F-5-03

Extended Abstracts of the 2018 International Conference on Solid State Devices and Materials, Tokyo, 2018, pp405-406

# Investigation of $BaSi_2$ homojunction solar cells on a $p^+$-$BaSi_2$/$p^+$-Si tunnel junction towards $BaSi_2$/Si tandem solar cells

Tianguo Deng[1], Zhihao Xu[1], Yudai Yamashita[1], Komomo Kodama[1], Takuma Sato[1], Kaoru Toko[1] and Takashi Suemasu[1]

[1] Univ. of Tsukuba
1-1-1, Tennodai, Tsukuba, Ibaraki 305-8577, Japan
Phone: +81-29-853-5472 E-mail: suemasu@bk.tsukuba.ac.jp

**Abstract**

**Towards a $BaSi_2$-pn/Si-pn tandem solar cell, a $p^+$-$BaSi_2$/$p^+$-Si tunnel junction (TJ) with a low resistance of 0.081 $\Omega cm^2$ is achieved by molecular beam epitaxy and a conversion efficiency of a 500-nm-thick $BaSi_2$ homojunction solar cell on TJ is simulated by automat for simulation of heterostructures (AFORS-HET). Large photoresponsivities experimentally obtained for $BaSi_2$ films formed on TJ indicates great potential for a $BaSi_2$-pn/Si-pn tandem solar cell.**

## 1. Introduction

It is important for solar cell materials to have a large absorption coefficient ($\alpha$), and a suitable band gap (*ca.* 1.4 eV) which matches the solar spectrum to achieve a high conversion efficiency ($\eta$). Materials composed of earth abundant and environmental friendly elements are also desirable. Si-based solar cells occupy more than 90% of the photovoltaic market. However, the band gap of crystalline Si (c-Si) is 1.1eV, which is 0.3 eV smaller than the ideal band gap considered suitable for solar cell applications [1]. We have focused much attention on semiconducting $BaSi_2$ because $BaSi_2$ is a material of choice for targeting $\eta$ > 30% in a Si-based tandem structure solar cell. The band gap of $BaSi_2$ is 1.3 eV, which matches the solar spectrum much better than c-Si[2], and can be increased by adding Sr, O, or C atoms [3-5]. Moreover, it has a very large $\alpha$ of $3 \times 10^4$ $cm^{-1}$ at 1.5 eV and can be epitaxially grown both on Si(111) and Si(001)[6]. An $\eta$ of over 25% can be expected for a 2 μm-thick $BaSi_2$ pn homojunction solar cell[7]. In our previous work, we grew boron (B)-doped p-$BaSi_2$ with a hole concentration ($p$) at $10^{18}$ $cm^{-3}$ as an emitter layer on a flat n-Si(111) substrate and a textured n-Si(001) substrate with a pyramid structure consisting of {111} facets to form p-$BaSi_2$/n-Si heterojunction solar cells and achieved an $\eta$ of 9.9 and 4.6%, respectively [8-9].

In this study, prior to the formation of a $BaSi_2$-pn/Si-pn tandem solar cell, we aimed to form a $p^+$-$BaSi_2$/$p^+$-Si tunnel junction (TJ), which is necessary to make the electrical contact between $BaSi_2$-pn and Si-pn solar cells sufficiently small. We also simulated the $\eta$ of a $BaSi_2$ homojunction solar cells on TJ, using automat for simulation of heterostructures (AFORS-HET)[10]. An $\eta$ of 16.5% was simulated in a 500-nm-thick $BaSi_2$ homojunction solar cell with an open-circuit voltage ($V_{OC}$) of 0.76 V, a short-circuit density ($J_{SC}$) of 25.8 $mA/cm^2$ and a fill factor ($FF$) of 83.9%. The TJ properties were confirmed by experiment, and the tunnel current density reached 18.3 $A/cm^2$ at a bias voltage of 1.0 V, showing great potential for $BaSi_2$ homojunction solar cells on a TJ.

## 2. Experiment

The solar cell characteristics and key parameters such as band alignment, the current density versus voltage (*J*-*V*) characteristics and suitable thickness of each layer were determined using the AFORS-HET (v2.5) simulation.

