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Numerical Modeling of Hydrogen Plasmas: Effects of Frequency and Pressure

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Abstract

The results of the numerical modeling of a capacitively coupled hydrogen plasma are presented. We report on the effects of frequency in the 13.56 - 40.68 MHz range and compare them to influence of the pressure in the range of 0.5-1.5 Torr. The results allow us to make a conclusion that both, pressure and frequency, have pronounced and somewhat similar influence on the parameters of the discharge.

I. INTRODUCTION

The increase of frequency has been reported as an effective way of increasing the deposition rate of hydrogenated amorphous silicon[1]. However, despite of a large amount of experimental data, the explanations for the higher efficiency of very high frequency (VHF) plasmas are rather contradictory. Some authors have invoked an enhanced surface reactivity of the film precursors (due to a larger flux of low energy ions) as the main reason for the increase in deposition rate, while others suggested an enhancement of gas phase processes with the excitation frequency.

On the other hand, it has been shown that the increase of the total pressure leads to an increase of the deposition rate of amorphous silicon, to values comparable to those achieved by VHF. Moreover, the increase of the pressure results in a reduction of the ion bombardment and an improvement of the properties of microcrystalline silicon films. It is interesting, that similar values for the deposition rate and for the efficiency of micromorph solar cells have been reported for depositions at 13.56 MHz and by the VHF technique[2,3]

This study of hydrogen plasmas is directly relevant to the growth of microcrystalline silicon by the layer-by-layer technique[4] , in which the deposition of amorphous silicon is decoupled from its exposure to hydrogen plasma.

II. MODEL FORMULATION

A symmetric RF plasma with one electrode driven and one grounded (no self-bias) is studied. Plasma is described by the system of one-dimensional fluid equations[5], which involves the continuity equations for positive and negative ions H^+, H^-, H_2^+, H_3^+ for electrons and neutrals H and H_2 .The flux of electrons is defined from “drift-diffusion” approximation of the full momentum transfer equation for the electrons. Electric potential is calculated from Poisson’s equation. The concept of “effective” electric field was used to describe the transport of ions. The temperature of the ions was supposed to be equal to that of the background gas. Off-line two-term expanded Boltzmann solver is used for the calculation of the electron-impact rate constants and electron transport coefficients. The mean electron energy can be still evaluated from a conservation equation similar to that used when Maxwellian EEDF is assumed.. The source terms for the continuity equations were calculated as a sum of loss and production terms of 27 chemical reactions.

III. RESULTS.

Constant RF voltage or constant dissipated RF power

The amplitude of RF voltage influences strongly the dissipated power as shown in Fig. 1(a).

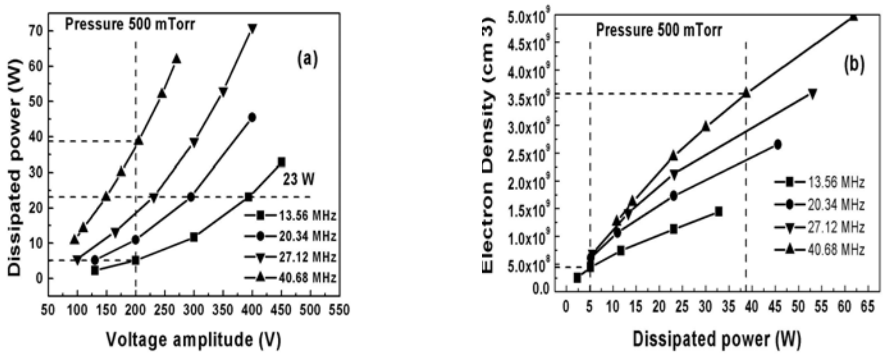

Fig. 1. The plots of the dissipated power versus voltage amplitude at the driven electrode (a) and max values of time-averaged electron density versus the dissipated power (b) for different values of the frequency.

If we keep constant the RF voltage, a substantial growth of the power dissipated in the plasma can be observed. Electron density n_e as a function of the power dissipated in the plasma is presented in Fig.1(b) for different values of the excitation frequency. When the RF power increases from 5 to 40 W n_e increases by about a factor of 7. The plots in Fig.1(a,b) show clearly that keeping constant the RF voltage masks the real frequency impact. These results are in good agreement with those, reported by E. Amanatides and D. Mataras [6].

Power dissipation as a function of frequency and pressure

The effects of frequency and pressure on the spatial time-averaged profiles of total RF power dissipated in the plasma, as well as its distribution between the power coupled to electrons and the power coupled to ions, are plotted in Fig. 2(a, b, c). Fig. 2(a) shows that at 13.56 MHz and 500 mTorr nearly half of the total power dissipated in the plasma is spent to accelerate the ions in the sheath region (ion bombardment).

The increase of pressure for the same frequency (Fig. 2(b)) results in a more spatially

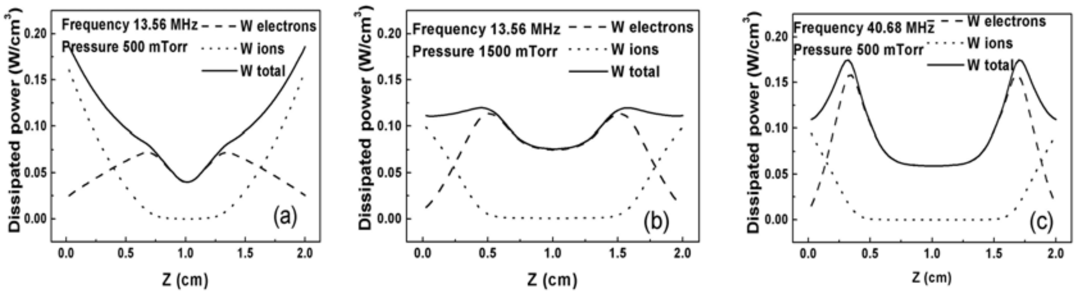

Fig. 2. Spatial distribution of the total dissipated power, and the power coupled to electrons and to ions for: (a) 13.56 MHz at 500 mTorr; (b) 13.56 MHz at 1500 mTorr ; and (c) 40.68 MHz at 500 mTorr.

