Materials Science in Semiconductor Processing 56 (2016) 344–348

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp

Microstructure evolution of amorphous silicon thin films upon annealing studied by positron annihilation

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ARTICLE INFO

Keywords:
Amorphous silicon
Thin films
Defects
Positron annihilation

ABSTRACT

Amorphous silicon (a-Si) thin films were prepared on glass substrates by plasma enhanced chemical vapor deposition (PECVD). Influence of annealing temperature on the microstructure, surface morphology, and defects evolution of the films were studied by X-ray diffraction (XRD), atomic force microscope (AFM) and positron annihilation Doppler broadening spectroscopy (DBS) based on a slow positron beam, respectively. The *S* parameter of the as-deposited a-Si thin film is high, indicative of amorphous state of Si film with many defects. The a-Si gradually grows into polycrystalline silicon with increasing temperature to 650 °C. For the films annealed below ~450 °C, positron diffusion lengths are rather small because most positrons are trapped in the defects of the a-Si films and annihilated there. With further rising the temperature to 600 °C, the diffusion length of positrons increases significantly due to the removal of vacancy-type defects upon annealing at a high temperature. The results indicate that the coalescence of small vacancy-type defects in a-Si thin film and the crystallization of a-Si occur around 450 °C and 650 °C, respectively.

1. Introduction

Solar cells have been widely used in many areas, for example, portable power [1], lighting equipment [2] and building-integrated photovoltaics [3]. Being one of the core materials of solar cell, amorphous silicon (*a*-Si) is a photovoltaic material with advantages of electrical and optical properties [4,5]. A-Si thin films possess high optical absorption coefficient and wide optical bandgaps [6] for extensive applications in liquid crystal displays (LCDs) [7], light emitting diodes (LEDs) [8], thin-film transistors (TFTs) [9] and photodetectors [10], especially in thin-film solar cells [11]. With such attractive features as mentioned above, a-Si has attracted enormous interests in semiconductor industry and it is a promising material for low-cost [12] thin film solar cells.

Numerous methods have been used to deposit a-Si thin films, and it is known that the film properties have a great dependence on their preparation conditions. Since the efficiency of a-Si thin film solar cells is closely associated with the preparation, various methods have been applied, such as radio-frequency magnetron sputtering [13], plasma enhanced chemical vapor deposition (PECVD) [14], hot wire chemical vapor deposition (HWCVD) [15] and microwave electron cyclotron resonance chemical vapor deposition (MWECR-CVD) [16]. PECVD, which can be applied to prepare thin films with large areas at a low coating temperature, is widely used for the deposition of a-Si thin films. For current application of thin films in solar cells, it is urgent to overcome the defect of “Steabler-Wronski effect” [17], i.e. the conversion efficiency decreases significantly in case the battery has been used for a long time. Generally, a post annealing is necessary for a-Si thin films to improve the converting efficiency [18]. A-Si thin films by heat treatment grow into polycrystalline silicon (polysilicon) thin films with fewer internal defects and lower internal stress [19,20], which can rectify the “Steabler-Wronski effect”. Polysilicon thin films are considered to be optimal solar cell materials for long lifetime and high efficiency [21]. However, monitoring defects in silicon thin films is often difficult by available conventional methods.

Positron annihilation spectroscopy is able to detect defects in materials [22,23]. Positron annihilation spectroscopies based on slow positron beams [24] were developed in the 1980s, and used to detect and analyze microstructures, thin films and sub-surfaces of materials [25,26] by varying the energy of incident positrons. It is a new non-detractive nuclear technology for unique measurements of sizes, concentration of defects and micro-phase of thin films [27]. The positron annihilation 511 keV γ-ray radiation Doppler broadening spectroscopy (DBS) usually represented by line shape parameters *S* and *W* [28], the value of *S* parameter qualitatively describes the state of defects while the *W* parameter represents the information of core electrons from surrounding atoms.

In this work, crystallization of a-Si films deposited on glass upon

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http://dx.doi.org/10.1016/j.mssp.2016.09.019
Received 20 March 2016; Received in revised form 27 August 2016; Accepted 17 September 2016
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different temperature annealing were studied by X-ray diffraction (XRD), atomic force microscope (AFM), the evolution of defects of a-Si thin films upon annealing were studied by positron annihilation Doppler broadening spectroscope based on a slow positron beam.

2. Experimental

A-Si thin films, supplied by AsiaTree Technology Co., Ltd, Taiwan, were deposited on glass substrates by PECVD technique. To prevent the oxidation of the thin film surface during annealing process, the as-deposited samples, cut from the same slice, were annealed in high-purity argon gas (99.999%) using a tube furnace. The thin films were annealed in high-purity argon gas (99.999%) for 2 h at various temperatures of 400 °C, 500 °C, 600 °C, 650 °C, 700 °C, respectively. The thicknesses of the silicon thin films were measured with an ellipsometer (α-*SE*, J.A. Woollam Co., Inc. Ellipsometry Solution), which showed the thicknesses of the deposited a-Si film and those annealed at 400 °C, 500 °C, 600 °C, 650 °C, 700 °C were about 430 nm, 403 nm, 379 nm, 386 nm, 313 nm, 310 nm, respectively. The distinct decrement in the thickness of the films annealed at 650 °C and 700 °C is indicative of crystallization of a-Si at high temperature. The crystallization behavior of the film samples was examined by XRD (Bruker AXS D8-FOCUS). The surface morphology and roughness of all the films were observed by AFM (SPM9500J3, SHIMADZU).

