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Theoretical Studies of the Electrical Discharge Characteristics of Sulfur Hexafluoride

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Abstract – This paper contains results of the theoretical studies of the electrical breakdown properties in sulfur hexafluoride. Since the strong interaction of high-energy electrons with the polyatomic sulfur hexafluoride molecule causes their rapid deceleration to the lower energy of electron capture and dissociative attachment, the breakdown is only possible at relatively high field strengths. From the breakdown voltage curves, the effective yields that characterize secondary electron productions have been estimated. Values of the effective yields are found to be more consistent if they are derived from the experimentally determined values of the ionization coefficient and the breakdown voltages. In addition, simulations were performed using an one-dimensional Particle-in-cell/Monte Carlo collision code. The obtained simulation results agree well with the available experimental data with an error margin of less than 10% over a wide range of pressures and the gap sizes. The differences between measurements and calculations can be attributed to the differences between simulation and experimental conditions. Simulation results are also compared with the theoretical predictions obtained by using expression that describes linear dependence of the breakdown voltage in sulfur hexafluoride on the pressure and the gap size product.

Keywords: Electrical discharge, Breakdown, Effective yield, Simulation

1. Introduction

Sulfur hexafluoride SF_6 is one of the most extensively and comprehensively studied molecular gases mainly because of its wide range of commercial and research applications [1-5]. The use of SF_6 has been established in the insulation of supervoltage generators in particle-accelerating machines, betatrons, neutron generators and other equipment used for radiation applications in scientific institutions, medicine and industry. Parallel to the development of SF_6 plant technology in the high-voltage sector, SF_6-insulated, high-voltage measuring instruments and calibrated power sources have also been produced. SF_6-fillings are also employed in instrument transformers, pressurized gas capacitors and surge arresters for super voltages. Nowadays, SF_6 is more and more used for the manufacturing of semiconductor devices such as IC (integrated circuits), flat panels, photovoltaic panels and MEMS (Micro-Electro-Mechanical-Systems) [6-9].

Studies of SF_6 breakdown characteristics have been performed in two aspects: experimentally and numerically. The experiments are usually done in order to obtain the breakdown value of voltage under different type of voltage and electrode geometry [10-15]. In numerical modelling, simulation models are built and solved to acquire some microscopic parameters of discharge and study the principles of the discharge [16-19]. Some phenomena in gas discharges can be explained by experiments but the details of the discharge happening and developing cannot be studied well by this method. Especially for SF_6 which is a polyatomic large molecule, a lot of physical and chemical reaction will happen during discharge. The strong interaction of high-energy electrons with the SF_6 causes their rapid deceleration to the lower energy of electron capture and dissociative attachment. SF_6-breakdown is therefore only possible at relatively high field strengths. Although SF_6 is the electric power industry's preferred gas for electrical insulation, still there is a little data about its electrical properties.

As complement to the experimental and numerical results, several theoretical approaches have been developed [20, 21, 22]. For low pressures, the electrical discharge characteristics of SF_6 are discussed in relation to the field dependence of the ionization coefficient and the electron attachment coefficient leading to a good agreement with the experimental results [23-25]. The concept of breakdown at a certain value of the reduced electric field E/p (electric field to the pressure ratio) in SF_6 previously observed experimentally has been established theoretically [26].

In this paper we investigate the discharge characteristics in SF_6 both for the standard gap sizes and microgaps. Beside the Paschen law, the breakdown voltage in SF_6 can be predicted by a simple expression describing the linear dependence of the breakdown voltage on the *pd* product (pressure times the gap spacing) derived in [26]. Based on the experimental conditions we also performed Particle-in-

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Cell/Monte Carlo simulations. There are very few attempts to model gas breakdown in SF_6, especially in micron scale gaps. The obtained simulation results for the breakdown voltage show a good agreement with the available experimental data [26, 27] as well as with the theoretical predictions. Based on the determined breakdown voltage curve, the effective yield of SF_6 has been estimated representing one of the crucial parameters in modelling. Values of the ionization coefficients in the standard gap sizes will be used for obtaining the α coefficients in smaller gap sizes. In addition, the obtained values will be fitted by semi-empirical expression.

