First demonstration of BaSi₂ pn homojunction solar cell

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Abstract

In this study, we aimed to confirm the operation of a BaSi₂ homojunction solar cell. To this end, we formed two types of solar cells for comparison, that is Sb-doped n⁺-BaSi₂/p-Si heterojunction solar cell and Sb-doped n⁺-BaSi₂/B-doped p-BaSi₂ homojunction solar cell. Under AM 1.5 illumination, it was demonstrated from the internal quantum efficiency spectrum of the homojunction diode, photogenerated carriers were originated from the p-BaSi₂ layer and they were separated by the built-in electric field of the pn junction. This is the first demonstration of a BaSi₂ homojunction solar cell.

1. Introduction

We have paid special attention to semiconducting BaSi₂ because BaSi₂ has attractive features as solar cell material from the viewpoint of a bandgap of 1.3 eV, a large absorption coefficient $\alpha = 3 \times 10^4$ cm⁻¹ at 1.5 eV, and a large minoritycarrier lifetime $\tau \sim 10 \ \mu s$, giving a large minority-carrier diffusion length $L \sim 10 \ \mu m$, which is sufficiently large for thinfilm solar cell applications [1]. Recently, we have achieved an efficiency $\eta = 9.9\%$ in B-doped p-BaSi₂/n-Si heterojunction solar cells [2]. But the open-circuit voltage $V_{\rm OC}$ was smaller than 0.5 V because the built-in potential of p-BaSi₂/n-Si is limited up to 0.2 eV. Therefore, to achieve the high efficiency solar cells, BaSi₂ homojunction solar cells are necessary. An $\eta > 25\%$ with an open-circuit voltage > 0.8 V can be expected in a BaSi₂ homojunction solar cell [3]. Furthermore, we can target BaSi₂-pn/Si-pn tandem solar cells to achieve η > 30%.

Contact resistance is one of the most important parameters that directly affects the η . In our previous work, contact resistance reached a minimum of 0.019 $\Omega \cdot cm^2$ in Al/Sbdoped n-BaSi₂, which is much smaller than that in Al/Bdoped p-BaSi₂ [4]. That's why we chose the structure where n-BaSi₂ was positioned at the surface side. Furthermore, we plan to use undoped BaSi₂ as an active layer of a BaSi₂ homojunction solar cell like sample A in Fig. 1(a). This is because undoped $BaSi_2$ has a large L, and this feature facilitates the collection of photogenerated carriers in an external circuit even though L degrades to some extent owing to extrinsic effects such as crystal imperfections and other causes. As a first step, however, we attempted to form samples B, C and D to confirm the operation of a solar cell. In this work, we first aimed to confirm the operation of a BaSi₂ homojunction solar cell.

2. Experiment

Schematics of solar cell samples are shown in Figs. 1(a)-(c). Sample A is ideal; however, we formed samples B, C and D to confirm the operation of a solar cell. In sample B, Sbdoped n-BaSi₂(300 nm, $n \sim 10^{19}$ cm⁻³) was formed on medium doped p-Si(111) ($\rho > 0.1 \ \Omega$ cm) by molecular beam epitaxy (MBE). On the other hand, in samples C and D, Sb-doped n-BaSi₂(50 nm, $n \sim 10^{19}$ cm⁻³)/B-doped p-BaSi₂(500 nm, $p \sim 10^{16}$ or 10^{17} cm⁻³)/B-doped p-BaSi₂(20 nm, $p\sim 10^{19}$ cm⁻³) was formed on low-resistivity p-Si(111) ($\rho < 0.01 \ \Omega cm$) by MBE. The difference of sample C and D is the hole concentration of the p-BaSi₂ absorber layer, $p \sim 10^{16}$ for sample C and 10^{17} cm⁻ ³ for sample D. Using such a low- ρ Si substrate, we can eliminate the contribution of photogenerated carriers in the Si substrate. These substrates have defects at the BaSi₂/Si interface caused by step-bunching upon the thermal cleaning of the Si substrate [5]. So high- η is not expected, but we use this substrate to achieve the purpose of this study. For all the samples, a 3-nm-thick a-Si passivation layer was deposited [6]. Finally, 80-nm-thick ITO surface electrode and 150-nmthick Al back electrode were made by sputtering. The crystallinity was investigated using θ -2 θ XRD and RHEED. The photoresponse properties and current density versus voltage (J-V) characteristics were measured at room temperature under AM 1.5 illumination.