For experiment, an ion-pumped molecular beam epitaxy (MBE) system with a base pressure of less than $10^{-8}$ Pa, equipped with an electron-beam evaporation source for Si as well as standard Knudsen cells for Ba, Sb and B was used. To make a $p^+$-$BaSi_2$/$p^+$-Si TJ, we set their $p$ values to exceed the effective density of states in the valence band for $BaSi_2$ ($2.0 \times 10^{19}$ $cm^{-3}$) and Si ($2.69 \times 10^{19}$ $cm^{-3}$). The procedure of the sample preparation is as follows. Si and B were co-deposited at a substrate temperature ($T_S$) of 500 ℃ to form a 40 nm-thick $p^+$-Si epitaxial layer ($p = 4.3 \times 10^{19}$ $cm^{-3}$) after thermal cleaning of the substrate. Afterwards, Ba was deposited at $T_S$ = 500 ℃ to form a 1 nm-thick $BaSi_2$ epitaxial template by reactive deposition epitaxy. This template works as a kind of seed crystal for subsequent layer. B, Ba and Si were co-deposited on the template at $T_S$ = 650 ℃ by MBE to form a 10 nm-thick $p^+$-$BaSi_2$ epitaxial film with $p = 2 \times 10^{19}$ $cm^{-3}$ on the $p^+$-Si layer on a p-Si(001) substrate with resistivity ($\rho$) of 2–5 Ωcm (sample A) and $\rho$ = 0.07 Ωcm (sample B) with a structure of $p^+$-$BaSi_2$/$p^+$-Si TJ. Subsequently, for sample C, $T_S$ was decreased to 600 ℃ to fabricate a 500 nm-thick p-$BaSi_2$ film with $p = 1 \times 10^{17}$ $cm^{-3}$. After that, a 10 nm-thick n-$BaSi_2$ epitaxial film with $n = 2 \times 10^{19}$ $cm^{-3}$ and a 3 nm-thick a-Si were grow. TJ properties of samples A and B were checked by *J*-*V* characteristics with 150 nm-thick sputtered Al electrodes with a diameter of 1 mm on the front side and full on the back side. The photoresponse spectra were measured using a xenon lamp with a 25-cm-focal-length single monochromator (Bunko Keiki, SM-1700A and RU-60N). All measurements were performed at room temperature.

## 3. Results and discussions

Figure 1 show the schematic diagram and the band alignment of a n-$BaSi_2$(10 nm, $n = 2 \times 10^{19}$ $cm^{-3}$)/p-$BaSi_2$(500 nm, $p = 1 \times 10^{17}$ $cm^{-3}$)/$p^+$-$BaSi_2$(10 nm, $p = 2 \times 10^{19}$ $cm^{-3}$)/$p^+$-Si (40 nm, $p = 4.3 \times 10^{19}$ $cm^{-3}$)/p-Si(500 μm, $\rho$ = 0.07 Ωcm) solar cell. From Fig. 1(b), the electron-hole pairs generate in the absorber p-$BaSi_2$ region, afterwards, electrons transport toward the n-$BaSi_2$ side by the build-in electric field and holes transport to the p-Si side across the $p^+$-$BaSi_2$/ $p^+$-Si TJ, leading to the operation of the solar cell.

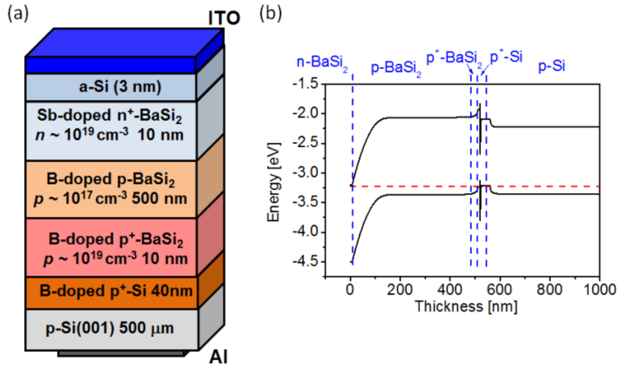


Fig. 1 (a) Schematic diagram and (b) band alignment of a $BaSi_2$ homojunction solar cell on a $p^+$-$BaSi_2$/ $p^+$-Si TJ.

Figure 2 shows the simulated *J-V* characteristics of the solar cell in the dark and under standard AM1.5 illumination. Good rectifying properties were achieved and an $\eta$ of 16.5% was obtained with a $V_{OC}$ of 0.76 V, a $J_{SC}$ of 25.8 mA/cm$^2$ and a *FF* of 83.9%.

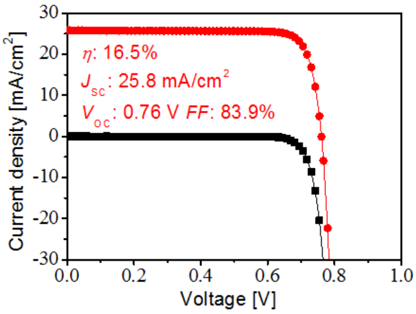


Fig. 2 *J-V* characteristics of the solar cell in the dark and under standard AM1.5 illumination.