2. Theoretical Background

It is well known that electrical breakdown of a gas takes place when sufficient free charges are present to generate a conducting plasma channel that bridges the electrode gap. Multiplication or avalanche of free charge is formed when the motion of an electron due to an applied electric field causes greater liberation than capture of other electrons. Since SF_6 molecule has the high electron affinity, an electron avalanche will develop in this gas when the ionization coefficient α exceeds the electron attachment coefficient η. The transition from an avalanche to a self-sustaining discharge can result from the Townsend secondary emission mechanism when new avalanches are generated by secondary processes. If each avalanche initiates on the average more than one new avalanche, the total amount of ionization will increase until breakdown.

With an applied electric field, discharges in the gas occur as a result of ionization leading to the breakdown of the gas:

$$\int_0^{x_c} (\alpha - \eta) dx = \ln N, \tag{1}$$

where N is the number of electrons in the avalanche, x represents the distance from the surface of the electrode and corresponding maximum electric field $E_{\max}$, while x_c represents values of x where $\alpha=\eta$. For $\alpha>\eta$, x_c is taken to be the gap length.

It was shown that the effective ionization coefficient of SF_6 can be approximated by the expression [26]:

$$\frac{\alpha-\eta}{p} = \kappa\left[\left(\frac{E}{p}\right) - \left(\frac{E}{p}\right)_c\right] \tag{2}$$

with κ as a numerical constant and $(E/p)_c$ as the critical reduced field of SF_6. It was shown that ionization α and the attachment η coefficients of SF_6 can be written as [25]:

$$\frac{\alpha}{p} = 1.12\times10^4 \times \exp\left(-2.74\times10^5 \frac{p}{E}\right), \tag{3}$$

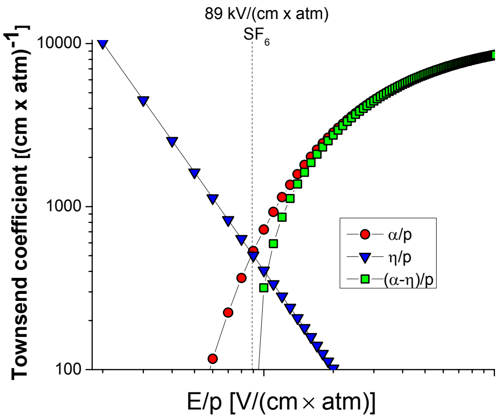


Fig. 1. The ionization (red circles), attachment (blue triangles) and the effective ionization (green squares) coefficients as a function on the reduced electric field. Dot line corresponds to the critical reduced field of 89 *kV/(cm × atm)* for SF_6.

$$\frac{\eta}{p} = 4.06\times10^{12} \times \left(\frac{p}{E}\right)^2 p. \tag{4}$$

Fig. 1 shows the dependence of the α/p (red circles), η/p (blue triangles) and the effective ionization coefficient $(\alpha-\eta)/p$ (green squares) on the reduced electric filed plotted in accordance to the expressions (3)-(4) [25]. The value of the reduced field at $\alpha=\eta$ for SF_6 is 89 kV/(cm x atm).

According the Townsend theory, the breakdown voltage can be determined from the well known Paschen law:

$$V_b = \frac{Bpd}{\ln pd + \varsigma} \tag{5}$$

where $\varsigma = \ln[A/(1+1/\gamma)]$, while the appropriate constants for SF_6 are A=0.94 $(\text{atm}\times\text{cm})^{-1}$ and B=21.608 V/(atm×cm) [26].

Another expression for the breakdown voltage in SF_6 has been derived in [26]:

$$V_b = \frac{\ln N_c}{\kappa} + \left(\frac{E}{p}\right)_c p\cdot d\,. \tag{6}$$

The expression (6) provides that the breakdown voltage of SF_6 is almost linearly proportional to the *pd* product. In contrast to many existing expressions for the breakdown voltage, derived expression (6) does not contain additional fitting parameters.

3. Simulation Technique

In this study calculations were performed using an one-dimensional Particle-in-cell (PIC) code with Monte Carlo

(MC) algorithm for collisional processes. An overall description of the code can be found in previous publications [28-30], so only the main characteristics of the code will be provided here.

In the standard PIC/MCC code scheme, the equations that correspond to the coupled system of charged particles and fields are solved. The particles are followed in a continuum space, while the fields are computed on a mesh. Interpolation provides the means of coupling of the continuum particles and the discrete fields [28]. At the beginning of the simulation, every charged particle is assigned a specific position on the grid, leading to a self-generated electric field. A certain potential is applied to one of the electrodes, giving rise to an external field. This field accelerates the particles, and the particles move to their new positions, changing the self-created field and, hence, changing the force acting on the particles. This is done every time step by first weighting the positions of the particles to the grid, yielding the charge densities on the grid point. The potential and electric field on the grid points are then determined from the calculated charges by solving the Poisson's equation. A weighting procedure is repeated again to obtain the forces on the positions of the particles from the previously obtained field on the grid points.

