Modelling spot patterns on cathodes of DC glow discharges

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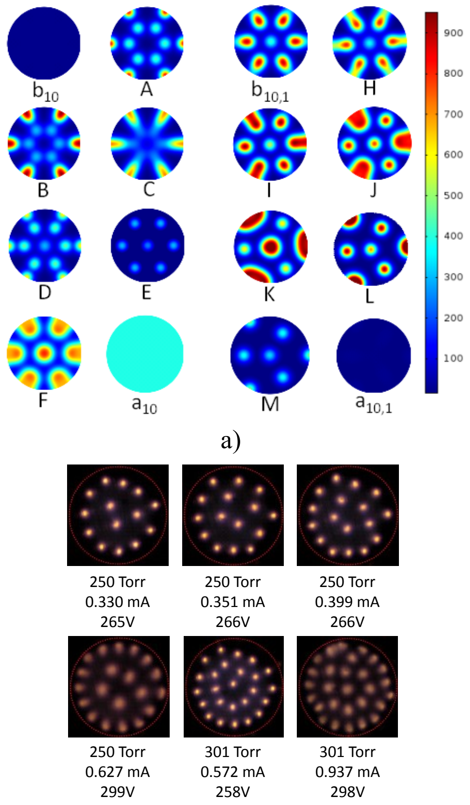
A summary and a discussion are given of recent results and techniques of the modelling of self-organization in DC glow discharges with bare electrodes. 2D (axially symmetric) and 3D solutions are given for different gases, different pressures, and different discharge configurations. A comparison of results obtained by means of stationary and time-dependent solvers is given. The possibility of the theory and modelling to guide experiments is illustrated. All the modelling is performed with the use of the basic package of commercial software COMSOL MultiPhysics; a discussion of delicate points of the use of this software will be presented.

1. Introduction

Self-organized patterns of cathodic spots in DC glow microdischarges have been observed for the first time a decade ago [1] and represent a very interesting and potentially important phenomenon. By now, a number of experimental reports on this phenomenon have been published, see review [2] for references, and a theoretical interpretation in terms of multiple solutions existing in the theory of glow discharge for the same value of discharge current has been given [2]. The cornerstone of the theory is the existence of bifurcations of steady-state solutions. It must be stressed that bifurcations are not an artificial mathematical construction or an elaborate numerical trick. There is a direct experimental proof of their existence in DC glow microdischarges, see [2,3] for a discussion and references. By now, modelling of self-organization in DC glow discharges has produced a substantial volume of results and has been successfully used as a guide for experiments [4].

An example of computed solutions is shown in figures 1 and 2, along with their experimental counterparts. The computed patterns of cathodic spots are in good agreement with the experiments, although the comparison has been merely qualitative up to now.

The modelling has shown that even the most basic self-consistent model of glow discharge, which takes into account a single ionic species and employs the local-field approximation, encompasses physical mechanisms responsible for self-organization, which are ionization and transport of charged particles. Modelling performed for different gases and under different conditions support this conclusion; it has also been found that the inclusion in the model of a detailed kinetic scheme and of non-locality of electron transport and kinetics not only does not affect the pattern of self-organization, but also increases the number of multiple solutions [5].



a)

b)

Figure 1: Computed (a) and experimentally observed (b) patterns in krypton. From [4].

A number of interesting questions have been triggered by the above-mentioned modelling, in particular: why were the multiple solutions not found before, or, why are they difficult to find when conventional modelling techniques of gas-discharge physics are employed? What does one need to do in order to compute such multiple solutions? The answer to these questions is multi-fold. There are

