Self-organization in DC glow microdischarges in krypton: 3D modelling and experiments

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The present work is aimed at finding, by means of modelling and experiments, whether self-organized patterns of cathodic spots can be observed in DC glow microdischarges in krypton. The modelling is performed in the framework of the simplest self-consistent model of glow discharge. The experiments are performed in a cathode boundary layer discharge (CBLD) configuration. It was found by modelling that several 3D modes exist provided that the product of the pressure by the interelectrode distance (*pd*) is high enough. Preliminary experimental results showed clear correspondence with the modes predicted in the modelling. Self-organization pattern formation in krypton favours higher *pd* than it is in xenon.

1. Introduction

Self-organized patterns of cathodic spots have been observed in DC glow microdischarges in xenon [1, 2]. These self-organized patterns appear at the transition from the normal mode to the abnormal mode and comprise two or more cathodic spots.

Modelling of microdischarges in xenon [3-5] has revealed existence of multiple solutions for the same value of discharge current. Some of these solutions describe normal discharges, others describe 2D (axially symmetric) patterns of cathodic spots, and still others describe 3D patterns similar to those observed in the experiments [1, 2]. This modelling represents the first step towards a self-consistent modelling of self-organization in DC glow discharges.

A very interesting question is why modes with self-organized patterns have been observed in DC glow microdischarges in xenon but not in other gases such as argon [6]. Modelling [7] suggests that self-organized patterns can, in principle, be observed in plasma-producing gases other than xenon provided that conditions are right.

The present work is aimed at finding, by means of experiments guided by the modelling, whether self-organized patterns of cathodic spots can be observed in DC glow microdischarges in krypton.

2. Modelling

2.1 The model

In this work the most basic self-consistent model of DC glow discharges is employed. It comprises equations of conservation of a single ion species and the electrons, transport equations for the ions and the electrons written in the so-called drift-diffusion approximation, and the Poisson equation:

$$\nabla . \boldsymbol{J}_i = n_e \alpha \mu_e E - \beta n_e n_i$$
$$\boldsymbol{J}_i = -D_i \nabla n_i - n_i \mu_i \nabla \varphi$$
$$\nabla . \boldsymbol{J}_e = n_e \alpha \mu_e E - \beta n_e n_i$$
$$\boldsymbol{J}_e = -D_e \nabla n_e - n_e \mu_e \nabla \varphi$$
$$\varepsilon_0 \nabla^2 \varphi = -e(n_i - n_e).$$

Here n_i, n_e, D_i, D_e, J_i, J_e, μ_i and μ_e are number densities, diffusion coefficients, densities of transport fluxes and mobilities of the ions and electrons, respectively; α is Townsend's ionization coefficient; β is the coefficient of dissociative recombination; φ is the electrostatic potential, $E = |\nabla\varphi|$ is the electric field strength; ε_0 is the permittivity of free space and e is the elementary charge.

Let us consider a cylindrical discharge vessel of a radius R and of a height h, and introduce cylindrical coordinates (r,ϕ,z) with the origin at the center of the cathode and the z-axis coinciding with the axis of the vessel. Then the boundary conditions read:

$$z = 0: \quad \frac{\partial n_i}{\partial z} = 0, \quad \boldsymbol{J}_{ez} = -\gamma \boldsymbol{J}_{\mathrm{iz}}, \quad \varphi = 0;$$

$$z = h: \quad n_i = 0, \quad \frac{\partial n_e}{\partial z} = 0, \quad \varphi = U;$$

$$r = R: \quad \frac{\partial n_i}{\partial r} = \frac{\partial n_e}{\partial r} = 0, \quad \boldsymbol{J}_{ir} - \boldsymbol{J}_{er} = 0.$$

Here U is the discharge voltage, the subscripts r and z denote radial and axial projections of corresponding vectors.

The input parameter for the model can be the discharge voltage U or the discharge current I, depending on the slope of the current-voltage characteristics (CVC); see discussion in [4].

