Plasma Edge Simulations by Finite Elements using COMSOL

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Abstract: Finite elements using the COMSOL software package have been used to simulate the edge plasma in a large area capacitively-coupled RF reactor. In order to reduce numerical difficulties simplified reactor edge geometries have been used. First results show the importance of electrostatic double layers within this plasma. In addition the non-uniform behaviour of the plasma sheath around convex and concave corners turns out to be a basic feature of the edge plasma. The plasma physics and plasma-wall interaction are strongly influenced by these elementary structures.
The simple model and simple geometry result in an important tool giving new insights and understanding into the physics of RF edge plasmas. The simulations help designing reactor walls to optimize the RF plasma in industrial reactors.

Keywords: RF plasmas simulation, Plasma edge design

1. Introduction

Capacitively-coupled RF plasmas play an important role in industrial applications such as the production of flat displays and thin film solar cells. In these prominent applications, large area coatings with homogeneous film thickness and film structure over large substrate areas must be obtained in order to satisfy the stringent material properties. Recently, large efforts have been made to obtain several square meters of surface coatings with sufficient homogeneity in thickness and film structure by careful design of the electrode of the RF reactor. However, the reactor edges and the resulting edge plasma still can lead to considerable perturbations in the coating properties. Inhomogeneities of plasma parameters lead to imperfection on the film and can also be responsible for the occurrence of nonlinear effects such as nano-particle formation in the plasma. In addition, the edge plasma is susceptible to triggering parasitic discharges leading to inhomogeneities, severe perturbations of the coating process, or even to the destruction of reactor components. The physics and chemistry induced by particular reactor edge designs are still unknown and not yet well investigated. In the present work, numerical simulations of the edge plasma produced in simplified reactor geometries are presented. Simplified design has been chosen in order to reduce the complexity of the numerical calculation and moreover to investigate the basic plasma physics of the reactor edge and its dependence on typical design parameters. Several simplified edge geometries such as an open electrode geometry, electrodes with corners and angles and also (a)symmetrical electrode configurations have been studied.

2. Model and simulation

The COMSOL Multiphysics software is used to simulate the RF edge plasma in the mbar pressure range with a simplified reactor geometry. At present an electropositive plasma excited by a RF frequency of 13.56 MHz is modeled by the well-known continuity equations for the electron and ion density and energy conservation equations closed by the Poisson equation and the corresponding boundary and initial conditions [1,2,3].

The basic idea of the present work was not to exactly reproduce the plasma in great detail but to have a flexible numerical tool describing correctly the plasma physics which then can be used for the reactor edge design of a capacitively-coupled RF reactor. Using simple expressions for the rate constants[4], the model was kept simple with the aim not to reproduce a true physical plasma but to investigate general plasma properties in various electrode configurations.

The following reactor parameters have been used and kept constant for all the cases presented: excitation frequency 13.56 MHz, RF voltage 200 V_{pp}, gas pressure 1 mbar and an electrode gap of 30 mm.

The chosen edge reactor geometries investigated so far are shown in Fig.1. The edge geometries were divided into asymmetric (a, b, c) and symmetric reactor edge design (d). For the asymmetric reactor design an open electrode design (a), and a corner with different width (1, 2, 3 and 4 cm) were investigated (b). In addition, different sized asymmetric constrictions of the electrode gap (c) have also been simulated .

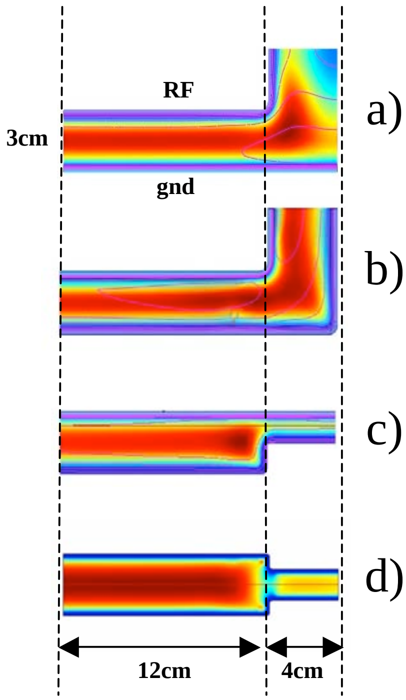

Figure 1. The RF reactor geometries considered in this paper. (Surface plot of the electron density and the contour plot of the electrical potential)

The typical geometrical dimensions of the investigated plasmas were chosen to be comparable to industrial RF plasma reactors.
The model was written for 2D geometry, meshed by quadrilateral elements, and solved by means of the time dependent Spoole solver given in the software package.

