Modelling and characterization of a low pressure capacitively coupled hydrogen discharge

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This paper presents a systematic characterization of a pure hydrogen capacitively coupled radio frequency discharge, produced in a parallel plate cylindrical setup, comparing experimental measurements obtained for such discharge with numerical simulations. A good agreement is found between simulation results and experimental measurements for the discharge main electrical parameters. A comparison of H atom absolute density LIF measurements with simulation results will also be presented.

1. Introduction

Parallel plate capacitively coupled radio frequency (CCRF) discharges are of great interest in plasma assisted material processing applications, as in the plasma enhanced chemical vapour deposition (PECVD) of silicon thin films using hydrogen based mixtures.

The present work is part of an effort to model and optimise an existing PECVD reactor for quality μ-Si:H deposition, using SiH_4-H_2 mixtures under high dilution conditions for silane. The RF reactor is similar to the GEC reference cell, with 6.2 cm radius and 3 cm inter-electrode distance, at pressures between 0.2 – 1 Torr, frequencies in the 13.56 - 80 MHz range and RF voltages 50 – 800 V. The gas temperature is assumed to be 323 K. We have started by studying a 13.56 MHz capacitively coupled RF discharge in pure hydrogen, using a two-dimensional (2D) fluid model to describe the dynamics of electrons, H^+, H_2^+ ,H_3^+ ions in the reactor under study [1]. However, model predictions [2,3] were found to be systematically underestimated with respect to measurements, which was attributed to both experimental uncertainties and the simple hydrogen kinetics considered. In order to clarify the importance of hydrogen kinetics, we have self-consistently coupled the previously developed charged particle transport model to a homogeneous kinetic model for hydrogen, including vibrationally and atomic exited hydrogen species [4].

A systematic comparison of experimental results with simulation predictions will be presented as a function of the gas pressure, excitation frequency and applied rf voltage, for the electron density, bias voltage, plasma potential, power coupled to plasma and H atom density.

2.Model description

The simulation results were obtained using a two-dimensional, time-dependent fluid model (describing the production, transport and destruction of electrons, positive ions H^+, H_2^+, and H_3^+, and negative ions H) [1,2], coupled to the two-term electron Boltzmann equation, and to a homogenous collisional-radiative (CR) model [4] for the populations of H(n=1-5) electronically excited atoms and $H_2(X^1\Sigma_g^+, \nu=0..14)$ vibrationally excited ground state molecules. The CR model takes in to consideration the following collisional processes: ground state elastic collisions and rotational excitations by electron impact; e-V, E-V through all singlet states, V-V and V-T excitations/de-excitations collisions; dissociation through triplet states (b^3, c^3, a^3, e^3); attachment and ionization for $H_2(\nu)$ molecules; excitation/de-excitation and ionization processes for H(n) atoms. The cross sections for the various electron-neutral collisional processes appearing in the Boltzmann equation were normalized in order to obtain a good fit between the calculated and experimental [5,6] available electron transport parameters.

The coupling between the models is made by running the CR model several times (typically every 5 RF periods), passing to it the average frequencies (in space and time) of gain and loss of each neutral specie with electrons, until overall convergence is achieved. The new chemical composition, obtained after each run of the CR model, is used to update the electron transport parameters and rate coefficients by solving the homogeneous time independent Boltzmann equation, before running again the charged species transport model. This self consistent coupling between charged species transport and

chemical kinetics was used successfully in other works [7].

3. Results and discussion

The model was run for applied RF voltages between 50-800V, gas pressures 0.2-1.0 Torr, excitation frequencies in the range 13.56-80.0 MHz, assuming a constant gas temperature of 323 K.

Figure 1 plots, as a function of the excitation frequency, the calculated and measured electron density obtained at the discharge axis. The dc self-bias voltage V_{dc} (calculated and measured) is plotted in figure 2, as a function of frequency. The simulation results shown were obtained using the complete hydrogen kinetics, described above, and a simplified version that does not consider vibrational and atomic excited species or negative H^- ions.

Figure 1 shows a qualitative agreement between experimental [8] and calculated results for the electron density, with a systematic overestimation of measurements with respect to model predictions. The increase of the electron density with frequency can be mainly attributed to the increase of the discharge confinement fields, associated with the reduction of the space-charge sheath thickness. Figure 2 shows that the model qualitatively reproduces the experimental [8] variation of the self-bias voltage on frequency. However, one can observe a 30% systematic overestimation of the calculated V_{dc} with respect to measurements. This kind of deviation between simulations and experiments can be partially attributed to experimental uncertainties. The use of the complete hydrogen kinetics can at most correct the calculated densities by 10% and bias voltage in 3 %.

The dissociation degree calculated with our hybrid model is in the range 10^{-4} – 10^{-3} and strongly depends on the H atom wall recombination probability considered [8]. The simulation results agree well with first LIF measurements of H atom absolute density.

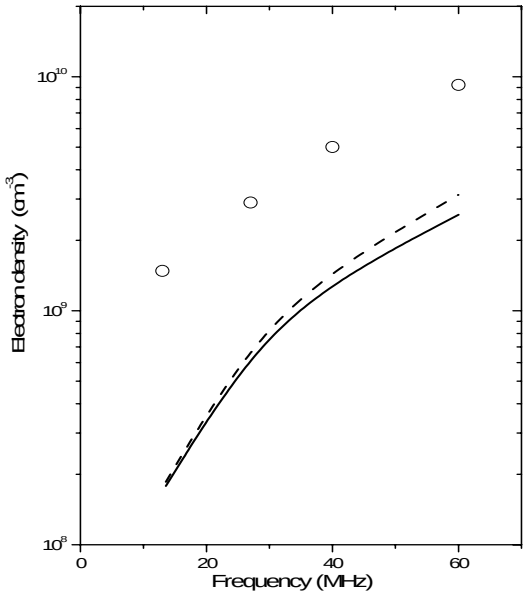

Fig. 1 Electron density vs frequency
(RF voltage=100V; Pressure= 300 mTorr)
(○ Experimental; —— Model with simplified kinetics;
– – – Model with full kinetics)

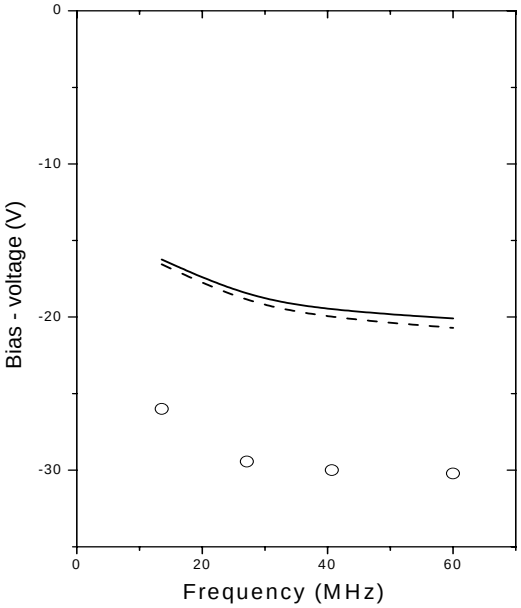

Fig. 2 Self-bias voltage vs frequency
(RF voltage=100V; Pressure= 300 mTorr)
(○ Experimental;—— Model with simplified kinetics;
– – – Model with full kinetics)

4. References

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