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Interfacial Super Structure between Epitaxial Si(111) Layers and B($\sqrt{3}\times\sqrt{3}$)/Si(111) Substrates Studied by Synchrotron X-Ray Diffraction

K.Akimoto, J.Mizuki, I.Hirosawa, T.Tatsumi, H.Hirayama, N.Aizaki and J.Matsui

Fundamental Research Laboratories, NEC Corporation
1-1 Miyazaki 4-chome, Miyamae-ku, Kawasaki, Kanagawa 213, Japan

A ($\sqrt{3}$x$\sqrt{3}$)R30° structure was observed in the sample of Si(111)/B($\sqrt{3}$x$\sqrt{3}$)/Si(111) by grazing incidence X-ray diffraction with use of a synchrotron radiation X-ray source. This is the first observation of the interfacial super structure between epitaxial layers. In the sample, a Si(111) epitaxial overlayer of 100 Å in thickness was grown on the ($\sqrt{3}$x$\sqrt{3}$)R30°-B (θ = 1/3 ML) surface structure on a Si(111) substrate at 650 °C and the surface structure of this Si(111) epitaxial overlayer was 7x7, which was confirmed by RHEED. Bragg peaks of X-ray diffraction from the super structure were observed at (2/3,2/3) and (-2/3,4/3) lattice points in a two-dimensional reciprocal lattice space. This ($\sqrt{3}$x$\sqrt{3}$)R30° structure must exist at the interface between the Si(111) epitaxial overlayer and the Si(111) substrate having the ($\sqrt{3}$x$\sqrt{3}$)R30°-B (θ = 1/3 ML) surface structure.

1.Introduction

Heterojunctions are widely used in semiconductor devices. In these systems, the interfaces often play an important role in the determination of physical characteristics. Although a reconstructed structure on a clean solid surface is well studied by many techniques, for example, LEED, RHEED, STM, it has not been clear so far that a reconstructed structure or a super structure does exist at an interface between two solid layers. This is because those techniques for surface studies are less powerful in investigation of interfaces.

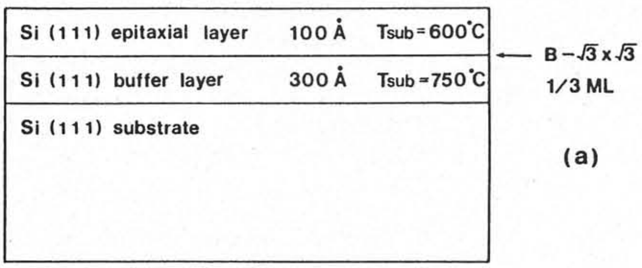
Recently, 7x7 interfacial super structure was observed at the a-Si/Si(111) interface by the TED technique [1]. And by the grazing incidence X-ray diffraction (GID) technique, the interfacial super structure of a-Si/Si(111)-7x7 [2], a-Si/$Ge_{0.2}Si_{0.8}$(111)-5x5 [3] and Al/GaAs(001)-4x6 [4] were observed. However, in these systems, Al or a-Si overlayers were deposited on the substrate at room temperature and these overlayer have an amorphous structure or a polycrystalline structure.

In this paper, we will show that the super structure exist at the interface between epitaxial layers. And we will discuss the possibility of a new structure for electrical devices using this interfacial super structure between epitaxial layers.

2.Experimental

Experiments of the sample preparation were performed in an ultra high vacuum (UHV) Si-MBE apparatus (ANELVA MBE-430). We briefly describe the sample preparation procedure as follows. A chemically pre-cleaned Si(111) substrate (a 100 mm diameter, p-type) was cleaned by deposition of an amorphous silicon and succeeding annealing at the substrate temperature of 800°C. A Si(111)-7x7 RHEED pattern was obtained after this surface cleaning process. A pure Si(111) buffer layer of 300 Å in thickness was grown on the cleaned Si(111) surface, whose temperature was 750°C. Boron from an HBO_2

crucible cell was deposited on the substrate at 750°C [5]. The $(\sqrt{3}x\sqrt{3})R30°$ RHEED pattern was observed at the coverage of 1/3 ML of boron. Finally, a Si(111) epitaxial layer of 100 Å in thickness was grown on this $(\sqrt{3}x\sqrt{3})R30°$-B (θ = 1/3 ML) surface structure at the substrate temperature of 650°C. The surface structure of this Si(111) epitaxial overlayer was the 7x7 reconstructed structure. The structure of this sample is shown in Fig. 1(a).