The well established cross sections data for SF_6 are shown in Fig. 2 [31, 32]. Simulation conditions were based on the experimental conditions mainly. Depending on the gas pressure, the time step was varied between and which consumed a lot of time for running each case. The gap pressure was varied between 1 atm and 6 atm.

One million computer particles was used as the initial number in the simulation. Since the gas pressure was on the order of few atmospheres, a lot of time is needed to compute each case. In order to determine the breakdown voltage, we employed the fact that the breakdown is not an instantaneous phenomenon. It occurs over a finite period of time which can be determined from the balance between creation of charged species by ionization and their losses via collisional processes and diffusion to the walls [33].

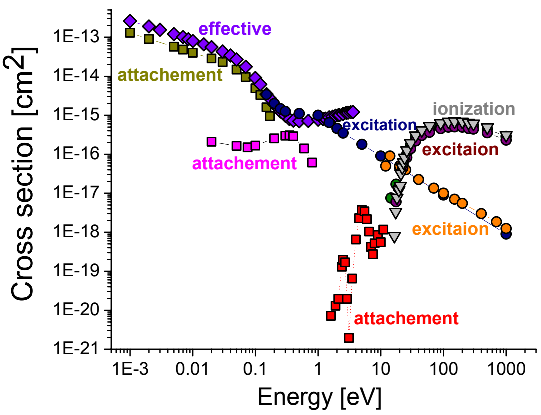


Fig. 2. Cross sections data for SF_6 taken from [31, 32].

For each value of the gas pressure, the dependence of the electron density was tracked, and depending on its increasing or decreasing nature, the interval in which the breakdown voltage lies could be found through trial error processes. For each value of the gas pressure, a several calculations were needed.

4. Results

As can be clearly seen from Fig. 3, the strong interaction of high-energy electrons with SF_6 molecule causes their rapid deceleration to the lower energy of electron capture and dissociative attachment. SF_6 breakdown is therefore only possible at relatively high field strengths. Good agreement is achieved between the experimental data for SF_6 (circles) taken from [26] and the theoretical prediction obtained by using 6) (line). In order to demonstrate differences between reduced field for air and SF_6 the experimental data for air [26] are shown by circles.

The breakdown voltage against the *pd* product (the pressure times the gap size) is given in Fig. 4. Several curves are plotted. The solid curve represents the theoretical predictions obtained by using the expression (6) while symbols show the experimental data taken from (red squares) [24] and (green circles) [35], respectively. Dot curve represents the values obtained by using Paschen law (5) with contains taken from [26]. Finally, our PIC/MCC simulation results are shown by crosses. Simulation results have the same trend as both experimental and theoretical results. The higher breakdown voltage obtained in the simulations as compared to the experimental data can be attributed to differences between the simulation and experimental conditions, especially secondary emission coefficients. Although the same gap size and the pressure are used in both cases, the temperature and electrode materials used in the experiments are unknown. Based on the good agreement between the theoretical, experimental and simulation results, we may conclude that the expression

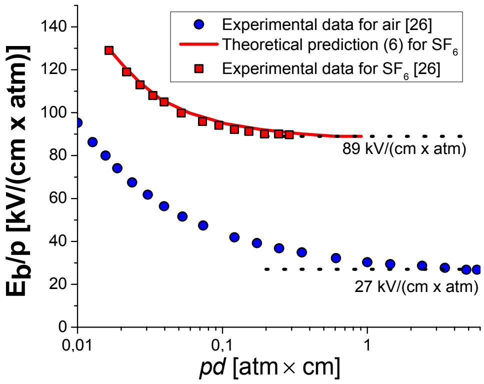


Fig. 3. Measured data taken from [26] and calculated by using expression (6) values of the breakdown fields strength versus the *pd* production for SF_6 (squares) and air (circles).

