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Influence of Power on the Microstructure and Optical Properties of Microcrystalline Si Films

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Abstract. Microcrystalline silicon films were deposited using Ar diluted SiH_4 gaseous mixture by electron cyclotron resonance plasma-enhanced chemical vapor deposition (ECR-PECVD). The effects of power on microstrcture and optical properties of microcrystalline silicon films were investigated. The results show that, with the increasing of the power, the crystallinity increased, but the concentration of hydrogen decreased monotonously. Furthermore, the absorption coefficient of the films increased monotonously, and the optical bandgap changed from 1.89eV to 1.75eV with the microwave power ranging from 400 W to 650W.

Introduction

Solar cells have been widely applied in aerospace applications including use at high altitude atmospheric environments, in earth orbital environments, and in interplanetary, lunar, and planetary environments. With the developments of the solar cells industry, microcrystalline silicon (μ-Si) films have attracted considerable attention for its high-efficiency and stability, which are strongly dependent on the films optical properties, e.g., optical constants, optical band gap and absorption [1]. Microcrystalline silicon films are widely produced using SiH_4+ H_2 gaseous system because it is believed that atomic hydrogen can balance the dangling-bonding defect and hydrogen ions can etch the weak Si-Si bonds, so as to promote stability and crystallinity of the films [2]. However, H_2 dilution would limit the deposition rate seriously [3] and great amount of H existing in the film would draw back the photoelectric efficiency of micro-Si film due to acceptor-like defect formation and light-induced defect creation [4].

In our previous researches, Ar was used instead of H_2, and the results demonstrated that the concentration of hydrogen in the films decreased dramatically, which would limit the creation of the light-induced defect in microcrystalline silicon and enhance the photoelectric efficiency of the films [3]. In present work, it is investigated that the effects of the power on microstructure and the optical properties of microcrystalline silicon films deposited with SiH_4＋Ar.

Experiment

The μ-Si films were deposited with SiH_4/Ar by ECR-PECVD. The source gas SiH_4 was diluted in Ar (SiH_4: Ar = 1:19) to guarantee the security. Pre-vacuum of the reaction chamber was 6×10^{-3}Pa. Substrate temperature was 300°C. The flow ratio of SiH_4 to Ar was F (SiH_4): F (Ar) = 10:70 which was the optimum result of the previous researches making the deposition rate highest. A sequence of microwave power was chosen as: 400W，500W，600W，and 650W. The films were deposited on glass and poly-Si substrate for different tests. The preferred orientations of the films were determined by X-ray diffraction (XRD). Fourier transform infrared spectroscopy (FTIR) was utilized to characterize the configuration of H existing in the films and estimate the concentration of hydrogen. PE Lambda900 UV－VIS transmission measurements in the 200-800nm range were used to estimate the optical constants and band gap.

Results and Discussion

Effects of Power on Film Microstructure. The preferred orientations of the films fabricated with different microwave power are characterized by XRD. As shown in Fig. 1, <111> orientation is the dominant crystal texture. According to Scherrer's formula, wider full width at half maximum (FWHM) of XRD peak means smaller grain size. With comparing FWHM of the <111> XRD spectra for the films, the grain size first increases and then decrease as microwave power increases. These results should be attributed excessiveness of ion bombardment under a power of 650W [5].

