Mathematical modelling of stability of 1D and 2D DC glow discharges with the use of COMSOL Multiphysics

P. G. C. Almeida, M. S. Benilov, and M. J. Faria

Departamento de Física, Universidade da Madeira, Largo do Município, 9000 Funchal, Portugal

Stability of 1D and 2D (axially symmetric) DC glow discharge against small perturbations is investigated in the framework of the linear stability theory with the use of software COMSOL Multiphysics. Conditions of current-controlled microdischarges in xenon are treated as an example. Variations of the increments of perturbations with discharge current are investigated for the 1D glow discharge and different modes of axially symmetric glow discharge. Both real and complex increments have been detected, meaning that perturbations can vary with time both monotonically and with oscillations. In general, results given by the linear stability theory confirm intuitive concepts developed in the literature and conform to the experiment. On the other hand, the theory provides suggestions for further experimental and theoretical work.

1. Introduction

Multiple solutions in the theory of DC glow discharges have been computed recently [1,2]. Some solutions describe modes with a normal spot and the others describe modes with patterns of multiple spots similar to those observed in DC glow microdischarges in xenon; e.g., [3]. In this abstract, stability of 1D and 2D fundamental modes, i.e., the ones which exist in a wide current range, is studied in the framework of the linear stability theory. Results on stability of non-fundamental modes are skipped here because of lack of space but will be presented at the conference. Software COMSOL Multiphysics is employed. Note that this software includes, in addition to powerful steady-state solvers, also an eigenvalue solver, which makes it fit for the task.

2. The model

2.1. System of equations and boundary conditions

In [4] self-organized patterns on DC glow cathodes have been studied by means of a model which accounts for atomic and molecular ions, non-equilibrium population of excited states, several ionization channels, and comprises an energy equation for the electrons. It was found that the effect of chemistry and non-locality of electron kinetic and transport coefficients does not cause qualitative changes in self-organization. Therefore, in this abstract, a simple model is used which takes into account a single ion species (molecular ions) and employs the local-field approximation.

The system of equations comprises equations of conservation of a single ion species and the electrons, transport equations for the ions and the electrons written in the drift-diffusion local-field approximation, and the Poisson equation:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot \mathbf{J}_i = w, \quad \mathbf{J}_i = -D_i \nabla n_i - \mu_i n_i \nabla \varphi, \tag{1}$$

$$\nabla \cdot \mathbf{J}_e = w, \quad \mathbf{J}_e = -D_e \nabla n_e + \mu_e n_e \nabla \varphi, \tag{2}$$

$$\varepsilon_0 \nabla^2 \varphi = -e(n_i - n_e), \tag{3}$$

where

$$w = n_e \alpha \mu_e E - \beta n_e n_i. \tag{4}$$

Here n_i, n_e, J_i, J_e, D_i, D_e, μ_i, and μ_e are number densities, densities of transport fluxes, diffusion coefficients, and mobilities of the ions and electrons, respectively; α is Townsend's ionization coefficient; β is the coefficient of dissociative recombination; φ is scalar potential; $E = |\nabla\varphi|$ is the electric field strength; ε_0 is the permittivity of free space; e is the elementary charge; and t is time.

Numerical results refer to a discharge in xenon under the pressure of 30 Torr. The transport and kinetics coefficients are the same that in [1]; in particular, constant values are assumed for the transport and dissociative recombination coefficients.

The discharge occurs in a vessel in the form of a right circular cylinder of a radius R = 1.5 mm and of a height h = 0.5 mm. Let us 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. Boundary conditions at the cathode and anode are written in the conventional form. One boundary condition at the (dielectric) lateral wall of the discharge vessel is zero of the radial component of the total electric current density. The boundary conditions of the charged particles at the wall are written under the assumption that all ions and electrons coming to the wall are absorbed.

The discharge is assumed to be current-controlled. Therefore, the discharge voltage U is found in the course of simulations.

The above stationary problem admits an axially symmetric (2D) solution, $F = F(r,z)$ (here F is any of the quantities n_i, n_e, and φ) which exists at all discharge currents: the fundamental mode. Under certain conditions, the problem admits also other 2D and 3D solutions, which exist in a limited current range. In this abstract, results on stability of the 2D fundamental mode are reported.

