

Orientation Control of Al-Induced Crystallized Silicon by Diffusion Barrier Layers

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1. Introduction

Most solar cells produced currently are silicon based. However, the optical absorption coefficient of crystalline Si is much smaller than those for GaAs and CdTe. Thus, Si with a thickness of at least 100 μm is required to form crystalline Si solar cells. Therefore, novel Si-based materials are of great interest for high-efficiency solar cells. We have focused on orthorhombic barium disilicide (BaSi_2) as an interesting and useful Si-based material for solar cells. This is because BaSi_2 , composed of abundant elements Ba and Si, has a band gap of approximately 1.3 eV, matching the solar spectrum. In addition, it has a very large optical absorption coefficient of approximately $3 \times 10^4 \text{ cm}^{-1}$ at 1.5 eV [1,2]. This value is approximately 100 times higher than that of crystalline Si. Although, BaSi_2 can be grown epitaxially on Si (111) [3,4], it is more favorable if we can grow high-quality BaSi_2 films on inexpensive SiO_2 substrates. Thin film crystalline Si on a glass wafer has been investigated intensively for many applications such as thin film transistors and solar cells [5,6]. For that reason, high-quality $\langle 111 \rangle$ -oriented polycrystalline Si (poly-Si) thin layers formed on SiO_2 is demanded for high-efficient and low-cost crystalline BaSi_2 solar cells. The Al induced crystallization (AIC) method is known as a method for obtaining large grained poly-Si thin layers [7], where amorphous Si (a-Si) layers on Al was transformed into crystalline phase via exchange between the Al and Si layers during the annealing. A preferential (111) orientation of the Si layers was reported, and this is favorable for the subsequent growth of BaSi_2 layers [8]. However, there still remains an open question about what determines the preferential orientation of AIC-Si layers. For examples, Kurosawa *et al.* reported that the preferential orientation of AIC-Si can be controlled by changing the air exposure time of Al, and proposed a model explaining that the orientation of AIC-Si is determined by the crystallinity of an Al oxide diffusion barrier layer [9]. In contrast, Jung *et al.* reported that the preferential orientation depends on the annealing temperature, and proposed a model stating that the growth rate of AIC-Si determines the preferential orientation [10].

In this study, we aimed to investigate factors such as diffusion barrier layer thickness, and the surface condition of a SiO_2 substrate, that may have decisive influence on the preferential orientation of AIC-Si.

2. Experiment

The growth conditions for AIC-Si are summarized in Table I. The fused silica (SiO_2) wafers, and those processed by fluorinated acid (HF) were used as a substrate. We also employed SiO_2 wafers covered with Al-doped zinc oxide (AZO) (Al_2O_3 :2wt%) by sputtering. First, a 100-nm-thick Al film was sputtered at room temperature (RT) on these substrates. Next, the SiO_2 layers was sputtered at RT as a diffusion barrier layer in samples A-D, or just air exposure was performed for 48 h in samples E-G to form a native Al oxide layer. Then, a 100-nm-thick Si film was sputtered at RT. All sputterings were carried out by a radio-frequency (RF) magnetron sputtering method. During sputtering the vacuum level was 0.2 Pa, and the RF power was 100 W. The AIC process was performed by annealing samples in dry- N_2 atmosphere at 500°C for 10 h. The surface morphology and the oxide layer were evaluated by atomic force microscopy (AFM), and its crystal orientation was characterized by electron backscatter diffraction (EBSD).

Table I. Sample preparation conditions

Sample	Substrate	Al (nm)	Diffusion barrier layer (nm)	Si (nm)
A	SiO_2	100	SiO_2 (2)	100
B	Covered with AZO (400 nm)	100	SiO_2 (2)	100
C	SiO_2	100	SiO_2 (10)	100
D	Covered with AZO (400 nm)	100	SiO_2 (10)	100
E	SiO_2	100	native Al-O	100
F	Covered with AZO (400 nm)	100	native Al-O	100
G	Processed with HF SiO_2 wafer	100	native Al-O	100

