Characterization of undoped-$BaSi_2$ on textured Si (001) substrate grown by molecular beam epitaxy

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Introduction Barium disilicide ($BaSi_2$) has attractive features for solar cell application such as a suitable band [1], and a large minority-carrier lifetime ($\tau \sim 10$ μs) [2] and a large minority-carrier diffusion length ($L \sim 10$ μm) [3]. Power conversion efficiency (η) was expected to be larger than 25% only in a 2-μm-thick $BaSi_2$ pn junction diode [4]. To ensure both light-trapping and epitaxy of $BaSi_2$ on Si(111) faces, textured Si(001) substrates with Si(111) faces were formed. In this study, we attempted to grow $BaSi_2$ on such a textured Si(001) substrate, and compared with the results obtained for $BaSi_2$ on Si(111).

Experiment Approximately 400 nm-thick undoped-$BaSi_2$ was grown by molecular beam epitaxy (MBE) for 5 hrs on textured Si(001) or a flat Si(111) substrate after reactive deposition epitaxy process, which was used to control the crystal orientation of $BaSi_2$ over layers. We employed the optimum growth condition for $BaSi_2$ on Si(111). Then, 3-nm-thick a-Si was prepared over the $BaSi_2$ layers as a capping layer to reduce oxidation of the film. The crystal orientation of $BaSi_2$ was investigated by XRD pole figure measurement for textured substrate with 2θ = 62.42°. Moreover, reflectivity of the film was measured by RU-60N diffusion reflection test unit.

Results & Discussions Schematic diagram of textured Si(001) substrate is shown in Fig. 1(a), the texture was constructed by four Si(111)-orientated faces. Fig. 1(b) shows the XRD pole figure image with 2θ = 62.42°, corresponding to the diffraction angle of $BaSi_2$(600). The fact that four points existed on the map indicates that *a*-axis of $BaSi_2$ was oriented normal to the (111)-oriented texture on the Si(001) substrate. Besides, reflectivity of the films on flat and textured substrate was compared in Fig. 2. It is obvious that the reflection of the film grown on the textured substrate was much lower than that on the flat one, indicating that light trapping took place. Based on these results, Si(001) textured substrates have a potential for $BaSi_2$ solar cell applications.

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[1] K. Toh, *et al.*, Jpn. J. Appl. Phys. **50** (2011) 068001. [2] K. O. Hara *et al.*, J. Appl. Phys. **112** (2012) 083108. [3] M. Baba, *et al.*, J. Cryst. Growth. **348** (2012) 75. [4]T. Suemasu, Jpn. J. Appl. Phys. **54** (2015) 07JA01.

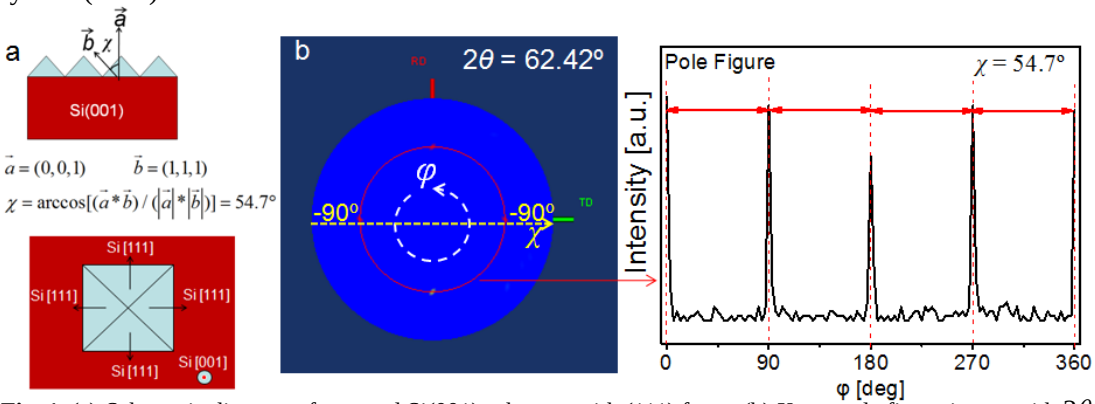

Fig. 1. (a) Schematic diagram of textured Si(001) substrate with (111) faces. (b) X-ray pole figure image with 2θ = 62.42°

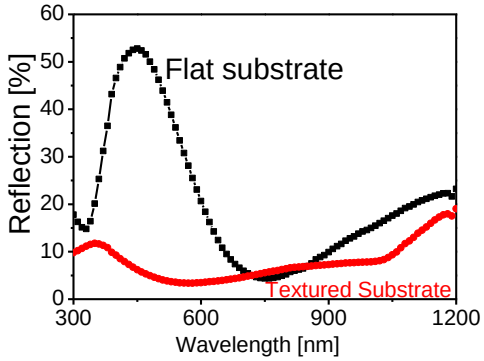

Fig. 2. Reflectance spectrum of undoped-$BaSi_2$ on flat substrate and textured substrate