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Silicon–hydrogen bond effects on aluminum-induced crystallization of hydrogenated amorphous silicon films

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ABSTRACT

The effects of hydrogen dilution on aluminum-induced crystallization (AIC) of hydrogenated amorphous silicon (a-Si:H) films have been studied. The Raman spectra showed that the short-range order (SRO) and the intermedium-range order (IRO) of the as-deposited a-Si films increased with the increase of the H_2 dilution from 0% to 20%. The optical microscope (OM) and X-ray diffraction (XRD) observation revealed that, compared to the a-Si:H film deposited in pure Ar, the a-Si:H films deposited with H_2 dilution in the range of 3–8% possessed a lower crystallization rate while the a-Si:H films deposited with high H_2 dilution in the range of 15–20% possessed a faster crystallization rate. It was found that majority of the hydrogen existed in the form of monohydride (SiH) bond in the a-Si:H films with H_2 dilution ratio of 3–8%, the bonding energy of which was higher than that of Si–Si bond, leading to a lower crystallization rate of a-Si:H films. While the dihydride (SiH_2) bond became dominant in the a-Si:H films with high H_2 dilution of 15–20%, the bonding energy of which was lower than that of Si–Si bond, thus accelerating the crystallization rate. Therefore, it was illustrated that not the hydrogen concentration but the form of silicon–hydrogen bond determined the AIC process of a-Si:H films.

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1. Introduction

Recently, growth of high-quality poly-Si films is one of the most important subjects due to the advantages of low cost thin-film technology and the superior optoelectronic properties of crystalline Si [1–4]. An attractive technique for the preparation of poly-Si films is aluminum-induced crystallization (AIC) because it offers a lower thermal budget than other crystallization methods, the possibility to use low-cost substrates and the generation of grains that are larger in size than the thickness of the poly-Si films [5,6]. In this process, annealing of glass/Al/a-Si structures at temperatures below the eutectic temperature of the Al–Si binary system (577 °C) leads to the formation of glass/poly-Si/Al (+Si) structures. The main parameters involved in the AIC process, i.e. the annealing temperature, time and atmosphere [7,8], the thickness and composition of interfacial oxide layer [9,10], the Al/Si thickness ratio and layer sequence [7,11], etc. have been intensively studied. However, for more complete elucidation of the mechanism of the AIC process, the influence of the precursor material characteristics on the crystallization process has to be revealed.

It was already demonstrated by Kim and Pihan et al. that the introduction of hydrogen in precursor a-Si films can reduce the crystallization temperature either by the method of solid phase crystallization [12] or aluminum-induced crystallization [13]. Prathap et al. [14] further reported that the hydrogen bonded as dihydride (SiH_2) in the a-Si:H films was a prominent factor for the faster crystallization process and the more the amount of dihydride (SiH_2) bond, the faster the crystallization process. In their experiment, majority of the hydrogen existed in the form of dihydride (SiH_2) in the a-Si:H film with a hydrogen dilution of 85%, the exchange of Al/a-Si:H layers has been observed at a lower annealing temperature of 425 °C. While Hossain et al. [15] reported that the crystallization initiation temperature was a function of the hydrogen bonded as monohydride (SiH) in the a-Si:H film and the monohydride (SiH) bond led to the decrease of crystallization temperature. Therefore, the mechanism of hydrogen on the AIC process of a-Si:H films was still controversial.

In this manuscript, the effects of hydrogen content and silicon–hydrogen bond in a-Si:H films on the AIC process of a-Si:H films were investigated. It was illustrated that the AIC process of a-Si:H films was determined not by the hydrogen content, but by the

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form of silicon–hydrogen bond. The AIC process was accelerated only in the a-Si:H film with majority of dihydride (SiH_2) bond.

2. Experimental details

Poly-Si films were prepared by AIC method. The film deposition was achieved using a JCP-350M2 magnetron sputtering system equipped with three magnetron sources and a biased substrate holder. Two different types of substrates were used for this study. One set was quartz glass. The other set was double-side polished silicon wafer which was only used for Fourier-transform infrared (FT-IR) measurement. First, Al layers were deposited directly on quartz glass with the following fixed conditions: base pressure of 3×10^{-4} Pa, RF power of 200 W, Ar pressure of 0.6 Pa, and substrate temperature of room temperature. Before the deposition of a-Si:H layers, the Al layers were kept in air for 24 h to form native oxide layers. Then the a-Si:H films were deposited on top of the Al layers and the double-side polished silicon wafer with the following fixed conditions: base pressure of 3×10^{-4} Pa, RF power of 300 W, substrate bias of -100 V, substrate temperature of room temperature and total gas pressure of 0.4 Pa. The H_2 dilution, which was defined as the flow ratio of Ar/H_2 gas, was ranged from 0% to 20%. The thicknesses of the Al and a-Si:H layers were set as 370 nm and 440 nm in order to supply enough Si atoms to form continuous poly-Si layers. After deposition, the glass/Al/a-Si:H structure was subjected to furnace annealing at 530 °C for 5 h in Ar atmosphere. During annealing, the Al and a-Si:H films experienced the layer exchange, and the a-Si:H films transformed into the poly-Si films. The Al precipitates on the surface were etched off by a standard Al etching solution (80% phosphoric acid, 5% nitric acid, 5% acetic acid and 10% deionized water at 50–55 °C) for the Raman measurements.

