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Fast and reliable simulations of argon inductively coupled plasma using COMSOL

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ABSTRACT

Inductively coupled plasma (ICP) reactors are widely used for microelectronic device fabrication. Numerical simulations of these devices are an important tool, which enables an improved understanding of ICP processes. Simulations based on fluid models have been reported in literature numerous times; however, in most cases high accuracies require expensive computational costs. We have checked in this work the applicability of COMSOL for plasma simulations, using a fluid model able to provide high accuracies with very low computational cost. A Boltzmann equation solver has been included in order to calculate the electron energy distribution function and the reduced electron mobility. Ions mobility has been calculated as a function of the reduced electric field. The results of the simulations have been benchmarked both against model and experimental results showing a high correlation with experimental values. This model approach can provide, in addition to high accuracy, fast simulations with an easy set-up of initial conditions, which allows flexible changes in the input variables in a short period of time.

1. Introduction

Inductively coupled plasma (ICP) reactors are widely used for microelectronic device fabrication, as they deliver high plasma densities and good uniformity. Within such reactors, it is possible to provide high fluxes of ions and radicals onto the wafer surface, and in addition, ions energy can be controlled independently of the plasma density. Numerical simulations of these devices have become an important tool, which enables an improved understanding of ICP processes and allows replacing measurements which would be expensive or difficult to achieve in an experimental setup. In recent years, self-consistent numerical codes appeared. These codes are based on implementing sub-models that can be assembled to form a particular self-consistent physical model. Some important examples of codes would be the hybrid plasma equipment model (HPEM) toolkit of Kushner and co-workers [1,2] or the Plasimo modelling framework developed at Eindhoven University of Technology [3]. Commercial multiphysics codes are becoming lately very important for the simulation of various types of non-equilibrium plasmas, for example, the Comsol-based studies in the group of Graves at Berkeley [4–8]. A recent summary about fluid, kinetic and hybrid plasma models can be found in Ref. [9]. Simulations based on fluid models have been proved to give valid approaches of plasma process for low Knudsen numbers (Kn < 0.2), which is the case for typical ICP chambers of pressures of 10 mTorr or higher [10–12]. In this paper, an ICP chamber is investigated by use of COMSOL software. COMSOL is a software package that provides since 2010 a plasma module with an ICP interface. As there is limited literature available with respect to applications of the plasma module of COMSOL, the objective of this paper is providing simulation results that can be quantitatively benchmarked against published results. We have already seen papers that use COMSOL to describe ICP chambers, for instance [13]. The model used there applied many simplifications, for instance, a Maxwellian electron energy distribution function. In this paper, a model with some new improvements is presented, such as a Boltzmann equation solver and a function to calculate ions mobility depending on the reduced electric field. In another paper [14] we have successfully used a similar model in order to simulate an ICP chamber with an applied bias voltage on an electrode. In this work, we will focus on the accuracy of this model comparing our simulation results with

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experimental and other model results, for discharge powers ranging from 6.25 to 200 W.

2. Material and methods

The ICP interface of the plasma module of COMSOL was used to run the main simulations. In addition, the Boltzmann equation solver interface was used, which is strongly recommended in order to achieve a high accuracy. To check our approach, prior to further calculations, we chose appropriate papers with experimental results [15,16] so as to compare our simulations with the outcomes shown there. To be able to compare, the geometry was the same used on those papers and it is shown in Fig. 1. A 2d axisymmetric simulation was chosen. The antenna is a five-turn coil placed below the quartz window, which has a thickness of 1.27 cm. All other dimensions of the chamber are described in Ref. [15]. A Faraday shield was used in the experiment ([15]) in order to reduce capacitive coupling. Thus, capacitive coupling from the coils was ignored in our model. This approach is common for this kind of simulations [17]. The walls surrounding the plasma were grounded (0 V). The external boundaries of the whole geometry (excepting the symmetry axis) were magnetically insulated ($\mathbf{n}\,\mathbf{A} = 0$, being $\mathbf{n}$ the surface normal and $\mathbf{A}$ the magnetic vector potential). The air surrounding the coils is considered to possess vacuum characteristics. The relative permittivity of the quartz window was considered to be 4.2.

A simple argon chemistry was chosen, which is shown in Table 1. The excited state of argon Ar(4s) is included. The electron-impact rate coefficients of reactions 1–5 in Table 1 are calculated using the electron cross sections data imported from Ref. [18] and the following equation [19]:

$$k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon \tag{1}$$

where k_k are the calculated rate coefficients, © equals $(2m_e/q)^{1/2}$, m_e is the electron mass, q is the electron charge, q is the electron energy, $f(\varepsilon)$ is the eedf (electron energy distribution function) and σk is the corresponding collision cross section.

