Modeling And Analysis Of The Breakdown Curve Of A High-Frequency Discharge In Hydrogen

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Abstract: The subject of this study is the construction of the breakdown curves of a RF discharge in hydrogen. Based on previously developed by the authors breakdown criteria, the breakdown curves of a discharge in hydrogen were analytically constructed for the first time. Very good coincidence between the proposed analytic breakdown criteria and known in literature experiment data is obtained. A comparison is made with other breakdown criteria, developed earlier. It is found that the positive and negative electric fields occurred in the discharge influence each other.

Index Terms: Analytic model, Breakdown curve, Gas discharge, Low-pressure discharge, Radio-frequency discharge.

1 INTRODUCTION

High-frequency (HF) discharges continue to find applications in various technological processes - processing of semiconductor materials, pad cleaning, determining the chemical composition of compounds, generation of oxide coatings. The increased interest in HF discharges also stems from the possibility of using these to study the properties of plasma and the interactions of electrons with gas ions and atoms. This type of discharge is also used to pump gas lasers and metal vapor lasers. For this reason, discharge excitation process continues to be of interest [1, 2]. As it known [2], in a HF field, electrons fluctuate at an amplitude many times smaller than the size of the gas discharge volume. The bulk of electrons does not reach the walls of the container and cannot be recombined with the positive ions. The main channel for electron loss is through diffusion to the walls of the gas discharge volume. If the gas is negatively charged, the additional loss of electrons is determined by the electrons which become attached to gas molecules. The deviation of positive and negative ions is even smaller than that of the electrons. A cloud of practically static ions is formed in the gas discharge, generating their own direct current fields. In a simple case, when the main reasons for electron loss are the processes of ionization and electron diffusion, the radio-frequency breakdown criterion has the following form:

\[ \frac{\nu_i}{D_e} = 1/A^2, \]  

where \( \nu_i \) is the frequency of molecule ionization by electrons, \( D_e \) is the electron diffusion coefficient, \( A \) – diffusion length, dependent on the geometry of the gas discharge chamber [3].

When deducing criterion (1), it is assumed that the diffusion coefficient of electrons is an isotropic function, i.e. it is not dependent on electron movement direction. For flat electrodes, the quantity \( A \) is given as follows:

\[ 1/A^2 = \left(\pi/d\right)^2, \]  

where \( d \) is the distance between electrodes. In accordance with [3], equation (1) assumes the form

\[ \exp\left(\frac{B_p}{2E}\right) = A_p d \left(1 - \frac{E/B_p}{C_d/d/\lambda}\right), \]  

where \( A, B \) and \( C \) are molecular constants, \( p \) is the gas pressure, \( \lambda \) is the vacuum wavelength of a HF field, \( E = E_d / \sqrt{2} \) is the efficiency of the HF field. Using known dependencies \( \nu_i = \alpha v_d = \alpha \mu_e E \) criterion (1) can be written as

\[ \frac{\alpha E}{D_e/\mu_e} = 1/A^2, \]  

where \( \alpha \) is the coefficient of gas volume ionization and \( v_d \) is the drift speed of electrons. Usually, criterion (2) may be represented in the form [1]

\[ \alpha / p = A \exp\left(-\frac{B}{E/p}\right), \]  

where \( A, B \) are constants.

Based on experiment data, the ratio \( D_e/\mu_e \) can be approximated by

\[ D_e/\mu_e = M + N E / p, \]  

using suitably defined constants \( M, N \). The diffusion length \( A \) for flat configurations is given by the expression

\[ 1/A^2 = \left(\pi/d\right)^2. \]  

In this manner, criterion (2) may be written as
\[ U_{pd} \exp \left( -\frac{Bpd}{U_{pd}} \right) \left( M + NU_{pd} \right) \] 
\[ - \pi^2 = 0 , \]  
(5)

where \( U_{pd} = E_d \) is the breakdown voltage of the layout.

This results in the non-explicit form \( F(U_{pd}, pd) = 0 \) for the breakdown condition as a function of the parameter \( pd \). It has been found through experiments that the application of weak external direct current voltage to a high-frequency discharge causes a notable increase of breakdown voltage in a HF discharge to the right side of the breakdown curve \([4]\). The additional direct voltage increases electron losses due to drift from electrodes. This leads to an increase in discharge pressure and voltage. The minimum of the breakdown curve shifts towards higher voltages and pressures. When a stronger external field is applied, the processes of additional ionization of the gas are accelerated at the expense of the external field. The discharge generation curves in a HF field are displaced towards lower voltages. In this case criterion (1) takes the following form \([4]\):

\[ U_{pd} \exp \left( -\frac{Bpd}{U_{pd}} \right) = \frac{1}{A^2} + \left( \frac{E_{dc}}{2D_{rf} \mu_e} \right)^2 , \]  
(6)

where \( \mu_e \) is the coefficient of electron mobility, \( E_{dc} \) is the intensity of the DC field.

