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Substrate temperature dependence of microcrystalline silicon growth by PECVD technique

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Abstract

Undoped hydrogenated silicon films have been prepared from a gas mixture of silane and hydrogen, varying substrate temperature from 180–380 °C in an ultrahigh vacuum system using RFPECVD technique. XRD and Raman measurements enable us to know that the films are microcrystalline throughout the substrate temperature range. Bond formation of the SiH films at different substrate temperature is studied through different characterisation techniques like Fourier transform infrared spectroscopy and hydrogen evolution study. The infrared absorption spectroscopy and hydrogen evolution study reveal two types of growth: the formation of a void rich material at low T_s (~180 °C) and a compact material at comparatively higher T_s.
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Keywords: Silicon; Thin films; Microstructure

1. Introduction

Hydrogenated microcrystalline silicon (μc-Si:H) deposited by plasma enhanced chemical vapour deposition (PECVD) is a widely acclaimed material for thin film devices viz. solar cells, TFT and sensors, etc. [1,2]. Intrinsic μc-Si:H is being considered seriously as an active layer in a-Si solar cell to improve its performance, viz. (a) to minimise the light induced degradation (b) to enhance spectral response in the longer wavelength region of the solar spectrum. Influence of deposition temperature on microstructure, hydrogen evolution and crystallinity of the films have been investigated systematically in the substrate temperature range 180–380 °C. Microcrystalline silicon at high temperature is widely studied [3,4], but its temperature dependent bond formation has not yet been studied in details. The objective of the present work is to investigate how deposition temperature influences the growth process and hence the hydrogen bonding and film characteristics.

2. Experimental details

Intrinsic silicon films were prepared from gas mixture of silane (SiH_4) and hydrogen (H_2) by RFPECVD technique. The substrate temperature (T_s) was varied from 180 °C to 380 °C keeping the hydrogen dilution H_2/SiH_4 fixed at 82. The chamber pressure, RF power density, and electrode configuration have been kept constant. The thicknesses of the films were between 5000 Å and 6000 Å. X-ray diffraction, Raman studies have been done to measure the crystallinity in Si films. The bonding configurations of hydrogen with silicon have been analysed by Fourier transform infrared (FTIR) spectroscopy. To know the details of the hydrogen release process from the Si films hydrogen evolution experiments have been done.

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3. Results

3.1. X-ray diffraction studies

Fig. 1 shows the X-ray diffraction spectra for the films deposited at different T_s. It is observed in figure that for $T_s = 180$ °C two peaks corresponding to the planes (1 1 1) and (2 2 0) of crystalline silicon are present. However, the peak corresponding to ⟨2 2 0⟩ can be observed only for $T_s \geqslant 250$ °C. Intensity of the ⟨2 2 0⟩ peak increases with the increase in T_s indicating that at higher substrate temperature crystallites revealed a preferred orientation. For the film deposited at 180 °C, the average crystallite size measured from FWHM was 45 Å. The crystallite sizes for the films deposited at 250 °C and 340 °C were 305 Å and 320 Å, respectively.

3.2. Raman studies

Fig. 2 shows the Raman spectra of the films deposited at different substrate temperatures. The individual spectrum in the range 420–550 cm^{-1} was deconvoluted into three peaks. Peak at 480 cm^{-1} is assigned to TO mode vibration of amorphous silicon and the peak near 520 cm^{-1} is attributed to TO mode vibration of crystalline silicon. The intermediate component 510 cm^{-1}, which is ascribed to grain boundary contribution arose due to presence of crystalline grains with localized stacking faults [5]. The results of deconvolution of spectra are summarized in Table 1. The crystalline volume fraction f_c is defined as $f_c = (I_c + I_b)/(I_a + I_b + I_c)$ where, I_c, I_b, and I_a are the integrated intensities of crystalline, intermediate and amorphous component, respectively [6]. At $T_s = 180$ °C, crystalline volume fraction f_c was estimated to be 84.0%. With the increase of substrate temperature f_c increases up to 89.2%.

