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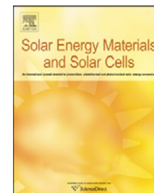

Structural and optical studies on hot wire chemical vapour deposited hydrogenated silicon films at low substrate temperature

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A B S T R A C T

Thin films of hydrogenated silicon are deposited by hot wire chemical vapour deposition technique, as an alternative of plasma enhanced chemical vapour deposition technique. By varying the hydrogen and silane flow rate, we deposited the films ranging from pure amorphous to nanocrystallite-embedded amorphous in nature. In this paper we report extensively studied structural and optical properties of these films. It is observed that the rms bond angle deviation decreases with increase in hydrogen flow rate, which is an indication of improved order in the films. We discuss this under the light of breaking of weak Si–Si bonds and subsequent formation of strong Si–Si bonds and coverage of the growing surface by atomic hydrogen.

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1. Introduction

It is well established that hydrogenated amorphous silicon (a-Si:H) and hydrogenated microcrystalline silicon (μc-Si:H) are very suitable materials for low cost and stable solar cell and other applications [1]. The extensively studied technique for the deposition of device quality a-Si:H and μc-Si:H is the plasma enhanced chemical vapour deposition (PECVD). This technique is widely used for industrial applications with RF frequency 13.56 MHz to deposit a-Si:H films with very good optoelectronic properties. However, low deposition rate, especially for μc-Si:H, offers hurdles to the cost-effective fabrication of the PECVD-deposited devices [2,3]. Another important drawback of this technique is that the bombardment by energetic ions on the growing surface creates lots of defects, which is undesirable [3]. As an alternative of plasma assisted deposition a new technology namely hot wire chemical vapour deposition (HWCVD) or catalytic CVD (Cat-CVD) is emerging to prepare device quality films [4–6]. In this method the precursor gases are decomposed with the help of hot filament by the process of catalytic cracking reaction, thus avoiding the disadvantages related to plasma assisted processes. The simplicity of design [7] is another added advantage. As this is a new technique and not as extensively studied as PECVD, there is a need of extensive research on the deposition of device quality a-Si:H, μc-Si:H, nc-Si:H, etc. by this process.

In this paper, we report preparation and structural studies of HWCVD silicon films deposited at low substrate temperature by varying the hydrogen and silane (SiH_4) flow rate. Both X-ray diffraction (XRD) and Raman scattering studies show that the deposited films range from amorphous to nanocrystallite-embedded amorphous in nature. Scanning electron microscopy (SEM) studies on the films also reveal that the surface of these films range from smooth to that having grains. Fourier transform infrared (FTIR) spectroscopic analysis shows that the films contain ~6–13% of atomic hydrogen. Further analysis shows that hydrogen is present in the network mostly in monohydride configuration, which is an important requirement for stable device applications.

2. Experimental details

The films were prepared at low substrate temperature (substrate temperature ~200 °C) in a load lock based HWCVD chamber by varying the hydrogen and silane flow rates (HFRS and SFRs) keeping other parameters fixed (filament temperature ~1700 °C, filament to substrate distance ~6 cm). The chamber is first evacuated to base pressure 3×10^{-6} Torr before the precursor gases are passed. Prior to the dissociation of the gases, the chamber pressure is set at about 55 mTorr, which decreased to about 47 mTorr when the dissociation took place except for samples #1 and 9 where the chamber pressure after dissociation became 30 and 25 mTorr, respectively. The chamber pressure decreases because of the dissociation of the gases into various

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Table 1
Deposition conditions, thickness and deposition rate of hydrogenated silicon films used in the present study

Sample #/Series #			Process pressure (mTorr)	SiH_4 flow rate (SCCM)	H_2 flow rate (SCCM)	Thickness (nm)	Deposition rate (Å s^{-1})
Sample #1	I		30	4	0	483	3.22
Sample #2	I		47	4	10	478	1.77
Sample #3	I	III	45	4	15	302	1.20
Sample #4		III	50	3	15	242	0.89
Sample #5	II	III	47	2	15	174	0.64
Sample #6	II		49	2	10	202	0.75
Sample #7	II		46	2	8	325	1.20
Sample #8	II		45	2	5	480	1.78
Sample #9	II		25	2	0	315	1.75

The films are prepared by varying either the hydrogen or silane flow rate keeping substrate temperature 200 °C and filament temperature 1700 °C. Samples #1–3 form Series I (SFR 4 SCCM), samples #5–9 form Series II (SFR 2 SCCM) and samples #3–5 form Series III (HFR 15 SCCM). Prior to the dissociation of the gases the chamber pressure is set at about 55 mTorr, which decreased after the dissociation took place.

radicals having different lifetimes. The whole set of samples were deposited on corning 7059 glass, ITO-coated glass as well as c-Si wafer substrates for carrying out different types of studies. The SFRs and HFRs are varied such that samples #1–3 form one series (Series I) and samples #5–9 form another series (Series II) with varying HFR at two different SFRs 4 and 2 SCCM, respectively; while samples #3–5 form another series (Series III) with varying SFR at constant HFR of 15 SCCM. The detailed deposition conditions are listed in Table 1.

