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Investigating the effects of microstructure on optical properties of different kinds of polysilicon thin films

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ABSTRACT

Flat, *B*-doped, low-stress and non-stress polysilicon (poly-Si) thin films were deposited by low pressure chemical vapor deposition (LPCVD). X-ray diffraction (XRD), combined with atomic force microscopy (AFM) and Raman system, UV-Raman measurements and spectroscopic ellipsometry, was used to study the microstructure, the morphology and optical properties of the films. The results indicate that the surface roughness is related to the grain size and the change in the microstructure. The *B*-doped poly-Si shows a tensile stress, while the flat poly-Si shows a high compressive stress. The bandgap of the *B*-doped poly-Si is the narrowest because of its most disordered microstructure.

1. Introduction

Polysilicon (poly-Si) thin films are widely used to fabricate different micromechanical structures in MEMS/NEMS [1–4]. Typically, poly-Si thin films are deposited by low pressure chemical vapor deposition (LPCVD). Different conditions during this process may affect the morphology, microstructure and optical properties of poly-Si thin films, which contributes greatly to the performance of devices [5]. So it is vital to determine the morphology, microstructure and optical properties of poly-Si films prepared under different deposition conditions.

Raman scattering spectroscopy is a nondestructive and stable tool for characterization of stress, defects and other chemical information of materials [6]. However, due to the optical diffraction limit, its conventional spatial resolution is limited to $1 \times 1\ \mu m^2$ [7,8]. The atomic force microscope (AFM) is used to investigate surface morphology and surface roughness with high resolution [9]. The integration of AFM and Raman enables the simultaneous measurements of the surface morphology and the enhanced Raman spectrum of poly-Si thin films.

Y.E. Strausser et al. [10] investigated the surface morphology of poly-Si by AFM with different temperatures and pressures. They found that the surface morphology is sensitive to deposition temperature and is not so sensitive to pressure. T. Jawhari [11] discussed the relationship between the Raman shift and the presence of stress, crystalline disorder and chemical impurities. Y.T. Cherng et al. [12] pointed out that the stresses in poly-Si thin films influence the device electrical and optical properties.

In this work, flat, *B*-doped, low-stress and non-stress poly-Si thin films were prepared by LPCVD using different deposition conditions. The latter two films were annealed under different temperatures after deposition. *B*-doped poly-Si was doped with boron ions. The film textures and grain sizes were analyzed using X-ray diffraction (XRD) measurement. The AFM-Raman system was used to measure the surface morphology and Raman spectra of the four thin films, simultaneously. UV-Raman measurements were carried out to get the information of poly-Si near the surface. Furthermore, we used the spectroscopic ellipsometry to acquire the optical properties of the four thin films. The results of this work provide new insight into the effects of microstructure on optical properties of different kinds of poly-Si thin films.

2. Experiment

Poly-Si thin films with the thicknesses of ~500 nm were deposited on crystalline silicon substrates by LPCVD. The pure silane (as gas source) flow rate was kept constantly at 75 sccm throughout the deposition process. For different samples, the deposition temperatures and pressures were pre-determined. Flat poly-Si thin film was grown at 650 °C with the chamber pressure of 233 mtorr. There was no subsequent treatment of this sample. By implanting boron ions from BF_3 with the dose of $4 \times 10^{15}\ cm^{-2}$ and the

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Table 1
The preparing process of the four polysilicon thin films.

Sample	Temperature (°C)	Deposition rate (nm/min)	Pressure (mtorr)	Post treatment
Flat poly-Si	650	108	233	/
B-doped poly-Si	650	108	233	*B* doped
Low-stress poly-Si	590	65	250	Annealing
Non-stress poly-Si	605	77	250	Annealing

energy of 60 keV, the *B*-doped poly-Si thin film was acquired. Low-stress poly-Si thin film was deposited at the temperature of 590 °C. Subsequent annealing was performed at the temperature of 950 °C in the furnace with nitrogen gas for 30 minutes. Non-stress poly-Si thin film was deposited at 605 °C, followed by subsequent annealing in N_2 and O_2 at 950 °C for 30 minutes and then in N_2 at 1100 °C for 4 h. Detailed preparing processes are given below (see Table 1).

The X-ray diffraction (XRD) measurements were carried out with Cu-K radiation, 40 kV anodic voltage, and 50 mA current at each stage of the processing. A small scanning step and a θ–2θ configuration were used. A wide range was scanned so that all the major diffraction peaks could be detected.

The AFM-Raman system used in this study consists of a confocal Raman system Nanofinder HE and an AFM. The integration of these two devices is realized to acquire Raman spectrum and AFM morphology simultaneously. The Si tip coated with Au was applied in tapping mode for the combined AFM-Raman measurements, which can provide a good optical access to the sample surface. In this AFM-Raman measurement, spatial resolution below 50×50 nm^2 can be achieved. The backscattered Raman light is diffracted by an 1800 g/nm grating. For Raman excitation, an argon-ion laser with the wavelength of 532 nm and the power of less than 2 mW is applied. The low power can prevent sample heating and crystallization of the films. The UV-Raman measurements were performed using a LabRam HR800 UV spectrometer. The 325 nm emission line was used for excitation. Spectroscopic ellipsometry measurements were taken in the spectra range of 250 nm to 650 nm to obtain the ellipsometric parameters using the SOPRA GES5. The incident angle was set at 75°.

