Thin Solid Films 519 (2011) 2863–2866

Contents lists available at ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

Spectroscopic ellipsometry studies on hydrogenated amorphous silicon thin films deposited using DC saddle field plasma enhanced chemical vapor deposition system

Jhantu Kumar Saha [a], Barzin Bahardoust [a], Keith Leong [a], Adel B. Gougam [b], Nazir P. Kherani [a,c,*], Stefan Zukotynski [a]

[a] Department of Electrical and Computer Engineering, University of Toronto, 10 King's College Road, Toronto, Ontario, Canada M5S 3G4
[b] Arise Technologies Corporation, 65 Northland Road, Waterloo, Ontario, Canada N2V 1Y8
[c] Department of Materials Science and Engineering, University of Toronto, 184 College Street, Toronto, Ontario, Canada M5S 3E4

ARTICLE INFO

Available online 21 December 2010

Keywords:
Hydrogenated amorphous silicon
Spectroscopic ellipsometry
DC saddle field

ABSTRACT

Hydrogenated amorphous silicon (a-Si H) films deposited on crystalline silicon substrates using the DC saddle field (DCSF) plasma enhanced chemical vapor deposition (PECVD) system have been investigated. We have determined the complex dielectric function, $\varepsilon(E)=\varepsilon_1(E)+i\varepsilon_2(E)$ for hydrogenated amorphous silicon (a-Si:H) thin films by spectroscopic ellipsometry (SE) in the 1.5–4.5 eV energy range at room temperature. The results indicate that there is a change in the structure of the a-Si:H films as the thickness is increased above 4 nm. This is attributed to either an increase in the bonded hydrogen content and, or a decrease of voids during the growth of a-Si:H films. The film thickness and deposition temperature are two important parameters that lead to both hydrogen content variation and silicon bonding change as well as significant variations in the optical band gap. The influence of substrate temperature during deposition on film and interface properties is also included.

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1. Introduction

Hydrogenated amorphous silicon (a-Si:H) films have been widely used for various electronic devices such as thin film solar cells [1], thin film transistors [2] and novel electronic devices, for example, quantum dot memory devices [3]. The optical properties have usually been determined by means of optical transmission measurements of thick films grown on a transparent glass substrate [4,5]. However, this is not possible for films grown as part of a device on a non-transparent substrate such as crystalline silicon (c-Si) in an amorphous-crystalline silicon heterojunction. Spectroscopic ellipsometry can be utilized to determine the real and imaginary parts of the dielectric functions of the a-Si:H layers directly. Ellipsometry is insensitive to light intensity fluctuations, temperature drifts, and macroscopic roughness [6]. For nanometer (nm) thin films, optical characterization becomes more sensitive owing to the possibility of large variations in film morphology [7] and optical properties [8–11]. In the present work, a-Si:H films deposited by the DC saddle field (DCSF) plasma enhanced chemical vapor deposition (PECVD) technique [12,13] are characterized by ultraviolet–visible (UV–VIS) spectroscopic ellipsometry (SE). The SE data are analyzed to obtain structural and optical properties of the a-Si:H films. In order to calculate the desired values (e.g., layer thickness, optical constants) from the measured data, a suitable optical model has to be applied. For amorphous semiconductors several models exist. In the present work, the widely accepted Tauc-Lorentz (TL) model is applied, a specific model for amorphous semiconductors combining the Tauc relation and Jellison–Modine's dispersion expression. These results have been analyzed to determine the influence of substrate temperature during deposition on film and interface properties.

