3 - 1 Modification of Structure and Optical Band-gap of nc-Si : H Films with High-energy Kr-ions

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Nc-Si : H films with thickness of about 1.0 μm were deposited on glass substrates by hot-wire chemical vapor deposition. And then, the samples were irradiated at room temperature with 30 and 196 MeV Kr-ions, which delivered by HIRFL, to fluences of 5.0×10^{13}, 1.0×10^{14} and 2.0×10^{14} Kr-ions/cm^2. The irradiation parameters are listed in Table 1.

Table 1 Irradiation parameters of incident Kr-ions in nc-Si : H films: ion energy (E), electronic (S_e) and nuclear (S_n) energy losses, projected range (R_p), as well as ion fluence (Φ)

E (MeV)	S_e (keV/nm)	S_n (keV/nm)	R_p (μm)	Φ (ions/cm^2)
30	6.15	0.08	8.18	(0, 5, 10, 20)$\times10^3$
196	9.48	0.017	27.51	

Fig. 1 shows the dependences of crystalline fraction (a), crystallite size (b) and bond angle variation (c) on the ion fluence. As seen from Fig. 1(a), when the ion fluence increases from 0 to 2.0 10^{14} ions/cm^2, the crystalline fraction (X_c) for Series I samples (30 MeV) decreases from 53.7% to 21.7%, and it for Series II samples (196 MeV) slightly decreases from 52.5% to 47.1%. It can be observed from Fig. 1 (b) that the crystallite size (d_{Raman}) for Series I samples decreases from 6.7 to 4.4 nm with the ion fluence increases. And in Series II, the d_{Raman} shows a small decline from 6.5 to 5.9 nm after irradiation. From Fig. 1(c), one can see that with the ion fluence increases, the bond angle deviation ($\Delta\theta$) for Series I samples gradually increases from 7.6° to 10.4°, whereas it for Series II samples increases from 7.5° to 9.1° when the ion fluence achieves to 5.0×10^{13} ions/cm^2 and then remains nearly constant.

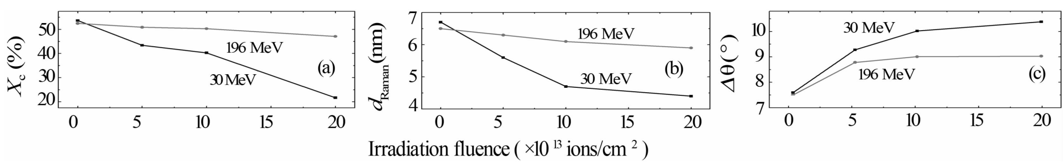

Fig. 1 Crystalline fraction, crystallite size and bond angle deviation varying with the ion fluence.

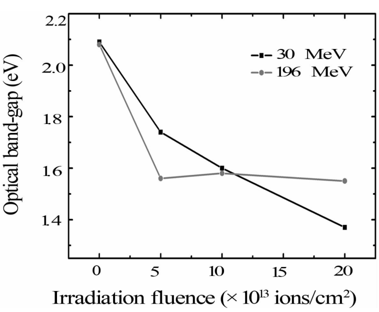

Fig. 2 Dependence of optical band-gap of nc-Si : H films on ion fluence.

Fig. 2 shows the optical band-gap (E_g) for nc-Si : H films irradiated with 30 and 196 MeV Kr-ions at different ion fluences. It can be seen that the optical band-gap of the samples irradiated with 30 MeV Kr-ions decreases gradually from 2.09 to 1.37 eV with the ion fluence increases. The optical band-gap of the samples irradiated with 196 MeV Kr-ions decreases significantly from 2.08 to 1.56 eV at ion fluence of 5.0×10^{13} ions/cm^2 and then remains nearly constant.

Since the nc-Si : H film is a two-phase material, structural modification induced by ion irradiation should be considered from both the crystalline and amorphous phases. For the crystalline phase, the reduction of crystalline fraction and crystallite size indicates that the incident ions cause the breakage of Si-Si bonds and the displacement of silicon atoms in the crystallites, which leads to the amorphization of crystalline phase at sufficiently high ion fluences[1]. And for the amorphous phase, the breakage of Si-Si or/and Si-H bonds in the amorphous network increases the bond angle variation and results in the reduction of short-range order[2].

