Power consumption effect on the microcrystalline silicon deposition process: A comparison between model and experimental results

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Abstract. A two dimensional (2D), time dependent fluid model was used to study the deposition of $\mu$-c-Si from low-pressure, capacitively coupled radio-frequency (RF), silane - hydrogen discharges. The model was applied for the simulation of a parallel plate, capacitively coupled plasma chamber, operating at frequency 27.12 MHz and conditions of low pressure, dust free regime. Qualitatively good agreement between the model and the experimental results was found for the electrical and chemical characteristics of the discharge. This agreement, allowed us to discuss the main effects of the discharge power on the species production and fluxes towards the substrate and to identify the most important parameters for microcrystal formation and the achievement of rather fast deposition rate.

1. Introduction
Properties such as high stability, carrier mobility and doping efficiency, made microcrystalline silicon ($\mu$-Si) a promising candidate in replacing amorphous silicon (a-Si:H) materials in thin film transistors and solar cell industry [1]. High quality $\mu$-c-Si thin films can be obtained by plasma enhanced chemical vapor deposition (PECVD) from hydrogen diluted silane (SiH$_4$) plasma at low pressures [2]. The material quality would be greatly improved by understanding its growth mechanism; however, a major problem in optimizing material properties is the complexity of the SiH$_4$/H$_2$ discharge chemistry, including the gas-phase and plasma-wall interaction as well as the deposition process at the substrate. Plasma models can provide valuable information about the physics and chemistry of the deposition process and they can be used as a cost effective way to optimize the process in terms of material properties and deposition rate [3]. A commercially available fluid code (CFDRC) has been used to simulate highly diluted SiH$_4$ in H$_2$ discharges in order to study the effect of the RF power and pressure, which are both strongly affecting the growth rate and the crystallinity of the films [4]. The model has been found to predict fairly well the influence of plasma parameters on the experimentally measured electrical and chemical characteristics of the discharge and this allowed the discussion concerning the effect of power a’t two pressures, on the species density, the composition of the radical flux reaching the surface and the film growth rate.

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2. Model formulation

A two dimensional (2D), time dependent fluid model was used to study the deposition of $\mu$-Si:H in low-pressure, capacitively coupled radio-frequency (RF), silane-hydrogen discharges.

The model describes the discharge by a combination of particle, momentum and electron energy conservation equations derived from Boltzmann equation, coupled with Poisson’s equation for a self-consistent calculation of the electric field. A detailed description of the model can be found in Ref. [5]. A set of 22 species together with a total number of 105 reactions (80 in the gas phase and 25 surface-gas interactions) were incorporated in the model, comprising electron - impact reactions with molecular species, neutral-neutral, and ion-neutral reactions. Cross sections data have been used for electron impact reactions description [6], while for reactions involving neutral species, calculated or experimentally measured rate constants were considered [7]. Plasma-surface interaction of the radicals i.e., the growth of $\mu$-Si:H is included through the use of sticking coefficients.

The model requires as input the geometry of the reactor and the applied voltage and provides as outputs the most important properties of SiH$_4$/H$_2$ discharges, such as the distribution of the electric field and voltage in the plasma, electron, ions and species densities, electron temperature, radical flux towards the substrates and the deposition rate.

3. Results and Discussion

The model was applied in a parallel plate, capacitively coupled plasma chamber, operating at frequency of 27.12 MHz, dust free and low pressure conditions. These conditions are typically used for the deposition of high quality, device grade $\mu$-Si:H thin films. The effect of the discharge power on the deposition process at two different gas pressures (0.5 and 1 Torr) was investigated and the model results were compared to experimental measurements performed in identical conditions [8].

![Figure 1](image1.png)

**Figure 1.** Total current of the discharge measured at the driven electrode as a function of power dissipated in 0.5 Torr 2% and 1 Torr 6% SiH$_4$ in H$_2$ discharges.