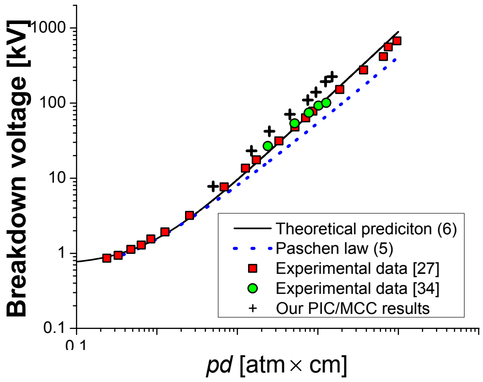


Fig. 4. The breakdown voltage curves for SF_6. Experimental data are given by red squares [34] and green circles [35]. Results obtained by expression (5) are shown by dot curve, while solid curve correspond to the theoretical prediction (6).

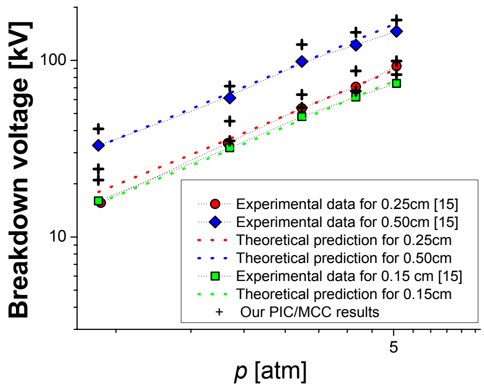
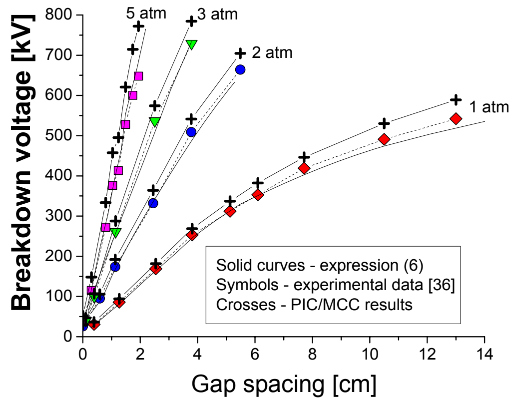
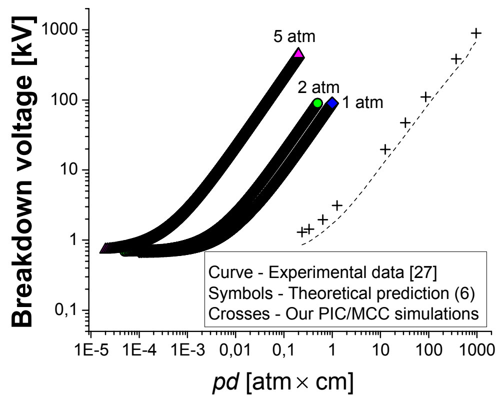


Fig. 5. The dependence of the breakdown voltage on the pressure for various gap sizes. Values obtained by using (8) (dot curves) are compared with the measured values [15] (symbols).



(a)



(b)

Fig. 6. The breakdown voltage of SF_6 in a homogeneous field as a function of: a) the distance between electrodes and b) the *pd* product at various gas pressures. Results obtained by the expression (6) are compared with the available results of measurements taken from [37] and [34], respectively.

(3) fits well the experimental data.

Fig. 5 displays comparison between results of measurements performed at a fixed gap size by varying pressure (symbols) [15] and results achieved by derived expression 6).The gap lengths were put to be 0.15 cm, 0.25 cm and 0.50cm, respectively. At each gap, the pressure was set from varied 1atm to 5atm by using 1atm increment. All SF_6 breakdown experiments were carried out at 30kHz. Theoretical values obtained by expression (6) are given by colored symbols, while crosses correspond to our PIC/MCC simulation results. Again, there is a good agreement between the results achieved by three different techniques. Since the breakdown strength of SF_6 is independent of frequency, it represents an ideal insulating gas for UHF equipment [36].

A good agreement between theoretical results (solid curves), PIC/MCC simulation results (crosses) and experimental data (symbols) [37] are presented in Fig. 6(a). Although the scaling law (6) is valid over a wide range of pressures, at higher pressures, however, deviations have been observed under certain conditions [37].

In addition Fig. 6(b) shows comparison between the theoretical predictions based on expression (6) and results of measurements taken from [34].

