Modelling the influence of frequency in a low pressure capacitively coupled hydrogen discharge

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This paper investigates the dependence of plasma density and self-bias voltage with excitation frequency (13.56-40.68 MHz) using a two-dimensional (2D) fluid model in a low pressure (300 mTorr) radio frequency (RF) capacitively coupled hydrogen discharge. A comparison with experimental results reveals that the model predicts the correct trends of density and self-bias voltage variation with driving frequency.

1. Introduction

Radio frequency capacitively coupled discharges driven at 13.56 MHz are routinely used in plasma assisted material processing applications, due to their low cost, scalable dimension and high repeatability. A strong effort is under way to optimise existing plasma processing tools, which may meet the increasing demand for higher throughput, lower damage, improved uniformity and film quality in the semiconductor industry. Such requirements demand low ion energies to minimize film damage and high plasma densities (and/or ion fluxes) to raise the deposition rates. An increase of the applied RF voltage, holding frequency constant, yields higher plasma densities but also causes an increase in both the plasma potential and the ion energy. Raising the pressure can also enhance the ion density, but there is an increased risk of dust particle formation in the discharge. Several studies [1] indicate that is possible to obtain higher plasma densities, while maintaining the ion energy, by increasing the RF excitation frequency and adjusting other operating discharge parameters (applied RF voltage, pressure).

The present work is part of an effort to model and optimise an existing plasma enhanced chemical vapour deposition 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 [2], operating at a pressure of 300 mTorr, RF voltage of 100 V and frequencies between 13.56 and 40.68 MHz.

The modelling starts by studying the charged particle transport in a capacitively coupled discharge in pure hydrogen for various excitation frequencies. The dependence of total ion density, self-bias voltage, plasma potential, mean ion energy and electron temperature, on the excitation frequency is presented. A comparison of the total ion density and self-bias voltage with available experimental results is also shown. Special attention is given to the relative population of hydrogen ions in the discharge. In particular, partial ionisation cross sections are considered, to account for the creation of H_2^+, H^+ from the electron impact ionisation of molecular hydrogen.

2. Model description

A 2D time dependent fluid type model was developed to describe the transport of electrons, H^+, H_2^+ and H_3^+ in the reactor under study [3]. The description, in space and time, of charged particle transport uses the corresponding continuity, momentum transfer and mean energy equations (the latter for electrons only), coupled with Poisson's equation.

The system of equations is discretized in a grid of 32x32 points using finite differences, and is solved subject to appropriated boundary conditions. Typically, 1000 time steps are used within each RF period, and a few hundred RF cycles are needed to reach convergence. Convergence is assumed if relative changes of particle densities, mean electron energy, plasma potential and self-bias voltage, between two consecutive periods is less than 0.1%.

We adopt the local electron mean energy approximation. The electron transport parameters are tabulated as a function of electron mean energy, by first solving the stationary, space-independent electron Boltzmann equation using the electron cross-sections compiled in references [4,5]. The ion mobilities are those of reference [6], with the field dependence proposed in [7].

3. Results and discussion

The model was run for an applied RF voltage of 100 V, pressure of 300 mTorr, excitation frequencies of 13.56, 27.12 and 40.68 MHz, assuming a constant gas temperature of 323 K.

Figure 1 plots, as a function of the excitation frequency, the calculated and measured (using a plane probe of 0.25 cm^2 surface) total ion density n_i, obtained at a distance of 4 cm from the discharge axis. The dc self-bias voltage V_{dc} (calculated and measured), the plasma potential V_p, the ion mean energy $<E_i>$ at grounded electrode (where a substrate is to be hold), and the electron temperature T_e are plotted in figure 2, as a function of frequency. The increase of the ion density and ion mean energy 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 1 shows a qualitative agreement between experimental and calculated results for the plasma density, with a systematic overestimation of measurements with respect to model predictions. This deviation can be partially attributed to experimental uncertainties.

Figure 2 shows that the plasma potential presents a weak dependence on frequency. This result, which agrees with observations presented in other works [1], combined with the strong increase of the plasma density with frequency can account for the small decrease of the electron temperature when the excitation frequency increases. Figure 2 also shows that the model qualitatively reproduces the experimental 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 was already reported [3,8] and can be associated to the enhanced difficulties in obtaining a correct estimation of the charged-particle current involving (light) hydrogen ions.

In an attempt to understand the disagreement between simulation and experiment we have tried to correct the predictions on hydrogen ion populations. We have considered partial ionisation cross-sections for molecular hydrogen by electron impact, thus discriminating in energy the production channels of H_2^+ and H^+. While the total ion density and the self-bias potential are only marginally affected by this correction, the H^+ density is strongly reduced.

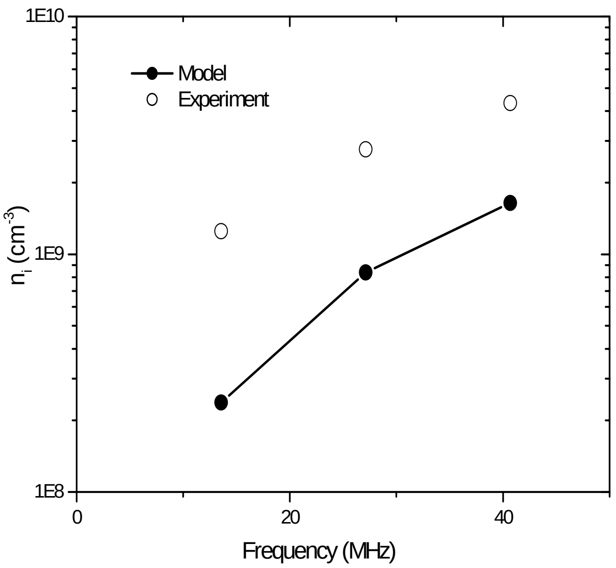

Fig. 1 Total ion density vs frequency

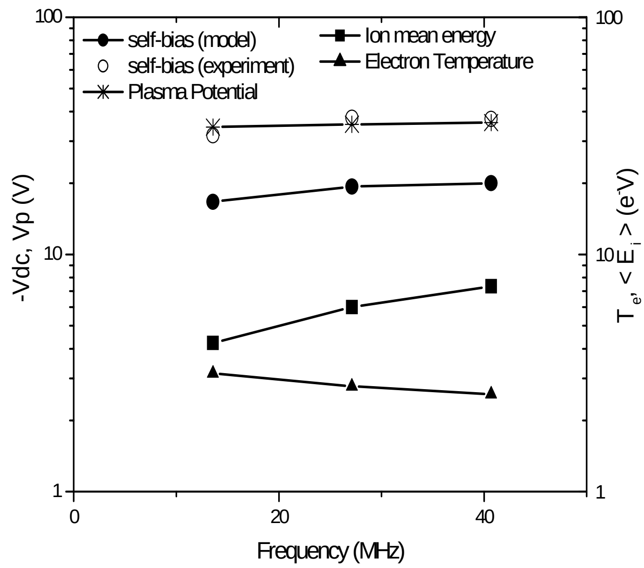

Fig. 2 Self-bias voltage, plasma potential, ion mean energy, electron temperature vs frequency

4. References

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