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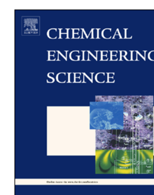

Multiscale modeling and operation of PECVD of thin film solar cells

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HIGHLIGHTS

- Novel microscopic model of thin film microstructure evolution.
- Multiscale PECVD model accounting for wafer grating.
- Novel operation policy for large-area thin film deposition.
- Uniform film thickness and surface microstructure that optimizes light trapping.

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ABSTRACT

This work proposes a multiscale modeling and operation framework for plasma-enhanced chemical vapor deposition (PECVD) of thin film silicon solar cells with uniform thickness and film surface microstructure that optimizes light trapping. Specifically, we focus on a single-wafer parallel-electrode PECVD process with showerhead arrangement and develop a multiscale model capturing both the gas-phase reaction and transport phenomena that lead to the deposition of the thin film across the wafer as well as multiple microscopic models that describe the evolution of the thin film surface microstructure at equispaced, discrete spatial locations across the wafer. While the modeling of chemical reactions and transport-phenomena (both diffusion and convection) in the gas-phase adopts the continuum hypothesis and is based on two-dimensional in space partial differential equations, a novel microscopic model is developed for the *a*-Si:H thin film surface evolution, which accounts for four microscopic processes: physisorption, surface migration, hydrogen abstraction and chemisorption. A hybrid kinetic Monte Carlo (kMC) algorithm is utilized to reduce computational requirements without compromising the accuracy of established chemical models that account for interactions amongst physisorbed radicals, and the microscopic model fidelity is established though calibration with experimentally obtained growth rates and surface morphology data. The results of the multiscale process model indicate that in order to produce a thin film with a diameter of 20 cm and a uniform thickness with surface microstructure that optimizes light trapping: (a) a sinusoidally grated wafer surface should be used in which the grating period and depth should correspond to values that lead to film surface roughness and height–height correlation length that are on the order of visible light wavelength range, and (b) the substrate temperature should be adjusted, along several concentric zones across the substrate, to compensate for a radially non-uniform deposition rate of the film on the wafer owing to gas-phase transport phenomena. Due to the dependence of film growth rate on substrate temperature, the wafer surface is separated into four concentric zones, each with an independent heating element. Extensive simulations demonstrate that the use of appropriate sinusoidal wafer grating and the regulation of substrate temperature provide a viable and effective way for the PECVD of thin film silicon solar cells with uniform thickness and film surface microstructure that optimizes light trapping.

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1. Introduction

Plasma enhanced chemical vapor deposition (PECVD) is widely used in the microelectronics and solar cell industries to deposit thin films from a mixture of gas-phase species onto a solid substrate (Kern, 1991). Specifically, in the solar cell industry, PECVD is broadly used in the production of thin film silicon solar cells to deposit amorphous silicon semiconductor layers due to low manufacturing costs via silane recycling (Kreiger et al., 2013), the possibility for extremely low operating temperatures ($\leq 250\ ^{\circ}C$) (Yang et al., 2000), and the desirable dielectric properties of amorphous silicon thin films (Rech and Wagner, 1999). However, even high quality amorphous silicon solar cells suffer from efficiencies (of solar power conversion) that are lower than their crystalline counterparts which has motivated significant efforts to improve other thin film light trapping attributes to increase solar power conversion (Green et al., 2014). In this direction, periodic surface textures have been recently proposed in an effort to increase light scattering on the thin film surface or interface and to obtain photocurrents from *a*-Si:H thin film solar cells competitive with other existing solar cell technologies (Eisele et al., 2001; Heine and Rudolf, 1995; Zeng et al., 2008; Sai et al., 2008). Optical simulations of thin films with periodic surface textures (grown on appropriately grated wafers) have demonstrated up to 35% more photocurrent when compared to traditional, flat interfaces (Campa et al., 2010), particularly when the surface roughness and height–height correlation length are comparable to visible light wavelength length scales. Although photolithographic fabrication techniques allow for the creation of grated wafer substrates (van-Erven et al., 2008), in practice, it is not easy to achieve consistent morphology of the surface of an absorbing layer due to the need to deposit thin films over a large area. Significant non-uniformity in final film thickness and variations in surface morphology may occur due to the consumption of reactants as process gases travel radially across the wafer, leading to radially varying deposition rates (e.g., (Armaou and Christofides, 1999; Stephan et al., 1999; Sansonnens et al., 2003)).

