Fabrication of $Ba(Si,C)_2$ films on Si(111) by plasma-assisted molecular beam epitaxy

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[Introduction]

We have been focusing on orthorhombic semiconductor, $BaSi_2$ as a potential material for solar cells. $BaSi_2$ is comprised of harmless and abundant elements in nature. The value of optical absorption coefficient α is 3×10^4 cm^{-1} at 1.5 eV, which is approximately 30 times larger than that of monocrystalline silicon [1]. In addition, the value of the band gap is approximately 1.3 eV, which matches the solar spectrum better than crystalline silicon [1]. Furthermore, $BaSi_2$ can be grown epitaxially on Si(111) [2]. Its application to multijunction solar cells of which efficiency occupies the lead among various kinds of photovoltaics is considered for an advanced step. For these reasons, band gap widening to 1.85 eV is a prerequisite since the highest efficiency of double-junction solar cell is expected to be obtained in the case that it consists of top junction with the value of band gap and silicon bottom junction (E_g=1.1 eV) [3]. According to Ref. [4], the band gap expansion is expected in $Ba(Si,C)_2$. This study, thus, aims to fabricate $Ba(Si,C)_2$ films on Si(111) substrate by plasma-assisted molecular beam epitaxy (MBE) and to clarify carbon composition dependence of band gap.

[Experiment]

A plasma generator (300W) was used for cracking propane (C_3H_8). Supply of carbon and its reaching to a substrate should be checked. First, the cracking of carbon was confirmed by observing the spectra of C-H species. Then, the C_3H_8 plasma was supplied to a high-temperature Si(111) substrate to form 3C-SiC.

For growth of $Ba(Si,C)_2$ films, template layer was grown by reactive deposition epitaxy (RDE) on Si(111) at 500˚C. After that, MBE growth involving simultaneous supplies of Ba, Si, and C was conducted on the template layer. Patterns of reflection high-energy electron diffraction (RHEED) were observed. Crystal quality of grown layers was characterized by X-ray diffraction (XRD) measurement.

[Results and discussion]

Figure 1 shows a spectrum of C_3H_8 plasma. The peaks such as CH and C_2 indicates that C-C bonds are well-cracked. As shown in Fig. 2, the θ-2θ XRD pattern of the sample fabricated with the supply of C_3H_8 plasma on Si(111) suggests the formation of 3C-SiC.

In Fig. 3, carbon composition ratio to Si in $Ba(Si,C)_2$ increases from S1 to S4, where S1 is an undoped $BaSi_2$ sample. The diffraction peak position of (600) gradually shifted to a higher angle with increasing C, meaning that the out-of-plane lattice constant decreases. This result indicates the incorporation of C atoms in the grown layers, and thereby the formation of *a*-axis-oriented $Ba(Si,C)_2$ films for the first time.

[Conclusion]

An availability of C_3H_8 plasma as a source of carbon atoms was confirmed by identifying the formation of 3C-SiC on Si(111). The addition of carbon atoms into $BaSi_2$ induced the XRD peak shift, suggesting the growth of $Ba(Si,C)_2$ films.

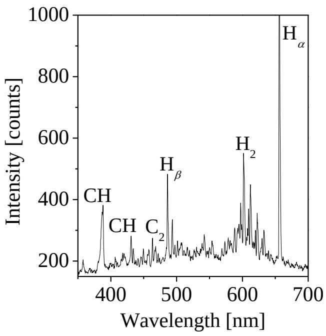

Fig. 1 Optical emission spectrum of C_3H_8 plasma.

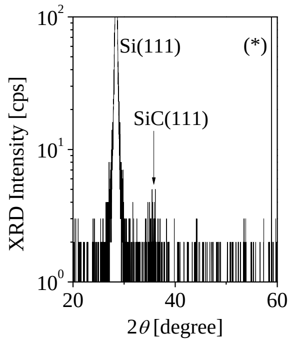

Fig. 2 θ-2θ XRD patterns of 3C-SiC.

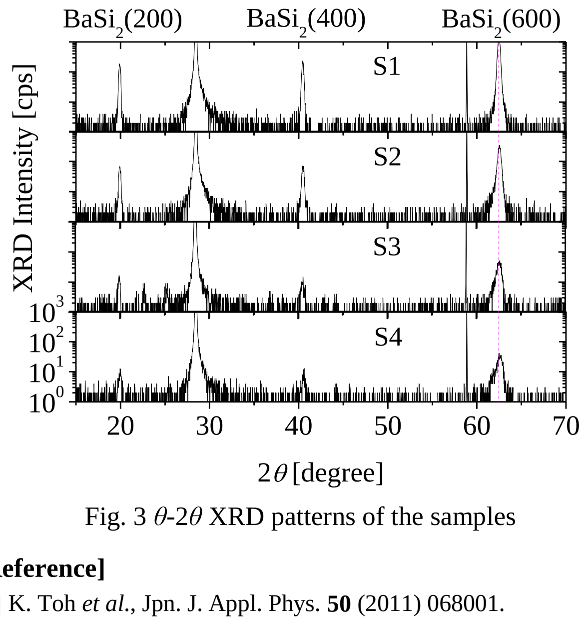

Fig. 3 θ-2θ XRD patterns of the samples

[Reference]

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