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Lattice distortion of an $In_{0.2}Ga_{0.8}As/GaAs$ superlattice

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Abstract

We investigated the elastic behavior of an $In_{0.2}Ga_{0.8}As/GaAs$ strained superlattice grown on a (001)-oriented GaAs substrate by molecular beam epitaxy. Using high-resolution X-ray diffraction, we found that the strained superlattice has monoclinic, and no longer tetragonal crystal symmetry. The measurements of the peak shift of X-ray Bragg reflections were performed using a diamond-anvil cell. The behavior of the system under hydrostatic pressure gave the magnitude of the stress from the monoclinic distortion. The experimental value of the stress was about 5 kbar. We propose the microscopic aspects of the $In_{0.2}Ga_{0.8}As/GaAs$ superlattice including elastic and structural aspects.

Keywords: Gallium arsenide; Indium arsenide; Molecular beam epitaxy; Superlattices; Surface stress; X-ray diffraction

1. Introduction

It is widely accepted that the changes in barrier height on group III–V semiconductors are induced by pressure [1]. Moreover, the performance of high electron mobility transistors (HEMT) using lattice-mismatched heteroepitaxies has improved drastically compared to lattice-matched heteroepitaxies [2–4]. Since the lattice strain plays a very important role in semiconductive devices, the measurement of lattice strain is at the center of wide spread interest.

A marked asymmetry in the dislocation density in the $[1\bar{1}0]$ and $[110]$ directions has been studied in some $In_{1-x}Ga_xAs$ single quantum wells on GaAs(001) substrates. The asymmetric dislocations generate an asymmetric lattice distortion of in-plane structure and the surface structure. The existence of an asymmetric lattice distortion has been reported in several papers [5–9]. For example, Breen et al. [8] claimed that the morphology of interfacial dislocations in $In_{1-x}Ga_xAs$ thin films on a GaAs (001) substrate undergoes a transition with increasing x from rectangular arrays, with dislocations lying in the $\langle 011 \rangle$ directions, to random tangled arrays, with a reduced preference for crystallographic orientation. The asymmetry is observed only in thin $In_{1-x}Ga_xAs$ films with a small value of x. However, no paper has yet been published on the magnitude of the strain generated quantitatively by asymmetric dislocation.

We observed similar behavior in an $In_{1-x}Ga_xA/GaAs$ multi-quantum well on a GaAs(001) substrate. In this paper, we carried out X-ray diffraction of an $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ strained superlattice. The morphology of the superlattice can be evaluated with simulated spectra using step-model calculations.

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Furthermore, high-pressure X-ray diffraction is a powerful method to obtain quantitatively the magnitude of the lattice strain. If the data of asymmetric strain from interfacial dislocations can be fed back to the film growth, we would obtain novel photonic and electronic devices.

2. Experimental

The superlattice film composed of $In_{0.2}Ga_{0.8}As/GaAs$ multilayers was grown on a GaAs(001) substrate by moelcular beam epitaxy (MBE) using a Riber MBE 2300 R&D. The growth chamber has an ultra-high vacuum system that consists of an ion pump and a titanium sublimation pump. Gallium arsenide (001) wafers were etched in an H_2SO_4: H_2O_2: H_2O = 5:1:5 (in volume) solution for 1 min to remove damaged layers induced during lapping. Then the substrates were introduced into a chamber. The surface oxide layer was removed by a thermal flash at 450°C. The base pressure of the chamber was 1×10^{-8} Torr. The details of the superlattice growth are described in Refs. [10,11]. The growth rates of crystals were determined by the period of the intensity oscillation in the specularly reflected electron beam. The intensity was measured through an optical fiber and a photomultiplier. The deposition rate of each layer was about 1 Å s^{-1}. After oxide desorption, 1000 Å buffer layer of $In_{0.1}Ga_{0.9}As$ was grown. Then 7 ML thick $In_{0.2}Ga_{0.8}As$ layers and 7 ML thick GaAs layers were grown alternatively. The indium concentration of the buffer layer was 0.1 to obtain the partially relaxed buffer layer. If the indium concentration is larger than 0.1, the buffer layer will be fully relaxed. By using the partially relaxed buffer layer, the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice is under the influence of the GaAs substrate.

