Photoresponse properties of low B-doped p-BaSi₂ on

P⁺ ion-implanted Si (111)

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[Introduction]

Semiconducting BaSi2 has an indirect band gap of approximately 1.3 eV, matching the solar spectrum, and has large absorption coefficients, reaching 3.0×10^4 cm⁻¹ at 1.5 eV [1,2]. We have successfully fabricated n-Si/B-doped p-BaSi2 heterojunction solar cells that achieved a conversion efficiency η of 9.9% [3]. In the work mentioned, we used an n-Si(111) substrate with $n \sim 10^{15}$ cm⁻³, and a 20-nmthick B-doped p-BaSi₂ layer with hole concentration $p = 2.2 \times 10^{18}$ cm⁻³ [3]. In order to utilize B-doped p-BaSi₂ as an active layer, we need to employ n-Si with higher electron concentration n and low p p-BaSi₂, so that the depletion region stretches toward the p-BaSi₂ layer. However, the rectifying current density versus voltage (J-V) characteristics degraded as we utilized heavily-doped n-Si substrate due to the defects around steps with 3-4 MLs (~1 nm) in height. They were formed during thermal cleaning due to step bunching, confirmed by TEM (Fig. 1). High impurity concentration near the surface is suspected to be one of the origins of this step bunching. In order to reduce this step bunching by maintaining low impurities at the surface, we implant P⁺ ions into the Si substrate to the depth of 50 nm to form heavily-doped n⁺-Si embedding layer. We then formed a low B doped p-BaSi₂ layer and measured the external quantum efficiency (EQE) as well as the J-V characteristics.

[Experiment]

We implanted P⁺ ions to the n-Si(111) ($n \sim 10^{15}$ cm⁻ ³) wafer at an acceleration voltage of 36.0 kV and a dose of 4.0×10^{12} cm⁻². We then annealed it at 550 \Box for 30 min, followed by RTA at 1050 \square for 10 s to recover the damage as well as P activation. The peak carrier concentration of $n=6.7\times10^{17}$ cm⁻³ is expected at a depth of 50 nm from the surface. We also prepared the same layered structure on an initially substrate $(n \sim 10^{18} \text{ cm}^{-3})$ heavily-doped for comparison. We then deposited a 5-nm-thick template layer by Ba deposition on a hot substrates $(T_{sub} = 500^{\circ}C, T_{Ba} = 555^{\circ}C)$. Next, Ba, Si, and B were coevaporated to form approximately 300-nmthick a-axis-oriented B-doped p-BaSi2 epitaxial films by MBE ($T_{sub} = 600$ °C, $T_{Ba} = 576$ °C, $R_{Si} = 2.0$ Å/s), followed by a-Si capping. The boron K-cell temperature $T_{\rm B}$ was set to 1000°C, corresponding to a p of 1.4×10^{16} cm⁻³. The front contact was formed by sputtering 1-mm-diameter and 70-nm-thick ITO, and the rear contact was made with Al by sputtering. The crystallinity of BaSi₂ was investigated by RHEED and θ -2 θ X-ray diffraction (XRD). EQE were evaluated at RT using a lock-in technique with a xenon lamp and a 25 cm focal-length single

monochromator (Bunko Keiki, SM-1700A).

[Results and discussion]

Figure 2 shows the EQE spectra under 0V bias voltage for samples formed on different substrates. Sample with P⁺ implanted substrate (sample A) produces higher photocurrent reaching an EQE of 3.5%. This value is a little higher than those of sample on initially heavily-doped substrate (sample B). Photocurrents flowing to the opposite direction in a short wavelength range are also suppressed in sample A, meaning that photocarriers produced near the surface of p-BaSi₂—far from p-BaSi₂/n-Si interface—are prevented to flow to the opposite direction. In the *J-V* characteristics (Fig. 3), both samples still have poor rectifying properties. Thus, further optimization of implantation condition are needed.



Fig. 1 Cross sectional TEM image of low $p-BaSi_2/n^+-Si(111)$ interface.



Fig. 2 EQE of sample with P^+ implanted n-Si(111) substrate (sample A) and sample with initially heavily-doped n-Si(111) substrate (sample B).



Fig. 2 J-V characteristics of sample with P⁺ implanted n-Si(111) substrate (sample A) and sample with initially heavily-doped n-Si(111) substrate (sample B).

[Reference]

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