3. Results and discussion

XRD technique was used to analyze the film textures and grain sizes of the flat, *B*-doped, low-stress and non-stress poly-Si thin films, and the measured X-ray spectra are shown in Fig. 1. (111), (220) and (311) components are all contained in the four thin films. Except for the low-stress poly-Si film, other films also have textures with (002) components. All the films showed (111) prefer orientation. As for the *B*-doped poly-Si film, the intensities of (111) and (220) are higher than the flat poly-Si film, while the (311) intensity is weaker. This is due to the formation of borosilicate molecular group (boride structures) after boron doping, and then the crystallite grains tend to form and become large. Both the low-stress and non-stress poly-Si thin films have been annealed at high temperature, and the intensities of (111) for both films significantly enhanced. It reveals that some defects of (111) disappeared and recrystallization took place after annealing treatment.

Grain sizes of the four thin films can be calculated using Scherrer's formula [13,14]:

$$D = \frac{k\lambda}{\beta \cos\theta}, \tag{1}$$

where D is the average crystallite size, λ (1.5406 Å) is the wavelength of the used X-ray, β is the full width at half maximum

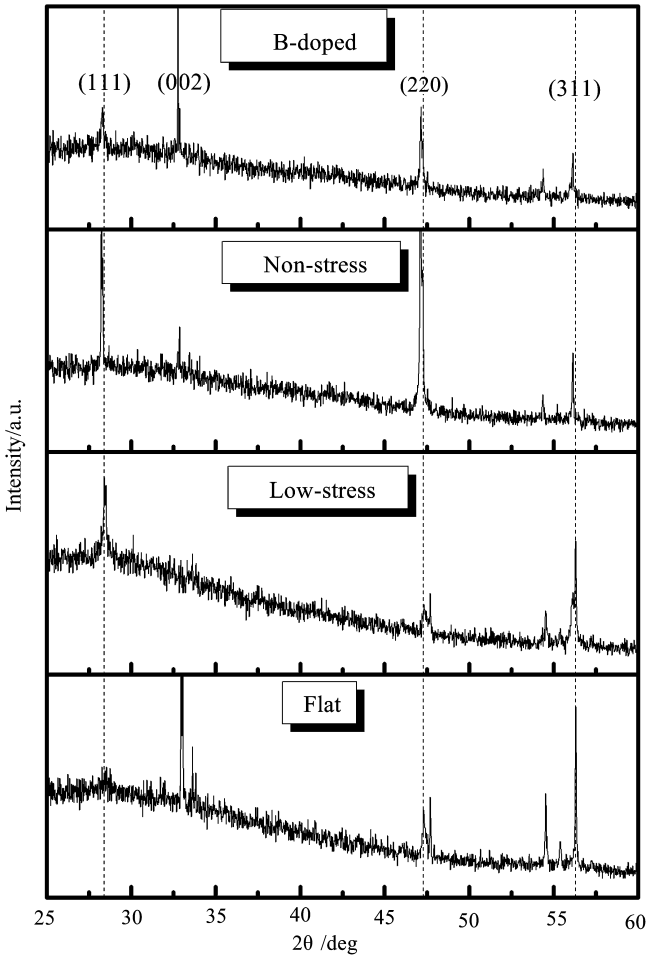

Fig. 1. XRD Spectra of flat, *B*-doped, low-stress and non-stress polysilicon films.

Table 2
The parameters for surface topography and micro-structure of the four polysilicon films.

Sample	R_a (nm)	Stress (MPa)	Grain size (nm)	FWHM (cm^{-1})	$\Delta\bar{\vartheta}$ (deg)
Flat poly-Si	2.57	−227	21.23	8.76	0.42
B-doped poly-Si	7.42	+345	46.96	11.55	1.35
Low-stress poly-Si	0.62	−102	36.86	5.42	/
Non-stress poly-Si	13.80	~0	77.13	8.34	0.28

(FWHM) of the measured peak in radians and θ is the angle of diffraction. k is a constant which is determined by the geometry of the crystallites and taken as 1. The grain sizes of the films were 21.23 nm, 46.92 nm, 36.86 nm, 77.13 nm, shown in Table 2. Boron doping changes the film's microstructure so that the grain size becomes larger. Considering the deposition conditions, flat thin film showed the minimum grain size because it was not annealed after deposition. Non-stress thin film's grain size is the largest due to long annealing time and high annealing temperature. The grain size of low-stress poly-Si is not so large because the annealing time is short.

Using the AFM-Raman system, we can get the surface morphology and Raman spectrum simultaneously. The surface morphologies of the poly-Si thin films imaged by AFM in tapping mode are shown in Figs. 2(a), 3, 4, 5(a). The surface grain sizes of brighter areas are larger than those of other areas. The mean square roughness (R_a) values of the films defined as the arithmetic mean of the deviation in height from the profile mean value can be calculated using the formula [15]: