Proceedings of the Mustansiriyah International Conference on Applied Physics (MICAP-2021)

Effect of Adding Krypton Gas to SF_6 Gas on Electronic Distribution Function and Electronic Transport Coefficients

KHALID S. JEBUR*

Iraqi Ministry of Education, General Directorate of Education, Rusafa 3, Baghdad, Iraq

Doi: 10.12693/APhysPolA.140.332

*e-mail: khaledsalman663@gmail.com

By using the EEDF program, the Boltzmann equation for the steady state was solved to study the electron energy distribution function f(u) and electron transport coefficients for SF₆ sulfur gas and its mixtures in different concentrations with the krypton gas. Krypton gas was used as an inert gas and mixed with SF₆ gas. The behavior of the gas varies depending on its concentration in the mixture and the strength of the reduced electric field. The difference in the type of gas and the type of mixture leads to a difference in the electronic energy distribution function and thus a difference in the electronic transport coefficients. The effect of reduced electric field strength E/N on f(u) and electron transport coefficients has also been studied numerically in the 10–600 Td range, where 1 Td = 1×10^{-17} V cm².

topics: EEDF program, krypton gas, SF₆ gas, electron transport coefficients

1. Introduction

Some noble gases, such as krypton, neon, helium, argon, as well as their mixtures containing specific gases such as chlorine gas or sulfur hexafluoride gas, are important in practical applications, e.g. plasma technology, electrical discharge, and the development of radiation detectors. This is because a monatomic noble gas and its atoms have a closed structure. The collision of an electron with a noble gas atom is the most common case of electron-atom collision [1]. In particular, plasma is an example of ionized gas [2]. In the plasma model, the distribution function f(u) plays a crucial role because of its importance in calculating reaction rates [3, 4]. The distribution function f(u) and electronic transition coefficients (ETC) are an essential part of glow discharge when the cross-sections for gases are known [5, 6]. The plasma density is limited by collisional de-excitation. The function of electron energy distribution can be determined by the balance between the gain of electron energy due to the increase in the electric field and its loss of energy due to collisions [7].

 SF_6 is a non-toxic substance so it can be inhaled without risk. Moreover, the SF_6 gas is not flammable. The thermal conductivity — one of the exceptional qualities of the gas — allows gas to be used to extinguish arcs by thermal transport [8]. At atmospheric pressure, the SF_6 gas possesses good properties, has a breakdown force three times that of air, is non-flammable and chemically inert. Due to its excellent physical and electrical properties, SF_6 is widely used in electric fields as insulation gas for high voltage equipment. Recently, however, many concerns arose about the fact that SF_6 is a powerful global greenhouse gas and so preventive efforts in this area should have been made. One of the possible solutions is to mix SF_6 gas with insulating gas. Among the gas mixtures with desire electrical insulation properties is a mixture of a SF_6 gas with a chemically inert gas such as nitrogen gas or CO [9, 10]. Therefore, there is an urgent need to obtain accurate data on engineering and electrical applications that use SF_6 gas.

In this study, we provide data for (SF_6+Kr) mixtures with varying percentages in a stable electric field by solving the Boltzmann equation with the EEDF program in order to determine the effects of these mixtures on the electron energy distribution function f(u) and electron transport coefficients.

2. Method

The Boltzmann equation (BE) plays a major role in electron transport and explains the physical phenomena that are of great importance to technology and engineering applications [11]. BE is a mathematical expression that describes the chronological evolution of the distribution function f(u) in the energy space. BE can be written as follows [12]

$$u^{1/2} f_0(u) \left(\frac{\mathrm{d}n_e}{\mathrm{d}t}\right) = I_E(u) + I_{\mathrm{ele}}(u) + I_{\mathrm{ine}}(u) + I_{\mathrm{ee}}(u).$$
(1)

The isotropic component of the electron energy distribution function is defined by $f_0(u)$. In (1), u is the electron energy, $I_E(u)$ denotes the heating of electrons in an electric field, $I_{ele}(u)$ is the elastic collision, $I_{\text{inele}}(u)$ is the inelastic collision, and $I_{\text{ee}}(u)$ is the electron–electron collision. The conservation of the electron density is represented in (1) by the portion $\left(\frac{\mathrm{d}n_e}{\mathrm{d}t}\right)$. It is defined as

$$\frac{\mathrm{d}n_e}{\mathrm{d}t} = n_e \left(v_{io} - v_{\mathrm{att}} - v_{\mathrm{rec}} \right),\tag{2}$$

where v_{io} , v_{att} and v_{rec} are the ionization, attachment and recombination frequencies, respectively, which can be expressed in terms of proper integration of $f_0(u)$.

The EEDF code allows solving the Boltzmann equation. Starting from (2), the calculated value of $\frac{\mathrm{d}n_e}{\mathrm{d}t}$ becomes the offset in (1), and the process is repeated iteratively to obtain the function f_0^{n+1} . The code is restricted to the standard value which ends the iterative procedures. The function f_0^{n+1} is the solution, and after the distribution function is present, the properties of plasma are calculated. The equations below are used in the program [12]. The mean of electron energy (\bar{u}) is given by

$$\bar{u} = \int_{0}^{\infty} \mathrm{d}u \, u^{3/2} f_0(u) \,. \tag{3}$$

The relationship between the distribution function and the electron diffusion coefficient is

$$D_C = \frac{2}{3m} \int_0^\infty \mathrm{d}u \, \frac{u^{3/2}}{q_m(u)} f_0(u),\tag{4}$$

where q_m is momentum transfer cross-section [cm²]. The characteristic energy (E_k) represents the ratio between the electron diffusion coefficient to the electron mobility, i.e.,

$$E_k = \frac{eD_C}{\mu_{el}}.$$
(5)

The ability of an electron to travel through a medium under the influence of the electric field Eis defined as the electron mobility $\mu_{el} \, [\mathrm{cm}^2/(\mathrm{V \ s})]$. This is given by the following relationship [13, 14]

$$\mu_{\rm el} = \frac{v_D}{E} = -\frac{1}{3N} \sqrt{\frac{2e}{m}} \int_0^\infty \mathrm{d}u \, \frac{u}{q_m(u)} \frac{\mathrm{d}f_0}{\mathrm{d}u}.$$
 (6)

By using the distribution function, we can obtain the speed of electronic drift given by the following relationship [12]

$$v_D = -\frac{E}{3N} \sqrt{\frac{2e}{m}} \int_0^\infty \mathrm{d}u \, \frac{u}{q_m(u)} \frac{\mathrm{d}f_0}{\mathrm{d}u},\tag{7}$$

where u is the electron energy [eV], N is the gas density $[cm^{-3}]$, and E/N is the reduced electric field in $[V \text{ cm}^2]$.

3. Results and discussion

Solving the Boltzmann equation requires knowledge of pure gas cross-sections and mixtures. The gas cross-section data is provided by the EEDF software which is used in conjunction with their references. Figure 1a and b displays the cross-sections



Fig. 1. The cross-sections [cm²] versus electron energy for (a) SF_6 and (b) Kr.



Fig. 2. (a) The f(u) as a function of u for dissimilar values of E/N in pure SF₆ gas. (b) Drift velocity versus Kr content for SF₆-Kr mixture. Pressure value of 760 Torr, the electron concentration $N = 1 \times 10^9$ cm⁻³ are used in the calculations.

of SF_6 sulfur gas and krypton gas vs the electron energy. One can see that the SF_6 gas possesses many cross-sections compared to pure krypton gas.

The distribution function f(u) vs the electron energy of pure SF_6 gas is shown in Fig. 2a, for several values of the reduced electric field 10-600 Td (color lines), where $Td = 1 \times 10^{-17} V cm^2$. It becomes obvious that changing the reduced electric field E/N has a significant impact on the distribution function.

The curves of the distribution function f(u)(see Fig.2a) are close to each other for low E/Nvalues because electrons obtain less energy from the



Fig. 3. (a) The distribution functions f(u) vs electron energy u in the 80% SF₆+ 20% Kr mixture for different E/N. (b) The distribution function f(u) vs electron energy u in 50% constituents of both SF₆ and Kr mixture, and (c) 20% SF₆+ 80% Kr mixture for different E/N. The concentration of N electron is 1×10^9 cm⁻³, and the pressure is 760 torr.

applied reduced electric field. Each curve reaches its maximum in the area of low values of u. For a fixed value of the reduced electric field E/N, the maximum value of f(u) is reduced with the increase of u. In turn, increasing the reduced electric field causes the curves of the distribution function f(u) to develop towards higher energy with higher rates due to the strong influence of the electric field in this regime. This warms the cold electrons, i.e., their energy increase [15].

The velocity of electron drift v_D is one of the important transport parameters that is affected by the difference in Kr concentration in the mixture (SF₆+Kr). The parameter v_D is shown as a function of Kr concentration in Fig. 2b. When the electric field stabilizes at E/N = 400 Td, the concentration of Kr in the mixture increases, resulting in a linear increase in v_D .

The effect of the SF_6 gas concentration on the mixture is evident in Fig. 3a–c. Due to the broad cross-sections of SF_6 , the reduction of the SF_6 concentration in the mixture with a constant value



Fig. 4. (a) The calculated mean electrons energy in the SF₆+ Kr mixture. (b) The characteristic energy E_k as a function of E/N for various gas mixture ratios SF₆:Kr.

of E/N causes the distribution function to curve away to the right with high energy rate. Now compared to Kr gas, the increase of the Kr atom number in the mixture reduces the frequency of electrons collision, and thus provides sufficient time to accelerate the electrons, and increase their kinetic energy due to the increase in the reduced electric field.

In Fig. 4a, the value of the reduced electric field, i.e, E/N = 200 Td, is a very important turning point in the behavior of mixtures and pure gases. When E/N value is less than 200 Td, a decrease in the SF₆ concentration causes an increase in the energy of electron, leading to an increase in E/Ndue to the lower number of collisions. Note that for a given electron energy value, the energy growth rate for a given concentration of SF₆ in the mixture increases linearly with E/N (according to (3)).

