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X-Ray Standing Wave Analysis of GaAs/Si Interface

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The GaAs/Si interfaces were analyzed by using X-ray standing wave technique. The adding effect due to large lattice mismatch between GaAs and Si can be avoided by using thin GaAs films. Two 4ML GaAs/Si(111) samples grown by MBE, and one 3ML GaAs/Si(100) sample grown by MOMBE were prepared. The results of X-ray standing wave analyses suggest that GaAs has a different structure on different initial Si(111) surfaces, that GaAs has an anti-phase structure on Si(100) even when the final GaAs film being single domain.

1 Introduction

The X-ray standing wave method is an interferometric technique for accurately determining the position of atoms at surfaces and interfaces. Despite the validity of this technique, it is seldom used to analyze buried heteroepitaxial interfaces,[1,2] because of the adding effect of overlayers. This effect is very significant in the GaAs/Si system because of its large mismatch there, about 4%. The calculated fluorescence yield profiles of Ga and As $K\alpha$ from GaAs films grown on the Si(111) substrate change markedly with increasing overlayer thickness, and the maximum thickness for X-ray standing wave analysis is estimated to be about 10 monolayers (Fig. 1). One way of solving this problem is by using thin GaAs overlayers, so that the adding effect can be neglected. For a GaAs/Si system exposed to air, a very thin, tough overlayer of GaAs has been reported,[3] suggesting the possibility of using these thin overlayers for GaAs/Si interface analysis.

This work studies the interface structure of thin GaAs/Si(111) and GaAs/Si(100) in air. Two kinds of GaAs/Si(111) samples with different initial surfaces , and an As passivated GaAs/Si(100) sample were investigated using the X-ray standing wave technique. The interface structure of GaAs/Si(111) and GaAs/Si(100) are discussed considering the calculation results, and the interface models are also described.

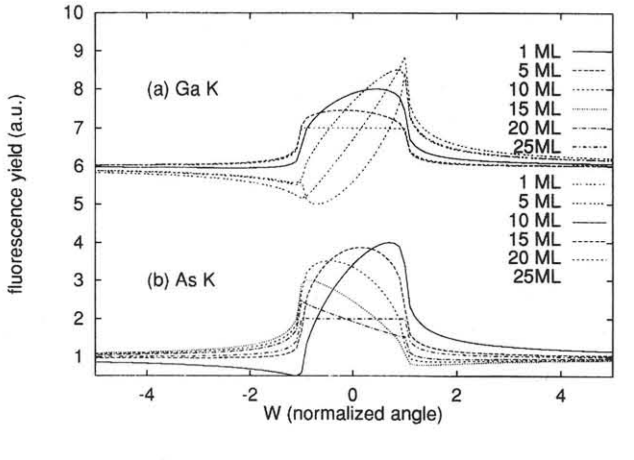

Fig. 1. Fluorescence yields of Ga and As $K\alpha$ as a function of reduced angle calculated for various overlayer thickness.

2 Sample Preparation

We used the X-ray standing method to investigate two kinds of GaAs/Si(111) and one GaAs/Si(100) sample. The GaAs/Si(111) samples were prepared by MBE to grow GaAs on different initial surfaces, one passivated by As atoms, and the other not passivated. The thickness of the GaAs overlayers was confirmed by high-resolution transmission microscopy to be about 4 monolayers. The GaAs/Si(100) sample was prepared by MOMBE with solid arsenic and triethylgallium (TEG). A Si(100) substrate 4^{o} off toward the < 110 > direction was used to prepare the single domain GaAs structure. The RHEED observation of the initial Si(100) surface and As passivated on Si(100) surface showed 1x2 and 2x1 patterns, which suggests a single domain structure during initial growth. The surface of the 4ML GaAs overlayers was protected by evaporating an additional 0.50 nm As layer onto it. Figure 2 shows a typical cross-sectional high-resolution transmission electron micrograph. The GaAs overlayer continues into the Si substrate. This confirms the suitability of using the X-ray standing wave technique for this sample.

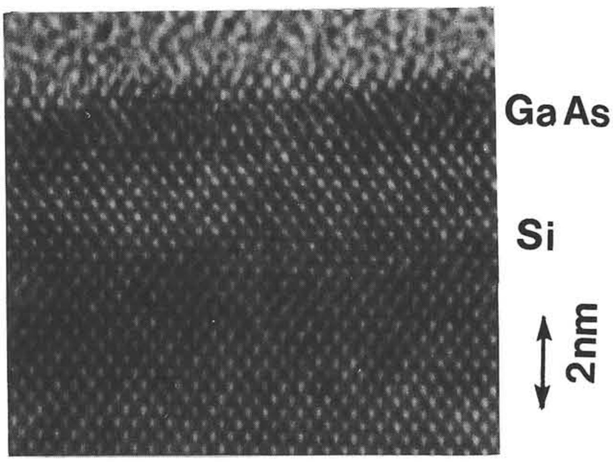

Fig. 2. The cross section of high resolution transmission electron microscopy.

3 Experimental

The X-ray standing wave measurements were performed on the Wiggler beamline BL-14B at the Photon Factory under the 4-crystal arrangement as shown in Figure 3. The selected wavelength was about 0.08 nm for excitation of Ga and As $K\alpha$ to avoid contamination from Compton and elastic scattering in the signals. The samples were rotated through the Bragg reflection region while the Ga and As $K\alpha$ fluorescence yields and Bragg reflection were measured. To avoid euivalent information from two sites, Si(111) planes were used for both the GaAs/Si(111) and GaAs/Si(100) samples. For the GaAs/Si(100) sample, the substrate was inclined 55.5 degrees from the vertical axis. Figure 3 shows the experimental arrangement for the GaAs/Si(100) sample.