Fig. 1 Schematics of samples.

3. Results and discussion

Figures 2 and 3 show (a) the θ -2 θ XRD and (b) RHEED for sample B and D, respectively. The XRD patterns show both samples contain *a*-axis-oriented BaSi₂ epitaxial films. From the RHEED patterns, streaky patterns are obtained after the deposition of every BaSi₂ layer and halo patterns are obtained after the deposition of a-Si layers.

Figs. 4(a)-(b) show the J-V characteristics and IQE spectrum of sample B. Rectifying properties was obtained.



Fig. 2 (a) RHEED and (b) XRD patterns of sample B, Sb-doped n-BaSi₂(300 nm, $n\sim 10^{19}$ cm⁻³)/p-Si(111) ($\rho > 0.1 \Omega$ cm) heterojunction solar cell.



Fig. 3 (a) RHEED and (b) XRD patterns of sample D, Sb-doped n⁺-BaSi₂(20 nm, $n\sim10^{19}$ cm⁻³)/B-doped p-BaSi₂(500 nm, $p\sim10^{17}$ cm⁻³)/B-doped p⁺-BaSi₂(20 nm, $p\sim10^{19}$ cm⁻³)/p⁺-Si(111) ($\rho < 0.01 \Omega$ cm) homojunction solar cell.

A short-circuit current density $J_{SC} = 11.8 \text{ mA/cm}^3$, an opencircuit voltage $V_{OC} = 0.22 \text{ V}$, a series resistance $R_S = 148 \Omega$, and $\eta = 1.5\%$ were obtained. The values of J_{SC} , V_{OC} and η are much smaller than those obtained in B-doped p-BaSi₂/n-Si heterojunction solar cells [6]. This is because there are large conduction-band and valence-band offsets at the n-BaSi₂/p-Si interface, which hinder the transport of photogenerated carriers. As shown in Fig. 4(b), the internal quantum efficiency (IQE) increases sharply at wavelengths $\lambda < 1200 \text{ nm}$, corresponding to the band gap of Si. On the other hand, the *IQE* is negligibly small in the short wavelength range $\lambda < 600 \text{ nm}$. This means that the photogenerated carriers in the 300-nmthick n⁺-BaSi₂ do not contribute to the photocurrent.

Figures 5(a) and 5(b) show the *J-V* characteristic of sample D and *IQE* spectra of samples C and D. The leakage current is so large in Fig. 5(a); however, rectifying properties is also obtained. In sample D, the *IQE* exceeded 30% at a wavelength λ of 500 nm. The *IQE* increases sharply at wavelengths $\lambda < 700$ nm in Fig. 5(b), while the *IQE* in the long wavelength range is very small. Considering that the absorption length (3/ α) at λ =500 nm is approximately 0.1 µm in BaSi₂, we can state that the



Fig. 4 (a) J-V characteristics and (b) IQE spectrum of sample B.



Fig. 5 (a) *J-V* characteristics of sample D and (b) *IQE* spectrum of samples C and D.

photogenerated carriers were separated by the electric field of the BaSi₂ pn junction diode in samples C and D. This is the first demonstration of a BaSi₂ homojunction solar cell. The η is very small at the moment because of large leakage currents, which are originated from defects at the BaSi₂/Si interface caused by step-bunching [5]. The η will be improved very soon by using an epitaxial p⁺-Si layer on p-Si.

4. Conclusions

We demonstrated the operation of a BaSi₂ pn homojunction solar cell in Sb-doped n⁺-BaSi₂(20 nm, $n\sim 10^{19}$ cm⁻³)/Bdoped p-BaSi₂(500 nm, $p\sim 10^{16}$, 10^{17} cm⁻³)/B-doped p⁺-BaSi₂(20 nm, $p\sim 10^{19}$ cm⁻³) on p⁺-Si(111) ($\rho < 0.01 \Omega$ cm) for the first time. The rectifying properties were obtained in the *J-V* characteristics though the leakage current was significantly large. From the *IQE* spectrum that increased sharply at $\lambda < 700$ nm, we can conclude that the photogenerated carriers were separated by the built-in electric field of the BaSi₂ pn junction. This is the first demonstration of BaSi₂ pn homojunction diode.

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