It is well known that such plasma simulations are complex due to the different physical time scales of the driving RF frequency and the much slower electron and ion diffusion times. Detailed studies concerning the convergence behavior of the plasmas simulations were carried out. It turned out that for correct interpretation of the simulations only well-converged cases allow an artefact-free vision of the ongoing plasma physics. In the present case to obtain a conveniently converged case at least 2000-3000 full RF cycles have been calculated.
Furthermore it has to be mentioned that the 2D meshing strongly influences the calculation; in particular it determines the required computer time till convergence of the model is reached. Optimisation of the 2D mesh has been made using the various options of the COMSOL software package. In particular, the boundary mesh options turned out to be helpful for convenient meshing of the plasma sheath near to the electrode surfaces. In addition, the convergence and numerical results of the 2D simulations were benchmarked against 1D calculations. Finally, the included post processing package was used for numerical diagnostics of the obtained simulations in order to obtain physical insight into the edge plasma physics of RF reactors.

3. Results

The post processing of the simulations show that in the open electrode cases and also in the symmetric case, electrostatic double layers exist beside the usual plasma sheaths.

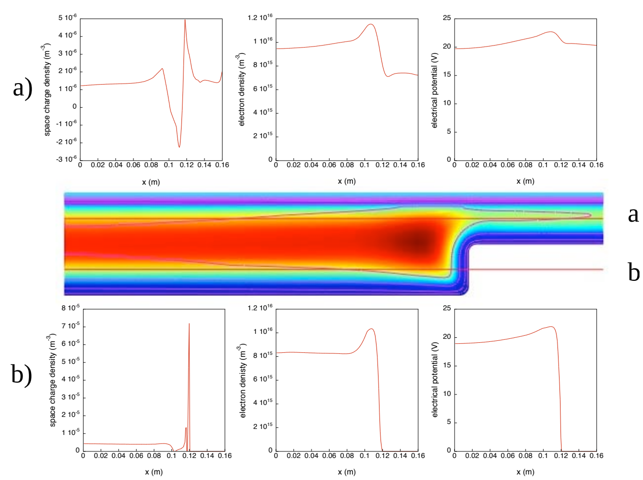

Figure 2. Presence of electrostatic double layers at two different locations within the discharge shown. The inserts show the space charge density, electron density and electrical potential at each location.

Fig. 2 shows the surface plot of the electron density and the contour plot of the electrical potential for the asymmetrical electrode case.

The inserts show the space charge density, potential, the electron density and electrical potential along the indicated lines. The space charge density shows the typical behaviour found in earlier investigations on electrostatic double layers.
The presence of the double layer in these RF plasmas has been reported earlier[1] and is still a point of ongoing research.

Of particular interest appeared to be the constricted symmetric reactor edge design (Fig. 1d). In this case the surface plot (Fig. 3) of the electron density clearly reveals the presence of two separated zones of different plasma density. The dense plasma in the main reactor part is separated by a electron density minimum from the less dense plasma in the constricted electrode gap. The electrical potential structure resembles the structures found in constricted DC discharges[5]. Furthermore, a local electron density maximum is found near to the two concave corner walls (see also Fig 4). Post processing also shows that the ionization rate is also peaked at this place.