Convective flux was not considered, and therefore no gas inflow and outflow were used. The model was filled with 30,284 mesh elements, most of them triangle meshes. Boundary layers have

Table 1
Important collision processes in the argon discharge.

No.	Process	Reaction	Hj (eV)	Rate coefficient[a]
1	Elastic collision	$Ar + e \rightarrow Ar + e$		k_{el}
2	Ground state excitation	$Ar + e \rightarrow Ar^* + e$	11.56	k_{ex}
3	Ground state ionization	$Ar + e \rightarrow Ar^+ + 2e$	15.7	k_i
4	Step-Wise ionization	$Ar^* + e \rightarrow Ar^+ + 2e$	4.14	k_{si}
5	Superelastic collisions	$Ar^* + e \rightarrow Ar + e$	−11.56	k_{sc}
6	Metastable pooling	$Ar^* + Ar^* \rightarrow Ar^+ + Ar + e$		$k_{mp}=6.2 \times 10^{-10}$
7	Two-Body quenching	$Ar^* + Ar \rightarrow 2Ar$		$k_{2p}=3 \times 10^{-15}$

[a] Rate coefficients for processes 1–5 are calculated using Eq. (1). Rate coefficients for reactions 6 and 7 are imported from Ref. [10]. Units are cm3/s. Ar* refers to the excited state Ar(4s).

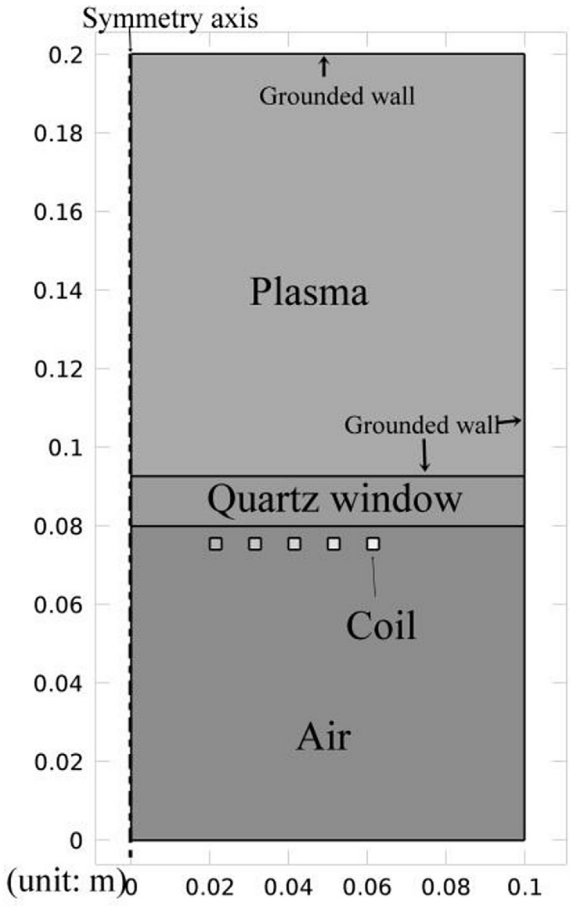

Fig. 1. Schematic diagram of the ICP chamber used in the simulation, adopted from Ref. [15].

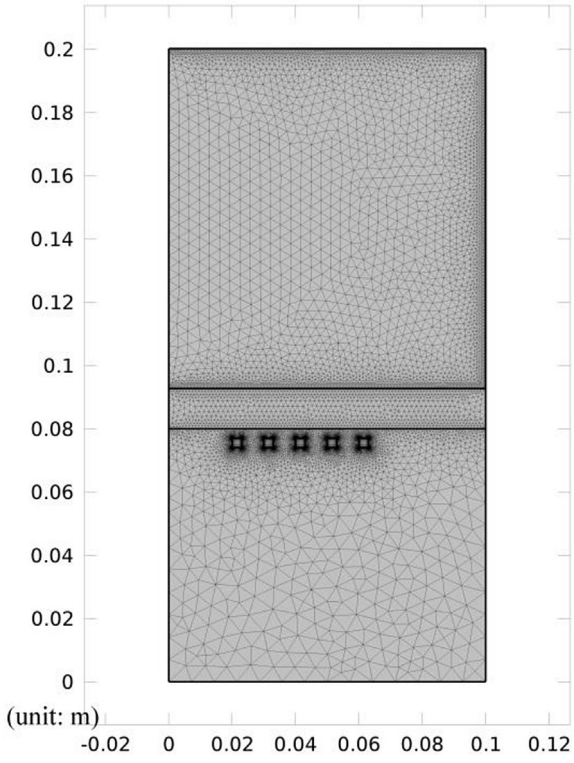

Fig. 2. Final mesh of the ICP chamber.