![Figure 2](image2.png)

**Figure 2.** Radical average number densities vs. power dissipated in 0.5 Torr 2% and 1 Torr 6% SiH$_4$ in H$_2$ discharges.

The variation of the total discharge current with the effective power density as calculated by the model as well as measured experimentally for both pressures is presented in figure 1. The model underestimates the power dissipated in the discharge as compared to the experimental values for both pressures but simultaneously an overestimation of the total current at the driven electrode is observed. The discrepancies between model and experimental results are less noticeable in the lower pressure and lower power dissipation case. This observation can lead to the estimation that the differences between model and experimental results may come from power dissipated to ions or to an underestimation of electron-molecule collision processes, which are both favored at high power – high pressure conditions. Nonetheless, the trends of discharge current and power dissipation are in a very good qualitatively agreement between the calculated and the measured values and this allow us to further discuss the results of the model concerning the gas phase chemistry and the deposition rate.
Thus, figure 2 shows the densities of the main radicals in silane - hydrogen discharges (H, SiH₃, SiH₂, Si₂H₅) as a function of the dissipated power. Species densities increase with the rise of power consumption, independently of the pressure, although they have different behavior at the different pressures. Silyl radical (SiH₃) has the highest particle density for all simulated conditions and it is about one order of magnitude higher than silylene (SiH₂). Even though H₂ is the main component of the discharge mixture (98% at 0.5 Torr, 94% at 1.0 Torr respectively), the hydrogen atoms density is lower than SiH₃ density, which is the result of the much lower cross section for H₂ compared to SiH₄ dissociation. However, as pressure decreases and higher powers are applied into the discharge, hydrogen atoms tend to become the most abounding species in the discharge. This mainly comes from the fact that each H₂ dissociation reaction produces two hydrogen atoms enhancing thus, the fast increase of H atoms density with the H₂ dissociation rate. The highly reactive SiH₂ radical is not favored by the pressure and silane concentration increase, which raises the probability of being consumed in secondary reactions with mono and poly-silane species. In addition, Si₂H₅ radical doesn’t show any noticeable variation at these two pressures, except of being present in lower concentration (about two orders of magnitude) than all other species of interest.

Figure 3. Radical fluxes ratio (Γ_{SiH₃}/Γ_{SiH₂} and Γ_{SiH₃}/Γ_H) as a function of the applied RF voltage in 0.5 Torr 2% and 1 Torr 6% SiH₄ in H₂ discharges.

Figure 4. Growth rate R_D as a function of the applied RF voltage in 0.5 Torr 2% and 1 Torr 6% SiH₄ in H₂ discharges.

Except of the species densities, a very important parameter during the deposition of μc-Si:H thin films is the flux of radicals towards the substrate. Actually, the radicals’ flux determines the deposition rate, the crystallinity and the electronic properties of the films. Thus, figure 3 shows the flux ratios of radicals having an important contribution to the film growth and to its quality, as a function of the applied RF voltage. The values plotted are averaged over the substrate area. As the applied voltage and consequently the power consumption is the only parameter that varies, no changes of the discharge mass transport properties are expected. Thus, the variation of these ratios can be only attributed to the modifications of the gas phase chemistry when we compare the results for the same gas pressure. Both radical fluxes ratios (e.g. R₁=Γ_{SiH₃}/Γ_H and R₂=Γ_{SiH₃}/Γ_{SiH₂}) decrease with applied voltage although they have different behavior as the pressure is modified. R₁ drop is the result of the fact that hydrogen atoms density increases faster than all the other species with the applied power as previously explained. On the other hand, the decrease of R₂ with the applied voltage can be attributed to the restriction of the SiH₂ consumption in the gas phase from the secondary reaction with silane. Namely, the increase of the applied voltage result to a continuous increase of the silane consumption in the discharge and consequently to a drop of the rate that SiH₂ radical is consumed through the reaction with silane. In such a manner, the density of the SiH₂ radical and consequently of the flux of this species appear to increase faster with the applied voltage compared to the rather low reactive SiH₃.