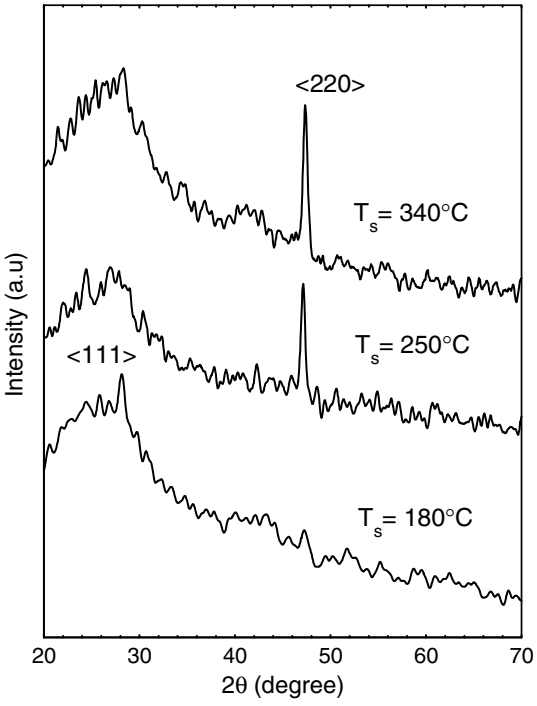

Fig. 1. X-ray diffraction spectra of Si:H films prepared at different substrate temperature (T_s).

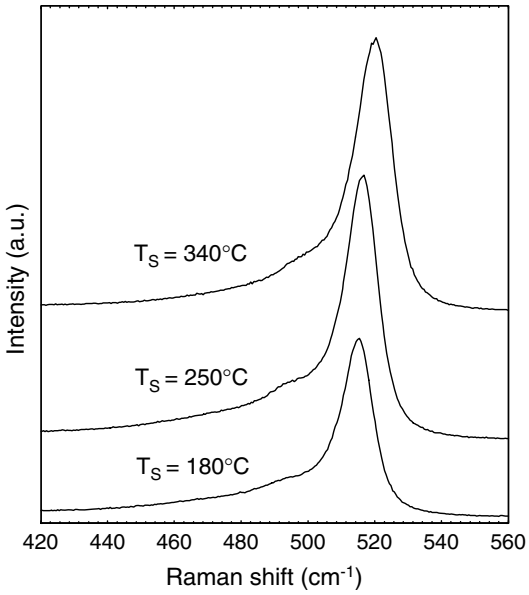

Fig. 2. Raman spectra of the μc-Si:H films prepared at different T_s.

3.3. Hydrogen content and its bonding configurations

The infrared spectra for the films deposited at different T_s in the range 1800–2300 $cm^{-1}$are presented in Fig. 3. The film deposited at 180 °C shows the SiH stretching mode vibration around 2100 cm^{-1}, which corresponds to di/polyhydride bonds of Si. Peak at 840 cm^{-1} corresponding to bending and scissors mode of $(SiH_2)_n$ was also observed for this film. This figure shows that, with increase in T_s, the relative intensity of 2000 cm^{-1} peak associated with monohydride bond of silicon increases over 2100 cm^{-1} peak but the total integrated area of SiH stretching mode decreases. It is to be noted that no such peak around 850 cm^{-1} and/or 890 cm^{-1} was observed for the films deposited at high T_s ($\geqslant$250 °C). For the film deposited at $T_s = 380$ °C, the stretching mode was observed at 2000 cm^{-1} but with very low intensity.

The total bonded hydrogen contents (C_H) for the films were calculated from the integrated area of the absorption spectra centered around 630 cm^{-1}corresponding to SiH wagging mode. Bonded hydrogen contents in the films deposited at different substrate is shown in the table (inset of Fig. 3). It is also evident from the table that with an increase in T_s, the C_H decreases.

3.4. Hydrogen evolution experiment

The hydrogen evolution process from Si:H depends on the hydrogen bonding configurations in the films. Fig. 4 shows the hydrogen evolution spectra of the films deposited

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