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Monte Carlo simulation of electron kinetics in a hollow cathode discharge

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Abstract. A kinetic model is reported computing the electron behavior in a hollow cathode discharge based on the Monte Carlo technique. It is a part of the PLASIMO modelling toolkit. The model allows the electrons to be closely followed while they travel and undergo collisions in the discharge. The Monte Carlo module was applied to the case of a HCD used as an excitation medium of atoms obtained by laser ablation. Results are obtained on the electron energy distribution function and the mean electron energy under typical discharge conditions. The output data and future development of the model and its applications are analyzed and discussed.

1. Introduction

The elemental composition of different materials can be investigated using a hybrid technique employing laser ablation (LA) and a hollow cathode discharge (HCD). The HCD in this so-called LA-HCD technique [1], is employed for additional excitation of the ablated material.

The focus of this work is modelling the processes in the plasma of a HCD. For this purpose we use the PLASIMO modelling platform [2], on which the HCD was already simulated by the MD2D model [3] - a time dependent two-dimensional multi uid model. The uid model calculates the spatial density distribution of various discharge species, the mean electron energy and the electrostatic potential. The results of the MD2D model are found to agree well with experimental and analytical observation [3,4,5].

In the HCD, there are regions, for instance in the cathode fall (CF), where the particles do not experience many collisions, or particles exist, such as pendulum electrons, whose free path exceeds the plasma size. This is why the kinetic approach is applied to simulate them. As the electrons are the main energy carriers from the field to the hollow cathode (HC) plasma, their behaviour is first simulated.

The aim of the present work is to develop a kinetic model for the electrons in a HCD and describe their behavior in terms of kinetic quantities, such as the electron energy distribution function (EEDF), the mean electron energy and the distribution of ionization events. The model is used for the optimization of the discharge; it provides guideline information for the fluid MD2D model.

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2. Operation parameters of the kinetic model

Figure 1 presents the geometry - a hollow cathode cylinder with length of 20 mm and inner radius of 4 mm. The spatial distribution of the electric field inside the cylinder is obtained from the fluid model and is used as input for the kinetic model. The operating gas is helium (He) at pressure of 1 Torr. In this environment, the simulated particles are the electrons. Their collision processes with the He ground state atoms are listed in table 1, while the cross-sections [6] used for these processes are taken from [7].

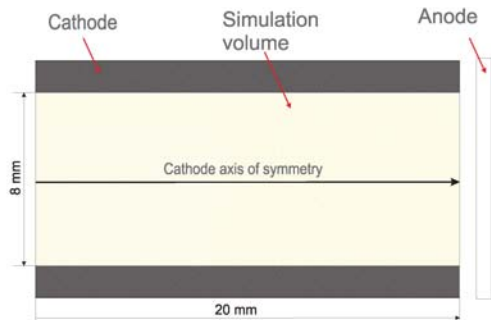


Figure 1. Scheme of the experimental HC with the simulation volume.

Table 1. Reactions used in the kinetic MC model for electrons.

Type	Reaction	Reaction threshold energy [eV]
Elastic collision	$\text{He} + e \rightarrow \text{He} + e$	0
Excitation	$\text{He} + e \rightarrow \text{He}^* + e$	19.8
Ionization	$\text{He} + e \rightarrow \text{He}^+ + 2e$	24.57

3. MC modelling results

3.1. MC simulations of wall secondary electron emission

The electrons emitted from the cathode wall are accelerated in the CF region and dissipate their energy in exciting and ionizing the plasma. However, some of the electrons can be accelerated to such an extent that their mean-free-path exceeds the plasma size. As a result, they can make multiple passes through the plasma with high velocity and are rejected by the CF on the opposite side. These electrostatically trapped electrons are known as pendulum electrons.

In order to observe the time evolution of the emitted electrons from the wall and the presence of pendulum electrons in the discharge, we inject 10^6 electrons at time $t = 0$ s from random points lying on the inner cathode wall. Since their transport is mainly radial, we impose only the radial electric field component.

Figure 2 shows the radial distribution of the ionization events involving the electrons. At the beginning of the simulation (figure 2a) the profiles of the ionization events have two pronounced peaks close to the walls, where the electrons have gained enough energies for ionization. At a later stage, these two peaks move towards the center of the HC (figure 2b) where they overlap (figure 2c). Finally, the ionization profile turns into a smooth curve with a sharp peak in the center (figure 2d).

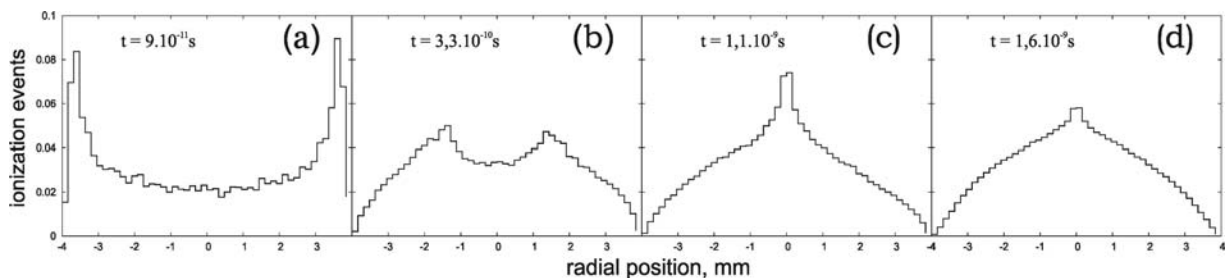


Figure 2. Time evolution of the ionization events obtained in the simulation of secondary emitted electrons.