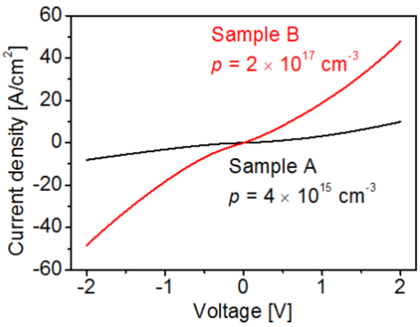


Fig. 3 *J-V* characteristics of samples A and B.

Figure 3 shows the *J-V* characteristics of samples A and B. Bias voltages were applied to the $p^+$-$BaSi_2$ layer with respect to the bottom p-Si substrate. The nearly linear behavior of sample B, which was grown on a p-Si(001) substrate with $\rho$ = 0.07 Ωcm, indicates that the sample works like a constant resistance under the bias voltage. Even under a very small bias voltage, the carriers could still tunnel through the $p^+$-$BaSi_2$/ $p^+$-Si TJ without being blocked. And the tunnel current density reached 18.3 A/cm$^2$ at a bias voltage of 1.0 V. Sufficiently small TJ resistance of 0.081 Ωcm$^2$ was achieved. In contrast, the sample grown on a medium resistive p-Si substrate showed high resistance especially around 0 V, which will block the transport of carriers.

Figure 4 shows the photoresponse properties of sample C under various forward and reverse bias voltages $V_{bias}$. The direction of the current flow changed between the reverse and forward bias conditions, as expected. Light absorption produces electron-hole pairs that are separated by the electric field between the electrodes, which leads to current flow in the external circuit as the photoexcited carriers drift before recombination. Photocurrents were increased at around 1000 nm, corresponding to the absorption edge of $BaSi_2$. The photoresponsivity reached 0.35 A/W at 850 nm at $V_{bias}$=1V, corresponding to an external quantum efficiency (EQE) of 54%. Next, we plan to form $BaSi_2$ homojunction solar cells on the TJ using the p-Si(001) substrate with $\rho$ = 0.07 Ωcm.

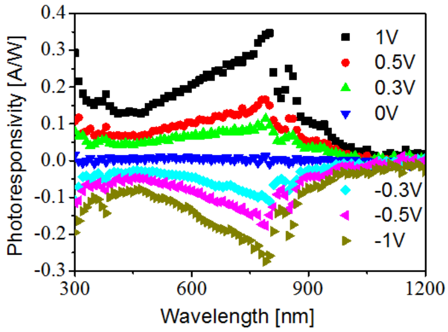


Fig. 4 Photoresponse properties of sample C under bias voltages.

## 3. Conclusions

A $BaSi_2$ homojunction solar cell on a $p^+$-$BaSi_2$/$p^+$-Si tunnel junction was simulated by AFORS-HET, and an efficiency of 16.5% was obtained. The tunnel properties of the $p^+$-$BaSi_2$/$p^+$-Si junction were confirmed, and the tunnel current density reached 18.3 A/cm$^2$ at a bias voltage of 1.0 V. Large photoresponsivity reaching 0.35 A/W at 850 nm at $V_{bias}$=1V, which corresponds to EQE = 54% show great promise of $BaSi_2$ on TJ for use in Si-based tandem solar cells.


## Acknowledgements

This work was financially supported by JSPS KAKENHI Grant Numbers 15H02237 and 17K18865, and JST MIRAI.


## References


[1] A. V. Shah *et al.*, Prog. Photovolt: Res. Appl. **12** (2004) 113.
[2] K. Toh *et al.*, Jpn. J. Appl. Phys. **50** (2011) 068001.
[3] K. Morita *et al.*, Thin Solid Films **515** (2007) 8216.
[4] W. Du *et al.*, Thin Solid Films **629** (2017) 17.
[5] Y. Imai *et al.*, Intermetallics **18** (2010) 1432.
[6] T. Suemasu and N. Usami, J. Phys. D: Appl. Phys. **50** (2017) 023001.
[7] T. Suemasu. Jpn. J. Appl.Phys. **54** (2015) 07JA01.
[8] S. Yachi, *et al.*, Jpn. J. Appl. Phys. **56** (2017) 05DB03.
[9] T. Deng *et al.*, J. Cryst. Growth **475** (2017) 186.
[10] R. Varache *et al.*, Sol. Energ. Mat. Sol. C. **141** (2015) 14.