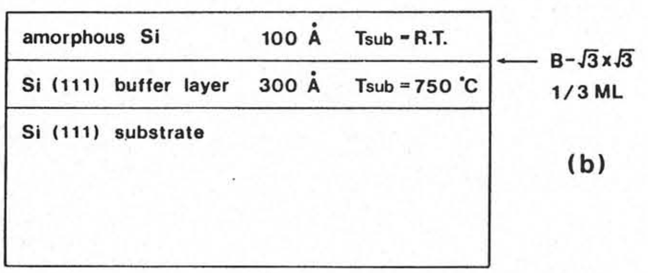


Fig. 1. The sample structure of Si(111)/B$(\sqrt{3}x\sqrt{3})$/Si(111) (a) and that of a-Si(111)/B$(\sqrt{3}x\sqrt{3})$/Si(111) (b).

As another sample, an amorphous Si layer of 100 Å in thickness was deposited on the $(\sqrt{3}x\sqrt{3})R30°$-B (θ = 1/3 ML) surface structure processed by the same procedure. The sample structure is shown in Fig. 1(b).

Experiments of X-ray diffraction were performed with synchrotron radiation at the beam line BL-9C, which is installed at Photon Factory (PF) in Tsukuba. A grazing incidence X-ray diffraction (GID) technique was employed to study the interfacial super structure. The X-ray beam was monochromatized by two Si(111) crystals which were set parallel to each other. The X-rays with a wavelength of 1.5 Å struck the sample at a grazing incidence angle of 0.2° and the diffracted X-rays were collected by a scintillation counter through 0.17° Soller slits. The scans for measurement were performed at several reciprocal lattice points with a θ-scan mode. A schematic drawing of GID experimental arrangement in this study is shown in Fig. 2.

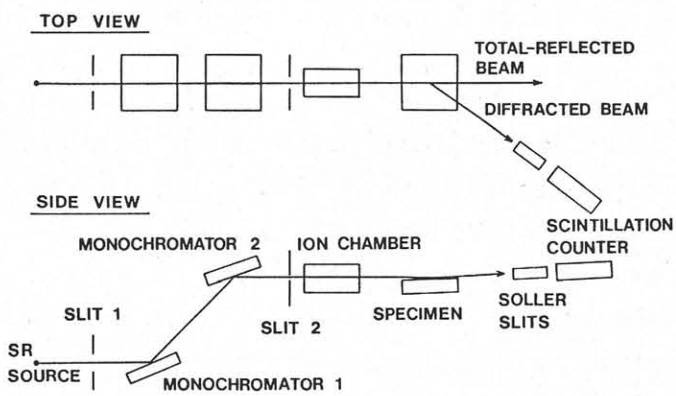


Fig. 2. Experimental arrangement.

3.Results and Discussion

The diffraction profiles from the sample of Si(111)/B$(\sqrt{3}x\sqrt{3})$/Si(111) are shown in Fig. 3. The direction and the center of the scan in the reciprocal lattice space are indicated on the right-hand side of each figure. The diffraction profiles in Fig. 3 are taken with θ-scans at the (2/3,2/3) and the (-2/3,4/3) fractional reciprocal lattice points in the two-dimensional lattice space. In the rest of this paper, we will refer to the 1/3(422) reflex in the three dimensional lattice space as (1,0) in the two dimensional one. These profiles show existence of $(\sqrt{3}x\sqrt{3})R30°$ super structure. The diffraction peaks were not observed at the (4/3,1/3), (5/3,2/3) and (-1/3,5/3) reciprocal lattice points.

This ($\sqrt{3}$x$\sqrt{3}$)R30° structure must exist at the interface between the Si(111) epitaxial overlayer and the Si(111) substrate. The reason is as follows. First,

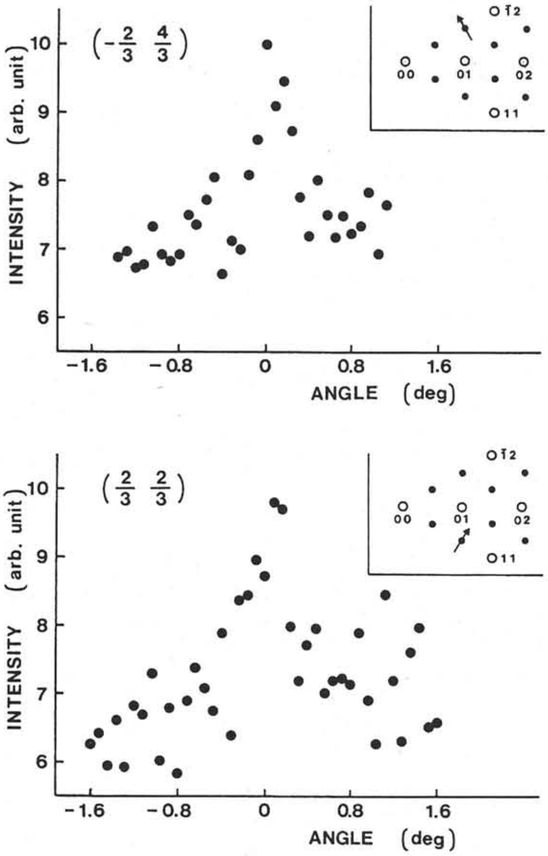


Fig. 3. X-ray diffraction profiles from the sample of Si(111)/B($\sqrt{3}$x$\sqrt{3}$)/Si(111).

