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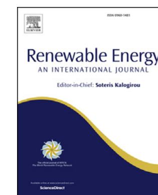

Multiscale modeling and run-to-run control of PECVD of thin film solar cells

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A B S T R A C T

In this work, we focus on the development of a multiscale modeling and run-to-run control framework with the purpose of improving thin film product quality in a batch-to-batch plasma-enhanced chemical vapor deposition (PECVD) manufacturing process. Specifically, at the macroscopic scale, gas-phase reaction and transport phenomena yield deposition rate profiles across the wafer surface which are then provided to the microscopic domain simulator in which the complex microscopic surface interactions that lead to film growth are described using a hybrid kinetic Monte Carlo algorithm. Batch-to-batch variability has prompted the development of an additional simulation layer in which an exponentially weighted moving average (EWMA) control algorithm operates between serial batch deposition sequences to adjust the operating temperature of the PECVD reactor to overcome drift in the electron density of the plasma. Application of the run-to-run (R2R) control system developed here is shown to reduce offset in the product thickness from 5% to less than 1% within 10 batches of reactor operation. Finally, we propose an extension of the EWMA algorithm to four independent, radial wafer zones in order to improve thickness uniformity in the presence of spatially non-uniform species concentrations. It is demonstrated that the produced thin films can be driven to the desired thickness set-point of 300 nm in less than 10 batches in the presence of both electron density drift and non-uniform deposition rate profiles.

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1. Introduction

Plasma enhanced chemical vapor deposition (PECVD) remains the dominant mechanism by which silicon based thin films are produced in both the microelectronics and solar cell industries [13]. Although moderate manufacturing costs and the possibility of extremely low operating temperatures ($\leq$525 K) allow for the widespread use of batch PECVD processing [16,31], two often neglected problems are persistent in the production of high quality amorphous silicon (a-Si:H) layers: the influence of reactor conditioning on the plasma chemistry [9], and the spatial non-uniformity in the thin film thickness [3] owing to gas-phase transport phenomena across the wafer. Specifically, during the initial operation of a clean PECVD reactor the plasma phase exhibits transient behavior as the interior surfaces become coated by the deposition species causing drift in the electron density profiles and in the film thickness. Second, at the reactor length scale (for example, a 20 cm wafer is used in this work) consumption and transport of deposition species across the wafer surface have been shown to cause growth rate differences greater than 19% [25,26]. Given that the efficiency of a photovoltaic absorber layer (e.g., an a-Si:H thin film) is strongly dependent on the film thickness [12], reduction of growth rate non-uniformities is of paramount importance. While preconditioning prior to thin film deposition (i.e., allowing the reactor surfaces to become fouled) is a well-established practice, this represents significant waste in both valuable resources and manufacturing time. In addition, the film uniformity within a single batch cannot be corrected via preconditioning alone, and has been shown to require advanced, in-situ processing techniques [6].

Recently much attention has been given to the development of model-based control schemes with the goal of improving solar cell performance through the production of textured surfaces (e.g., thin film grating) [10,11]. These models typically rely on kinetic Monte

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Carlo (kMC) algorithms to simulate deposition processes and therefore focus on the evolution of surface microstructure in nano- to micrometer length scales. As a result, these models are unable to capture the reactor scale dynamics and cannot be applied to the problems mentioned previously which pertain to both the macroscopic and microscopic domains of batch PECVD reactor operation. Fortunately, advances in high-performance computing have made possible the modeling of multiscale processes with complex behavior and large system sizes [14,22,30]. In a pervious work of our group [6], we developed a multiscale model which provided fundamental understanding of the dynamics involved in the PECVD of *a*-Si:H thin films and allowed for quantitative prediction of product quality. In the present work, we present improvements to our original model, as well as an additional simulation domain that allows for run-to-run (R2R) control of the batch process in an effort to counteract both batch-to-batch and spatial variations in the film thickness.

More specifically, this work proposes a multiscale modeling and operation framework which is capable of not only capturing the interdependence of the gas-phase and film growth phenomena, but also allows for multi-batch operation under the implementation of a run-to-run (R2R) control algorithm. Within a single batch simulation a standard gas-phase model is used; however, the microscopic model, describing the *a*-Si:H thin film surface evolution, has been developed from the work of Tsalikis et al. [28] to be computationally efficient and account for the four dominant microscopic processes: physisorption, surface migration, hydrogen abstraction, and chemisorption. As opposed to traditional kMC formulations, surface migration has been decoupled from the other microscopic surface processes owing to its faster rate to allow for simulations on the order of thousands of monolayers without compromising fidelity to established chemical models.