The structural properties of as-deposited a-Si:H films and the annealed Si films were characterized by a Renishaw inVia micro-Raman system excited by 532 nm Ar^+ laser, the incident laser power of which was set below 1.2 mW to avoid local crystallization. The hydrogen content and Si–H bonds of as-grown a-Si:H layer on silicon wafer were characterized by FT-IR spectroscopy. The morphology variations such as nucleation and grain growth were investigated using a LEICA optical microscope (OM). The structures of the annealed Si films were also characterized by Bruker AXS D8 Advance X-ray diffraction (XRD) using Cu $K\alpha$ radiation ($\lambda=0.154$ nm) at 40 kV and 40 mA.

3. Results and discussion

3.1. Hydrogen in the a-Si:H film

The hydrogen introduced during film deposition has an effect on the network structure of a-Si films [16]. Raman scattering has been widely used to characterize the network structure of a-Si thin films due to its sensitivity to the structural disorder in solids. The Raman spectra of the as-deposited a-Si:H films grown at H_2 dilution of 0–20% are shown in Fig. 1(a). Usually, the Raman spectrum of a-Si:H thin films consists of four characteristic peaks: the peak at 480 cm^{-1} related to transverse optical (TO) mode, the peak at 410 cm^{-1} related to longitudinal optical (LO) mode, the peak at 300 cm^{-1} related to longitudinal acoustical (LA) mode, and the peak at 180 cm^{-1} related to transverse acoustical (TA) mode. The TO peak is sensitive to the short-range order (SRO) of

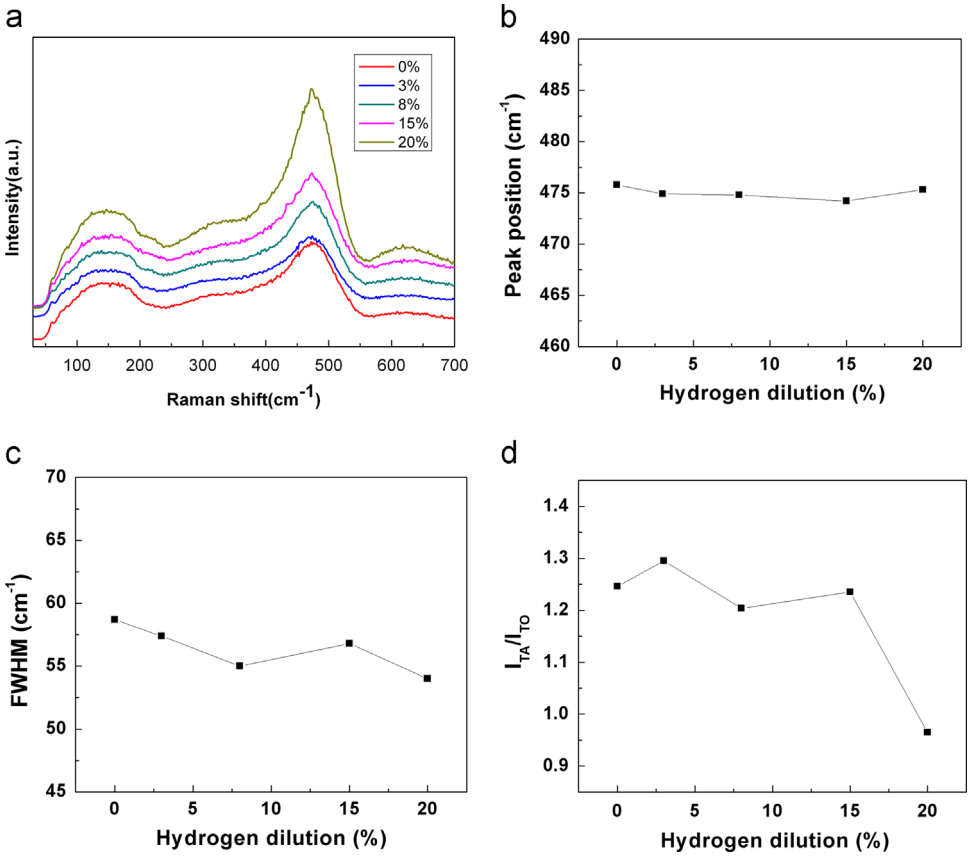

Fig. 1. (a) The Raman spectra, (b) the peak position, (c) the FWHM of the TO mode around 480 cm^{-1} and (d) I_{TA}/I_{TO} of the as-deposited a-Si:H films prepared at H_2 dilution of 0–20%.

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