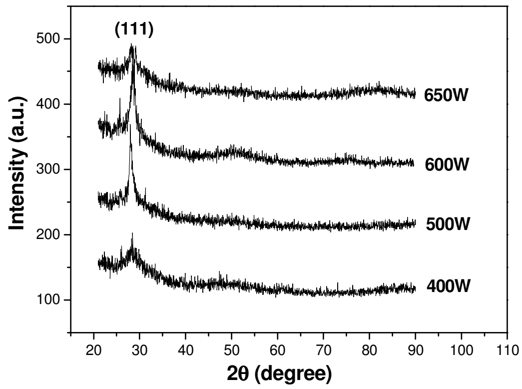

Fig.1 XRD spectra of the films deposited with different power

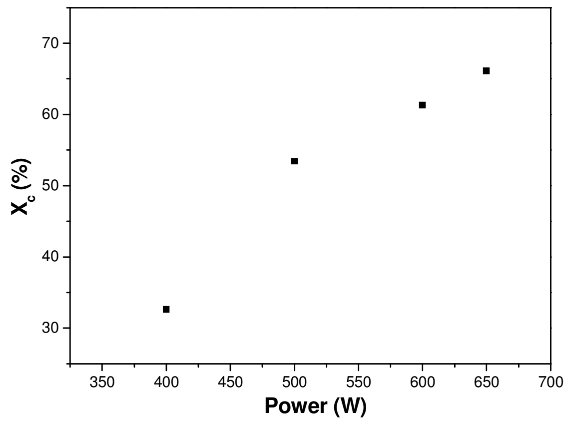

Fig.2 Crystallinity of the films deposited with different power

In order to obtain the crystalline volume fraction in films, Raman spectra for the films deposited with different microwave power are used. The crystalline volume fraction x_c is given by

$$x_c = \frac{I_c}{I_c + I_a}. \tag{1}$$

where I_a and I_c are Raman intensity of amorphous and crystalline phase centered at 480 cm^{-1} and 520 cm^{-1} respectively. The values of crystalline Si volume fraction of the films are demonstrated in Fig. 2. It is shown that with the increase of the power, the crystalline volume fraction increases monotonously. The results could be interpreted that with increasing power, superior Ar^+ etching on the film surface would participate in the growth process which would remove the weak Si-Si bond.

Fig. 3 plots the FTIR spectra of the films deposited with deferent power. The absorption bands are found to locate at 620 cm^{-1}, 650 cm^{-1}, and 850—890 cm^{-1}. The peaks centered at 620 cm^{-1} and 650 cm^{-1} are assigned to wagging vibration modes of Si-H bonding, and the peaks centered at 850—890cm^{-1} are related to Si-H_2 bonding [6]. Comparing the results of FTIR spectra, the intensity of Si-H and Si–H_2 bonds decrease with the increasing microwave power, which means the less hydrogen concentration. It is proposed that more energetic active radicals would break the Si–H and Si–H_2 bonds, and the concentration of hydrogen would decrease. Consequently, the stability of the films would be improved.

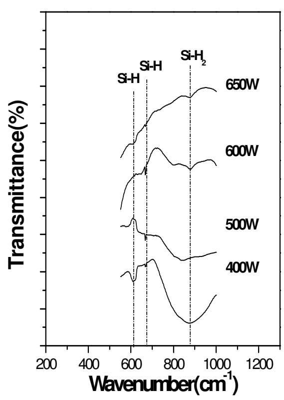

Fig.3 FTIR spectra from silicon films deposited with different power

Effects of Power on Film Optical Properties. Transmission and reflection spectra were recorded in the wavelength range 200-800nm by means of PE Lambda900 UV－VIS spectrophotometer. Transmittance T and reflectance R are given by

$$T = (1-R)^2 \exp(\frac{4\pi kd}{\lambda}). \tag{2}$$

$$\alpha = 4\pi k / \lambda . \tag{3}$$

where k is extinction coefficient, d is the film thickness, and α is the absorption coefficient. So α chould be calculated from Eq.(2) and Eq.(3). As shown in Fig. 4, with the increase of the power, the film absorption coefficient also increases. It is confirmed that the absorption coefficient would be improved with the decrease of the hydrogen concentration, which was proved by Futako[7].

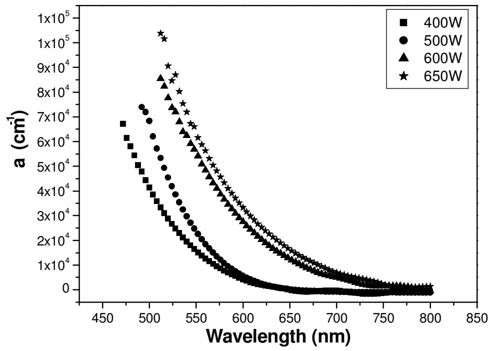

Fig. 4 Optical absorption coefficient spectra of films deposited with different power

From the Tauc relation shown in Eq. (4)

$$\alpha(\upsilon) = \begin{cases} B(h\upsilon - E_g)^2 / h\upsilon & h\upsilon \geq E_g \\ 0 & h\upsilon < E_g \end{cases} . \tag{4}$$

where α is absorption coefficient, hν is photon energy, E_g is optical band gap and B is coefficient relevant to the shape of band edge. Optical band gap (E_g) has been calculated by a linear extrapolation of the plot of (ahν)$^{1/2}$ versus hν for the prepared samples with different power and the results can be seen from Fig. 5.