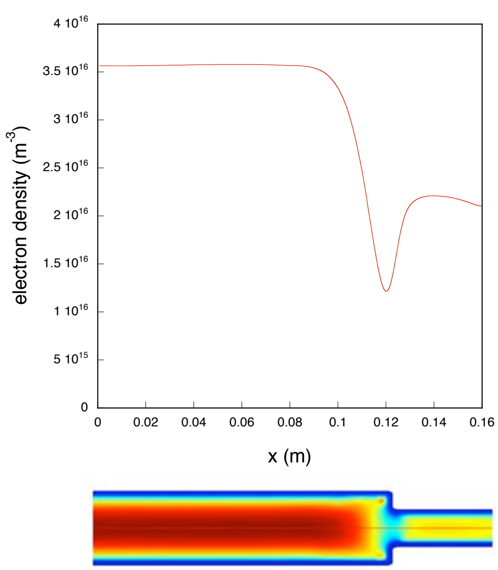

Figure 3. The symmetrically constricted RF plasma (Surface plot: electron density)

All the various simulations of edge plasmas revealed the importance of corners in the metallic reactor wall. Fig. 4 shows a zoomed view of the corners in the symmetric plasma edge design. The concave corner leads to a strong increase of the electrical potential amplitude as well as to a peaking of the particle densities and therefore to a focalization of the ionization rate. Conversely the convex corner leads to a decrease of the electrical potential and consequently to a decrease of the local electron density.

The different post processing options of the software package were also used to visualize the fluxes of the different plasma species and plasma currents within the plasma and onto the reactor walls. In the case of constricted electrodes the electron and ion flux to the electrodes has been calculated using the domain plot processing option.

Here it should be mentioned, that similar observations on the behavior of the plasma sheath around concave and convex corners have been made in plasmas applied for nitriding of complex substrates, using high ion energy[6,7,8,9]. The plasma sheath thickness, respectively the electron density and the step size are important parameters governing the plasma physics around corners. If the plasma sheath thickness is much smaller than the step dimensions, the plasma sheath follows the step conformally. However, if the sheath thickness and the step size are comparable, large changes in the plasma are expected. The behaviour of the plasma sheath around a corner is a basic feature of plasma physics and of first importance for the

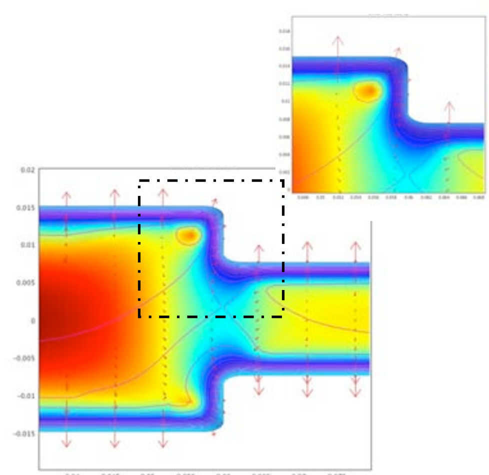

Figure 4. Influence of corners in the reactor wall on the edge RF plasma. Surface plot: electron density, contour plot: electrical potential, and arrows: total electron density flux.

design of RF plasma edge in modern plasma processing. The present simulations revealed the very basic influence of the reactor boundaries on the local plasma environment.

4. Discussion

Reliable results of the RF plasma behaviour can only be obtained after extensive calculations, typically after more than a few thousand RF cycles. Careful meshing turned out to be important to avoid artefacts due to numerical instabilities. First results on simplified reactor geometries indicate that, besides the traditional plasma sheath, electrostatic double layers play an essential role in these different types of RF plasmas investigated.

The particular design of the reactor edge also influences important plasma parameters such as the ionization rate in particular at the corners and edges.

5. Conclusions

These still very preliminary results clearly demonstrate that numerical simulation of edge plasmas with reasonable computing time using finite elements is a valid way to optimize modern RF plasma reactors.

The present simulations might be considered as a first step towards more detailed calculations of the plasma parameters in the RF reactor edge. This includes the simulations of more realistic reactor walls including metallic and dielectric elements. It is foreseen to test further reactor edge designs and to increase the details of the reactor design. Inclusion of the negative ions in order to take account of the electronegative nature of most reactive plasmas used in processing is a next step in the chain of improvement of the simulations. This should be followed by the inclusion of chemical reactions in order to finally simulate the influence of the reactor edge design on the resulting deposition or etching.

The simulations turned out to give interesting new insight and understanding in the physics of the RF edge plasma, and might lead to new advanced design of the crucial reactor edge.

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