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Epitaxial Growth and Photoresponse Properties of $BaSi_2$ Layers toward Si-Based High-Efficiency Solar Cells

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1. Introduction

Over 90% of solar cells presently in production are silicon based. However, the band gap of Si is approximately 0.3 eV smaller than the band gap considered suitable for solar cells. In addition, the optical absorption coefficient, α, is only 10^3cm^{-1} at 1.5 eV, so that Si with thickness of at least 100 μm is required. Therefore, novel Si-based materials have been of great interest for solar cells. We have focused on semiconducting silicide $BaSi_2$ as an interesting and useful alternative material. The band gap of $BaSi_2$ was found to reach the ideal value of approximately 1.4 eV by replacing half of Ba atoms with isoelectric Sr atoms [1-3]. In addition, both experimental and theoretical studies have revealed that $BaSi_2$ has a very large α of over 10^5 cm^{-1} at 1.5 eV [1,4], which is more than 100 times larger than that of crystalline Si. However, there have been no reports on the photoresponse properties of $BaSi_2$, which is very important when we discuss a quantum efficiency of solar cells. In this study, we report on the photoresponse properties of $BaSi_2$ epitaxial films on Si(111) substrates.

2. Experimental

MBE growth of $BaSi_2$ was performed as follows. Firstly, a 20-nm-thick *a*-axis-oriented $BaSi_2$ epitaxial film was grown on Si(111) substrate at 550 °C by Ba deposition, and this film was used as template for $BaSi_2$ overlayers. Next, Ba and Si were co-evaporated on the $BaSi_2$ template at 600 °C to form 850-nm-thick undoped-$BaSi_2$, followed by approximately 50-nm-thick Sb-doped n^+-type $BaSi_2$. Finally, Cr and Au were evaporated on the surface to form 1.5-mm-spacing striped electrodes. The same striped electrodes were also formed with Al on a 500-μm-thick *n*-type FZ-Si substrate (ρ=1000~6000 Ω·cm) for comparison. Both samples were not covered with an antireflection coating.

3. Results and discussion

Figure 1 shows the θ-2θ XRD pattern of the $BaSi_2$ layers. No peaks other than those from (100)-oriented $BaSi_2$ were obtained. The RHEED pattern shown in Fig.2, which consists of alternating intense and weak streaks, reveals that the *a*-axis-oriented $BaSi_2$ has three epitaxial variants rotated by 120° to each other in the surface normal direction, due to the three fold symmetry of Si(111). These results show that *a*-axis-oriented multidomain $BaSi_2$ epilayers were grown.

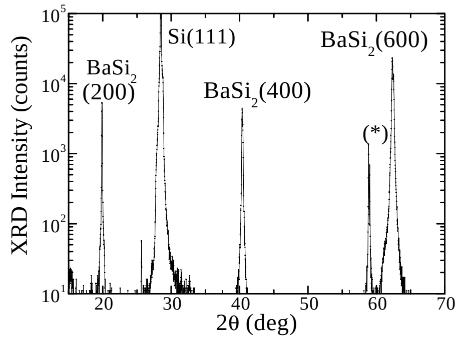

Fig. 1 θ-2θ XRD pattern of the $BaSi_2$ layer on Si(111).

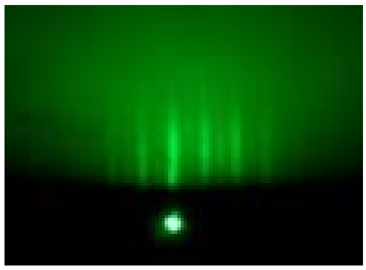

Fig. 2 RHEED pattern of MBE-grown $BaSi_2$ layer observed along Si[1-10].