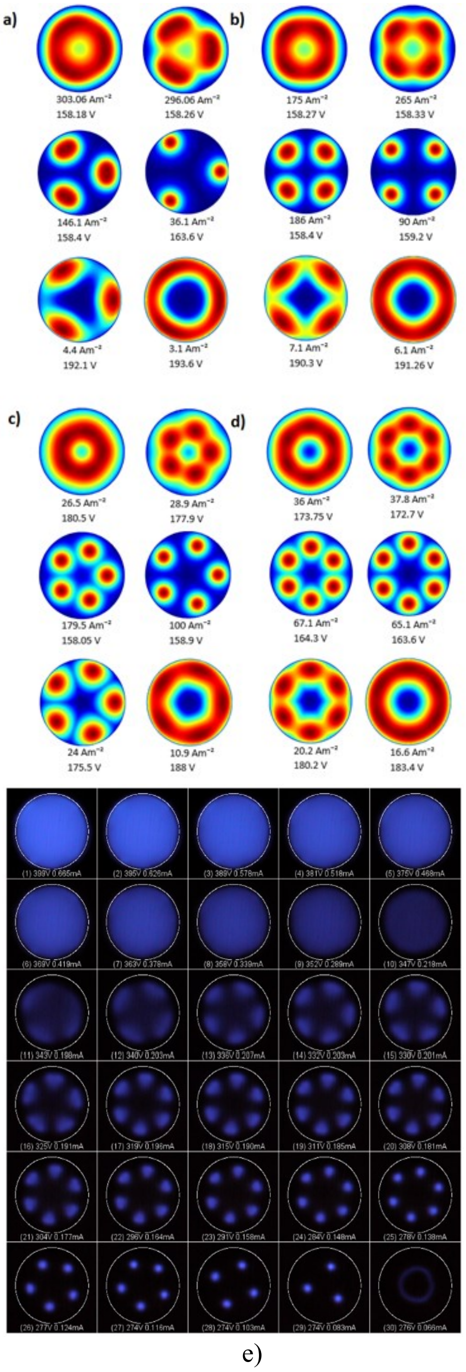


Figure 2: Computed patterns on the cathode of a cathode boundary layer discharge in xenon (a-d, from [8]) and experimentally observed patterns (e, from [10]).

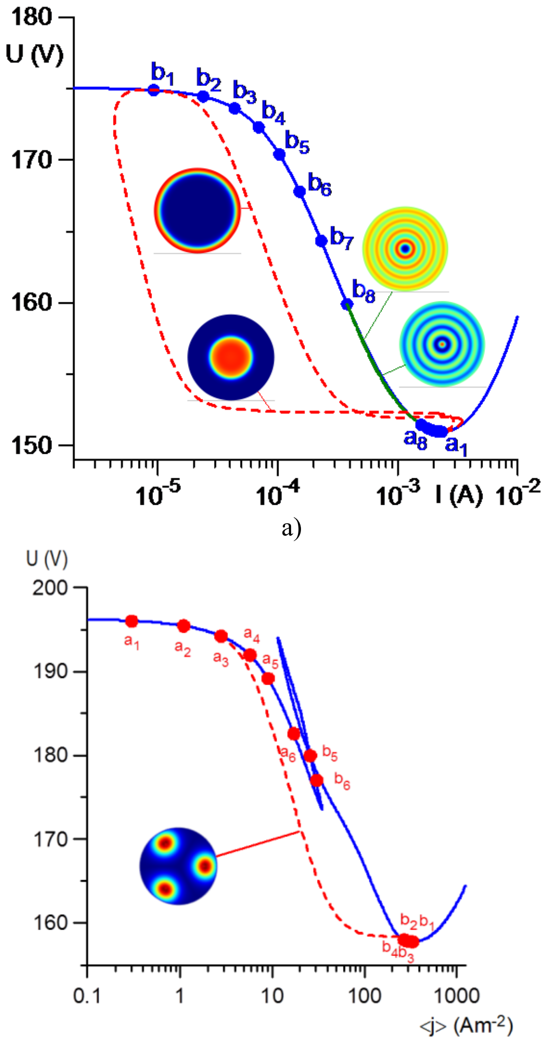
three key points in the modelling.The first is the use of a steady-state solver, as opposed to the standard practice in the modelling of gas-discharges of employing a time-dependent solver. Another key point in the computation of multiple solutions is the need to know where to look for these solutions and what do they look like. The final key point is the need to switch easily and seamlessly between discharge current and discharge voltage as the input parameter.

A powerful and convenient modelling tool that allows systematic computation of self-organized spot patterns on cathodes of DC glow discharges are steady-state solvers of the basic package of commercial software COMSOL Multiphysics. This software offers the possibility of representing the anode potential in terms of discharge current without the need to introduce in the model an external circuit, thus allowing for seamless switching between discharge current and voltage as the control parameter.