For the characterization of the films we used various tools like XRD, SEM, Raman spectroscopy, FTIR absorption spectroscopy, photoluminescence (PL) and UV–Vis–NIR transmission spectroscopy. XRD studies were done on the samples deposited on Corning 7059 using Siefert XRD 3003 TT X-ray diffractometer in 2θ mode at grazing angle of incidence 2–4°. Raman scattering experiments were done on the films deposited on both Corning 7059 and ITO-coated glass using Olympus BX41 Raman spectrometer with excitation wavelength of 514.532 nm in scan range 400–1000 cm^{-1}. SEM studies were performed using Leo 1430 VP scanning electron microscope on the films deposited on Corning 7059 glass. FTIR spectroscopic measurements were done in transmission mode in the wave number range 450–4000 cm^{-1} on films deposited on c-Si substrates with the help of Perkin Elmer Spectrum I and used for the calculation of bonded hydrogen content as well as the percentage of hydrogen in the monohydride mode. UV–Vis–NIR transmission measurements in the 400–1100 nm range were used to estimate the band gap, thickness and optical constants, following Swanepoel [8]. PL measurements are done at room temperature using Aminco Bowman Series 2 Luminescence Spectrometer with excitation wavelengths 300 nm (4.13 eV), 350 nm (3.54 eV) and 375 nm (3.30 eV), while the luminescence is recorded in the range 500–900 nm (2.48–1.38 eV).

3. Results and discussions

The thickness of the films as calculated from UV–Vis–NIR transmission data is found to be in the range of 175–480 nm. The band gap (E_G) of the films, calculated by plotting $\sqrt{\alpha h\nu}$ vs. $h\upsilon$ (Fig. 1), is estimated to be in the range of 1.7–1.9 eV. There is a general trend of increase in the band gap with the increase in HFR in the two series of samples with constant SFR. In Series I, E_G increases from 1.78 to 1.81 eV when HFR is increased from 0 to 15 SCCM, while in Series II, it increases from 1.7 to 1.9 eV. The change in E_G with increases in HFR is more for low SFR. However, with the variation of SFR no specific trend in the band gap variation is

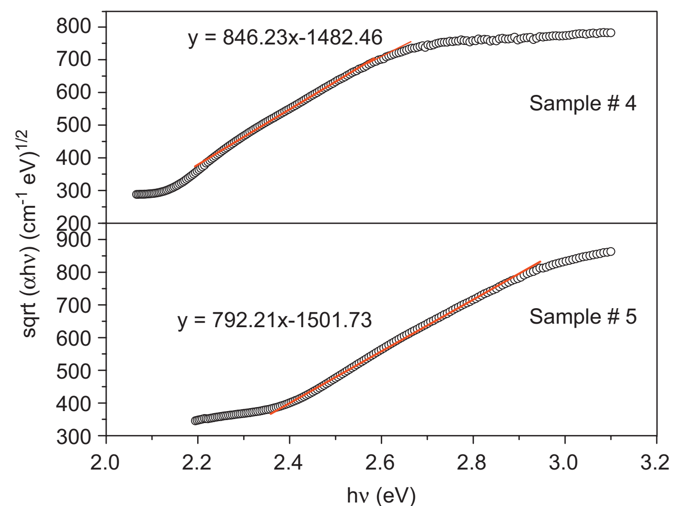

Fig. 1. Plot of $\sqrt{\alpha h\nu}$ vs. $h\upsilon$ for two samples to show the variation of absorption near the band gap. The intercept of the fitted line (in red colour) in the energy axis gives the band gap of the films.

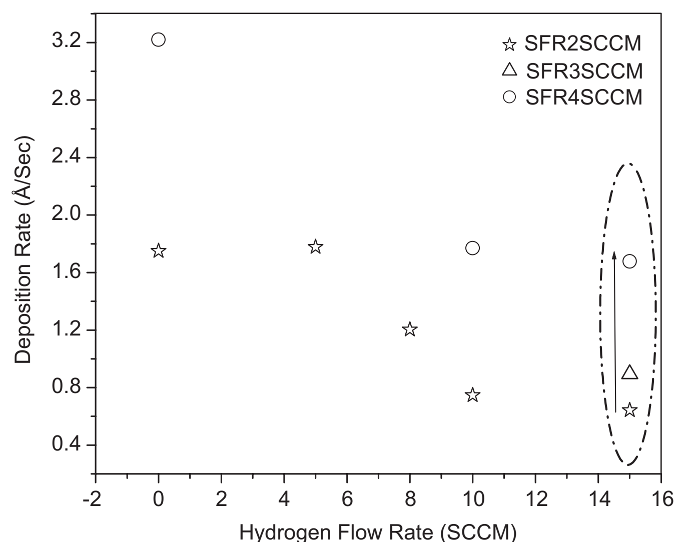

Fig. 2. Deposition rate vs. hydrogen flow rate (HFR) for the films prepared by varying HFR and silane flow rate (SFR). The encircled points correspond to Series III, with SFR increasing in the direction of the arrow.

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