Plasma Enhanced Chemical Vapor Deposition of Silicon Under Relatively High Pressure Conditions

E. Amanatides, B. Lykas, and D. Mataras

***Abstract*—A two-dimensional self-consistent model of highly-diluted SiH_4 in H_2 discharges used for the deposition of microcrystalline silicon thin films is presented. The promising high-pressure regime (1–10 torr), that has been shown experimentally to lead at high growth rates and high crystalline volume fraction, is examined. The main effects of the pressure increase on the power dissipation, the electron density, and the species distribution in the discharge are presented and discussed.**

***Index Terms*—Microcrystalline silicon, plasma enhanced chemical vapor deposition, radio frequency discharges, self-consistent modeling, silane, solar cells.**

PLASMA enhanced chemical vapor deposition (PECVD) is the standard technique for depositing both amorphous (a-Si:H) and microcrystalline silicon (μc-Si:H). The later is increasingly used to replace partially or totally a-Si:H in thin film solar cells due to its interesting optoelectronic properties [1]. The main disadvantage of using μc-Si:H is the still quite low film growth rate, especially when high crystallinity is required. Recently, the possibility to use highly diluted SiH_4 in H_2 discharges at relatively higher total pressures (>1 torr) was proposed to partially overcome these limitations [2]. However, the regime-specific mechanisms and the limits of this technique still need to be clarified.

In this direction, we present a two dimensional (2-D) simulation of PECVD of μc-Si:H from highly diluted SiH_4 in H_2 discharges operating in the so called high-pressure depletion regime (1–10 torr with dilutions between 0.25%–2.5%). The model uses the fluid flow approach, i.e., consists of particle, momentum, and energy balances obtained from moments of the Boltzmann transport equation, coupled with Poisson's equations for a self consistent calculation of the electric field. The formulation of the model is described in detail in [3]. Special attention is given in implementing an accurate description of the gas phase and surface chemistry of SiH_4/H_2 discharges. Thus, the model includes 33 species (neutrals, electrons, positive, and negative ions) participating in 107 gas phase and 23 surface reactions. The complete set of the gas phase and surface reactions used can be found in [4].

The results presented here concern the application of the model for the simulation of a small area capacitively coupled UHV reactor that has been used for the deposition of μc-Si:H thin films under similar conditions. Particularities of the specific configuration are that the grounded electrode is smaller than the powered electrode and that the deposition electrode consists of a grounded part and a dielectric part.

Fig. 1(a) and (b) presents the spatial distribution of power dissipation in the discharge at two different phases of the radio frequency (RF) cycle ($\pi/2$ and $3\pi/2$) for the pressures of 1 and 10 torr, respectively. Significant differences can be observed on the distribution of power consumption between the two pressures. In the 1 torr case, during the cathodic phase [Fig. 1(a)] most of the power is consumed close to the grounded electrode. At 10 torr the situation is the same but with no difference between the two areas. On the other hand, during the anodic phase [Fig. 1(b)], the power consumption is higher near the RF electrode and its shield for both pressures. In addition, if one compares power dissipation between the two phases of the RF cycle, it is evident that at 1 torr, most of the power is deposited close the RF electrode while at 10 torr, the difference between the powered and the grounded electrodes is very small. In both cases, a significant amount of energy is spent in the area close to the edge of the powered electrode.

Fig. 2 presents the time-averaged spatial distribution of electron density for the two pressures. At 1 torr, the electrons spread out of the discharge volume thus leading to the creation of a local density maximum between the edges of the two electrodes. This is mainly a result of the asymmetry of the system combined with the diffusive electron losses at the reactor walls which are high at this pressure. To the contrary, electrons are much better confined between the two electrodes at 10 torr since their diffusion toward the walls is hindered still their concentration at the electrode edges remains high.

Finally, Fig. 3(a) and (b) presents the spatial distribution of two species [SiH_2 Fig. 3(a) and SiH_3 Fig. 3(b)] at the pressures of 1 and 10 torr. These species play a very important role in the deposition of μc-Si:H thin films while having quite different gas phase and surface reactivities. This difference is naturally reflected on the spatial distribution of their density. Thus, the highly reactive, highly sticking SiH_2 radicals are well confined between the two electrodes while having a much lower but important concentration compared to SiH_3. On the other hand, the spatial distribution of SiH_3 radicals which are much less reactive in the gas phase and have a quite low sticking coefficient with the surface, is mainly determined by diffusion as well as by their initial production in high field areas between the two electrode edges. Concerning the differences between the two pressures, the density of SiH_2 [Fig. 3(a)] is much higher for the 1-torr case, while the density of SiH_3 is not significantly affected. This observation indicates that relatively high pressures favor the contribution of low sticking radicals to the film growth.