Results reported in this work refer to a krypton discharge under the pressure of 60, 100 and 120 Torr, the interelectrode gap and radius, R, of the discharge vessel are $5 \times 10^{-4}\,m$. The (only) ionic species considered in the modelling is Kr_2^+. The mobility of the ions is given by the formula $\mu_i = 1.21 \times 10^{-4} kT))/p\ ms^{-1}$ [8], where $T = 300K$ is the gas temperature. The mobility of the electrons is given by the formula $\mu_e = 0.421 \times 10^{24} kT/p\ ms^{-1}$; Townsend's ionization coefficient was evaluated by means of the formula $\alpha = C\rho \exp(-D(p/E)^{1/2})\ m^{-1}$ [9] where $C = 3.57 \times 10^3 m^{-1} Torr^{-1}$ and $D = 2.82 \times 10^2 V^{1/2} m^{-1/2} Torr^{-1/2}$. Diffusion coefficients were evaluated by means of Einstein's law, $D_{i,e} = kT_{i,e}\mu_{i,e}/e$, where k is Boltzmann's constant and $T_e = 1eV$ is the temperature of the electrons. The coefficient of dissociative recombination of molecular ions Kr_2^+ was taken as $2 \times 10^{-13} m^3 s^{-1}$ [10]. The effective secondary emission coefficient was set to equal to 0.03.

The modelling was performed in COMSOL Multiphysics using the interfaces *Transport of Diluted Species* and *Electrostatics*. The mesh used in 3D models contains 8400 to 26460 elements; symmetry considerations are used to reduce the computation time by modelling only part of the vessel. (For example, the computational domain for a 3D mode with period $\pi/2$ corresponds to 1/8 of the vessel.) The solver employed is a direct stationary solver, and the equations are fully coupled.

It must be stressed that in order to find 3D modes, one must know what they look like and where to find them. This information can be obtained by means of bifurcation analysis. In this work, bifurcation points for krypton were computed by the same method employed in [3].

2.2 Results

The discharge in krypton under the same conditions of the modelling [4,5], 30 Torr and interelectrode gap of 0.5 mm, is obstructed, i.e., there is no falling section of the current density-voltage characteristics (CDVC) and self-organization is not present. If pressure is increased to 60 Torr, a falling section and bifurcation points appear. The 1D mode, which is termed the fundamental mode, and bifurcation points computed under the pressures of 60 and 120 Torr are shown in figure 1 for two different radii of the discharge vessel: 0.5mm and 1.5mm. (In the figure, $< j >$ is the average value of the axial component of the

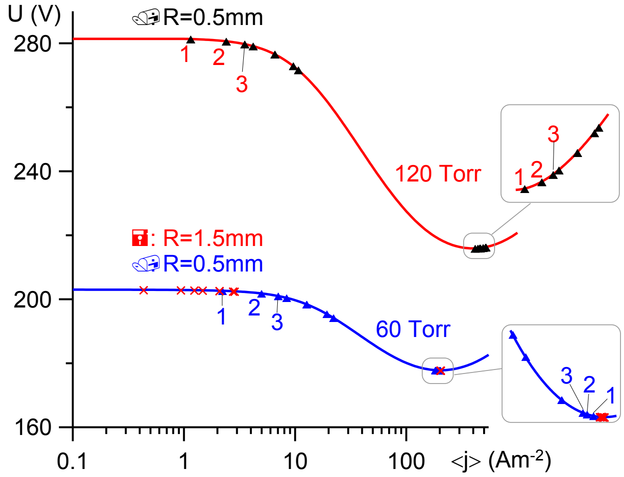


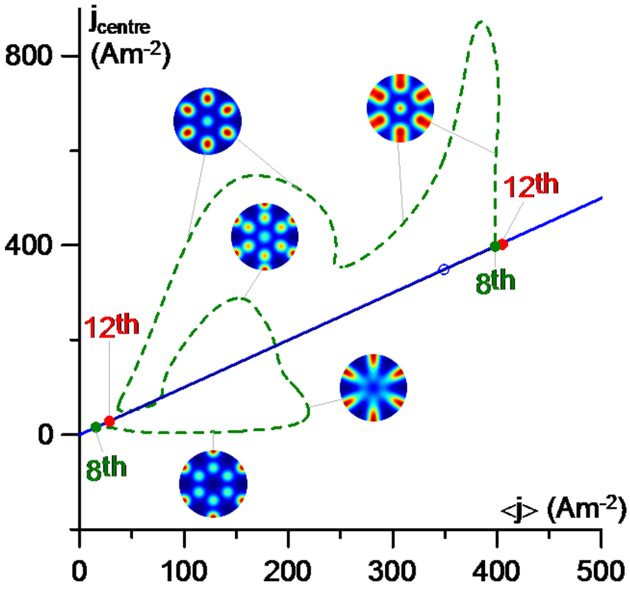
Figure 1: CVCs, Kr, fundamental mode. Crosses, triangles: bifurcation points.

electric current density evaluated over the whole cathode surface.) Each 3D mode possesses two bifurcation points: the first is positioned at low currents and the second at high currents, near the point of minimum of the CDVC. The mode which branches off from the first bifurcation point at lower currents is termed the 1st mode; the mode which branches off from the second bifurcation point is termed the 2nd mode; and so on.