In the context of thin film surface morphology control, several model-based control schemes have been applied to deposition process models with the goal of improving solar cell performance through the achievement of periodic film surface textures (e.g., (Huang et al., 2012a,b)). These models typically rely on kinetic Monte Carlo (kMC) algorithms to simulate deposition processes, focusing on evolution of thin film surface microstructure in nano- to micrometer length scales. The concept of using grated wafers to impart periodic surface textures to thin films has existed for some time (Geis et al., 1979), and over the past three decades extensive efforts have been made in optimizing grating shape for the purposes of light trapping (Campa et al., 2010; Eisele et al., 2001; Heine and Rudolf, 1995; Zeng et al., 2008; Sai et al., 2008). Four parameters define the final shape of textured thin films: periodic shape (e.g., rectangular wave, pyramidal, sinusoidal, etc.), height H, period P, and film thickness τ. Given that film growth is driven by the formation of dangling bonds, surface migration has little effect on the shape of thin films beyond local roughness, and as a result, grated wafers can consistently impart optimized textures to thin films. However, practical applications of the existing modeling and control approaches to deposit thin films with tailored surface textures need to address the fact that the film deposition takes place over a large area, leading to the possibility of non-uniformity in film thickness at the reactor scale. Specifically, non-uniformity in reactant and product gas phase species concentrations is negligible on the scale of a single grating period (on the order of hundreds of nanometers), nullifying the need for spatially controlled film thickness at the nanoscale. However, at the reactor length scale (e.g., a 20 cm wafer is used in this work) consumption of reactants across the wafer surface has been shown to yield growth rate differences greater than 19% (Armaou and Christofides, 1999; Stephan et al., 1999; Sansonnens et al., 2003), prompting the need for reactor scale control.

In addition to film thickness uniformity control, the physics of the gas-phase species and film surface interactions should be carefully modeled in the microscopic film growth model when the film growth takes place in a PECVD process. Specifically, due to the vast number of species introduced by the presence of plasma, microscopic modeling of film growth by PECVD is a challenging task. Often the level of modeling detail must be compromised in lieu of simulation efficiency: for example, Novikov et al. (2009) developed a kMC algorithm capable of simulating films several hundred monolayers thick, however, important surface phenomena such as diffusion (migration) were ignored. Conversely, Pandey et al. (2009) conducted more detailed kMC simulations that included diffusion of surface radicals, and although their results appeared in good agreement with experimental data, their work was limited to a relatively small number of monolayers. A close look in the literature indicates a broad agreement of accounting for microscopic events such as the physisorption, migration, and chemisorption of surface radicals in the modeling of the nanostructure of growing thin films in PECVD.

Motivated by the above considerations, this work proposes a multiscale modeling and operation framework for plasma-enhanced chemical vapor deposition (PECVD) of thin film amorphous silicon solar cells. The interdependence of the gas phase and film growth phenomena means that neither can be ignored; as an example, the film growth rate and roughness are strongly tied to the rate of physisorption of surface radicals, which in turn is governed by the inlet concentration of silane and hydrogen gases. Conversely, hydrogen abstraction from the surface into the gas phase influences the overall concentration of reactive radicals. Given the computational challenge of using a single microscopic model to describe the entire PECVD process behavior, the disparity in scales necessitates the need for a multiscale model capable of capturing both the macro- and microscopic phenomena involved in thin film growth processes. Therefore, a multiscale model is developed capturing both the gas-phase reaction and transport phenomena that lead to the deposition of the thin film across the wafer as well as multiple microscopic models that describe the evolution of the thin film surface microstructure at equispaced, discrete spatial locations across the wafer. While the gas phase model is standard, the microscopic model, describing the *a*-Si:H thin film surface evolution, is computationally efficient and accounts for four microscopic processes: physisorption, surface migration, hydrogen abstraction, and chemisorption. Specifically, a nanoscale hybrid kMC scheme originally developed by Tsalikis et al. (2013) is applied to the growth of silicon films with periodic surface textures in an effort to maintain fidelity to established chemical models while allowing for practical computational requirements. The model considers the two dominant species involved in the growth of amorphous silicon films, H and SiH_3 (Perrin et al., 1998; Gallagher, 1988), and four corresponding surface processes: physisorption from the gas phase, hydrogen abstraction by SiH_3, chemisorption onto dangling bonds, and migration across neighboring, hydrogenated lattice sites. As opposed to traditional kMC formulations, surface migration is handled in a decoupled manner from the other processes allowing for efficient simulations in excess of 1000 monolayers. The results of the multiscale process model indicate that in order to produce a 20 cm thin film of uniform thickness with surface microstructure that optimizes light trapping: (a) a sinusoidally grated wafer surface should be used in which the grating period and depth should correspond to values that lead to film surface roughness and height–height correlation length that are on the order of

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