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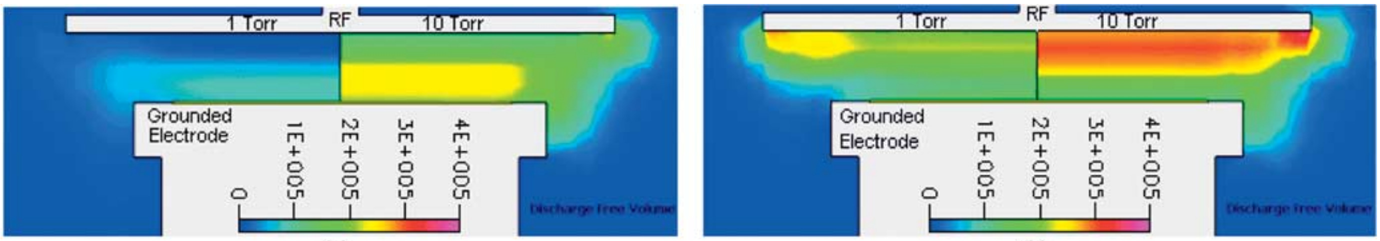


(a) (b)

Fig. 1. Spatial distribution of power dissipation (W/m^3) in 1-torr 2.5% SiH_4 in H_2 discharges and 10-torr 0.25% SiH_4 in H_2 discharges at (a) $\pi/2$ and (b) $3\pi/2$.

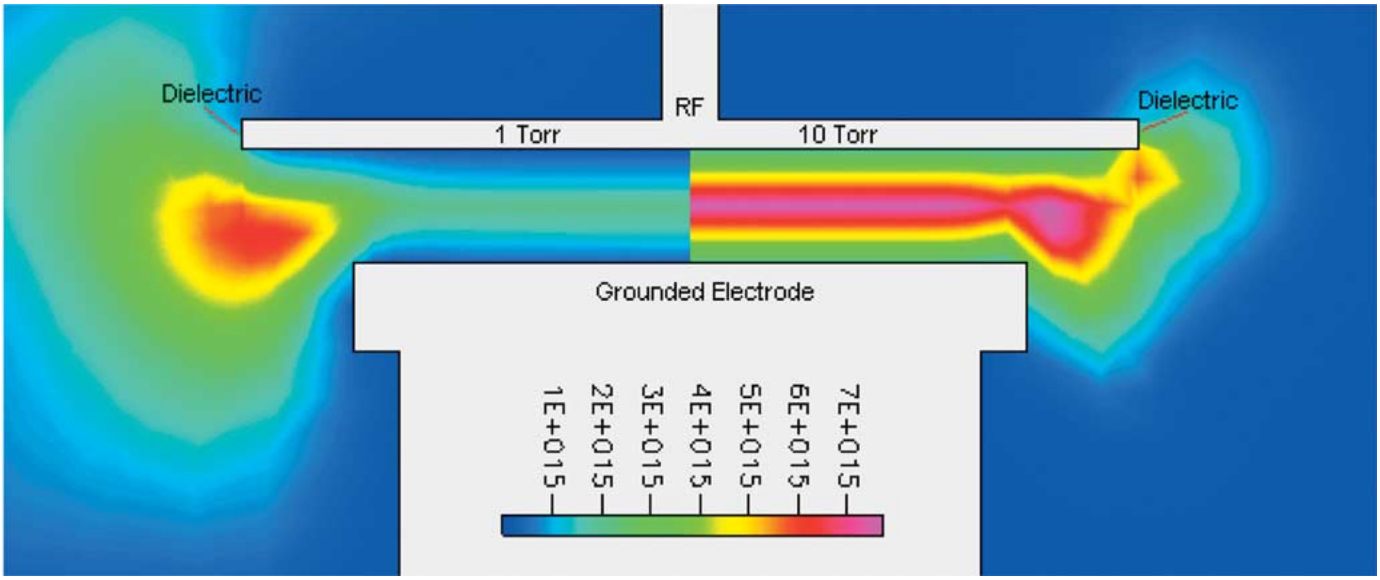
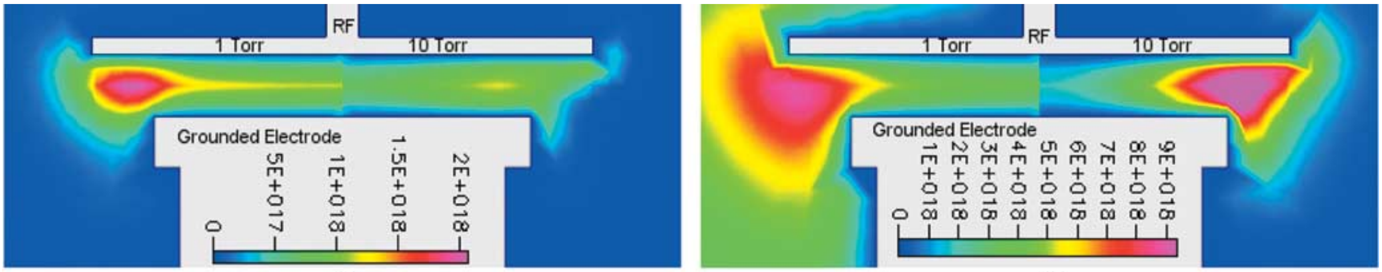


Fig. 2. Time-averaged electron density distribution (m^{-3}) for 1-torr 2.5% SiH_4 and 10-torr 0.25% SiH_4 in H_2 discharges.



(a) (b)

Fig. 3. Spatial distribution of (a) SiH_2 radicals and (b) SiH_3 radicals for 1-torr 2.5% SiH_4 and 10-torr 0.25% SiH_4 in H_2 discharges.

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