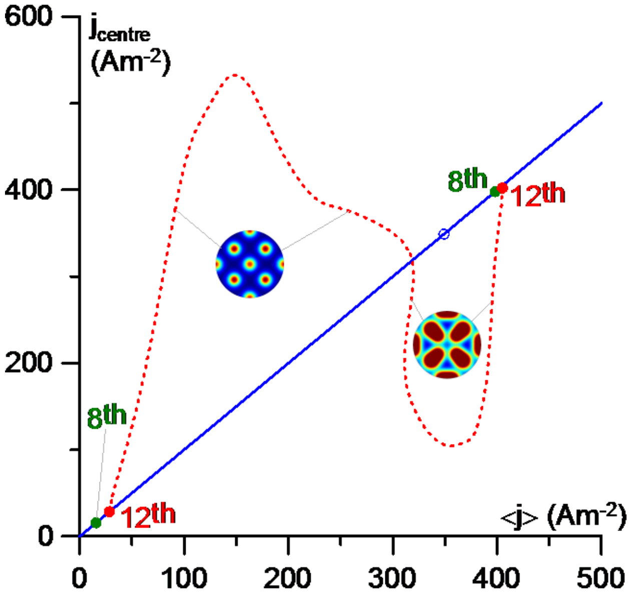
An increase of the pressure to 120 Torr results in the appearance of bifurcation points over the rising section of the CDVC (a result very interesting theoretically). Moreover, the first bifurcation point at low currents is paired with the first bifurcation point after the point of minimum; this pair is marked with the number 1 in figure 1. The second bifurcation point at low currents is paired with the second bifurcation point after the point of minimum; this pair is marked 2 in figure 1, and so on. Hence, the range of existence of the 3D modes does not decrease as the order of the modes increases; in fact modes of higher order may have a wider range of existence than modes of lower order. This is the opposite of what happens at 60 Torr.

An increase of the radius of the discharge vessel has the effect of increasing the range of existence of the 3D modes.

Two 3D modes have been computed for krypton under the pressure of 100 Torr and $R = 0.5$ mm. The CVCs of the modes are overlapping and in some ranges of discharge current almost coincident with the 1D mode, which is typical of modes with many spots. The modes are more conveniently represented in the coordinates $(< j >, j_{centre})$, where j_{centre} is the current density at the centre of the cathode surface. The resulting diagram is called a bifurcation



(a)



(b)

Figure 2: Bifurcation diagrams, Kr, 100 Torr, $R = h =$ 0.5 mm. Solid: fundamental mode. Dashed: 8th 3D mode. Dotted: 12th 3D mode. Full circles: bifurcation points. Open circles: point of minimum of the CVC of the fundamental mode. (a): 8th mode. (b): 12th mode.

diagram. In figure 2 the 8th and 12th 3D modes are shown, respectively. The schematics in these figures represent the cathodic spot patterns associated with each mode. For each 3D mode there are two states for which the discharge parameters become one-dimensional. These states belong not only to the 3D mode in question, but also to the fundamental mode: the bifurcation points. One can see that each mode possesses two bifurcation points, one of these points being positioned at low currents and the other near the point of minimum of the fundamental mode, which is in agreement with results from bifurcation analysis. For both modes the second bifurcation point is positioned at the rising section of the CVC of the fundamental mode. Both 3D modes exhibit complex behaviour in the form of backward sections. Some of the backward sections are accompanied by a change in the spot patterns associated with the corresponding mode (e.g., a spot at the centre of the cathode may disappear beyond a turning point). In other words, more than one pattern of spots may be associated with each 3D mode.