All the modelling reported in this work has been performed with the use of the basic package of COMSOL MultiPhysics. Simulation results are reported for two discharge configurations: the classical case of a cylindrical vessel with plane parallel electrodes and the so-called cathode boundary layer discharge (CBLD). CBLD has an electrode geometry consisting of a planar cathode and an anode with a circular opening, separated by a dielectric (cf. Fig. 1 of [4]).

2. How to compute the multiple solutions?

The general procedure for finding multiple solutions is as follows. The first step is computing the fundamental mode, i.e., the solution that exists for all values of discharge current. The second step is to find bifurcation points, i.e., states of the fundamental mode at which non-fundamental modes branch off. This is accomplished by means of an analysis of the linear stability of the fundamental mode against 2D and/or 3D perturbations. The perturbations are assumed to grow or decay exponentially in time; the azimuthal period of the perturbations being specified. A formal description of the procedure is skipped for brevity; it can be found in [7]. Broadly speaking, an eigenvalue problem for the increment of each perturbation can be formulated and conveniently solved in COMSOL Multiphysics by means of an eigenvalue solver, without making any substantial change to the equations of the model. The bifurcations are detected as the states belonging to the fundamental mode for which the real part of the increment of the perturbations changes signal. By repeating the procedure for each azimuthal period of the perturbation, one gains information on the values of current for which non-fundamental modes branch off from the fundamental one, and on the symmetry of the branching mode – for example, the simplest 3D mode with period 2π comprises one spot; the



a)

b)

Figure 3: Computed CVCs of different modes, xenon at 30 Torr. Solid: fundamental mode. Dashed: non-fundamental modes. Circles: bifurcation points. a) cylindrical discharge between parallel plane electrodes. Radius is 1.5mm and interelectrode gap 0.5mm. From [7] b) CBLD, radius and electrode separation of 0.5mm, from [9].

simplest mode with period π comprises two spots, etc. In other words, after a bifurcation analysis one will know where on the fundamental mode to search for multiple solutions and what they look like.

In figure 3, two examples are shown of computed current voltage characteristics (CVC) of fundamental modes and bifurcation points. (In the figure, *I* is discharge current and <*j*> is average current density.) Also shown in the figure is the CVC of non-fundamental modes. The schematics illustrate the spot patterns associated with these modes.

3. Time-dependent vs. stationary solvers

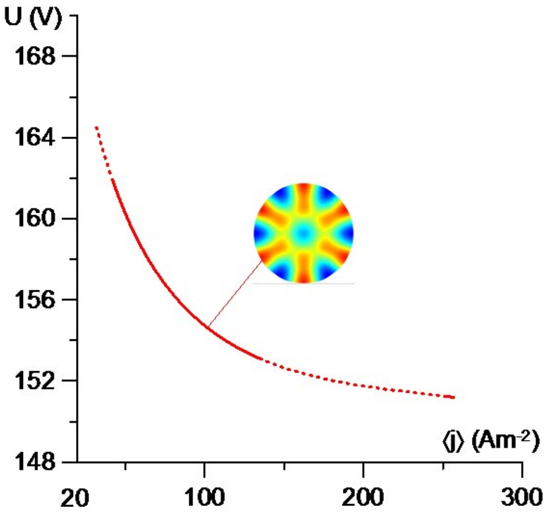


Figure 4: CVC of a 3D non-fundamental mode in a cylindrical discharge between parallel plane-electrodes in xenon at 30 Torr. Radius and interelectrode gap of 0.5mm. Solid: time-dependent solver. Dashed: stationary solver. From [9].

The most commonly used solvers in the modelling of gas discharges are time-dependent. However, time-dependent solvers do not allow decoupling questions of numerical and physical stability. Therefore, a complete and systematic study of retrograde sections and complex behaviour (cf. figure 3b) can hardly be performed by means of time-dependent solvers. In fact, multiple solutions in the theory of DC glow discharges have been computed using stationary solvers.

