Fabrication of low B-doped p-BaSi$_2$/n$^+$-Si heterojunction solar cells

M. Emha Bayu$^1$, R. Takabe$^1$, S. Yachi$^1$, K. Toko$^1$, T. Suemasu$^1$

$^1$Univ. of Tsukuba, Inst. Appl. Phys.
E-mail: s1620378@u.tsukuba.ac.jp

[Introduction]
Semiconducting BaSi$_2$ has attracted attention as a future absorber-layer material for thin-film solar cells. It has an indirect band gap of approximately 1.3 eV, matching the solar spectrum, and has large absorption coefficients, reaching $3.0 \times 10^4$ cm$^{-1}$ at 1.5 eV [1,2]. We have successfully fabricated n-Si/B-doped p-BaSi$_2$ heterojunction solar cells that achieved a conversion efficiency $\eta$ of 9.9% [3]. In the work mentioned, B-doped p-BaSi$_2$ $(p = 2.2 \times 10^{18}$ cm$^{-3}$) with an optimum thickness of 20 nm acts as a hole transport layer [3]. The deterioration of $\eta$ in thicker p-BaSi$_2$ layers is suspected due to the small minority-carrier lifetime $\tau$ of p-BaSi$_2$. In previous work, we confirmed that $\tau$ strongly depends on the hole concentration $p$ of p-BaSi$_2$. We measured that low doped p-BaSi$_2$ with $p = 1.4 \times 10^{16}$ cm$^{-3}$ has a $\tau$ of 2.0 $\mu$s, two orders higher than sample with $p = 3.9 \times 10^{18}$ cm$^{-3}$ [4]. In order to utilize B-doped p-BaSi$_2$ as an active layer, we need to employ n-Si with lower resistivity (higher electron concentration $n$), so that the depletion region stretches toward the p-BaSi$_2$ layer, and that the device has a sufficient built-in potential at the junction.

In this work, we fabricated 300-nm-thick low-doped p-BaSi$_2$ on the Si substrates with various resistivities and examined the electrical properties using $J$-$V$ characteristics. We then evaluated the result from the crystallinity point of view.

[Experiment]
Briefly, a 5-nm-thick template layer was grown by Ba deposition on a hot n-Si(111) substrates ($T_{sub}$ = 500°C, $T_{ba}$ = 543°C) with resistivity $\rho$ varied from 0.01–0.1 to 0.1–1.0 and 1.0–4.0 $\Omega$cm. Next, Ba, Si, and B were coevaporated to form approximately 300-nm-thick $a$-axis-oriented B-doped p-BaSi$_2$ epitaxial films by MBE ($T_{sub}$ = 600°C, $T_{ba}$ = 569°C, $R_{si}$ = 2.0 Å/s). The boron $k$-cell temperature $T_b$ was set to 1000°C which correspond to a $p$ of $1.4 \times 10^{16}$ cm$^{-3}$. Finally, the samples were capped with a 5 nm-thick a-Si as a passivation layer. The crystallinity of BaSi$_2$ was investigated by RHEED and $\theta$-2$\theta$ X-ray diffraction (XRD). The current density versus voltage ($J$-$V$) curves were measured under standard AM1.5, 100 mW/cm$^2$ illumination at 25°C. We also measured the FWHM of the X-ray rocking curve using BaSi$_2$(600) diffraction.

[Results and discussion]
Figure 1 shows the $J$-$V$ characteristic of sample with different substrate $\rho$ values. In Fig. 1, we see that the rectifying characteristics in the $J$-$V$ curves gradually disappears as $\rho$ decreases. The $J$-$V$ characteristic shows a clear ohmic-like behavior when the substrate $\rho$ is less than 0.1 $\Omega$cm even though the depletion region in the $p$ layer are calculated to be less than 200 nm, thinner than the p-BaSi$_2$ layer thickness.

The FWHM values obtained from an $\omega$-scan x-ray rocking curve using a BaSi$_2$(600) diffraction peak of sample with different substrate $\rho$ values are plotted in Fig. 2. In Fig. 2, the degree of preferred $a$-axis orientation degraded as we decreased the substrate $\rho$. The decrease of the crystalline quality is probably one possible driving forces behind the degradation of rectifying characteristics in $J$-$V$ curves. We plan to conduct TEM observations to see what happens around the p-BaSi$_2$/n-Si interfaces to gain further information.

[Acknowledgments] This work was financially supported in part by JST-CREST and JSPS (15H02237).

![Fig. 1 $J$-$V$ characteristic of p-BaSi$_2$/n-Si of samples with different Si substrate $\rho$.](image1)

![Fig. 2 FWHM values obtained from an $\omega$-scan x-ray rocking curve of BaSi$_2$(600) fabricated on n-Si(111) with different $\rho$ values.](image2)

[Reference]