

Modeling and experiments of microcrystalline silicon film deposited via VHF-PECVD

Yongsheng Chen^{*}, Xiping Chen, Yuechao Jiao, Xiuli Hao, Jingxiao Lu, Shi-e Yang

Key Lab of Material Physics, Department of Physics, Zhengzhou University, Zhengzhou 450052, China

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Abstract

A 1-D plasma model coupled with a well-mixed reactor model was used to simulate the growth properties of hydrogenated microcrystalline silicon film deposited by very high frequency plasma-enhanced chemical vapor deposition from SiH_4 and H_2 gas mixtures. Plasma parameters of the former, such as electron density and electron temperature, were determined and used as input values for the latter, in which concentrations of gas phase species, crystalline orientation, hydrogen content, surface fraction of dangling bonds, and deposition rate were calculated. Simultaneously, a series of in situ optical emission spectroscopy measurements and film depositions were carried out to investigate the correlation between the model and the experiments. Desired agreements between both were achieved. © 2013 Elsevier Ltd. All rights reserved.

Keywords: Hydrogenated microcrystalline silicon film; Plasma enhanced chemical vapor deposition; Simulation; Optical emission spectroscopy

1. Introduction

Hydrogenated microcrystalline silicon ($\mu\text{c-Si:H}$) films have attracted potential application in several kinds of devices, such as solar cells and thin film transistors in liquid crystalline display, because of their high optical absorption, high carrier mobility, and stable behavior under illumination compared with hydrogenated amorphous silicon (a-Si:H). Plasma-enhanced chemical vapor deposition (PECVD), especially excited with very-high frequency (VHF) power source, has become the most widely used method for deposition of device-grade $\mu\text{c-Si:H}$ films (Yamamoto et al., 2004; Klein et al., 2004; Vetterl et al., 2001). Thus, researchers focus on realizing controlled film growth as well as understanding the relationship between the deposition parameters and the film properties.

Theoretical simulation is extremely useful to verify the effects of the external parameters on the film deposition process.

Bhandarkar et al. (2000) and Bleecker et al. (2004) investigated the nucleation of silicon hydride clusters in a silane discharge, and found that anion-neutral reactions are the main pathway that leads to cluster formation. Kushner (1988) and Nienhuis et al. (1997) presented a model for radio-frequency glow discharges sustained in silane/hydrogen gas mixtures for the PECVD of a-Si:H , and discussed the relation between the external settings and the resulting composition of the gas and the deposition rate. In 2005, Satake and Kobayashi established a numerical model, composed of two linked simulations, namely, 1-D drift-diffusion plasma simulation, as well as gas-phase and surface chemistry simulation in well-mixed reactor, to study the correlation between $\mu\text{c-Si:H}$ properties and deposition operating parameters. However, the relationship between the numerical and experimental results was only limited to the deposition rate, which is not enough to verify the correction of the simulation.

^{*} Corresponding author.

E-mail address: chysh2003@zzu.edu.cn (Y. Chen).

The present paper implements a model that considers the electron-impact, gas phase, and surface reactions within a 1-D plasma model and a well-mixed reactor model to understand the effect of VHF power and deposition pressure on film properties. In situ optical emission spectroscopy is used to investigate the plasma optical properties. The $\mu\text{c-Si:H}$ thin films are prepared under model conditions for comparison with the model results.

2. Numerical model and experimental details

2.1. Numerical model

The numerical model considers the electron-impact, gas-phase, and surface phase reactions within a plasma model and a well-mixed reactor model. Plasma parameters, such as the electron density and electron temperature, are determined through a 1-D plasma model provided in the Plasma Module of COMSOL 4.2a, and used as inputs for the reactor model (Meeks et al., 1996; Kee et al., 1996). In this plasma model, 24 electron collision reactions with H_2 , H , and SiH_4 are considered including electron-neutral collision processes, such as elastic, ionization, excitation, dissociation, and attachment (<http://www.lxcat.laplace.univ-tlse.fr>). The secondary electron emission due to ion impact is set to zero, and H_2^+ , SiH_4^+ , and SiH_2^+ ions are considered as completely neutralized upon arriving at the electrodes. The excited H_2 and SiH_4 molecules and H atoms are set to revert to their ground states when they come in contact with the walls, and the dissociated H atoms and SiH_2 particle react with one another to form H_2 and SiH_4 molecules on the surface of the walls. The gas temperature, plasma frequency, SiH_4 concentration, and electrode distance are 400 K, 75 MHz, 3%, and 1.5 cm, respectively.

