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# Monte Carlo simulation of a sputtering hollow-cathode discharge for laser applications

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**Abstract.** We report on a kinetic model that computes the electron behaviour in a hollow cathode discharge. It is a part of the PLASIMO toolkit and is based on a Monte-Carlo technique. The model is tested by varying the input parameters and by comparing the output with the output obtained by the freeware Boltzmann equation solver BOLSIG+. The results show that the Monte-Carlo model gives reliable information about the behavior of the electrons in the discharge. The Monte-Carlo module is applied to the case of a hollow cathode discharge for laser applications. Analysis of the output data and its adequateness is done. Future developments of the model are discussed.

## 1. Introduction

In a hollow cathode discharge (HCD) device the closed cathode shape results in more efficient use of the charged particles: the higher ion current to the cathode give rise to higher second electron emission and higher cathode sputtering rate. These characteristics make the HCD appropriate for a variety of applications: atomic spectrometry, UV light generation, plasma processing, ion sources, laser technologies and others. One of the important applications of HCDs is as excitation medium of ion metal vapour lasers using cathode sputtering for metal atom production.

The research of these lasers has for long time engaged modeling techniques side by side with experiments. Two main modeling approaches exist: fluid and kinetic. The fluid approach is often very accurate when sufficient collisions take place in the plasma [1], i.e. when the particles mean free path is smaller than the plasma size.

A number of models simulating HCD have been published so far (see [1] and references therein). One of them developed in recent years is PLASIMO's simulation platform MD2D model [2] - a time dependent two-dimensional multi-fluid model. The results of the MD2D model are found to agree well with experimental and analytical observations on HCD [3]. However not all discharge phenomena can be simulated with a pure fluid model – e.g. “fast” electrons kinetics, ion inertia in cathode fall region, sputtering yield dependence on ion energy. In order to investigate these issues and to test their influence on the simulation results a kinetic model is required. Such model provides description of the discharge by closely following a large number of simulated particles, which is possible at the expense of a long simulation time. The kinetic model can be used in two ways. First, it can be employed as a



stand-alone model where the simulated particles move and collide in plasma with defined properties. Such a PLASIMO Monte Carlo (MC) sub-module has been previously developed to simulate drift-diffusive plasma [4]. Second, the kinetic model can be used in hybrid simulations [5]. In this case, some of the characteristics of the studied system are described by a fluid model while others are delegated to the MC module.

As a first attempt in the field our aim is to develop a stand-alone MC PLASIMO sub-model for the electrons in a HCD for laser applications. By closely following the electrons in both cathode fall and bulk regions, the kinetic model will provide as output more accurate data for the electron energy distribution function and the mean electron energy. These values are supposed to be used for input by the fluid MD2D model. In such a way the kinetic model will enable the development of a more realistic model of the HCD.

## 2. Theoretical and experimental setup

The developed kinetic model is based on the MC statistical technique. This technique is usually applied for gas discharges, in which one or more of the particle species are far from thermodynamic equilibrium [4]. In HCD plasma the electrons are such species.

The model requires as input the discharge geometry, the profile of the electric field, a list of species and a set of reaction among the defined species. As electrons are the followed particles, the model treats only reactions in which they participate: the simulated electrons undergo excitation, ionization and elastic collisions with the buffer gas particles and ionization and elastic collisions with the sputtered metal atoms.

The environment buffer gas is a mixture of He and 5% Ar with pressure of 2.7 kPa [1]. The sputtered Cu metal atoms percentage is varied from 0÷2%.

The number of electrons in the simulations is chosen to be  $10^9$  and it is based on data for the electron density from the fluid model [3] and the cathode volume.

The kinetic model is engaged in the performing of two distinct experiments. The first aims to verify the kinetic model by comparing it with a known model. The second experiment is the actual simulation of the HCD.

### 2.1. Drift experiment - Infinite "vessel" with uniform electric field

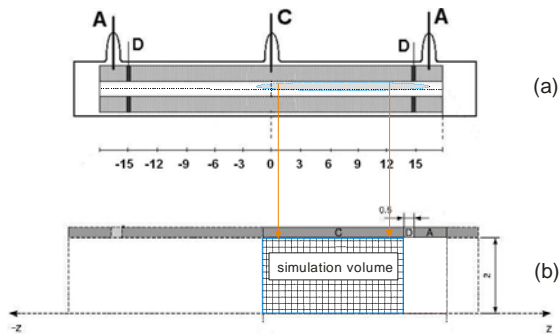
The kinetic model is compared with the freeware Boltzmann equation solver BOLSIG+ [6]. There are two main reasons for this comparison. First, Boltzmann equation solvers are an alternative of the kinetic models in solving the Boltzmann equation (BE). Second, so far BOLSIG+ is used to deliver the electron energy distribution function (EEDF) for the fluid model, which uses the EEDF to obtain electron rate and transport coefficients.

The conditions for the comparison are: infinite "vessel" and uniform electric field. The value for the electric field is varied between 0÷2000 Td.