At the completion of each batch simulation, a novel R2R control algorithm is applied in order to predict appropriate operating conditions for the upcoming batch. In other words, post-batch measurements of the film thickness at various radial positions are fed to an exponentially weighted moving average (EWMA) algorithm which in turn updates the temperature of the PECVD reactor within discrete zones. It is demonstrated that through appropriate tuning of the multiscale model, and application of the proposed R2R operation strategy, the thin film product can be driven to the desired thickness set-point regardless of radial position and drift within the PECVD reactor.

The structure of the manuscript is as follows: first, a detailed description of both the macroscopic gas-phase and microscopic surface models are provided. Next, extensive simulations demonstrate strong agreement between experimentally grown *a*-Si:H films and those resulting from the multiscale model proposed in this work. A total of 40 serial batch simulations conducted using the nominal process parameters (i.e., $T = 475$ K and $P = 1$ Torr) then reveal drift in the product away from the desired film thickness of 300 nm. The proposed EWMA algorithm is then applied within a single reactor zone and shown to successfully reduce film offset to within the process noise level. Finally, four concentric reactor zones are defined, each with a corresponding R2R controller and initial gas-phase concentration. In the presence of both plasma variation caused by conditioning of the reactor and spatial non-uniformity caused by consumption of the process gas, the proposed control scheme demonstrates significantly improved thickness uniformity regardless of radial position within the reactor.

2. Process description and modeling

The process under consideration in this work is a parallel plate PECVD reactor utilizing two charged electrodes designed to deposit thin films onto a single wafer placed on top of the lower electrode; see Fig. 1 (left). We employ a showerhead arrangement to distribute the influent gas stream consisting of a 9:1 mixture of hydrogen (H_2) and silane (SiH_4) throughout the chamber. Thin film growth proceeds through the production of plasma by a radio frequency (RF) power source which generates a chemically reactive mixture of radicals. These radicals (namely, SiH_3 and H) are transported to the surface via diffusion and convection where they react to form amorphous silicon (*a*-Si:H). Successful deposition requires the uniform growth of a 300 nm thick *a*-Si:H film on a wafer with a diameter of 20 cm.

Two distinct simulation regimes exist within this framework: the macroscopic gas phase which includes mass and energy balances, as well as the complex, microscopic surface interactions that dictate the structure of the silicon film of interest. Fig. 1 highlights the multiscale character of this process and the need to capture the dynamics at both scales due to the codepedency between the macroscopic and microscopic regimes. The following sections detail both the macroscopic gas-phase model and the microscopic surface model.

2.1. Gas-phase model

The twelve dominant species that lead to film growth and their corresponding thirty-four gas-phase reactions are accounted for throughout this work. A complete listing of the reactions, mechanisms and rate constants are available in Table 1. The first set of results presented in this work, within the open-loop operation section, assume that the process gas is well mixed and the rate constants do not depend on temperature. For this case a differential mass balance is used to numerically integrate the species concentrations forward with time and the resulting values are used without reference to the spatial location within the PECVD reactor. The following differential equation demonstrates the possible contributions to the mass balance for a given species:

$$\frac{dc_i}{dt} = \frac{c_i^{in}}{t_{in}} - \frac{c_i}{t_{out}} + \left[\sum_j \nu_i^j R^j\right] - \frac{1}{N_a V} r_{phys,i} + \frac{1}{N_a V} r_{abs,i}, \quad (1)$$

where c_i is the concentration in mol/cm^3 of species i, t_{in} is the inlet gas time constant defined as the reactor volume over the flow rate into the reactor, t_{out} is the outlet stream time constant defined as the reactor volume over the flow rate out of the reactor, ν_i^j is the stoichiometric coefficient for reactant i in reaction j as listed in Table 1, $r_{phys,i}$ is the rate of physisorption of species i, and $r_{abs,i}$ is the rate of abstraction of species i from the wafer surface.

The second set of results presented in this work, those referring to spatial non-uniformity in film growth, utilize a gas-phase model that includes energy and momentum balances in addition to the differential mass balance presented above. Under the assumptions of axisymmetric flow and continuum in the gas phase, mass, energy and momentum balances allow for the detailed modeling of the gas phase required in order to investigate spatial non-uniformities. The governing equations have been developed at length for CVD-type applications (e.g., [5,21,29]); however, here we apply the formulation by Armaou and Christofides [3] as radial dependence of species concentrations is needed to be accounted for due to the strong dependence of thin film thickness on photovoltaic efficiency. The mathematical model of the PECVD reactor consists of a flow velocity profile and four nonlinear dynamic diffusion-convection-reaction equations in two (radial and axial) dimensions (a set of four coupled parabolic PDEs). By treating the gas-phase as a three-dimensional stagnation flow, the evolution of the flow velocity profile within the PECVD reactor is computed from the Navier-

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