uniform distribution of the total power. The power consumed by the ions strongly decreases to quarter of total power. The increase of the frequency for a constant pressure, as in Fig.2(c), also reduces the power spent for the acceleration of ions to 17 percent of total. However, the increase of the frequency leads to a less spatially uniform power dissipation in the discharge.

Increasing pressure or frequency leads to similar results on the spatial distribution of time-averaged primary ionization rate (H^+ and H_2^+) as depicted on Fig. 3. The increase of the

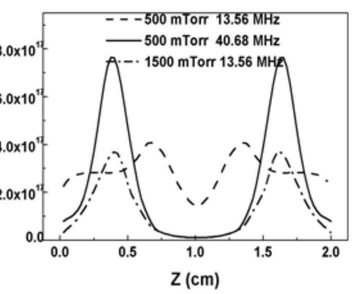

Fig. 3. Time-averaged ionization rate versus position between electrodes for different values of pressure and frequency.

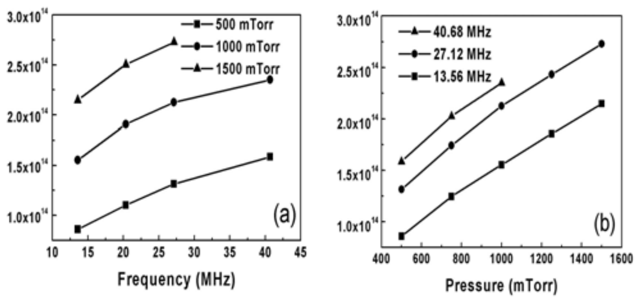

Fig. 4. Maximum values of time-averaged atomic hydrogen density versus frequency (a) and pressure (b)

pressure from 500 mTorr to 1500 mTorr at 13.56 MHz drastically changes the shape of the ionization rate, which shifts to the electrodes and resembles the ionization rate obtained at 40.68 MHz and 500 mTorr. However the maximum values of the ionization rate at 1500 mTorr and 13.56 MHz are lower by a factor of two than those achieved at 40.68 MHz.

Effects of frequency and pressure on plasma parameters

Increasing both, driving frequency and pressure, at equal level of dissipated power leads to the drop of time-averaged plasma potential and to the shrinking of sheath region, though, in a second case, those trends are less pronounced. Within the studied range of parameters at fixed dissipated power, the values of n_e differ at most by a factor of two. This is a surprising result, which does not explain the large effects observed on the deposition rate[1].

Effects of frequency and pressure on discharge chemistry

The spatial profiles of time-averaged densities of primary ionization products H_2^+ and H^+ are very similar to that of the ionization rate given in Fig. 3, where it is shown that the increase of frequency enhances the production of H_2^+ and H^+ ions; while the increase of pressure limits the production of those ions. H_3^+ is the main ion, by several orders of magnitude higher than for H_2^+ and H^+, in hydrogen plasmas for the studied ranges of parameters. The density profile of H_3^+ is quite smooth and shows a maximum in the center of the discharge.

Fig. 4 shows the effect of frequency and pressure on the maximum values of the density of H-atoms in the center of the discharge. In both cases we observe an increase in the production of H-atoms with increasing pressure or frequency. While the hydrogen density in the bulk of the discharge obtained at 1500 mTorr and 13.56 MHz is nearly twice greater than that, obtained at 500 mTorr and 40.68 MHz, the fluxes of H-atom onto the electrodes are almost equal in both cases.

IV. CONCLUSIONS

Both, pressure and frequency, have pronounced and similar influence on the parameters of hydrogen discharges: sheath thickness, ratio between power transferred to ions and electrons, concentration of H atoms and its fluxes to the surface.

The increase of pressure leads to a more spatially uniform dissipation of power by electrons, whereas increase in frequency keeps high amount of power dissipated in the sheath. The increase of frequency at *constant power dissipation* leads to moderate increase of electron concentration. Moreover, the increase of pressure or frequency at constant power dissipation enhances the fluxes of atomic hydrogen fluxes. Our results suggests that the efficiency of H_2 plasma as a source of hydrogen for etching loosely bonded Si material can be improved in a similar way by either the increase of the excitation frequency range of 13.56 MHz up to 40 MHz, or a the increase of pressure in the range of 500 – 1500 mTorr.

References

[1] H. Curtins, N. Wyrsch and A. Shah, Electron.Lett. **23,** 228 (1987).

[2] T. Roschek, T. Repmann, J. Müller, B. Rech, H. Wagner, JVST, A**20**, 492 (2002).

[3] H. Keppner, J. Meier, P. Torres, D. Fischer, A. Shah, Applied Physics A, **69,** 169 (1999).

[4] N. Layadi, P. Roca i Cabarrocas, B. Drévillon, I. Solomon, Phys. Rev. B **52,** 5136 (1995).

[5] J.-P. Boeuf, , Phys. Rev. A **36**, 2782 (1987)

[6] E. Amanatides and D. Mataras, J. Appl. Phys., **89**(3), 1556 (2001).