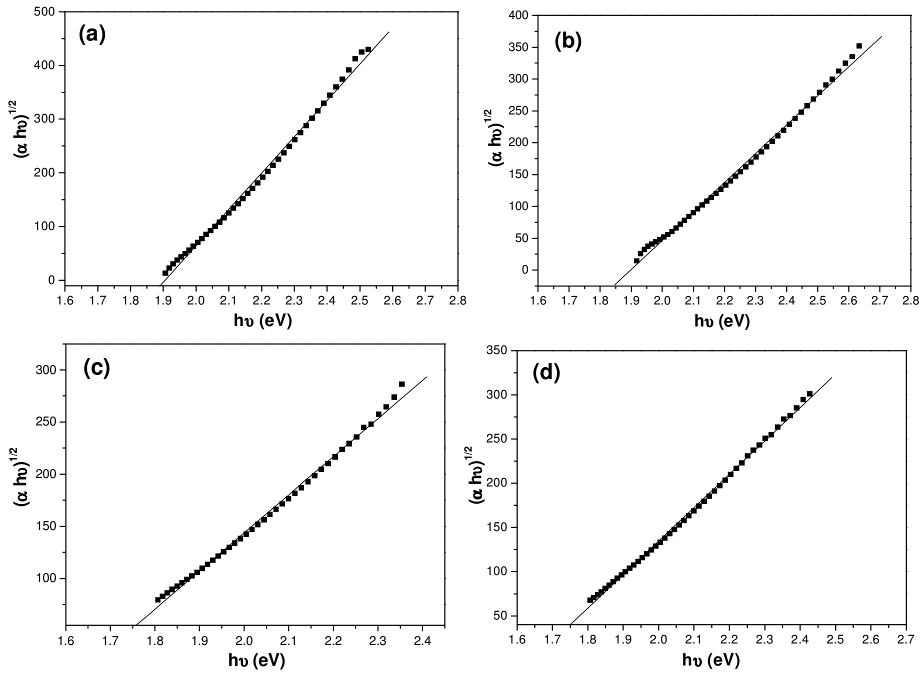

Fig. 5 $(\alpha h\upsilon)^{1/2}$～$h\upsilon$ curves of films deposited with different power (a) 400W, (b) 500W, (c) 600W, (d) 650W

A comparison of these curves shows a decrease in the optical band gap from 1.89eV to 1.75eV with increasing power from 400W to 650W. This can be explained as follows: since the band gap of crystalline silicon is 1.1eV in contrast to a 1.7eV of amorphous silicon, the band gap would be cut down when the film crystallinity is improved with the increase of the power [8]. On the other hand, it is proved that hydrogen in the films could saturate the dangling bond and balance the stress existing in the Si crystal lattice. When the hydrogen concentration in the films decreases, Si crystal lattice would compress and the band gap would be cut down [9,10]. So less hydrogen concentration with increasing power is also beneficial to the improved band gap.

Above all, it is confirmed that the film crystallinity and the hydrogen concentration play important roles for the film optical properties.

Conclusions

The effects of the microwave power on microstructures and optical properties of μ-Si films deposited by ECR-PECVD using SiH_4+Ar were studied. The results indicate that microstructure and optical properties of the deposited films would be affected remarkably by the microwave power. With the increase of the power, the crystallinity would increase, in contrust to the decrease of the hydrogen concentration. Consequently, the absorption coefficient of the films at visible region would be enhanced, accompanying the cuting down of the band gap. Based on these results, higher microwave power is suggested to prepare the micro-Si films with advanced stability ,compromised crystallinity, and favorable optical properties.

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