Effects of pulse laser annealing on the crystallinity and electrical properties of B-doped BaSi₂ epitaxial thin films

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[Introduction]

Semiconducting BaSi₂ is considered one of the promising materials for solar cells. It has an indirect band gap of approximately 1.3 eV, matching the solar spectrum, and has large absorption coefficients comparable to CIGS, which is 30 times larger than that of crystalline silicon [1,2]. The formation of highly-doped p-type BaSi2 on the undoped n-type BaSi₂ layer ($n = 5 \times 10^{15}$ cm⁻³ [1]) is necessary to complete a BaSi₂ pn junction solar cell. In the previous studies [3], it was confirmed that boron(B)doped BaSi₂ exhibits *p*-type conductivity. We also managed to control the hole concentration by changing the temperature of the B Knudsen cell crucible. The enhancement of activation rate of the B can be achieved by increasing the growth temperature or by post annealing at 800°C in Ar [3]; however, such methods induced the formation of cracks in the layers. This is probably caused the difference in thermal expansion coefficient between BaSi₂ and Si.

We proposed pulse laser annealing (PLA) as an alternative annealing method for BaSi₂, which reportedly can increase the B activation ratio in Si published elsewhere [4]. High temperature annealing can be performed in a very short period of time by PLA, which is favorable to the B activation without the formation of cracks. In this study, we evaluated the effect of PLA on the hole concentration and the crystallinity of B-doped BaSi₂. **[Experiment]**

Briefly, a 5 nm-thick template layer was grown by Ba deposition on a hot FZ n-Si(111) substrate (T_{sub} = 500°C, T_{Ba} = 540°C). Next, Ba, Si, and B were coevaporated to form approximately 50 nm-thick aaxis-oriented B-doped BaSi2 epitaxial films by MBE $(T_{sub} = 600^{\circ}C, T_{Ba} = 573^{\circ}C, T_{B} = 1300^{\circ}C)$, followed by capping with a 5 nm thick a-Si layer. After MBE growth, we conducted PLA in vacuum, using 10 pulses of 10 Hz Nd: YAG laser with a pulse duration of 7 ns and a wavelength of 532 nm for several samples. The laser energy density F was varied from 4.10 mJ/cm² to 59.5 mJ/cm². We evaluated the crystal quality of the samples using X-ray rockingcurve measurement. We then conducted Hall measurement at room temperature using Van der Pauw method to analyze the electrical properties.

[Results and discussion]

Figure 1 shows the FWHMs of $BaSi_2(600)$ peak measured by X-ray rocking-curve as a function of *F*. The FWHM increased as the *F* increased, meaning that the degree of preferred *a*-axis orientation

degraded with increasing F. It is important to consider the maximum possible F to perform PLA in order to keep the crystal quality in a good condition. According to the experimental result, the safe region to perform PLA is to set the F to be less than around 8.00 mJ/cm².

Figure 2 displays the carrier density as a function of *F*. The hole concentration, *p*, of as-grown sample was 3.12×10^{17} cm⁻³. *P* was increased by approximately 6 times to 1.8×10^{18} cm⁻³ at *F*=4.10 mJ/cm². The increase of *p* was achieved without the formation of cracks. The conductivity type changed from p to n-type in the samples annealed for *F* more than around 8.00 mJ/cm². This is in line with the crystallinity degradation in Fig.1. PLA with *F* less than around 8.00 mJ/cm² brings out *p*-type conductivity with improvement in carrier density.



Fig. 1 FWHM of $BaSi_2(600)$ peak measured by X-ray rocking-curve as a function of energy density.



Fig. 2 Carrier density as a function of energy density.

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