Investigation on p-BaSi₂/n-Si heterojunction solar cells using a Si(001) substrate

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Introduction
Barium disilicide (BaSi₂) shows great potential in solar cell applications as it has attractive features such as a suitable band gap, a large absorption coefficient, a large minority-carrier lifetime (τ ~ 10 μs) and a large minority-carrier diffusion length (L ~ 10 μm) [1]. In our previous work, we successfully grew boron (B)-doped p-BaSi₂ on a flat n-Si(111) substrate and a textured Si(001) substrate with a pyramid structure consisting of {111} facets to form pn junction solar cells with an efficiency (η) of 9.9% and 4.6%, respectively [2][3]. To explore the potential of a Si(001) surface for p-BaSi₂/n-Si heterojunction solar cells, in this study, we fabricated p-BaSi₂ films on a Si(001) substrate.

Experiment
B-doped p-BaSi₂ films were grown on a Si(001) substrate (resistivity ρ = 1–10 Ωcm) by molecular beam epitaxy (MBE) with layer thickness (d) ranging from 20 to 60 nm. The crucible temperature of the B K-cell (T_b) was set at 1170°C for all samples to set at p = 1.1 × 10¹⁸ cm⁻³. The current density versus voltage (J-V) characteristics was carried out under AM1.5 illumination with 80 nm-thick indium-tin-oxide (ITO) and 150 nm-thick Al electrodes on the front and back surface, respectively. Furthermore, the out-of-plane and in-plane XRD measurements were performed to obtain a, b, and c-axis lattice constants (a, b, and c) using the Nelson-Riely relationship.

Results & Discussions
Figure 1 shows the J-V curves of p-BaSi₂/n-Si solar cells. The solar cell performance changed depending on d and the largest η was obtained at d = 40 nm. It shows an η = 9.8%, with a short-circuit current density J_sc of 37.0 mA/cm², an open-circuit voltage V_oc of 0.44 V, and a FF of 59.7%, which is comparable to that on Si(111). We can see from Fig. 1 that as the d increased from 20 to 60 nm, the η improved first and then degraded for larger d because of a significant decrease in J_sc. In addition, V_oc almost saturated when d > 30 nm. Figure 2 shows strains (Δa/a, Δb/b, and Δc/c) as a function of d normalized using those of sample with d = 440 nm. Surprisingly, the values of Δa/a, Δb/b, and Δc/c were all negative when d was equal to or smaller than 60 nm, which is different from that on Si(111). Their magnitude decreased monotonically and approached 0, indicating that BaSi₂ films were under compressive strain.

References

Fig. 1. J-V characteristics of p-BaSi₂/n-Si solar cells.

Fig. 2. Normalized strains as a function of d.