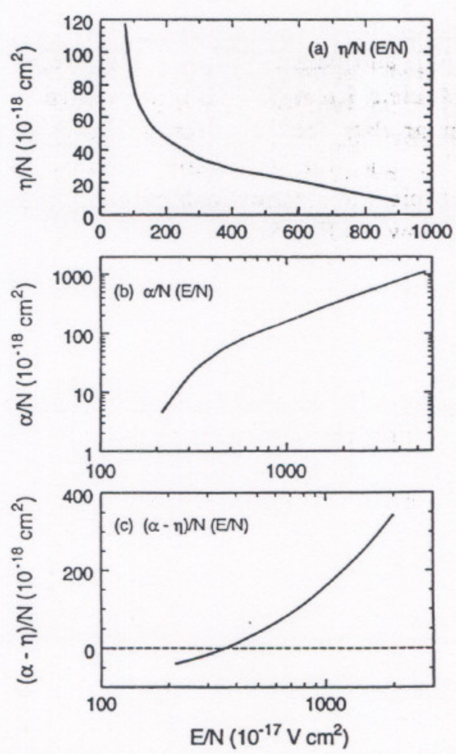

Fig. 4. Recommended or suggested values of the coefficients η/N (E/N), α/N (E/N), and $(\alpha-\eta)/N$ (E/N) for SF_6.

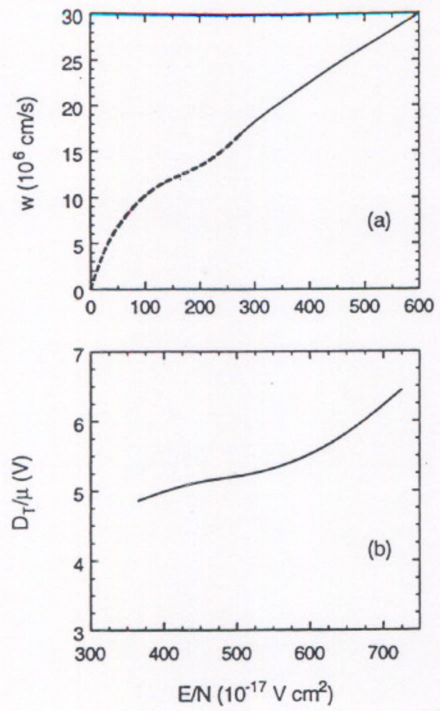

Fig. 5. (a) Recommended (—) and suggested (- - -) values of the electron drift velocity, w (E/N), in SF_6. (b) Suggested values of the transverse electron diffusion coefficient to electron mobility ratio, D_T/μ (E/N), as a function of E/N for SF_6.

reduced electron attachment coefficient [η/N (E/N)], and density-reduced effective ionization coefficient [$(\alpha-\eta)/N$ (E/N)] are shown in Fig. 4. Similar data for the electron drift velocity, w (E/N), and the transverse electron diffusion coefficient to electron mobility ratio, D_T/μ (E/N), are shown in Fig. 5.

CONCLUSIONS

The work described in this paper and in Ref. [1] indicates a rather simple pattern in the electron-interaction cross sections of the SF_6 molecule, which can be summarized as follows:

1. Elastic electron scattering is the most significant electron scattering process over the electron energy range from approximately 0.01 eV to 1000 eV.
2. Below 15 eV the most distinct inelastic energy-loss process is vibrational excitation – direct dipole excitation involving the ν_3 mode and indirect vibrational excitation via negative ion states involving the ν_1 mode.
3. Below ~0.1 eV electron attachment forming SF_6^- is the most dominant interaction (along with elastic scattering). Above this energy, the cross sections for dissociative electron attachment forming fragment anions [principally SF_x^- (x = 3, 4, and 5) and F^-] are appreciable, with the room temperature total electron attachment cross section dominated by the formation of SF_5^- between ~0.3 eV and 1.5 eV and by the formation of F^- ions beyond 2.0 eV.
4. Above ~16 eV dissociative ionization sets in generating principally SF_x^+ (x = 3, 4, and 5) and F^+ positive-ion fragments.
5. Electron-impact dissociation into neutral fragments SF_x (x = 1, 2, and 3) and F occurs above ~15 eV, with cross section values potentially exceeding those for ionization near 20 eV.
6. The total electron scattering cross section exhibits distinct structure due to negative-ion resonances at about 0.0 eV, 2.5 eV, 7.0 eV, and 11.9 eV.

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