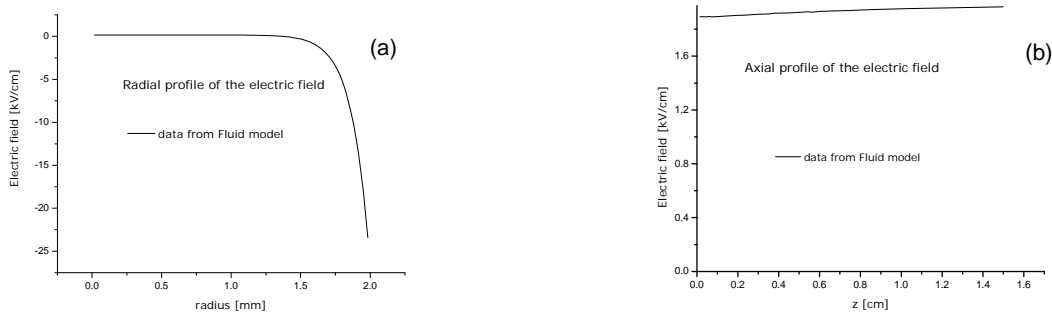
### 2.2. HCD – Cylinder with non-uniform electric field

The simulated HCD is active medium of a copper vapour laser [3]. The experimental realization of this HCD consists of an anode-cathode-anode configuration of the type shown in figure 1(a). Due to the existing symmetry the model simulates just one fourth of the cathode – figure 1(b). The sizes of the cathode are the following – inner diameter 4 mm and length 30 mm.

The electric field in HCD plasma is not uniform [1,3]. The profile of the applied electric field is constructed out of numerical data from the fluid model. It is decomposed in two projections: axial and radial – figure 2, which are fitted with appropriate functions and used in that form in the MC simulation.



**Figure 1.** Experimental setup: (a) anode-cathode-anode configuration of HCD; (b) the simulated part of the cathode volume.

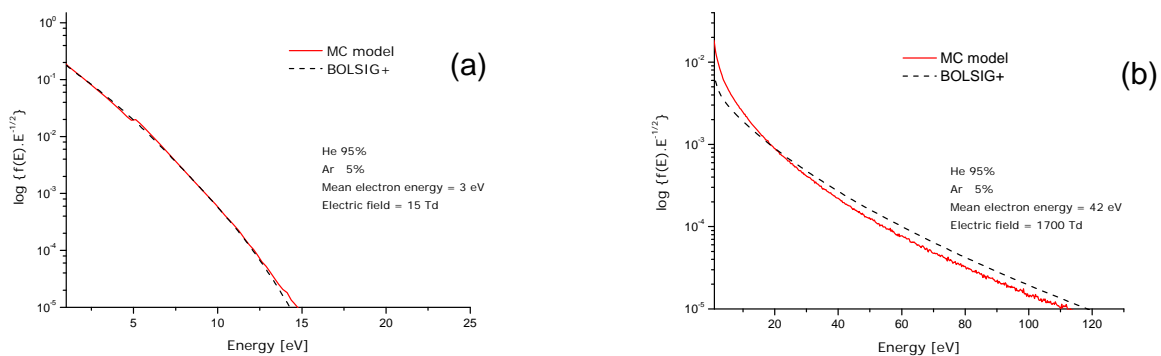


**Figure 2.** Applied profiles of the electric field in the simulation: (a) radial profile; (b) axial profile.

### 3. Results

#### 3.1. Comparison of MC model and BOLSIG+

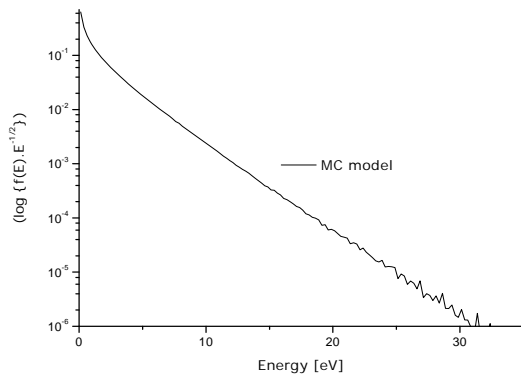
In order to verify the kinetic model we compare it with a known model as stated in section 2.1 under constant electric field. The electric field value is chosen according to the typical values for HCD. As known the HCD comprises of almost field-free negative glow (NG) with electric field in the order of 10 Td and cathode fall (CF) region with much higher field – 1500 Td. We present comparison results for the two typical cases in figure 3: NG with 15 Td and CF with 1700 Td. There is reasonable agreement between the results of the two models. It is better for small values of the electric field – figure 3(a). For large values of the electric field – figure 3(b), we probably go out of the region of validity of the two-term approximation, which is used by BOLSIG+ [6]. That is most likely the reason for the discrepancy between the BOLSIG+ and MC model in figure 3(b).



**Figure 3.** Comparison of MC model and BOLSIG+ EEDFs under constant electric field: (a) 15 Td; (b) 1700 Td.

### 3.2. Simulation of HCD cylinder tube

The simulations are carried out under the set of conditions described in section 2.2. The EEDF, obtained from the simulation under optimal lasing conditions, is shown in figure 4. From this EEDF the mean electron energy (MEE) is computed.



**Figure 4.** EEDF obtained from the kinetic model under optimal lasing conditions

The EEDF obtained from the kinetic model is a better source for input data for the fluid MD2D model. This is due to the fact that the MC model takes into account the strong non-uniformity of the electric field and the specific cathode geometry of the HCD for lasing. Moreover, the values that the MC model produces are supposed to be more accurate in the region of high electric fields and according high particle energies.

### Conclusions

The development of a kinetic Monte-Carlo model for the calculation of electron behaviour in HCD for laser application is presented. The model is a part of the PLASIMO toolkit. The MC model is capable of obtaining the EEDF and from it the MEE for the HCD.

The model was compared to a Boltzmann solver – BOLSIG+. As both methods provide a solution of the BE, the comparison provided the opportunity of validating the kinetic model. There is good agreement for small values of the electric field, as for the case of high electric fields the differences are analyzed.

The future development of the model is mainly oriented towards the creation of a hybrid model for the HCD by joining it with the fluid MD2D model. Moreover, the kinetic model can be used independently for the analysis of the behaviour of every kind of charged species in the discharge – e.g. to obtain sputtering yield, second electron emission coefficients.

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