This focusing effect of ionization events in the center of the discharge is attributed to the presence of pendulum electrons. As for them, it is more probable that they will pass through the center of the HC and, accordingly, it is more probable that they ionize there, which results in the sharp peak. Similar results have been reported earlier [8, 9] indicating the presence of pendulum electrons in HCDs.

3.2. MC simulations of HCD

For the simulation of the HCD setup, we impose the radial and axial electric field components obtained from the uid model. The axial electric field component has an important role for the electron transport to the anode [5]. The secondary electron emission from the wall is simulated by a continuous injection of electrons from the cathode wall at a rate of 1×10^{14} electrons/s. This value is also taken from the uid modelling results.

The output from the simulation are the EEDF and the spatially resolved EEDF. Figure 3 shows the EEDF obtained. The EEDF can be viewed as consisting of three parts. The first part comprises the low energy electrons with energies in the range $0 \div 40$ eV. These electrons are localized in the bulk of the discharge and are undergoing predominantly elastic collisions as their energy is not sufficient for more than one inelastic collision. Thus, the Maxwellization of these electrons is mainly due to elastic collisions. The presence of Maxwellization is indicated by the smooth line formed by the lower energy electrons in the EEDF. The second part consists of electrons in the range $40 \div 250$ eV. This group of high energy electrons is characteristic for the HCD. Electrons with such energies can excite not only atomic but also ionic states of the He atoms. The last part includes the electrons which have energies up to the full CF potential energy - 350 eV. This is the group of secondary emitted electrons and pendulum electrons. The secondary emitted electrons have just been ejected from the cathode and still carry the energy absorbed in the CF. The pendulum electrons tend to have low number of collisions and oscillate between the opposite CFs.

Figure 4 presents the spatially resolved EEDF. It is obtained by dividing the whole volume of the HC to a number of coaxial sub-volumes in which the EEDF is determined. The middle part of the EEDF in sub-volume 4 is higher than what is found for other regions. This is due to the fact that sub-volume 4 overlaps with the CF region, where a high radial electric field is present. The radial electric field is negligible in the other three sub-volumes, which results in similar shapes of the EEDF. However, some differences of sub-volumes 1 to 3 exist. The electrons in sub-volume 3, coming with high energy from the CF, start spending their energy in

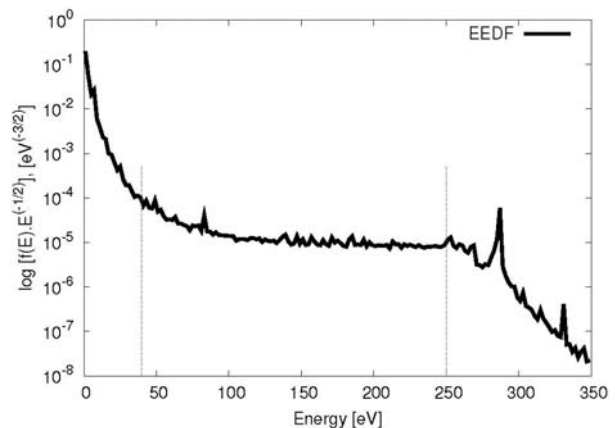


Figure 3. EEDF, obtained by MC simulations of all electrons in the HCD.

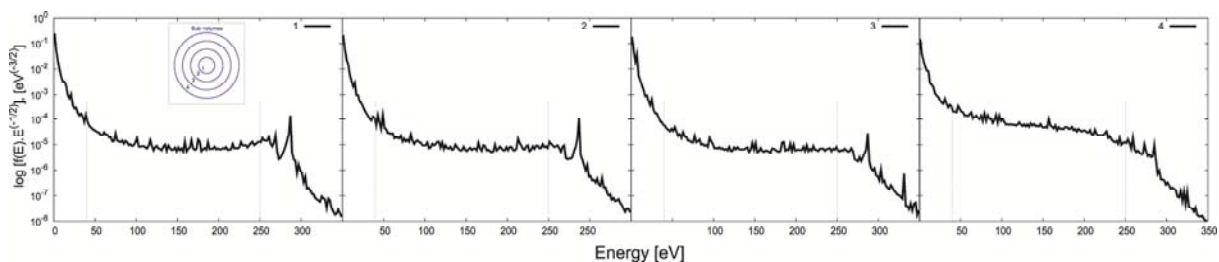


Figure 4. Spatially resolved EEDFs obtained in the MC simulation. The scheme of the fourth sub-volumes is shown in the graph.

effective impact ionization with the He atoms, so the EEDF has a lower number of highly energetic electrons. The EEDFs of the two inner sub-volumes are a little higher than in sub-volume 3. This is ascribed to the influence of the axial electric field. The electrons which have reached the inner part of the HC start to absorb energy from the axial electric field, which is accelerating them in the direction of the anode. The influence of the axial field is discussed in [5].

The EEDFs show high concentration of highly energetic electrons that are more abundant in the outer regions of the discharge and, due to the presence of strong radial field, enter in the central part of the discharge.

Conclusions

A kinetic model is developed simulating the behavior of electrons in the HCD. It is demonstrated that the ionization distribution has a radial profile with a sharp peak in the center of the HC. The steepness of the peak is ascribed to the pendulum electrons which predominantly pass through the axis of symmetry. A high concentration of energetic electrons in the whole volume of the HCD is found, thus the inelastic processes (excitation and ionization) are very probable. This shows that the HCD is indeed an appropriate medium for the excitation and ionization of ablated atoms.

In the future the kinetic model can be joined together with the uid MD2D in a hybrid model for the HCD.

Acknowledgments

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