It is of interest to consider also the case where all charged particles coming to the wall are reflected rather then absorbed. The fundamental mode of the discharge becomes 1D: all the parameters vary only in the axial direction, i.e., $F = F(z)$. This is the 1D form of glow discharge to which the classical von Engel and Steenbeck theory refers. The pattern of stability of this mode is the simplest and the easiest to understand. Besides, investigation of its stability includes a determination of points of bifurcation of steady-state modes, which are important for understanding the pattern of multiple steady-state modes [5] and calculation of these modes [1]. For this reason, stability of the 1D glow discharge is investigated as well.

2.2. Eigenvalue problem describing stability

Perturbations of 2D (1D) stationary states can be 2D or 3D (or 1D). In the framework of the conventional formalism of the linear stability theory, a solution to the above-described problem is sought as sum of a steady-state solution and small perturbations with exponential time dependence. Taking into account that the 3D perturbations are harmonic with respect to the azimuthal angle ϕ, one can write

$$n_{i,e}(r,\phi,z,t) = n_{i0,e0}(r,z) + e^{\lambda t} n_{i1,e1}(r,z)\cos m\phi + \ldots, \quad (5)$$

$$\varphi(r,\phi,z,t) = \varphi_0(r,z) + e^{\lambda t}\varphi_1(r,z)\cos m\phi + \ldots, \quad (6)$$

$$U(t) = U_0 + e^{\lambda t} U_1 + \ldots. \quad (7)$$

Here the first term on the rhs (right-hand side) of each expansion represents a solution describing the stationary state stability of which is being studied; the second term represents a perturbation of this state; λ is the increment of growth of the perturbation; and $m = 0, 1, 2, \ldots$. If $m = 0$, the perturbation being considered is 2D (or 1D). If $m = 1, 2, \ldots$, the perturbation is 3D with period in ϕ equal to $2\pi/m$.

Substituting expansions (5)-(7) into equations of the above-problem, linearizing, and equating linear terms, one obtains a linear eigenvalue problem, λ being the eigenvalue. By means of solving this problem for a given m, one will determine a set of eigenvalues λ (spectrum) associated with this m. By means of repeating this procedure for each m and joining the obtained spectra, one will find the whole spectrum of the stationary state being treated. If real parts of all eigenvalues are non-positive, the state is stable; if at least one eigenvalue has a positive real part, the state is unstable.

Numerical results have been performed with commercial software COMSOL Multiphysics, version 4.0a. The procedure is not quite straightforward and will be presented in detail at the conference.

3. Stability of the 1D fundamental glow discharge

The current-voltage characteristic (CVC) of the 1D glow discharge is shown in figure 1. A large number of different perturbation modes have been found, which are real or complex conjugate.

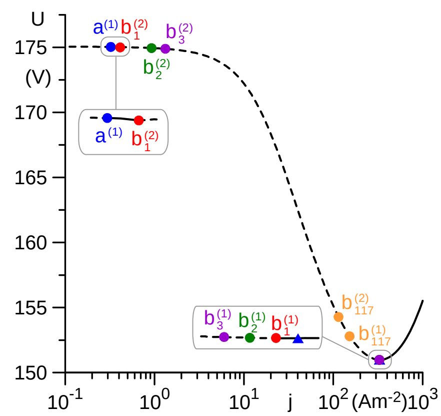

Figure 1 - CVC of the 1D glow discharge. Solid: stable sections. Dashed: unstable sections. Circles: points of change of stability against a mode of real perturbations or against two complex conjugate modes. Triangle: point of minimum of the CVC.

It is convenient to introduce "quantum numbers" in order to identify different modes of perturbations. Dependence of perturbations of 1D stationary states on r and ϕ is given by $J_m(j'_{ms}\, r/R)\cos(m\phi)$, where $J_m(x)$ is the Bessel function of the first kind and j'_{ms} is the sth zero of the derivative of the Bessel function of order m, $m = 0, 1, 2, \ldots$, $s = 1, 2, 3, \ldots$. So m and s are natural candidates. One more "quantum number" is needed in order to distinguish between perturbation modes associated with the same pair (m, s) but with different dependences on z. Let us number such perturbation modes in the order of decrease of Re λ; in the case of a pair of complex conjugate perturbations, the one associated with an increment with a positive imaginary part is counted first. Let us designate this number by l and use as the missing "quantum number".

