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Gas-phase and surface kinetics suitable for 3d simulations of SiH₄-H₂ discharges used in photovoltaic applications

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The present work deals with capacitively coupled SiH₄-H₂ discharges in conditions relevant for thin film photovoltaic industry. We aim here to provide practical but still accurate descriptions of gas-phase mechanisms and surface-reaction processes during the deposition of amorphous and micro-crystalline silicon films. Predicted densities of film precursors and the deposition rates as obtained from fluid simulations are compared against independent calculations and experimental values. The gas-phase and surface kinetics are further exploited to provide information about discharges sustained at 40 MHz in a parallel-plate configuration.

1. Introduction

With introduction of high performance amorphous and micro-morph (a-Si:H/ μ c-Si:H tandem solar cells) technologies Oerlikon Solar reached a top position within the market of thin film solar cells manufacturing solutions. This impressive commercial success relies heavily on plasma reactor design and its capabilities.

At Oerlikon Solar, along the years, several scientific aspects have been understood, solved through innovative approaches and the acquired knowledge transferred to our standard reactor KAI-1 1200, which allows the manufacturing of high efficient solar panels with 1.4 m² area [1].

2. Results

This work reports simulation results for SiH₄-H₂ discharges sustained at 13.56 and 40 MHz, in cylindrical and parallel plate configurations. The calculations have been performed for pressures between hundreds of mTorr to a few Torr. The SiH₄ dilutions correspond to gas mixtures leading to amorphous and micro-crystalline layers suitable for solar cell applications.

The commercial package CFD-ACE-Plasma is used to self-consistently describe the gas-flow, the charged particle dynamics and radical transport, as well as the formation of bulk material at the substrate. The software uses transient simulations, advancing radio-frequency cycle and flow with different time steps. Plasma module adopts a standard fluid framework and the sticking coefficient formulation is used to account for surface reactions.

Here, we first validate a coupled set of gas-phase mechanisms and surface reactions used later in standard simulations. The gas-phase description includes about 80 mechanisms while deposition and surface processes are represented by about 15 reactions.

Electron induced processes have been treated by means of collision cross sections. We report mainly results obtained with collision cross section taken from [2]. Since the dissociation pattern of SiH₄ molecule is unknown, several branching rates have been tested [3], and the results discussed. We analyze also the impact of several mechanisms, such as H atoms extraction, silylene insertion or silyl association, on the overall result. Attention is paid to reaction paths leading to the formation of poly-silane up to Si₄H₁₀.

Standard runs use the values of sticking coefficients proposed in [4]. We evaluate the individual contribution to film thickness of SiH₃, SiH₂, SiH and Si radicals, as well as the importance of ion fluxes, H atoms, disilyl and disilene incoming fluxes.

The calculated values of deposition rate and the densities of film precursors have been compared with that ones measured and computed in [3]. An overall good agreement is found. This validation has been performed for H₂ dominated discharges, in a cylindrical set-up, at 13.56

MHz excitation frequency. In table 1 we compare the present results with calculations and measurement reported in [3]. Note that in [3] the deposition rate has been measured through profilometry and the absolute densities of SiH_n ($n=1-3$) radicals have been measured using the threshold ionization mass spectrometry at the substrate center.

	A	B	C
DR [A/s]	1.7	2	5
SiH_3 [cm^{-3}]	4.2×10^{11}	4.5×10^{11}	3.6×10^{11}
SiH_2 [cm^{-3}]	6.3×10^{10}	7.1×10^{10}	1.3×10^{10}
SiH [cm^{-3}]	1.2×10^{10}	2.1×10^{10}	1.7×10^9

Table 1. Deposition Rate (A/s) and densities of film precursors (cm^{-3}) as predicted in this work - column A, and the values measured and calculated in [3] – column B and C, respectively.

The gas-phase and surface kinetics have been further used in three dimensional (3d) simulations of SiH_4 - H_2 discharges, in a parallel plate configuration, at 40 MHz frequency. In Figure 1 we plot the calculated values of the deposition rate in a parallel direction with the gas flow (toward outlet), and perpendicular with the flow (toward reactor wall). The differences which can be observed are a combination between pumping and reactor edge effects.

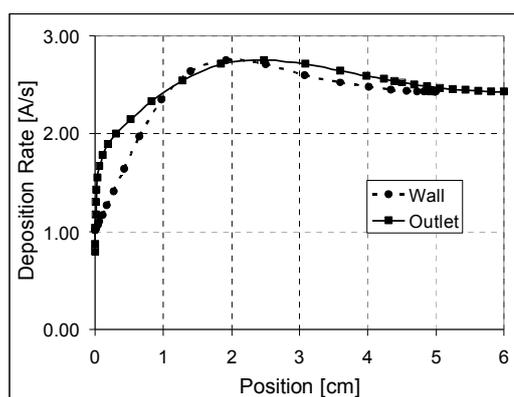


Figure 1. The deposition rate perpendicular to the gas flow (dotted line) and parallel with the flow – in front of the outlet (full line). Both wall and gas-outlet are located at position zero.

3. Conclusions

All the simulations here presented assume a Maxwellian electron distribution function. This may affect our calculations performed at low pressures. This limitation can be easily alleviated by using the look-up table technique. We conclude however that, for a given set of cross section, there are only a few gas-phase mechanisms with a considerable impact on the deposition rate. Changes of sticking coefficients do affect both deposition rate and film precursors in gas-phase. The cross section sets available in literature, as well as the silane dissociation pattern may influence the converged solution considerably. For a parallel plate configuration, the deposition rate can exhibit variations in directions parallel and perpendicular to the flow.

3. References

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