3. Results and discussion

After the annealing, layer exchange between the a-Si and Al layers occurred in all the samples. Figures 1(a)-1(g) show the inverse pole figures obtained for samples A-G, respectively. The Al top layers were etched away prior to the EBSD measurements. As shown in Fig. 1(e), AIC-Si layers in sample E, grown with a conventional AIC method on SiO₂, showed $\langle 111 \rangle$ -orientation as previously reported [11]. Similar results were obtained in sample G. In contrast, when we inserted a 2-nm-SiO₂ diffusion barrier in sample A, the preferential orientation drastically changed from $\langle 111 \rangle$ -orientation to $\langle 100 \rangle$ -orientation even on SiO₂, as shown in Fig. 1(a). When the SiO₂ barrier layer was increased to 10 nm, in sample C, the AIC-Si was preferentially $\langle 111 \rangle$ -oriented. Therefore, it can be said that the preferential orientation of AIC-Si is influenced by the thickness of a SiO₂ diffusion barrier.

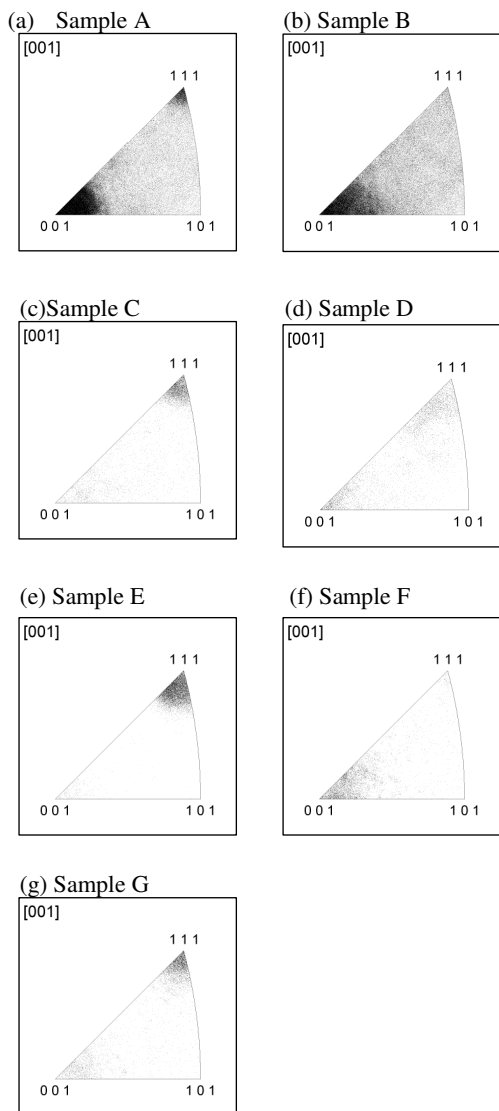


Fig.1 Inverse pole figures of AIC-Si (a) sample A, (b) sample B, (c) sample C, (d) sample D, (e) sample E, (f) sample F and (g) sample G.

At present, we don't have enough data to discuss the thickness of the native Al oxide layer in sample E. But, if this layer is found to be thicker than 2 nm by transmission electron microscopy, we can say that with increasing a SiO₂ diffusion-barrier layer thickness, the AIC-Si layer becomes preferentially $\langle 111 \rangle$ -oriented.

We next discuss the crystal orientation of AIC-Si layers formed on SiO₂ substrates capped with AZO layer. In sample F, even prepared with a conventional AIC method, $\langle 100 \rangle$ -orientation becomes dominant. This result is different from that obtained in sample E. We can say that the preferential orientation of AIC-Si may change depending on a substrate used. However, with increasing SiO₂ diffusion barrier layer thickness from 2 nm in sample B to 10 nm in sample D, the preferential orientation of AIC-Si changed from $\langle 100 \rangle$ -orientation to $\langle 111 \rangle$ -orientation as shown in Figs. 1 (b) and 1(d). This tendency is almost the same as we observed for the AIC-Si layers on SiO₂ substrate without AZO capping layers in samples A and C. On the basis of these results, it can at least be stated that as the SiO₂ diffusion layer thickness increases, the AIC-Si layers becomes $\langle 111 \rangle$ -oriented.

4. Conclusions

The crystal orientation of AIC-Si was investigated by EBSD. It was found that $\langle 111 \rangle$ orientation became dominant for both AIC-Si layers formed on SiO₂ and also those on SiO₂ capped with crystalline AZO layers.

Acknowledgements

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