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 $\alpha$ is $3 \times 10^4$ 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 value of the band gap is approximately 1.3 eV, which is approximately 30 times larger than that of monocrystalline silicon [1].

[Experiment]

A plasma generator (300W) was used for cracking propane (C$_3$H$_8$). 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-Benzene species. Then, the C$_3$H$_8$ 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$_3$H$_8$ plasma. The peaks such as CH and C$_2$ indicates that C-C bonds are well-cracked. As shown in Fig. 2, the $\theta$-2$\theta$ XRD pattern of the sample fabricated with the supply of C$_3$H$_8$ 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$_3$H$_8$ 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.

[Reference]