Based on the structural results mentioned above, the variation in optical band-gap of nc-Si : H films irradiated with 30 MeV Kr-ions can be explained in two aspects. One is the decrease of crystallite size from 6.7 to 4.4 nm widens the optical band-gap due to the quantum size effect[3]. The other one is the increase of bond angle variation from 7.6 to 10.4°, which represents the reduction in short-range order of amorphous phase, widens the band-tails of valence and conduction bands, and then results in the decrease of optical band-gap[4]. Considering both the effects of crystallite size and short-range order, the reduction of optical band-gap should be considered as a combined result of the structural damages of crystalline and amorphous phases induced by the irradiation. And for samples irradiated with 196 MeV Kr-ions, the ion irradiation just results in a slight change of the crystalline fraction and crystallite size. Such a small structural change of crystalline phase in the films does not influence the optical band-gap significantly (Fig. 2). Therefore, we consider that the decrease of optical band-gap for samples irradiated with 196 MeV Kr-ions is mainly attributed to the reduction in the short-range order of amorphous network.

References

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3 - 2 Raman Scattering Analysis of a-Si : H Films Irradiated with 500 keV He-ions

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As one of the most important semiconductor materials, hydrogenated amorphous silicon (a-Si : H) film has been widely applied in solar cells and thin film transistors due to its remarkable photoelectric property and the low cost. Ion irradiation is an effective tool to modify the structural, optic, electronic and mechanical properties of materials. Studies about the irradiation effects of a-Si : H film induced by energetic heavy-ions possess not only the important significance but also the potential application prospects.

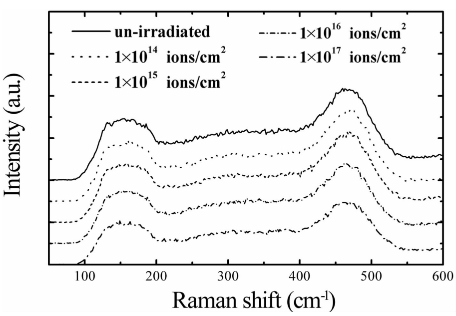

Fig. 1 The Raman spectra of a-Si : H films irradiated with different fluences.

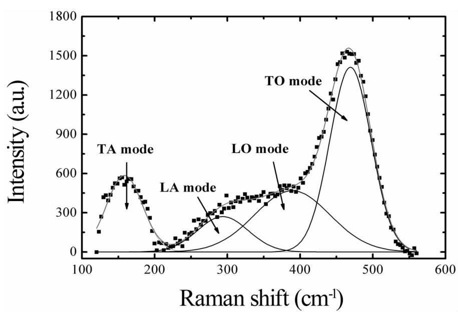

Fig. 2 The deconvoluted Raman spectrum for the un-irradiated a-Si : H film.

In present work, a-Si : H films with thickness of 300 nm were deposited on glass substrates by using radio-frequency magnetron sputtering. And then, the samples were irradiated at room temperature with 500 keV He-ions. The irradiation fluences are 1.0×10^{14}, 1.0×10^{15}, 1.0×10^{16} and 1.0×10^{17} ions/cm^2, respectively. Raman spectroscopy and UV-Vis transmission spectra were used to study the structural changes induced by the irradiation. Fig. 1 shows the Raman spectra of a-Si : H films irradiated with different fluences. As is well known, the Raman spectrum of a-Si : H film is consisted by four bands, which includes the transverse acoustic (TA) mode at 150 cm^{-1}, the longitudinal acoustic (LA) mode at 310 cm^{-1}, the longitudinal optic (LO) mode at 380 cm^{-1} and the transverse optic (TO) mode at 480 cm^{-1}[1]. The deconvoluted Raman spectrum of un-irradiated a-Si : H films is shown in Fig. 2. The ratios of integrated intensities of TA and LA peaks over that of TO peak (TA/TO, LA/TO) and the FWHM of TO peak varying with the irradiation fluence are presented in Fig. 3. With the fluence increases from 0 to 1.0×10^{17}