Figure 4b shows characteristic energy relationship with the reduced electric field for different ratios of a mixture (SF₆ + Kr) and the same condition as in Fig. 4a. It is noted that the characteristic energy curve of the krypton gas is higher than the SF₆ and also higher than the rest of the mixture. The behavior of the mixture varies with the different concentration of SF₆ in the mixture (according to (5)).



Fig. 5. (a) The drift velocity v_D of pure Kr and SF₆, and their mixtures, is dependent on E/N at 760 Torr and 273 K. (b) At similar conditions, the mobility (μ_{el}) of Kr, SF₆, and their mixtures is dependent on E/N.



Fig. 6. Diffusion coefficient D_C as a function of E/N in various mixture ratios SF₆:Kr.

Figure 5a shows the relationship between the drift velocity with the reduced electric field and the concentration of SF_6 gas in the mixture. A slight effect of the change of the concentration behavior of SF_6 appears in the vicinity of the point E/N = 200 Td. A significant and clear effect of the SF_6 concentration behavior is seen when E/N > 200 Td. Reducing the concentration of SF_6 in the mixture

leads to a distinct increase in the speed of electron drift, which is due to a decrease in the number of the inelastic collisions in this range, on the one hand, and an increase in the electric field, on the other hand. In all cases, the increase of E/N leads to the increase in the drift speed of all mixtures used. This results from heating and the increase of the kinetic energy of electron (according to (7)).

Figure 5b shows the opposite decrease in the electron mobility as the reduced electric field increases up to E/N < 200 Td. This is due to the fact that electrons lost their energy during inelastic collisions with neutral atoms. This decrease is more pronounced for higher SF₆ concentration values in the mixture, which is equivalent to having large cross-sections, which become larger as a result of collisions, and hence electron energy losses (according to (6)).

Figure 6 shows a variation in the behavior of the electronic diffusion coefficient D_C according to the concentration of SF₆ in the mixture and the strength of E/N, where E/N < 200 Td. The decrease of the electronic diffusion coefficient D_C with an increase in E/N appears for mixtures with a high concentration of SF₆. When E/N > 200 Td, the electron diffusion coefficient increases with decreasing concentration of SF₆ in the mixture and increasing E/N (according to (4)).

4. Conclusion

Boltzmann equation for the stable state was solved using the EEDF program. The results showed that the behavior of the pure gases and the mixtures used are affected by both the electric field strength and the gas concentration in the mixture. Reducing the concentration of SF_6 in the mixture leads to the distancing of the distribution function curves towards the high energy tail and then the electron transport parameters are affected by that, i.e., in particular when E/N > 200 Td. As the amount of SF_6 in the mixture is reduced, the electron drift increases, raising the curves of the electronic diffusion coefficient as E/N increases. In turn, when E/N < 200 Td, the reduction of the SF_6 in the mixture raises both the electron energy rate and the characteristic energy. The mobility decreases dramatically with the increased SF_6 concentration in the mixture within this range as E/N increases due to dominance of the inelastic collisions.

References

- D.M. Xiao, L.L. Zhu, X.G. Li, J. Phys. D Appl. Phys. 33, L145 (2000).
- [2] D. Szabo, S. Schlabach, *Inorganics* 2, 468 (2014).
- [3] R.J. Shul, S.J. Pearton, Handbook of Advanced Plasma Processing Techniques, Springer, Berlin 2000.

- [4] V. Demidov, C.Jr. DeJoseph, A. Kudryavtsev, *IEEE Trans. Plasma Sci.* 34, 825 (2006).
- [5] A. Pahl, Electron Energy Distribution Function, COMSOL Blog, (2014).
- [6] J. Komppula, O. Tarvainen, *Plasma Sources Sci. Technol.* 24, 045008 (2015).
- [7] A. Albert, D. Bošnjakovic, S. Dujko, J. Phys. D Appl. Phys. 54, 135202 (2021).
- [8] Wei Liu, Zhenxi Su, Jiong Qi, Feng Zhu, Yue Zhao, Fengxiang Ma, Xiaofang Yuan, Ying Chen, *IOP Conf. Ser. Earth Envi*ronm. Sci. 69, 012002 (2017).
- [9] C.T. Dervos, P. Vassilliou, J. Air Waste Manage. Assoc. 50, 137 (2000).
- [10] M.J. Pinheiro, J. Loureiro, J. Phys. D Appl. Phys. 35, 3077 (2002).

- [11] D.S. Abdul, B.J. Hussein, M.K. Jassim, J. Phys. Conf. Ser. 1003, 012116 (2018).
- [12] S.J. Khalid, A.J. Enas, K.J. Mustafa, AIP Conf. Proc. 2123, 020051 (2019).
- [13] R. Hippler, H. Kersten, M. Schmidt, K.H. Schoenbach, Low Temperature Plasmas: Fundamentals, Technologies, and Techniques, 2nd ed., Wiley-VCH, Weinheim 2008.
- [14] A.F. Borghesani, M. Folegani, P.L. Frabetti, L. Piemontese, J. Chem. Phys. 117, 5794 (2005).
- [15] I.H. Salih, M.M. Othman, S.A. Taha, ARO
 Sci. J. Koya Univ. 8, 22 (2020).