Switching of perturbations of different modes between decay and growth is illustrated by figure 2. At $j \geq j_{\min}$, where $j_{\min}$ is the current density at the minimum point of the CVC, real parts of the increments of all perturbation modes are negative, so the discharge is stable. As j decreases, real parts of the increments increase and eventually one of them turns positive. This happens at j slightly below $j_{\min}$, the corresponding state is designated $b_1^{(1)}$, and the perturbation that becomes growing is one with $m = s = 1$. As j decreases further, real parts of the increments of other perturbations turn positive. This happens in the order of increase of the value of $j_{ms}^{'}$. Altogether, 117 perturbation modes become growing between the point of minimum of the CVC and the state $b_{117}^{(1)}$, with 8 of these modes being 2D

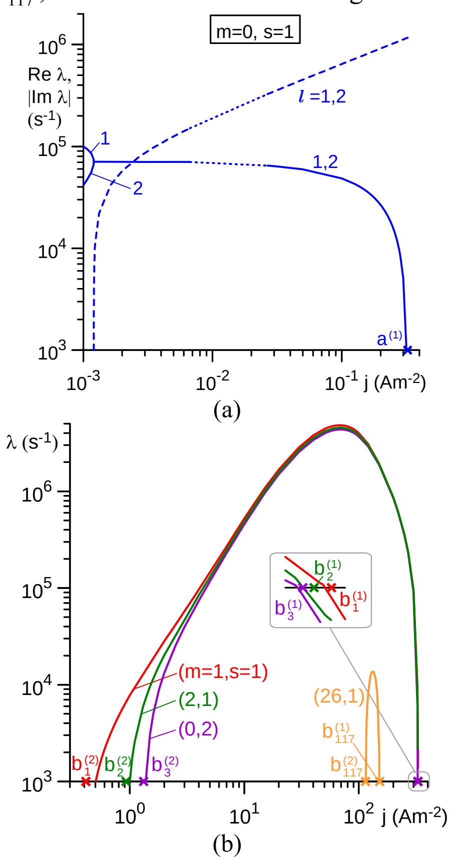

Figure 2 - Increments of growing perturbations of the 1D glow discharge. Solid: real part of the increment. Dashed: modulus of the imaginary part. Dotted: increments unknown. Crosses: values of j where stability changes against a mode of real perturbations or against two complex conjugate modes. a) 1D perturbations. b) Axially symmetric and 3D perturbations.

and 109 being 3D.

As j decreases further, real parts of the increments of all growing perturbation modes return to negative values. This happens in the order of decrease of $j_{ms}^{'}$. The discharge has regained stability at state $b_1^{(2)}$. However, the stability is lost once again at state $a^{(1)}$, where the real part of the increments of two conjugate perturbation modes with ($m = 0$, $s = 1$), which are 1D, becomes positive. As current decreases further, no more stability changes occur and the discharge remains unstable.

4. Stability of the 2D fundamental glow discharge

The CVC of the 2D fundamental mode is shown in figure 3.

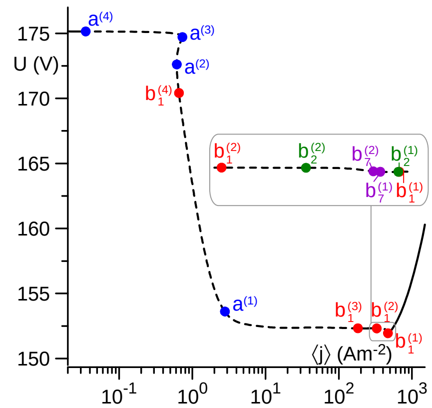

Figure 3 - CVC of the axially symmetric glow discharge. Solid: stable sections. Dashed: unstable sections. Circles: points of change of stability against a mode of real perturbations or against two complex conjugate modes.

Dependence of perturbations of axially symmetric stationary states on ϕ is given by $\cos(m\phi)$. In order to distinguish between perturbation modes associated with the same m but with different dependences on r and z, we once again number such perturbation modes in the order of decrease of Re λ and designate this number by q.

Switching of perturbations of different modes between decay and growth is illustrated by figure 4. At $\langle j \rangle \geq 469$ Am^{-2}, real parts of the increments of all perturbation modes are negative and the discharge is stable. As $\langle j \rangle$ decreases, real parts of the increments increase and eventually Re λ of two complex conjugate perturbation modes with $m = 1$ becomes positive. This happens at $\langle j \rangle \approx 469$Am^{-2}; state $b_1^{(1)}$. As $\langle j \rangle$ decreases further, real parts of the increments of other perturbation modes turn positive. This happens in the order of increase of the value of m. The last perturbation mode to becomes growing has

m = 7 (at state $b_7^{(1)}$). As $\langle j \rangle$ decreases further, real parts of the increments of all growing perturbation modes return to negative values.