The positron annihilation γ-ray energy spectra were measured with a high-purity Ge detector as a function of the incident positron energy E using a monoenergetic positron beam in Wuhan University. The beam based Doppler boarding positron annihilation spectroscopy benefited additionally from the well-defined positron energy prior to injection into the films, which governed their implantation depth, and allowed to probe to the desired depths beneath the surfaces. This made it ideally suit the study of thin films, near-surface structures and buried interfaces [29,30]. The positron annihilation Doppler boarding line shape parameter S for 511 keV γ-annihilation peak was defined as the ratio of the annihilation events of the central region (511 keV ± $|\Delta E_\gamma|$, where $|\Delta E_\gamma| \sim 0.76$ keV) to the total area of the peak. The line shape parameter W was defined as the ratio of the annihilation events of the wing regions (1.44 keV ≤ $|\Delta E_\gamma|$ ≤ 4.81 keV) to the total area of the peak [31].

The resulting positron implantation was fitted by VEPFIT program [32]. The implantation profile is the Makhov distribution, proposed by Valkealahti and Nieminen [33],

$$P(E, z) = \frac{mz^{m-1}}{z_0^m} \exp\left[-\left(\frac{z}{z_0}\right)^m\right] \tag{1}$$

$$z_0 = \bar{z}/\Gamma(1 + \frac{1}{m}) \tag{2}$$

$$\bar{z} = \frac{A}{\rho} E^n \tag{3}$$

Where m=2, Γ is the Gamma function, ρ (g/cm^3) means the sample density. In this study, the empirical parameters A and n are 3.0 μgcm^{-2}keV^{-n} and 1.6, respectively [34,35].

3. Results and discussion

3.1. Microstructure and surface morphology

The XRD patterns of as-deposited a-Si thin film and those upon annealing at different temperatures are shown in Fig. 1. Generally, for a-Si films, there is no characteristic diffraction peak due to the irregular arrangement of atoms. However, diffraction peaks appear for crystalline silicon because of the spatial periodical of Si atoms. No diffraction peak can be seen for the as-deposited a-Si thin film and those annealed for 2 h below 600 °C. As the annealing temperature is increased to

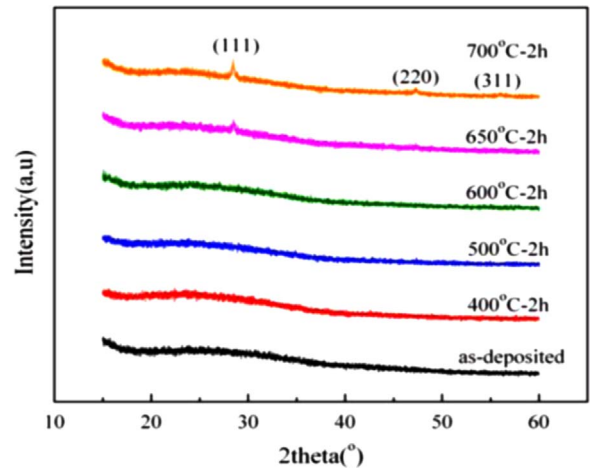

Fig. 1. The XRD patterns of amorphous silicon thin films as a function of different annealing temperatures.

650 °C, a clear diffraction peak of (111) around 28.4° is observed. And with further increasing the annealing temperature, the intensity of diffraction peak increases, which indicates the occurrence of crystallization of a-Si. From the main diffraction peaks, Debye-Scherrer formula is applied to calculate the crystallite size of the films annealed above 650 °C. The crystallite size of micro-crystal is ~60 nm for the film annealed at 650 °C. Then it shows a slight increase to ~90 nm with increasing the annealing temperature up to 700 °C. The results indicate that the crystallite size grows larger with increasing the annealing temperature higher enough.

Fig. 2 shows AFM images of (a) as-deposited amorphous silicon thin film and those annealed for 2 h at (b) 400 °C, (c) 500 °C, (d) 600 °C, (e) 650 °C, (f) 700 °C, respectively. Island-like structures, corresponding to the grains, are observed on the Si film surfaces. From the AFM images, the average sizes of grains are estimated to be 85 nm, 95 nm, and 100 nm for the as-deposited thin film, those films annealed at 650 °C and 700 °C, respectively. It seems that grain sizes are almost the same in the silicon films annealed at different temperatures. Nevertheless, it is noted that for the samples annealed at 650 °C, the estimated sizes of the grain from AFM are relatively larger than the crystallite sizes obtained from XRD analysis. This is because the grain may contain several crystallites with various defects. The surface of the as-deposited film is rough, and the average roughness and the square average roughness are about 1.7 nm and 2.2 nm, respectively. With the annealing temperature increasing to 700 °C, the surface roughness and the square average roughness decrease to approximately 1.466 nm and 1.851 nm. The results of AFM indicate that the thermal treatment can effectively eliminate crystallite boundaries and enlarge crystalline grain, and also enhance the uniformity of the film. In order to study the evolution of defects of a-Si thin films, positron annihilation Doppler broadening spectroscope based on a slow positron beam was preformed for each silicon thin film.

3.2. Defects evolution studied by DBS

Fig. 3 shows variations of S parameter as a function of positron incident energy E for the silicon thin films annealed at different temperatures. The lines denote the fitting results by VEPFIT program in two layers mode. For a typical S-E curve of the as-deposited film, the S parameter near the film surface (E ~0 keV) is relatively low due to the back diffusion to the surface of the low energy positrons, which then annihilate therein. The S parameter rises to a maximum value with increasing the position energy to around 1 keV, and it almost keeps a constant value at E=1–4.5 keV, which attributes to the annihilation of most positrons implanted in the silicon thin film. Finally, the S parameter rapidly drops down as the positron energy increases beyond

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