the surface structure of the Si(111) epitaxial overlayer was not the ($\sqrt{3}$x$\sqrt{3}$)R30° but the 7x7 reconstructed structure. Second, in the bulk crystal of Si (an epitaxial layer and a substrate), a super structure must not be newly formed. If this ($\sqrt{3}$x$\sqrt{3}$)R30° structure (θ = 1/3 ML) is a simple interstitial or a substitutional structure of boron, the ($\sqrt{3}$x$\sqrt{3}$)R30° structure is allowed to exist only as the two-dimensional structure. If this two-dimensional ($\sqrt{3}$x$\sqrt{3}$)R30° structure were stacked three-dimensionally according to the symmetry of the bulk diamond structure, the diffraction peaks of super structure should not be observed.

The diffraction profiles from the sample of a-Si/B($\sqrt{3}$x$\sqrt{3}$)/Si(111) are shown in Fig. 4. The diffraction peaks were observed at the (-2/3,4/3) and the (-1/3,5/3) fractional reciprocal lattice points.

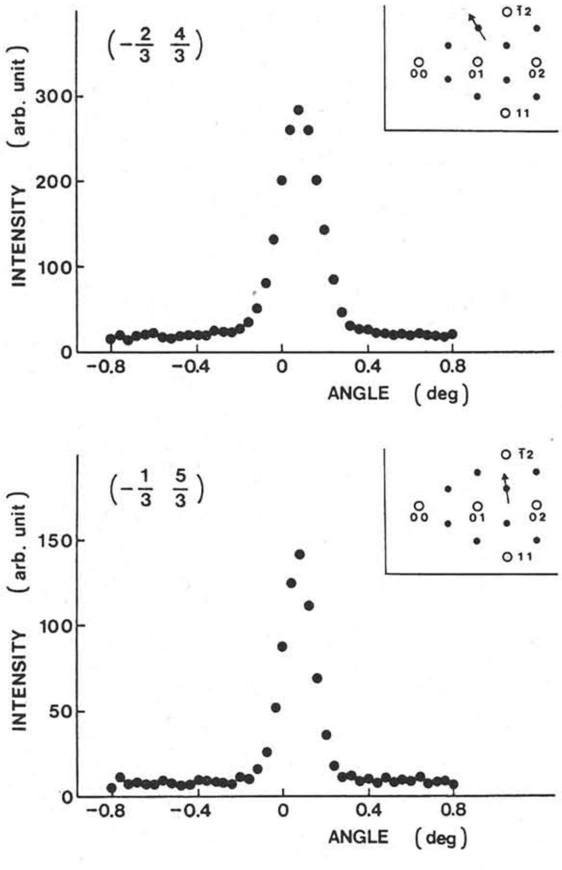


Fig. 4. X-ray diffraction profiles from the sample of a-Si/B($\sqrt{3}$x$\sqrt{3}$)/Si(111).

Intensity of these peaks is higher than that of the diffraction peaks from the interfacial super structure between epitaxial layers. This is because the interfacial super structure between the epitaxial layers may be partially destroyed, relative to the super structure between an amorphous layer and a substrate. If this $(\sqrt{3}x\sqrt{3})R30°$ structure ($\theta = 1/3$ ML) is a simple interstitial or a substitutional structure of boron, the $(\sqrt{3}x\sqrt{3})R30°$ structure may diffuse partially three-dimensionally at the interface. Since the diffraction peak at the (-1/3,5/3) reciprocal lattice point was not observed in the sample of $Si(111)/B(\sqrt{3}x\sqrt{3})/Si(111)$, the interfacial super structure between epitaxial layers is differnt from that between an amorphous layer and a substrate. Further experiments are required in order to determine each structure and the difference of these structures in detail.

Using this interfacial super structure, a three-dimensional super structure can be formed. The process is as follows. Firstly, an epitaxial layer is grown on a surface reconstructed structure of a substrate. A two-dimensional interfacial super structure can be stacked by repetition of this process above-mentioned. If this stacking is regular, a three-dimensional super structure can be formed. And using this interfacial super structure, a two-dimensionally monolayer doping (boron doping in this case) can be realized.

4.Conclusion

We have observed the $(\sqrt{3}x\sqrt{3})R30°$ structure at an interface between the Si(111) epitaxial overlayer and the Si(111) substrate having the surface structure of ($\sqrt{3}x\sqrt{3})R30°$-B (θ = 1/3 ML). This interfacial super structure between epitaxial layers will add a new and important participation to electronic devices.

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