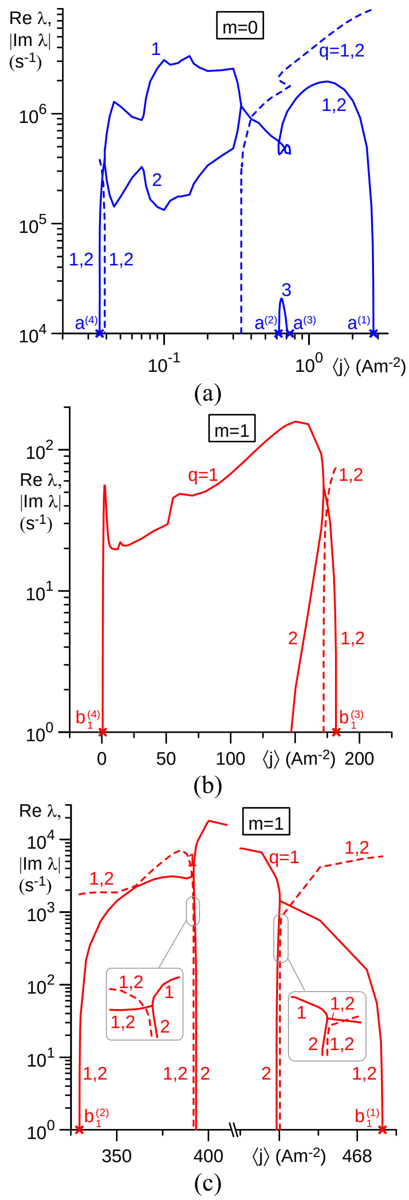

Figure 4 - Increments of growing perturbations of the axially symmetric glow discharge. Solid: real part of the increment. Dashed: modulus of the imaginary part. Crosses: values of $\langle j \rangle$ where stability changes against a mode of real perturbations or against two complex conjugate modes. a) Axially symmetric perturbations. b), c) 3D perturbations with m = 1.

After having regained stability at state $b_1^{(2)}$ ($\langle j \rangle \approx$ 330 Am^{-2}), the discharge remains stable until state $b_1^{(3)}$ ($\langle j \rangle \approx$ 182 Am^{-2}) where two modes with m = 1 become growing. One of these perturbations returns to being decaying at $\langle j \rangle \approx$ 141 Am^{-2} and the other at $\langle j \rangle \approx$ 0.66 Am^{-2} (state $b_1^{(4)}$). Since there are two growing perturbation modes with m = 0 in the current range 36 mAm^{-2} < $\langle j \rangle$ < 2.8 Am^{-2}, i.e., between states $a^{(1)}$ and $a^{(4)}$, the discharge become stable only for currents below 36 mAm^{-2}.

5. Conclusions

A pattern of stability of 1D and 2D glow discharges was established. Both real and complex increments of perturbations have been detected, meaning that perturbations can vary with time both monotonically and with oscillations. The 1D glow discharge is stable in the current range where the CVC is rising and unstable where the CVC is falling. The 1D Townsend discharge is unstable at low current. The 2D fundamental mode is stable when it operates in the abnormal regime and in a certain current range in the normal regime. The subnormal discharge is unstable. Loss of the charged particles at the lateral wall stabilizes Townsend discharge at low currents. In general, results given by the linear stability theory confirm intuitive concepts developed in the literature and conform to the experiment. On the other hand, the theory provides suggestions for further experimental and theoretical work.

6. Acknowledgments

The abstract was performed within activities of the project PTDC/FIS/68609/2006 of FCT, POCI 2010 and FEDER and of the project Centro de Ciências Matemáticas of FCT, POCTI-219 and FEDER. P. G. C. Almeida and M. J. Faria appreciate PhD Fellowships from FCT through grants SFRH/BD/30598/2006 and SFRH/BD/35883/2007.

7. References

[1] P. G. C. Almeida, M. S. Benilov and M. J. Faria, Plasma Sources Sci. Technol. 19 (2010) 025019.

[2] P. G. C. Almeida, M. S. Benilov and M. J. Faria, IEEE Trans. Plasma Sci. 39 (2010) to appear.

[3] K. H. Schoenbach, M. Moselhy and W. Shi, Plasma Sources Sci. Technol. 13 (2004) 177-185.

[4] P. G. C. Almeida, M. S. Benilov and M. J. Faria, Proc. 63rd Gaseous Electronics Conf. and 7th Int. Conf. on Reactive Plasmas 55 (2010) 166.

[5] P. G. C. Almeida, M. S. Benilov, M D Cunha and M. J. Faria, J. Phys. D: Appl. Phys. 42 (2009) 194010.