3. Experimental

The discharge device employed in the experiments consists of a molybdenum foil as the anode, an alumina plate as the dielectric spacer and another molybdenum foil as the cathode. The thickness of each layer is 250 µm. A single circular hole of 750 µm in diameter is prepared on both the anode and the dielectric spacer, and aligned before assembling to the cathode with *Torr Seal*®. After a careful cleaning and annealing process, the device is installed in a vacuum chamber, which is then evacuated to a base pressure of ~0.2 mTorr. Research grade krypton (99.999%) is used to fill the chamber to a pressure of 50-1200 Torr. A Glassman® direct current high voltage power supply is used to drive the device through a 100 kΩ ballast resistor. Current is calculated through voltage measured across a 1 kΩ current monitoring resistor connected in series in the circuit. Voltage across the device is recorded directly through a multimeter.

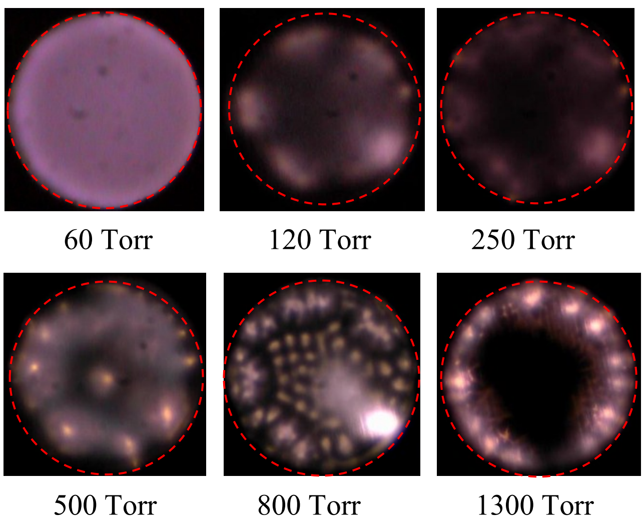
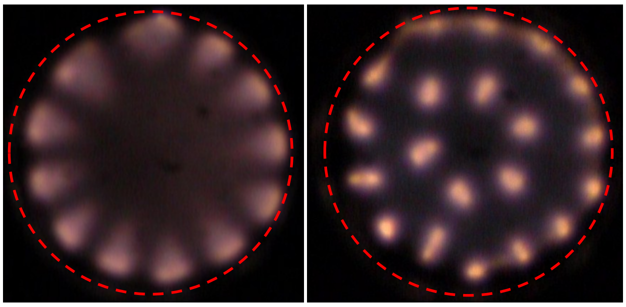


Figure 3: Exemplary visible photographs of CBLD operated in krypton at pressures from 60 to 1300 Torr. Pattern formation can be clearly seen from pressures of 120 Torr and beyond.

A few exemplary visible photographs of CBLD operated in krypton at pressures from 60 to 1300 Torr are shown in figure 3. No self-organization was observed in krypton at 60 Torr. At pressures above 120 Torr, clustered light emission was observed, despite that they were not as nicely patterned as in xenon. These clusters became confined to smaller areas at higher pressures with higher overall discharge currents. These preliminary results are in good correspondence with the trend predicted by the modelling results: at a given interelectrode distance (i.e. 250 microns in the current case), self-organized pattern formation in krypton favours higher pressure than what is usually required for xenon.

It should also be noted that self-organization in krypton seems to be more sensitive to the surface condition of the cathode than in xenon. The device aforementioned used an "as-is" cathode, i.e. the molybdenum cathode was cleaned following a standard cleaning protocol but was not polished. In another device, the cathode was polished following a three-step polishing procedure with a polishing machine. The final step is carried out on a polishing cloth with 3 micron polycrystalline diamond paste to achieve a mirror-like cathode surface condition. The result at 250 Torr is quite similar to the xenon case (at a pressure of ~150 Torr). Two visible photographs at different discharge currents are shown in figure 4 below, representing two different modes of operation.



(a)

Figure 4: Self-organized pattern formation in krypton at 250 Torr at discharge current of (a) 0.647 mA and (b) 0.535 mA.

4. Conclusions

Bifurcation analysis has predicted the existence of self-organization in krypton discharges provided that the product of pressure by interelectrode distance is high enough. This prediction has been confirmed both by modelling and experimentally. Bifurcation points computed by means of bifurcation analysis and those computed explicitly by means of full 3D modelling exhibit the same trend. The appearance of self-organized patterns of cathodic spots in DC glow microdischarges in krypton is demonstrated. Experimental results are in good correspondence with modelling predictions.

On a side note, we mention that COMSOL Multiphysics has proved to be an adequate tool for modelling self-organization in DC glow microdischarges.

Acknowledgements

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