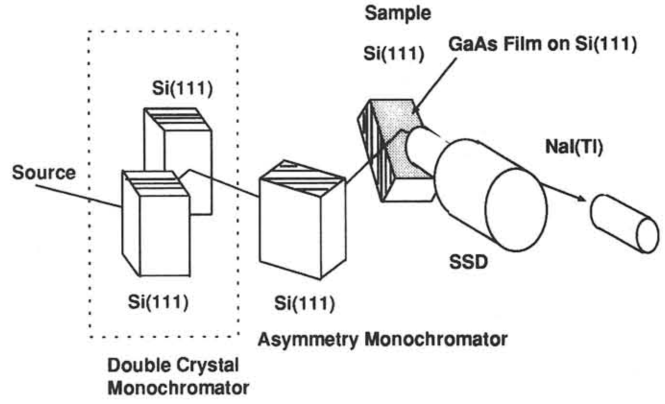

Fig. 3. Experimental arrangement of X-ray standig wave measurement.

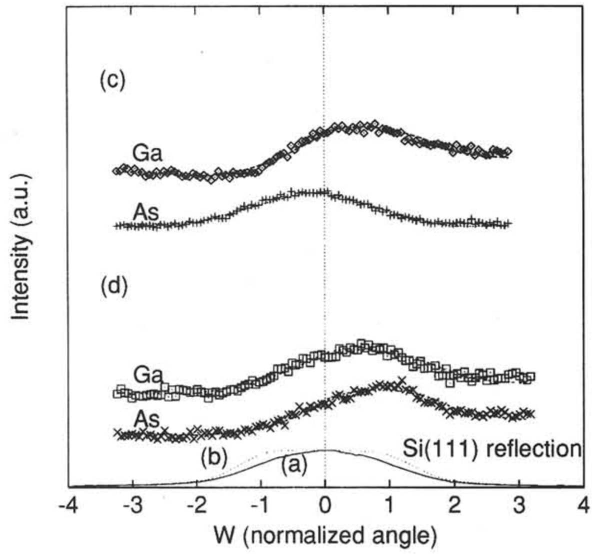

Fig. 4(a). Fluorescence yields of As $K\alpha$ and Ga $K\alpha$ from 4ML overlayers on Si(111) substrate.

Figure 4(a) shows the Bragg reflection profiles of an (a) As-passivated and (b) unpassivated GaAs/Si(111) surface, and the Ga and As $K\alpha$ fluorescence yield profiles from samples grown on an (c) As-passivated and (d) unpassivated surface. Least squares fitting revealed that on the As passivated surface, GaAs overlayers grow with a Si-As-Ga-As combination, but that without passivation, both Si-Ga-As-Ga and Si-As-Ga-As bonds exist(Fig. 4(b),(c)). These results suggest that some Ga atoms and As atoms are interchanged at the interface of GaAs/Si(111).[4)]

Figure 5 shows the Ga $K\alpha$ fluorescence yields of the GaAs/Si(100) sample and the calculated profiles by changing the ratio of Ga atoms between site A and site B. The cases of site A=1.0 and site B=1.0 mean that anly Ga atoms existed at one site and only As atoms existed at the other side. This situation was expected from the single domain and the single phase of GaAs overlayers. However, the Ga Kα fluorescence yield profile suggests that half of the Ga atoms existed at one site and the rest at the other site. This suggests the existence of an anti-phase domain during the initial stage of GaAs growth.

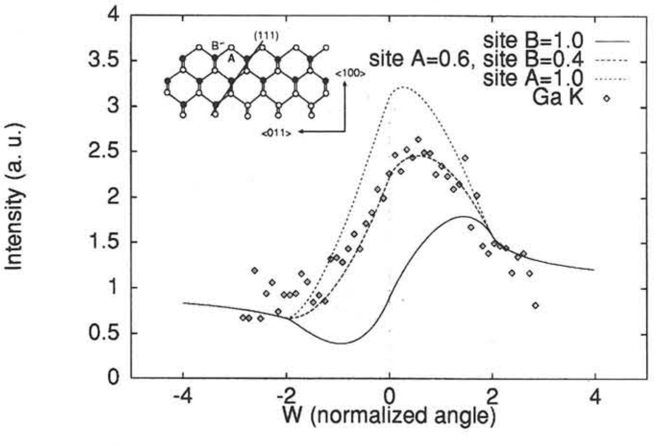

Fig. 5. Fluorescence yields of Ga Kα from 3 ML overlayers on Si(100) substrate, and the calculated fluorescence profiles as a function of Ga atoms ratio between site A and site B.

4 Conclusion

The interface structures of thin GaAs overlayers on Si(111) and Si(100) were analyzed by using X-ray standing wave technique in air. For GaAs/Si(111) with on As passivated initial surface, the interface structure was mainly a Si-As combination corresponding to the result of Patel.[3] Although Ga atoms were deposited first on an unpassivated initial surface, the interface compriseed both Si-As and Si-Ga combinaitons. This suggested the substitution of Ga and As atoms.

The situation for GaAs/Si(100) was similar to GaAs/Si(111) with an unpassivated initial surface. Despite of the RHEED observation, the measured fluorescence yield profiles corresponded to profiles calculated assuming that Ga atoms are found at both sites. This suggested the existence of an anti-phase domain during the initial stage of GaAs growth.

References

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