X-ray diffraction measurements were carried out using a four-circle X-ray diffractometer. First, an as-grown sample was measured with Cu K_α radiation (40 kV, 240 mA) monochromatized by a pyrolytic graphite (002) crystal to obtain the satellite reflections. Diffraction patterns were measured with a conventional geometry. A schematic layout of our experimental set-up is shown in Fig. 1. Next,

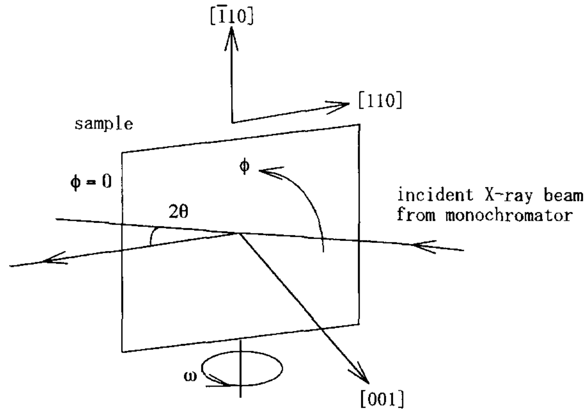

Fig. 1. Schematic drawing of our experimental set up of the X-ray diffraction of normal, high-resolution and high-pressure measurements.

a germanium (111) crystal was used as a monchromator to carry out high-resolution X-ray diffraction. Finally, the superlattice was measured under high-pressure with Mo K_α radiation (50 kV, 240 mA) monochromatized by a curved graphite crystal. We used a diamond-anvil cell (DAC) specially designed for X-ray diffraction. The specimen was trimmed to 0.5 mm × 0.5 mm. The DAC was mounted on the four-circle X-ray diffractometer. The scattering geometry was the same as shown in Fig. 1. Pressure was estimated from the lattice parameter of the GaAs substrate.

3. Results

3.1. X-ray diffraction with a graphite monochromator

First in this section, we present the diffraction pattern in $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ scanned along the perpendicular (layer stacking) direction operated with a $2\theta/\omega$ mode. The profile around the (004) reflection is shown in Fig. 2 (open circles). The fundamental peak of the $[(In_{0.2}Ga_{0.8}As)_7(GaAs_7]_{250}$ superlattice is so sharp that the peak splits into two (from Cu $K_{\alpha1}$ radiation and Cu $K_{\alpha2}$ radiation). The average lattice parameter of the superlattice is 5.704 Å.

In order to evaluate this sample, we calculated the X-ray diffraction intensity using the step model.

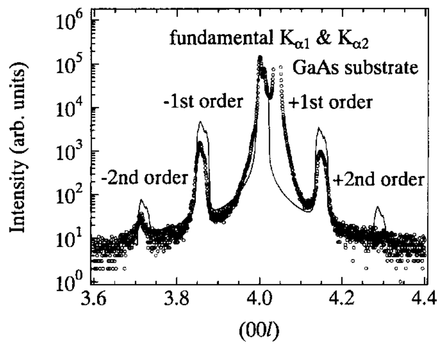

Fig. 2. Typical X-ray scattering profile around the (004) reflection in $[(In_{0.2}Ga_{0.8}As)_7/(GaAs)_7]_{250}$. Open circles are the observed intensity, and the solid line is the calculated intensity using the step model.

The lattice constants of bulk GaAs and $In_{0.2}Ga_{0.8}As$ are 5.654 and 5.735 Å, respectively. If the lattice strain did not exist in this superlattice, the designed modulation length of this superlattice would be 39.86 Å; the satellite reflections of first order can be seen around $(0,0,\pm3.857)$. The scattered X-ray amplitude of a superlattice along the [001] growth direction in $[(In_{0.2}Ga_{0.8}As)_7]_{250}$ is simply written by a periodic step function as follows.

$$A(00l)=\sqrt{I_e}\sum_j f_j\, e^{2\pi ilz}=\sqrt{I_e}\left\{F_A\sum_{s=0}^{n-1} e^{2\pi i(s+1/2)d_A/d_0} + F_B\, e^{2\pi ilnd_A/d_0}\sum_{s=0}^{m-1} e^{2\pi i(s+1/2)d_B/d_0}\right\}\times\sum_p e^{2\pi il(n+m)p},$$

where,

$$d_A=d_{GaAs(001)}/2,$$

$$d_B=d_{In_{0.2}Ga_{0.8}As(001)}/2,=(d_{InAs(001)}\times0.2+d_{GaAs(001)}\times0.8)/2, d_0=\frac{(nd_A+md_B)}{(n+m)},$$

$n=7$, $m=7$, and $p=250$.

The calculated intensities of the satellite reflections are also shown in Fig. 2 (solid line). The observed intensities would be almost explained by the step model. Therefore, the superlattice grew into a single-crystal with good film quality, as we designed. However, strictly speaking, the intensities and positions of satellite peaks are no longer calculated by a cubic system. The satellite reflections of first order are found around $(0,0,\pm3.854)$. That is, the observed modulation length $\Lambda=$ 39.32 Å, implying that the modulation structure is distorted to reduce the lattice-strain energy.