2. Experimental

The ultrathin a-Si:H films were deposited by the DCSF PECVD method onto double sided polished (100) orientated 280 µm n-type (P doped, FZ) wafers with resistivity of 1~2 Ω cm. The samples were RCA cleaned and the native oxide was etched off in a dilute HF solution (5%) for 60 s. Subsequently, the samples were immediately transferred to the load lock of the deposition system. Silane (SiH_4) was used as a source gas for the deposition. Chamber pressure was fixed at 160 mTorr, the silane flow rate was 30 sccm, and the anode current was 34.5 mA. The substrate temperature, T_s, was varied from 120 °C to 240 °C, and deposition time, t_d, was varied from 5 min to 30 min. The time interval between removal of the silicon samples from the deposition chamber and the ellipsometric measurements ranged between 1 and 5 h.

Surface morphology of the a-Si:H films was studied by means of an atomic force microscopy (AFM), using a multimode scanning probe microscope. The AFM image was acquired in the contact mode and in

* Corresponding author. Department of Electrical and Computer Engineering, University of Toronto, 10 King's College Road, Toronto, Ontario, Canada M5S 3G4. Tel.: +1 416 946 7372; fax: +1 416 946 8734.
E-mail addresses: jk.saha@utoronto.ca (J.K. Saha), kherani@ecf.utoronto.ca (N.P. Kherani).

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doi:10.1016/j.tsf.2010.12.074

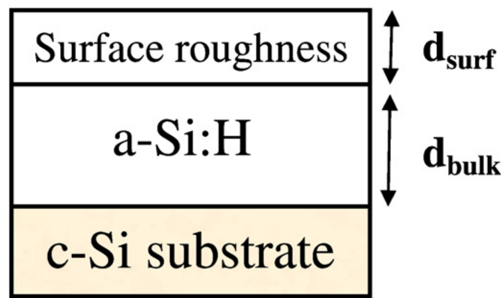

Fig. 1. The optical model used in SE analysis.

the repulsive force regime with a constant of the order of 1 nN between the AFM tip and sample surface.

The SE measurements were carried out over the spectral range of 1.5–4.5 eV using an ex-situ spectroscopic ellipsometer (Sopra model GES5-E) equipped with goniometer at incident angles of 65°, 70°, and 75°. The incident angles were chosen in order to attain maximum reflected intensity from the sample and large oscillations in cos(Δ) values within the measured spectrum. Data acquisition and analysis was performed using WINELL II software (version 2.2.0.6) [14,15]. The analysis of SE data was carried out by screening several realistic physical models for amorphous semiconductors [16–20]. In the present work, the widely accepted Tauc–Lorentz (TL) model [18,21] is applied for the parameterization of the optical functions for amorphous semiconductors and insulators. In order to represent a mixed amorphous–crystalline phase for films showing epitaxial character, the Bruggeman model (also the effective medium approximation (EMA)) was used [22,23].

In order to verify the thickness values obtained from the SE analyses, high-resolution (HR) cross-sectional transmission electron microscopy (TEM) micrographs were obtained for the a-Si:H/c-Si heterostructure samples using the HRTEM JEM2010F.

3. Results and discussion

3.1. AFM observations

We used AFM to evaluate the surface morphology of a 1 μm^2 surface of a 5-nm-thick a-Si:H sample grown on a c-Si substrate, as shown in Fig. 1. The root mean square (rms) roughness obtained from the AFM image is approximately 0.23 nm. This roughness is comparable to the reported value obtained for polished, HF-etched Si (111) wafers as measured by scanning tunneling microscopy (STM) (0.12–0.18 nm) [24]. It is noteworthy that surface micro roughness can have a significant effect on ellipsometric measurements [25].

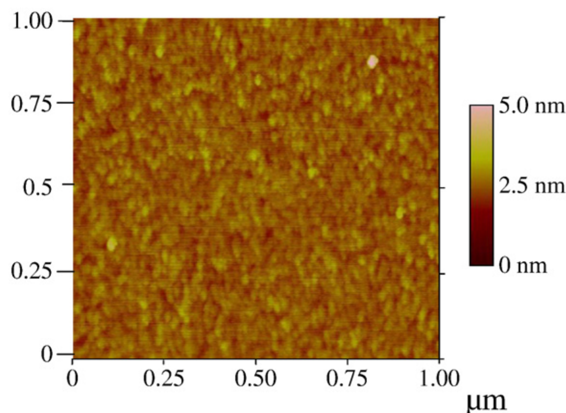

Fig. 2. AFM image (1 × 1 μm^2) for a-Si:H sample. The root mean square (rms) roughness obtained from this image is ~0.23 nm.