The well-mixed reactor model is composed of gas-phase and surface reactions in the AURORA module of the CHEMKIN software. The former includes 15 gas-phase neutral species (SiH_4 , H_2 , Si_2H_6 , Si_3H_8 , Si_4H_{10} , Si_5H_{12} , Si_6H_{14} , SiH_3 , SiH_2 , SiH , H_3SiSiH , Si_2H_5 , Si_3H_7 , Si_4H_9 , H) and 42 electron-neutral and neutral-neutral reactions, whereas the latter includes 43 surface reactions for each facet of (100) and (111) Bhandarkar et al., 2000; Kushner, 1988; Satake and Kobayashi, 2005; Moravej et al., 2004. The surface species is denoted by (S) and the bulk species by (B). The SSSS(B), SSSH(B), and SSHH(B) comprise fourfold silicon atom, monohydride, and dihydride in the bulk, respectively. The surface site densities of Si(100) and Si(111) surfaces are 1.12×10^{-9} and 1.3×10^{-9} mol/cm², respectively. The surface temperature and total gas flow are fixed at 493 K and 100 sccm, respectively.

2.2. Experimental details

All $\mu\text{c-Si:H}$ films were deposited on quartz glass substrates in a cluster PECVD system (Chen et al., 2010,2008) at a frequency of 75 MHz, with an electrode area of 78.5 cm², and similar deposition parameters as

those of the simulation. The structural properties of the deposited films were characterized with Raman spectroscopy and X-ray diffraction (XRD), whereas the thicknesses of the films were measured by spectroscopic ellipsometry. Discharge properties of the plasma were monitored online by optical emission spectroscopy (ANDOR, SR-500) performed at the middle of the electrode gap. The emission light was collected by a lens with a focusing distance of 50 mm and guided to a monochromator with a grating of 1200 L/mm. The emission peak intensities of three species of H_α (656 nm), H_β (486 nm), and SiH^* (414 nm) were detected, respectively.

3. Simulation results and discussion

Fig. 1 shows the spatial distribution of the electron density (n_e) and electron temperature (T_e) between the

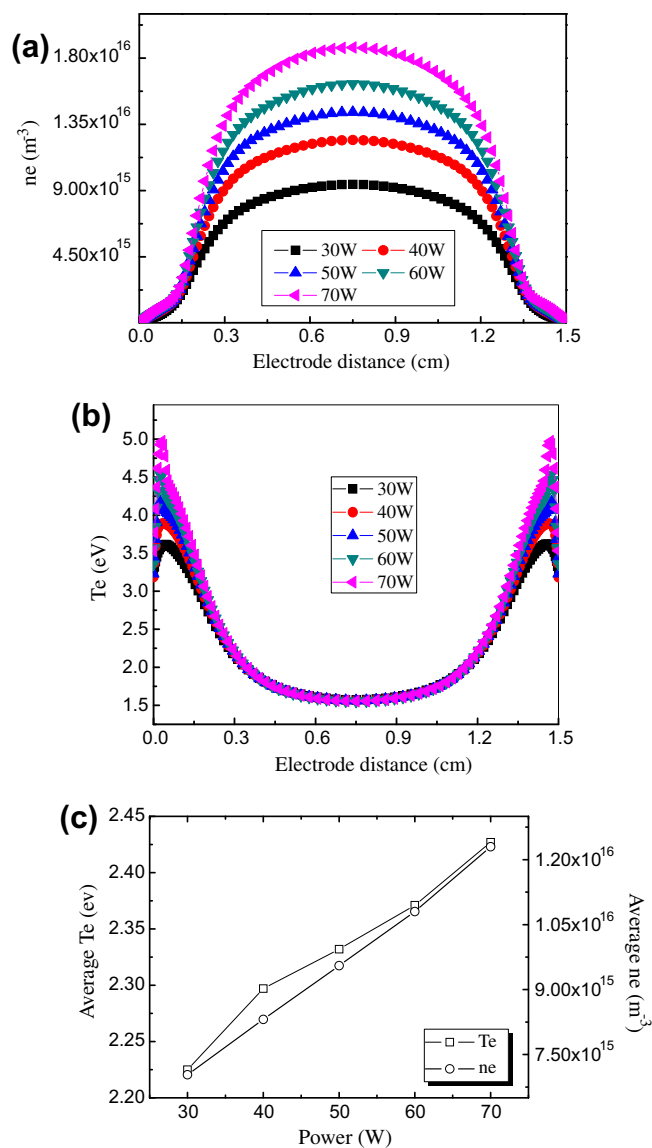


Fig. 1. Spatial distribution of (a) n_e , (b) T_e , and (c) space-averaged n_e and T_e with power at 2 Torr.

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