

Characterizations of crystalline quality and electrical properties of nitrogen-doped BaSi₂ films on Si(111)

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Introduction BaSi₂ has many advantages such as a band gap of 1.3 eV, matching the solar spectrum, a large absorption coefficient of $3 \times 10^4 \text{ cm}^{-1}$ at 1.5 eV, exceeding those of CIGS [1], and a minority-carrier diffusion length of ca. 10 μm [2]. Because of these excellent properties, BaSi₂ is considered to be a good material for pn junction solar cells. BaSi₂ doped with group 15 element such as P, As, and Sb shows n-type conductivity. However, there has been no report on N-doped BaSi₂. Thereby, we have attempted to dope nitrogen into BaSi₂ (N-doped BaSi₂) using radio-frequency (RF) plasma N source. Previously we reported that the hole concentration was not determined by a beam equivalent pressure of N₂ but plasma intensity of N atom. We can control its carrier type (p or n) by plasma intensity. However, the carrier concentration seems not to depend on the plasma intensity. This phenomenon may be caused by crystal quality. Thus, in this study, we attempted to evaluate the crystal quality of N-doped BaSi₂ by various methods.

Experiment We grew N-doped BaSi₂ thin films on high resistivity n-Si (111) ($\rho > 1000 \Omega \cdot \text{cm}$) with different N plasma intensities. First, we deposited Ba on a Si (111) substrate by reactive deposition epitaxy. Second, we co-deposited Ba, Si and N on the template at 580 °C to grow approximate 190 nm thick N-doped BaSi₂ to examine its crystal quality. The reflection high energy electron diffraction patterns were observed during the growth. The RF plasma power for nitrogen was set to 70 W. The plasma intensity with a wavelength of 747 nm indicates the amount of N atom [3]. To change the amount of N, we varied the plasma intensity from 560 to 1100 arbitrary unit (a.u.). X-ray diffraction (XRD) and secondary ion mass spectrometry (SIMS) measurement were carried out to characterize their crystalline quality and N concentrations.

Results & Discussions Figures 1 shows an example of N SIMS profile in N-doped BaSi₂. This sample was fabricated under the intensity of 655[a.u.]. The hole concentration was approximate 10^{17} cm^{-3} at room temperature. It was found from the SIMS result that the N was uniformly distributed and its concentration is around 10^{20} cm^{-3} . Similar results were obtained for other samples. Figure 2 shows the dependence of carrier type on plasma intensity. As reported previously, the carrier type was changed from p to n when the intensity is large (over 750). Figure 3 shows the dependence of plasma intensity and the XRD FWHM of BaSi₂(600). The FWHM increased with increasing the N plasma intensity. This means that the more nitrogen doped in BaSi₂, the poorer crystal quality becomes.

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Reference [1] K. Toh, *et al.*, Jpn. J. Appl. Phys. **50** (2011) 068001. [2] M. Baba, *et al.*, J. Cryst. Growth **348** (2012) 75. [3] H. Okumura, *et al.*, J. Cryst. Growth **198** (1998) 390.

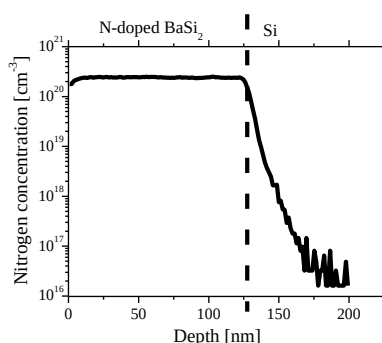


Fig 1 Example of N SIMS profile in N-doped BaSi₂.

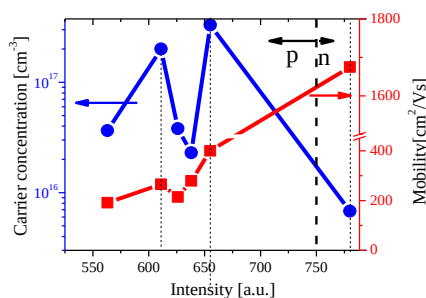


Fig 2 Dependence of N-plasma intensity ($\lambda=747\text{nm}$) and carrier con. and mobility of N-doped BaSi₂.

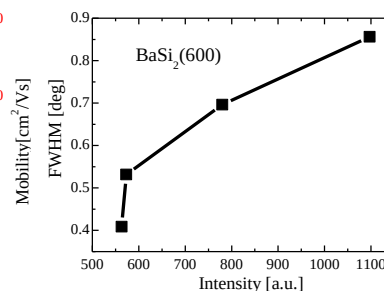


Fig 3 Dependence of N-plasma intensity ($\lambda=747\text{nm}$) and XRD FWHM of BaSi₂(600) peak in N-doped BaSi₂.