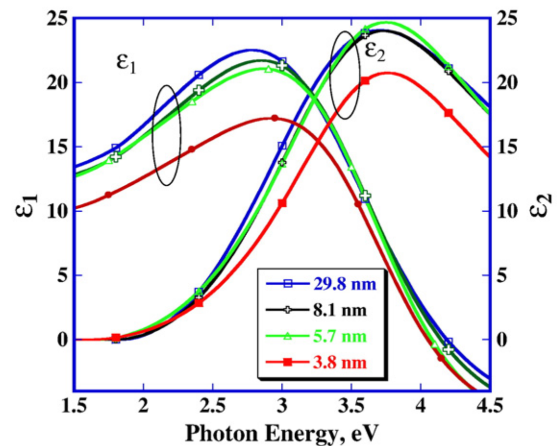

Fig. 3. Spectra for real (ε_1) and imaginary (ε_2) parts of dielectric functions of a-Si:H films for different thicknesses.

3.2. SE measurements and analysis

The dielectric function, $\varepsilon(E) = \varepsilon_1(E) + i\varepsilon_2(E)$, for hydrogenated amorphous silicon (a-Si:H) thin films is determined by SE in the 1.5–4.5 eV photon-energy range at room temperature using an optical model that assumes a perfectly flat surface. A two-layer model comprising of a thin a-Si:H layer and a native oxide (SiO_2) surface layer is used, as shown in Fig. 2; here the native oxide surface layer also substitutes for the surface roughness. The statistical measure of the quality of fit attained for the ellipsometric measurements performed on our films was fairly high (regression coefficient, $R^2 > 0.99$, mean -squares deviation, $\sigma < 0.001$).

Fig. 3 shows the real (ε_1) and imaginary (ε_2) parts of dielectric function spectra of a-Si:H for different thicknesses deposited by DCSF PECVD at substrate temperature of 170 °C and at working pressure of 160 mTorr. A single broad band peak in the $\varepsilon_2(E)$ spectrum is typically observed in amorphous tetrahedral semiconductors [25]. The experimental data of a-Si:H deposited by DCSF PECVD give a maximum value of ε_2~24.2 near E~3.6 eV. In contrast, ε_2~26.6 at E~3.45 eV was obtained for self-implanted a-Si [26], and ε_2 ~30 at 3.7 eV was obtained for LP-CVD a-Si [27]; the reported peak energy values bracket the peak energy value reported here. Closer observation of the of ε_1, ε_2 spectra in Fig. 3 show a marked drop as the film thickness decreases below 4 nm, indicating a change in the structure of the a-Si:H. This change can be attributed to an increase in the bonded hydrogen content and/or a decrease of voids during the growth of a-Si:H films on a bare c-Si substrate [28]. Table 1 summarizes typical fitting results as obtained from SE modeling using the two-layer structure. This includes the oxide layer thickness and the inferred Tauc gap, E_g, for the samples.

In order to investigate the effect of substrate temperature on the interface structure, a series of a-Si:H layers were deposited at temperatures between 120 °C and 240 °C with a deposition time of

Table 1
Effect of film thickness on optical properties of thin a-Si:H films measured by means of SE.

$t_{deposition}$ (min)	a-Si film thickness (nm)	SiO_2 layer thickness (nm)	E_g (eV)	Quality of fit, (R^2, σ)
5	3.8	0.58	1.62	$R^2 > 0.99$, $\sigma < 0.001$
8	5.7	0.42	1.65	
10	8.1	0.73	1.80	
30	29.8	1.14	1.83	

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