Optical properties improvement of lightly and heavily boron-doped $BaSi_2$ by atomic H passivation

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Introduction

Semiconducting $BaSi_2$ has many advantages for solar cell applications, such as a suitable band gap of 1.3 eV, a large absorption coefficient of 3×10^4 cm^{-1} at 1.5 eV, and a large minority-carrier diffusion length of ca. 10 μm [1]. The first-principle calculation predicts Si vacancies to be most likely to occur as point defects in $BaSi_2$ regardless of Si rich or Si poor growth conditions and lead to the degradation of the minority-carrier properties of $BaSi_2$[2]. Therefore, we try to passivate defects in undoped $BaSi_2$ films by atomic hydrogen (H). The photoresponsivity of undoped $BaSi_2$ films is enhanced markedly by irradiation of atomic H after the growth of $BaSi_2$ films for 15 min thanks to the improvement of minority carrier lifetime [3]. The basic solar cell structure is *pn* junction. Thus, passivation of impurity-doped p- or n-$BaSi_2$ films is of particular importance. In this study, we investigate the effect of atomic H passivation on the photoresponsivity property of lightly ($p = 7 \times 10^{16}$ cm^{-3}) and heavily ($p = 3 \times 10^{18}$ cm^{-3}) boron (B) -doped p-$BaSi_2$.

Experiment

Approximately 500 nm-thick B-doped $BaSi_2$ epitaxial films were formed at 600 ℃ on the low-resistivity (ρ) Czochralshi (Cz) n^+-Si(111) substrate (ρ = 0.01 Ωcm) for photoresponsivity measurement. The crucible temperature of B (T_B) was set at 1100 ℃ and 1230 ℃, wherein the hole concentration (p) were 7×10^{16} cm^{-3} and 3×10^{18} cm^{-3}, respectively. Second, we supplied the atomic H by using a plasma generator with various H supply durations (t_H) at the same substrate temperature of the first step. Here, the power of plasma generator was set at 10 W and the vacuum level was kept at 10^{-3} Pa. Finally, a 3 nm-thick amorphous Si (a-Si) layer was formed to prevent oxidation. Reference sample was undoped $BaSi_2$ films formed with t_H = 15 min, which showed the highest photoresponsivity among undoped $BaSi_2$ films. For the photoresponsivity measurement, 80 nm-thick indium-tin-oxide (ITO) electrodes and 150 nm-thick Al were sputtered on the front and back side of samples, respectively. A bias voltage of 0.3 V was applied to the front ITO electrode with respect to the Al electrode to extract photogenerated electrons at the front ITO electrode.

Results & Discussions

Figure 1 shows the t_H dependences on photoresponsivity of lightly B-doped $BaSi_2$ from samples 1-4. The photoresponsivity of samples with t_H of 5 and 10 min was significantly improved and reached a maximum of approximately 4 A/W at a wavelength of 800 nm. This value is almost twice as large as the value of the reference. We attribute this enhancement to defect reduction in $BaSi_2$ not only by atomic H but also by B. The photoresponsivity was degraded over the wide wavelength range at t_H = 15 min. We speculate that more defects are generated in $BaSi_2$ films by excess H atoms. Figure 2 shows the photoresponse spectra of heavily B-doped $BaSi_2$ films from samples 5-7, where t_H was varied in the range of 0-5 min. In contrast with samples 1-4, the photoresponsivity exhibited degradation with increasing t_H, showing that H passivation is not suitable to improve the photoresponsivity of heavily B-doped $BaSi_2$ films. The photoresponsivity of sample 1 is lower than sample 5, indicating that lightly B-doped $BaSi_2$ has more defects than heavily B-doped $BaSi_2$.

Reference [1] T. Suemasu, *et al.,* J. Phys. D. Appl. Phys. **50** (2017) 023001. [2] M. Kumar, *et al.*, J. Mater. Chem. A **5** (2017) 25293. [3] Z. Xu, *et al.*, Phys. Rev. Mater. **3** (2019) 065403.

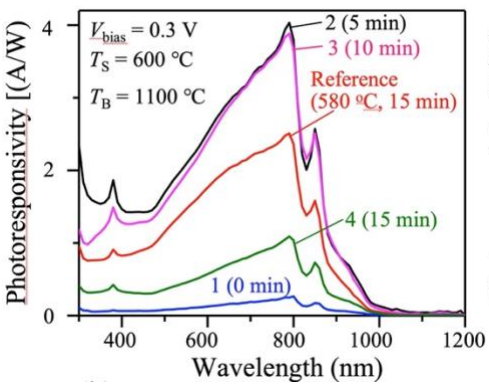

Fig. 1. Photoresponsivity spectra of 500 nm-thick lightly B-doped $BaSi_2$ layers passivated by atomic H with various t_H.

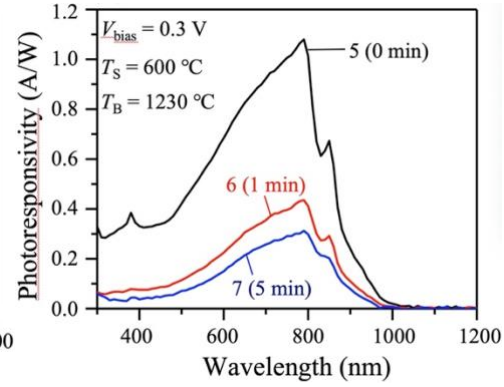

Fig. 2. Photoresponsivity spectra of 500 nm-thick heavily B-doped $BaSi_2$ layers passivated by atomic H with various t_H.