Fabrication of nitrogen-doped $BaSi_2$ films on Si(111) by molecular beam epitaxy

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Introduction $BaSi_2$ is a good candidate for future solar cell material, because its band gap is 1.3 eV, suitable for the solar spectrum. Besides, it also has a large absorption coefficient 3×10^4 cm^{-1} at 1.5 eV [1]. The minority-carrier diffusion length of undoped $BaSi_2$ is approximately 10 μm [2]. On the basis of these results, we aim to realize $BaSi_2$ pn junction solar cells. For n-type $BaSi_2$, we once attained the electron concentration of 10^{20} cm^{-3} for Sb-doped $BaSi_2$[3], whereas Sb is easy to diffuse into other layers [4], which might destroy a sharp pn junction required for solar cell. Therefore, exploring alternative donor impurity is very important. $BaSi_2$ films doped with a Group 15th element (P, As, Sb) except N have been grown, which all exhibit the n-type conductivity. In this study, we attempted to form N-doped $BaSi_2$ films and characterized their properties.

Experiment We used MBE method to grow N-doped $BaSi_2$ films on high resistivity p-Si (111) (ρ=1000-10000 Ω·cm). First, we deposited Ba on the hot Si (111) substrate for 5 min as a template layer by reactive deposition epitaxy (RDE). Second, we co-deposited Ba, Si and nitrogen on the template at 580 °C. The radio frequency (RF) plasma power for nitrogen was set to 70 W. In order to change the amount of N, we varied the beam equivalent pressure (BEP) of N_2 as 1×10^{-4} to 5×10^{-3} Pa. Reflection high energy electron diffraction (RHEED) and X-ray diffraction (XRD) with Cu Kα radiation were performed to evaluate the crystal quality of $BaSi_2$. The carrier concentration of N-doped $BaSi_2$ was measured by the Van der Pauw method.

Results & Discussions Figures 1 show the RHEED pattern observed after (a) RDE and (b) MBE at BEP = 5×10^{-3} Pa. Sharp streaky patterns from $BaSi_2$ are observed. Figure 2 shows the θ-2θ XRD pattern of the same sample. Diffraction peaks of *a*-axis-oriented $BaSi_2$ such as (200), (400), and (600) were found, meaning that we succeeded to fabricate N-doped $BaSi_2$ epitaxially on Si (111). Figure 3 shows the dependence of carrier type and carrier concentration of the grown films. When BEP was around 10^{-4} Pa, the grown film showed the n-type conductivity with the electron concentration of the order of 10^{17} cm^{-3}. For BEP > 5×10^{-3} Pa, however, N-doped $BaSi_2$ showed the p-type conductivity, differently from our prediction, and the hole concentration exceeded 10^{18} cm^{-3} with increasing BEP. Further studies are mandatory to understand what happens in N-doped $BaSi_2$.

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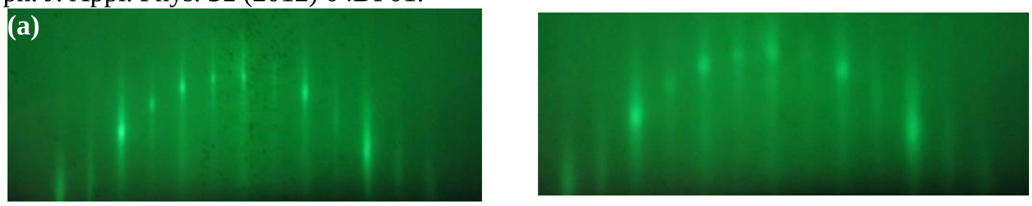

Fig 1. RHEED pattern after RDE and MBE, observed along Si [11-2].

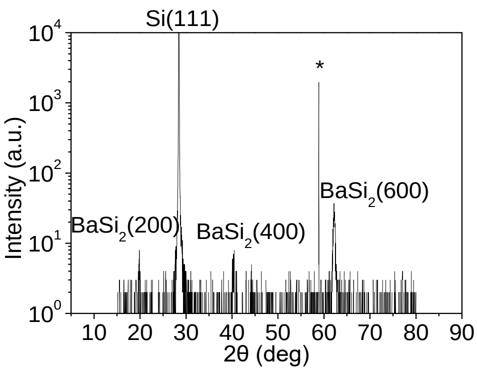

Fig 2 θ-2θ XRD pattern of $BaSi_2$.

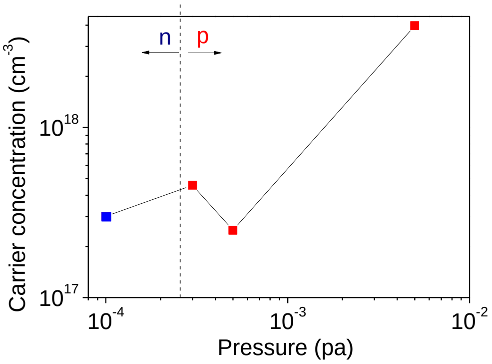

Fig 3 Dependence of carrier type and carrier concentration of N-doped $BaSi_2$ on N_2 BEP.