Figures 3(a) and 3(b) show the photoresponse spectra of $BaSi_2$/Si and FZ-Si bulk, respectively, measured under various bias voltages. Light absorption produces electron-hole pairs that are separated by the electric field between the electrodes, leading to current flow in the external circuit as the photoexcited carriers drift before recombination. The photocurrent was observed for photon energies greater than 1.25 and 1.05 eV for the $BaSi_2$/Si and FZ-Si, respectively, increasing sharply with increasing photon energy to reach maximums at approximately 1.70 and 1.25 eV, respectively. The contribution of photoexcited carriers originating from the Si substrate to the measured photoresponse spectra can be excluded. The α value of $BaSi_2$ exceeds 10^5 cm^{-1} at 1.70 eV [1]; therefore, almost all the photons at 1.70 eV are absorbed within the $BaSi_2$ film. Figure 4(a) shows the bias voltage dependence of the external quantum efficiency for $BaSi_2$. The external quantum efficiency decreased with increasing the photon energy, because as the photon energy becomes higher, more photons are absorbed in the region of the heavily-doped defective n^+-$BaSi_2$ due to the large α. Thus, the photocurrent was limited by the high surface recombination velocity. The external quantum efficiency at 1.70 eV increased with bias voltage and reached 7 % at 7 V as shown in Fig. 4(b). This value is higher than the highest values ever reported for semiconducting silicides by more than two orders of magnitude. In this work, photoexcited carriers drifted in the lateral direction, and therefore they were likely to experience grain boundaries. In the case of the $BaSi_2$ *pn* junction, an enhanced external quantum efficiency can be safely expected, because a much larger built-in electric field (~10^4 V/cm) exists around the junction, and also the distance that the carriers must travel is much shorter (~1μm) than that in the present case (1.5 mm).

4. Conclusion

We have investigated the photoresponse properties of semiconducting $BaSi_2$ epitaxial films on Si(111). Photocurrents were clearly observed for photons with energies greater than 1.25 eV under bias voltages applied between striped electrodes on the surface. It increased sharply with increasing photon energy and attains a maximum at approximately 1.70 eV. The external quantum efficiency increased with bias voltage and reached approximately 7% at 1.70 eV when the bias voltage was 7 V.

Acknowledgements

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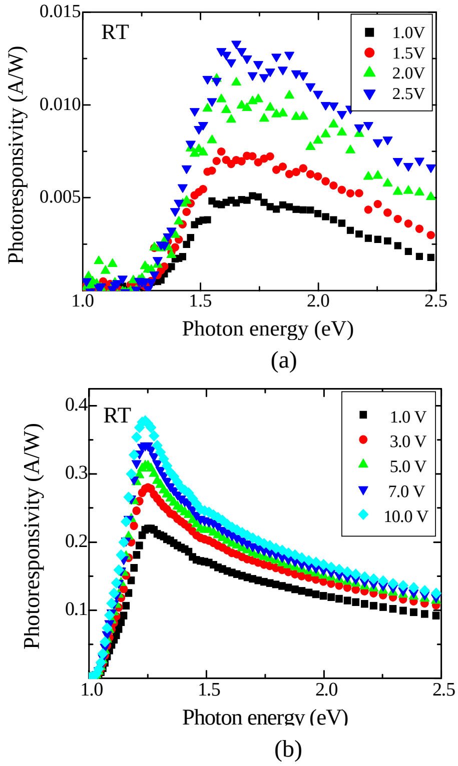

Fig. 3 Photoresponse spectra measured at room temperature for (a) $BaSi_2$/Si and (b) FZ-Si bulk.

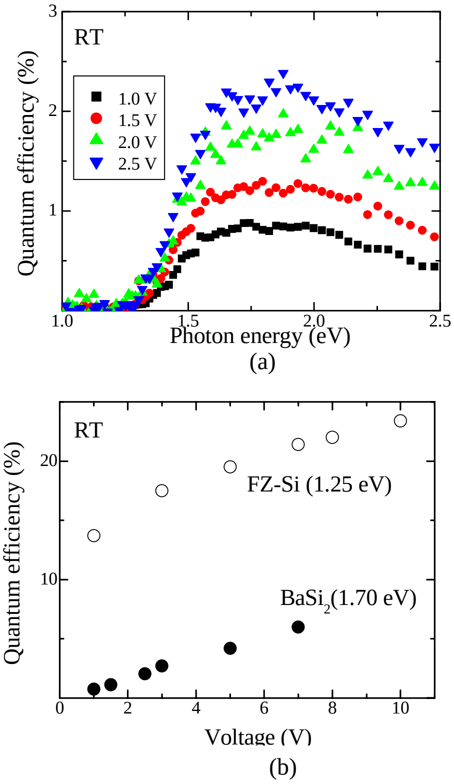

Fig. 4 (a) External quantum efficiency vs photon energy for $BaSi_2$ (b) bias voltage dependence of the external quantum efficiency for $BaSi_2$ and FZ-Si at 1.70 eV and 1.25 eV.