Starting from the breakdown voltage curve obtained by derived expression (6) (shown by solid curve in Fig. 4), the effective electron yield can be estimated and given by red diamonds in Fig. 7. Values of the effective yield are found to be more consistent if they are derived from experimentally determined values of the ionization coefficients and the breakdown voltage curves [38-40]. In order to demonstrate that a small differences in the breakdown voltages can cause a large discrepancies between the values of the effective yield, we also determined the yield (blue circles) from the Paschen curve (shown by dot curve in Fig. 4). As can be observed, a small discrepancy between solid and dot curves in Fig. 4, may cause a large differences in the corresponding yields (red diamonds and blue circles, respectively) indicating that the precise determination of the breakdown voltage is required.

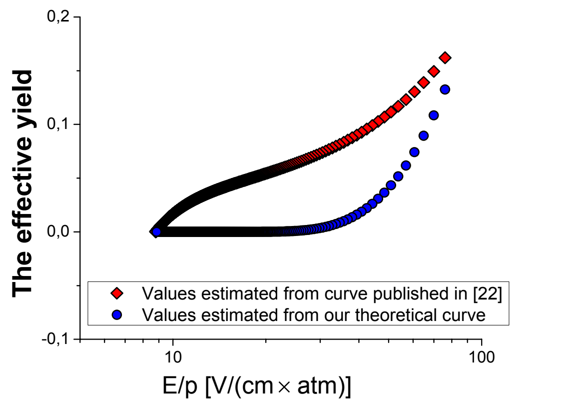


Fig. 7. The effective yield against the reduced filed of *E/p*. Diamonds and circles show values estimated from various breakdown voltage curves.

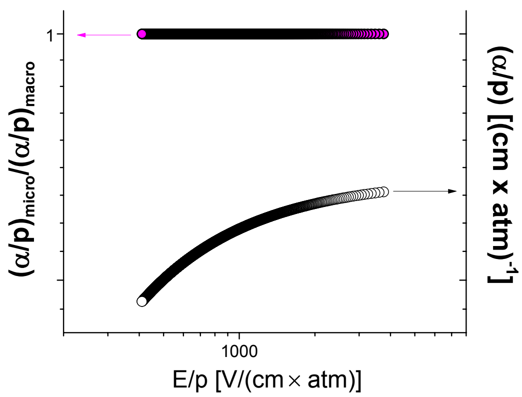


Fig. 8. The ionization coefficient in microgaps in accordance with (7) normalized to the ionization coefficient that correspond to the macroscale.

The values of the ionization coefficient in microgaps can be estimated based on the values measured in macrogaps in accordance with the relation [41]:

$$\left(\frac{\alpha}{p}\right)_{micro} = \left(\frac{\alpha}{p}\right)_{macro} \cdot \left\{1 - \exp\left[-\left(\frac{V/IP - 1}{3.1}\right)^{0.8}\right]\right\}, \qquad (7)$$

where *IP* is the ionization potential for gas under consideration. As can be seen from Fig. 8, the ionization coefficients in microgaps agree well with the values obtained for the standard size discharges indicating that the Townsend phenomenology does not need extension to describe microdischarges and that the ionization coefficients for such discharges obey the similarity law $\alpha/p = f(E/p)$ [42, 43].

5. Conclusion

In this paper, Particle-in-cell/Monte Carlo collision (PIC/MCC) simulations have been extensively used to investigate the discharge characteristics of SF$_6$ gas. Simulation parameters were based on the experimental conditions mainly. The strong interaction of high-energy electrons with SF_6 molecule leads to their rapid deceleration to the lower energy of electron capture and dissociative attachment. Consequently, the breakdown in SF_6 is only possible at relatively high field strengths it can be used in place of solid and liquid insulators. On the other hand, the breakdown strength of SF_6 is independent of frequency and therefore it can be considered as an ideal insulating gas for UHF equipment. The obtained simulation results are in a good agreement with the measured data with an error margin of less than 10% confirming that the PIC/MCC technique could be used for precise prediction of the discharge characteristics. The simulation results also make it possible to estimate the values of the effective secondary yields. We found that the effective yields of SF_6 are less than 0.2. Simulation results are also in a agreement with the derived expression for breakdown voltage [26] confirming that the breakdown voltage in SF_6 is linearly proportional to the pressure and the gap size product.

Results for the ionization coefficients in micro gap sizes are in good agreement with the values obtained at lower pressure but same reduced field indicating that the standard Townsend phenomenology is applicable down to a few micrometers.

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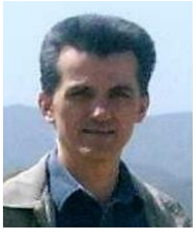

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