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Crystallization of as-deposited amorphous silicon films on glass prepared by magnetron sputtering with different substrate biases and temperatures

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ABSTRACT

The rapid thermal annealing (RTA) crystallization of sputtered amorphous silicon (a-Si) films on quartz glass deposited with different substrate biases (0–150 W) and at different substrate temperatures (100–400 °C) has been investigated in detail by an X-ray diffractometer, and Raman and transmission electron microscopes. It was found that only the a-Si film deposited under the optimal condition (substrate bias: 100 W, substrate temperature: 300 °C) attained noticeable degrees of crystallization during the post-deposition RTA at 750 °C. The RTA crystallized a-Si film deposited under optimal condition possessed crystalline fraction of 94.1%, and was proved to be polycrystalline in nature. Furthermore, it was revealed that the structural property of Si film improved with post-deposition RTA time or temperature.

1. Introduction

Polycrystalline silicon (Si) films are considered as one of the most promising materials for thin-film solar cells [1–3] because of their superior electrical properties and stability compared with amorphous silicon (a-Si) materials. Solid-phase crystallization using a-Si films as precursor is the commonly used technique to obtain polycrystalline Si films [4–6]. It is well known that the crystallization kinetics and the properties of polycrystalline Si films strongly depend on the properties of the as-deposited a-Si films [7], such as pre-existing nuclei for crystallization [8], impurities [9,10], defects, and stress state [11].

Magnetron sputter deposition is a particularly attractive method for Si film preparation because of its capability for large area deposition and process controllability [12,13]. Apparently, the deposition condition can affect the structure of as-deposited a-Si films, leading to difference in the crystalline Si film properties. Among these conditions, substrate bias [14–18] and substrate temperature [19–21] are thought to be the predominant parameters, both of which are capable of influencing the behavior of Si ad-atoms on the film surface through ion bombardment or heating, which cause various a-Si film networks. Jun et al. [17] found that substrate bias made a-Si films dense with few defects and, moreover, enhanced crystallization during the subsequent furnace annealing and the grain size in the resulting polycrystalline Si film [18]; however, these studies did not investigate how the a-Si films crystallization was influenced by different substrate biases. Substrate temperature has been reported to have an effect on the electrical properties and microstructures of a-Si films [19,20]; however, its effect on the subsequent crystallization process has not been reported. Therefore, an extensive investigation into the effect of different substrate biases and temperatures on the a-Si films crystallization is needed for a better understanding of the crystallization mechanism in a-Si films.

In this work, rapid thermal annealing (RTA) is chosen as the crystallization technique for its small thermal budget, high throughput, and process automation [22,23]. The a-Si films were deposited by magnetron sputtering with different substrate biases (0∼150 W) and at different substrate temperatures (100∼400 °C), followed by RTA crystallization. The effects of a-Si film deposition condition, in terms of substrate bias and temperature, as well as the post-deposition RTA time and temperature, on the RTA crystallization of sputtered a-Si films were intensively investigated.

2. Experiment

A J-sputter8000 magnetron sputtering system, equipped with six magnetron sources and a heated and biased substrate holder, was used for a-Si films deposition on quartz glass substrate. Firstly, the substrates were immersed in the ultrasonic baths of

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acetone and distilled water for about 15 min each. They were then blow-dried with nitrogen gas, after which the substrates were immediately transferred to an ultrahigh vacuum chamber for a-Si films deposition. The a-Si films were deposited under the following fixed conditions: RF power of 120 W, base pressure of 5×10^{-5} Pa, argon gas pressure of 0.21 Pa, and deposition time of 3 h, while the substrate temperature was varied in the range of 100∼400 °C, and the substrate bias in the range of 0∼150 W (corresponding to 0∼125 V). To investigate the effect of a-Si film deposition condition on the annealed Si film structural property, all the a-Si films were subjected to a five-step RTA at 750 °C for 60 s in Ar atmosphere with the cooling rate of 20 °C/s; to investigate the RTA crystallization process of sputtered a-Si film, the a-Si film deposited under optimal condition was subjected to different steps of RTA at 750 °C for 60 s in an Ar atmosphere at the cooling rate of 20 °C/s, and two-step RTA at 900 °C for 30 s in Ar at the cooling rate of 20 °C/s.

The structural properties of the annealed Si films were characterized using a Bruker AXS D8 Advanced X-ray diffractometer (XRD) with the Cu K_α radiation (λ=0.154 nm; electron beam condition: 40 kV, 40 mA); the reflectance of the annealed Si films was measured using a J.A. Woollam M-2000DI spectroscopic ellipsometer; the Raman spectra of the annealed Si film was measured using a Jobin Yvon Labor HR-800 Raman excited by Ar laser with wavelength of λ=514.5 nm; the surface and cross-section morphologies of the annealed Si films were observed using a Veeco Dimension 3100V atomic force microscope (AFM) in contact mode and an FEI Tecnai F20 transmission electron microscope (TEM) operating at 200 kV.