It has long been known that a HF discharge has constant positive potential \([2]\). This is the reason for the sputtering of electrodes in a HF discharge, analogically to DC. Ions are accelerated by the direct current field and sputter the electrode by bombarding it. This lies at the core of all ion-plasma technologies which employ a HF field. Based on experiment data \([1]\), the following empirical dependency was found:

\[ U_{dc} = U_{pd} / \pi , \]  
(7)

For this reason, criterion (6) can be applied without employing a formal external electric field. Following some simplifications, using (7), criterion (6) assumes the form

\[ U_{pd} \exp \left( -\frac{Bpd}{U_{pd}} \right) \left( M + NU_{pd} \right) \frac{2}{\pi^2} \left( M + NU_{pd} \right) = 1 . \]  
(8)

For the first time criterions (5) and (8) were developed and applied for the examination of the breakdown curve in argon \([5]\). It has been established that taking into account the self-generated electric field (7) and applying criterion (8) provides the best description of known experiment results for the breakdown curve in argon. Criterion (8) yields the best fit when compared with criterion (5), and criterion (3). The main conclusion which was drawn in \([5]\) is that the existing own electric field must always be taken into consideration and it is recommended that criterion (8) is applied. The objective of this paper is to examine the breakdown curve in hydrogen by applying criteria (5) and (8). There have been no such investigations for hydrogen until now. The behavior of the breakdown curve will be analyzed and simulated by the model criterions. Obtained results are compared to known experiment data and other existing modeling results.

2 Problem Setup

As it is known, hydrogen is an electronegative gas. The mechanisms of electron attachment and the formation of negative hydrogen ions are different. The highest probability is assumed for the process with disassociation attachment of the electron according to scheme \([6]\):

\[ H_2 + e^- = H^- + H , \]  
(9)

One possible but less likely process is \([6]\):

\[ e^- + H = H^- + h\omega , \]  
(10)

where \( h \) is the reduced Planck constant or Dirac constant, and \( \omega \) is angular frequency. In this way, two differentiated zones with positively and negatively charged hydrogen molecules are formed in the hydrogen discharge. Two own electric fields arise in the hydrogen discharge - a positive and a negative one. Up to now, the interactions between these electric fields have not been studied. There has been no investigation to establish which of the proposed criterions, (5) or (8) is more suitable for application with regard to a discharge in electronegative gases. The objective of this paper is to apply criterions (5) and (8) in the case of discharge in hydrogen, and to compare the obtained theoretical breakdown curves against known experiment results.

3 Results from Computer Simulations and Their Analysis

The computer simulation using the criteria (5) or (8) were performed by solving every of these nonlinear equations with respect to \( U_{pd} \) for different values of the parameter \( pd \). The calculations were carried out by means of authors own code in Wolfram Mathematica.
Fig. 1. Breakdown curve in discharge of hydrogen: Series 1 – experiment data from [7, 8]; Series 2 – simulated results by using proposed analytic criterion (8).

Fig. 2. Breakdown curve in discharge of hydrogen: Series 1 – experiment data from [7, 8]; Series 2 – simulated results by using proposed analytic criterion (5); Series 3 – breakdown curve from classical Kihara criterion (3) (see [7]).

Fig. 1 shows the breakdown curve based on experiment results for hydrogen in accordance with [7, 8], Series 1. This is compared with the breakdown curve constructed under criterion (8). It is observed a good coincidence between the two curves in Fig. 1 in the region of the minimum of the curves for $0.5 \leq pd \leq 2$. In Fig 2, the breakdown curve in hydrogen has been constructed once again using experiment data from [7, 8], Series 1. The same figure shows a breakdown curve obtained using criterion (5), Series 2. For comparison, a breakdown curve has been constructed by applying criterion (3), Series 3, given in [7]. The computer simulations were performed for the first time. These indicate that criterion (5) provides the best description of experiment results for the breakdown curve of hydrogen. This is different from the results obtained for argon, [5] where the best criterion was (8). Therefore, the positive and negative ions in the hydrogen discharge create electric fields which neutralize each other. As a result, criterion (5) proves to be the most accurate. Fig. 1 and Fig. 2 show that the proposed criteria (5) and (8) are significantly more accurate than criterion (3), suggested for the first time by Kihara [3].

4 CONCLUSION
For the first time, criteria have been proposed and applied for the representation of the breakdown curve of a RF discharge in hydrogen. The mutual influence of the obtained positive and negative electric fields has been examined. Based on the comparison of suggested criteria for the construction of the breakdown curve, it has been established that the two fields neutralize each other.

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