On the other hand, some sections of these solutions can be computed by means of time-dependent solvers. As an example, a comparison of the computation of a 3D mode using a time-dependent and a stationary solver is shown in figure 4. It can be seen that a significant section of the 3D mode cannot be computed with the time-dependent solver. Results not shown here suggest that this is indeed a general feature of time-dependent solvers and that such solvers cannot be used for a systematic study of multiple solutions. An in-depth discussion can be found in [9].

4. Theory and modelling as a guide for experiments

Until very recently, self-organization in DC microdischarges had only been observed in xenon and not in other gases like argon; see [5] for a discussion and references. The theory and modelling, however, predict that this kind of self-organization is a general phenomenon not exclusive of xenon; it should be observable in other gases provided that conditions are right. More specifically, the pressure must be high enough so that a falling

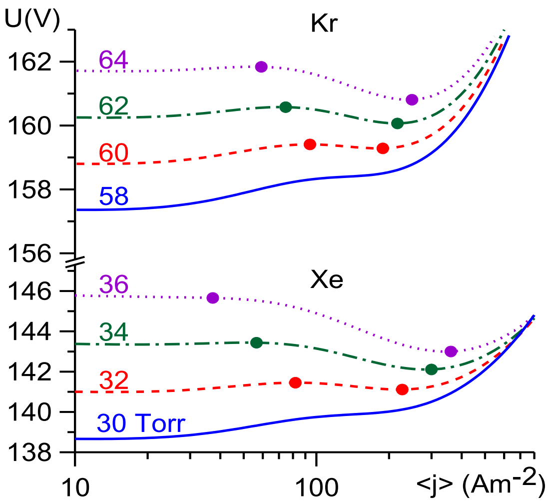


Figure 5: CVC of the 1D fundamental mode computed for xenon and krypton at different pressures. Circles: bifurcation points of the first non-fundamental mode. Radius of 0.375mm and interelectrode gap of 0.250mm. From [4].

section of considerable size is present in the CVC of the fundamental mode [5]. The required pressure can be found by means of bifurcation analysis, an approach used to guide experiments designed to finding self-organization in krypton CBLD. In figure 5 the computed CVC of the (1D) fundamental modes for xenon and krypton are shown for different pressures. Also shown are the bifurcation points of the first 3D mode. It has been found that the minimum pressure for the onset of self-organization in krypton should be roughly twice as high as that of xenon; a prediction that was confirmed experimentally [4].

In figure 6 examples of the computed 3D modes for krypton are mapped in the plane ($<j>$, j_c), where j_c is the current density at the centre of the cathode. It has been found that third generation 3D modes exist for krypton, i.e., 3D modes that branch off from other 3D modes through period-doubling bifurcations. One of such second-generation modes is the 3D mode $a_{10,1}$ $b_{10,1}$, which branches off from the mode a_{10} b_{10}. The evolution of the patterns associated with these modes is shown in figure 1a); the azimuthal period of mode $a_{10,1}$ $b_{10,1}$ is indeed twice that of mode a_{10} b_{10}.

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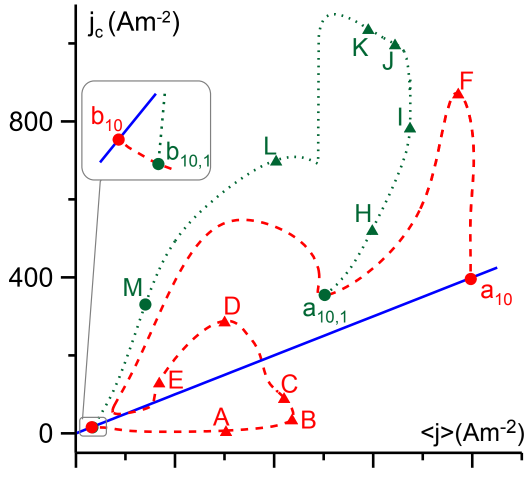

Figure 6: 3D modes in a cylindrical discharge in krypton at 100Torr. Solid: 1D. Dashed: second generation 3D mode. Dotted: third generation 3D mode. Circles: bifurcation points. Triangles: states for which spot patterns are shown in figure 2a)-d). Radius and interelectrode gap of 0.5mm.

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