3. Results and discussion

Fig. 1 shows the XRD patterns of the a-Si films deposited with different substrate biases or at different substrate temperatures subjected to five-step RTA 750 °C/60 s. As shown in Fig. 1(a), although the substrate bias during deposition significantly influenced the RTA crystallization, only the film deposited with a substrate bias of 100 W (100 V) showed Si characteristic peaks at 2θ=28.5°, 47.5°, and 56.3°, corresponding to (1 1 1), (2 2 0), and (3 1 1), respectively; in contrast, the films deposited with no substrate bias, a low substrate bias of 50 W (60 V), or a high substrate bias of 150 W (125 V) showed no characteristic peaks. Enhanced crystallization of substrate-biased a-Si film is in accordance with the previous result [18]; how a particular substrate bias value was required in our experiment will be discussed below. The effects of different substrate temperatures, as shown in Fig. 1(b), were as follows: at a low temperature of 100 °C, no Si characteristic peaks existed; at an increased temperature of 200 °C, the Si characteristic peaks with a low intensity appeared; further increasing the temperature to 300 °C resulted in increased intensities of XRD peaks; however, when the substrate temperature is increased to 400 °C, the XRD peaks suddenly disappeared. These observations suggest that the precursor a-Si film structure, which depends on the deposition conditions, significantly influences the subsequent RTA crystallization.

Fig. 2 shows the UV reflectance spectra for the same samples presented in Fig. 1. The change in the profile and the shift in the peaks in the UV spectra indicates the modification of the electronic density of states as a result of the long-range order. For

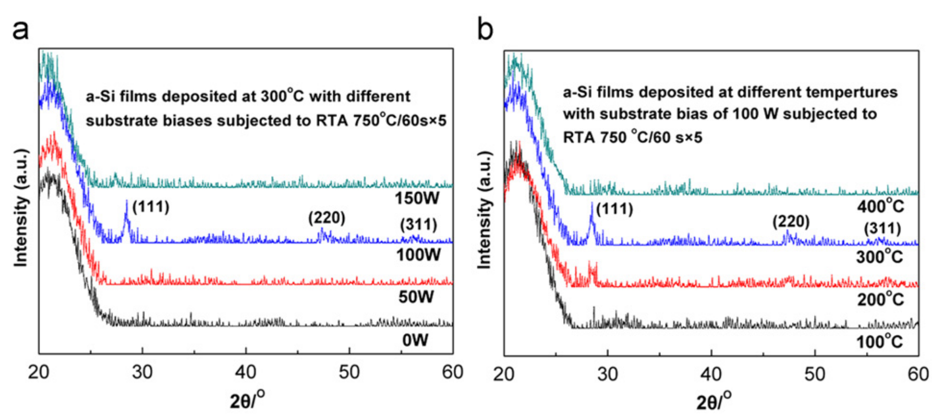

Fig. 1. XRD patterns of the Si films deposited under different substrate biases (a) or substrate temperatures (b), followed by five-step RTA 750 °C/60 s in Ar.

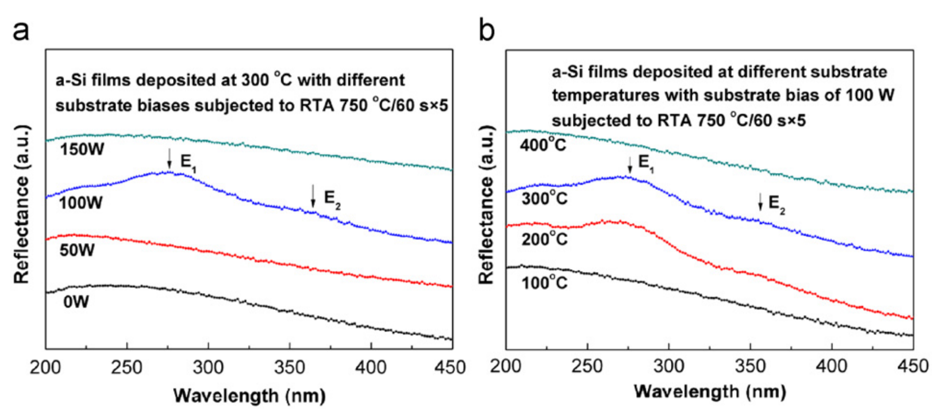

Fig. 2. UV reflectance spectra of the Si films deposited under different substrate biases (a) or substrate temperatures (b), followed by five-step RTA 750 °C/60 s in Ar.