As for the pressure effect on the composition of the species reaching the growing surface, we can observe that the increase of pressure mostly favors the flux of SiH₃ radical. Namely, R₁ and R₂ are
significantly higher at 1 Torr and this can be fully explained by the enhanced consumption of H atoms and SiH₂ radicals in the gas phase through secondary gas phase reactions, which are favored by the pressure increase. Furthermore, the variation of the relative species fluxes with either the total power dissipation or the total gas pressure can be further used in order to extract useful information concerning the species that are mainly responsible for the growth of microcrystalline silicon. Namely, the increase of power [9] and the decrease of pressure [4] were found to enhance the crystallinity percentage of the deposited films. At such conditions, our model predicts that H atoms flux is favored relative to all other radical, indicating a significant role of this species to the microcrystal formation. On the other hand, the fact that SiH₂ is favored relative to SiH₃ at high power - low pressure conditions indicate that the kind of silicon hydrides that reach the growing surface does not play a significant role in the film crystallization if a rather high hydrogen flux is maintained.

Finally, concerning the deposition rate (figure 4), the model can very well predict the significant increase of the film growth rate with the pressure and power, although its values tend to be overestimated in most of the conditions. The increase of the deposition rate with pressure is basically the result of the higher SiH₃ density in these conditions but also of the enhanced contribution of higher silanes (Si₂H₅) to the film growth (figure 2). Furthermore, this overestimation indicates that electron-molecule collisions processes are not very well predicted as in the case of the power dissipation. Different sets of cross sections and electron energy distribution functions will be applied in the future, together with comparison with in experimental results in a wider range of conditions in order to eliminate the discrepancies between model and experiments.

4. Conclusions
An investigation of the applied RF voltage effect on the deposition process of microcrystalline silicon thin films from highly diluted SiH₄ in H₂ discharges was carried out at two total pressures of 0.5 and 1.0 torr. A 2D self-consistent fluid model was applied for the investigation and the results of the simulation were compared with the experimental measurements.

The simulation reproduces fairly well the effect of the applied voltage on the electrical properties and on the deposition rate but quantitative discrepancies was found. The differences were attributed to the ambiguous prediction of the power spend by ions or to the calculation of the electron molecule collision processes.

However, the qualitatively agreement between model and experimental result, allowed as to discuss the effect of pressure and power on the gas phase chemistry of SiH₄/H₂ discharges and the deposition rate. The increase of the applied voltage was found to enhance the production and flux of all species towards the substrate. Hydrogen atoms were mostly favored, explaining thus, the beneficial effect of the increase of power consumption on the microcrystalline growth. Finally, the simultaneous increase of pressure and power leads to rather fast growth rate mainly because of the increase of SiH₃ flux towards the substrate and the enhanced contribution of higher silanes.

5. References
[1] Meier J, Fluckiger R, Keppner H and Shah A 1998 Appl. Phys. Lett. 65 860
[2] Schroop R and Zeman M 1998 Amorphous and Microcrystalline silicon solar cells (Dordrecht: Kluwer Academic Publishers) p 16-23 & 47-56
[3] Kushner M 1988 J. Appl. Phys. 63 2532
[4] Kondo M, Fukawa M, Guo L and Matsuda A 2000 J. Non-Cryst. Solids 84 266-269
[5] Lyka B, Amanatides E, Mataras D 2004 to be appeared in Proc. of 19th European Photovoltaic Solar Cell Energy Conf. and Exhibition (Paris)
[6] Janev R K and Reiter D 2003 Contrib. Plasma Phys. 43 401
[7] Perrin J, Leroy O and Bordage M C 1996 Contrib. Plasma Phys. 36 1, 3-49
[8] Amanatides E, Stamou S and Mataras D 2001 J. Appl. Phys. 90 5786
[9] Torres P, Keppner H, Meier J, Kroll Beck N and Shah A 1997 Rapid Research Notes: Physica Status Solidi R 9 163