3.2. X-ray diffraction with a germanium monchromator

From simulated spectra using the step model, the superlattice was found to be distorted. The symmetry of the superlattice would be monoclinic, like $In_xGa_{1-x}As$ monolayer films as mentioned before. If the lattice is strained uniformly in the growth plane, the symmetry of the superlattice is tetragonal. On the other hand, if the lattice undergoes an asymmetric strain in the growth plane, the symmetry of the superlattice is no longer tetragonal but monoclinic. The monoclinic distortion is caused by anisotropic strain relief.

High-resolution X-ray diffraction was carried out to observe peak broadening. The peak broadening was determined from the transverse scan operated with ω mode through the (004) fundamental peak to be 0.1979° (maximum) and 0.1448° (minimum) (compared with the full-width at half maximum (FWHM) of 0.078° for the GaAs substrate). Fig. 3a shows that the two rocking curves of this sample for minimum and maximum FWHM (corresponding to the sample orientations $\phi=0°$ and 100°) are remarkably different. Fig. 3b displays the experimental values of FWHM as a function of ϕ. The FWHM of the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice shows an oscillation with a periodicity of 180° as a function of the azimuthal orientation ϕ of the sample. These data indicate that the lattice symmetry of the strained superlattice is monoclinic.

3.3. X-ray diffraction with the DAC

After sample evaluation, diffraction measurements were carried out using the DAC. From the shift of peak positions, the lattice parameters are obtained as a function of pressure. From the previous experiment, the lattice parameters of the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice and GaAs substrate are given. Therefore, the compressibility

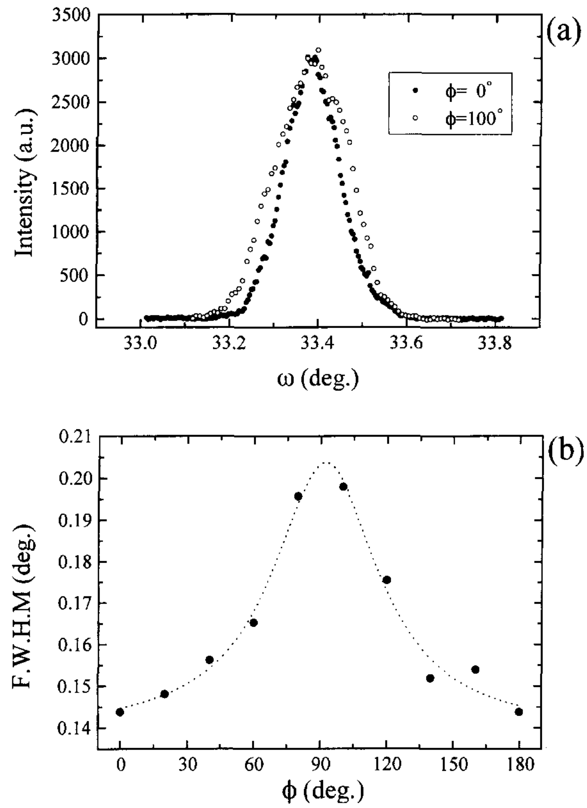

Fig. 3. (a) X-ray diffraction rocking curves for different azimuthal orientations ϕ of the sample. (b) Full width at half-maximum of the fundamental peak reflection as a function of the sample orientation.

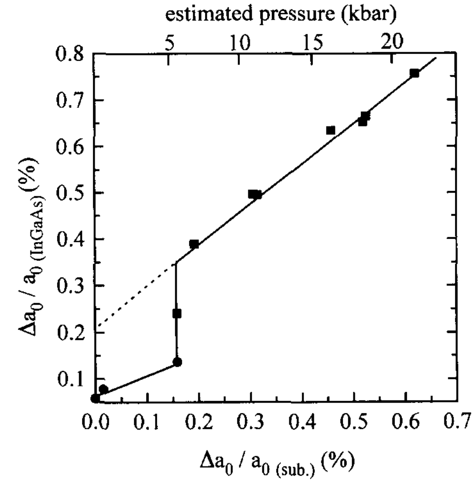

Fig. 4. Linear compressibility of $[In_{0.2}Ga_{0.8}As)_7/(GaAs)_7]_{250}$ as a function of the compressibility of the GaAs substrate. The upper axis is the estimated pressure calculated using the lattice parameter of GaAs substrate. The broken line is the compressibility extrapolated to 0 kbar using the high pressure range.

of the superlattice is obtained as a function of the compressibility of the GaAs substrate, as shown in Fig. 4. The lattice parameters of $a_{0(\mathrm{film})}$ and $a_{0(\mathrm{sub.})}$ are the values under atmospheric pressure of the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice and GaAs substrate, respectively, measured without the DAC. p denotes the applied pressure. We defined that the linear compressibility is zero under atmospheric pressure ($p=0$). The linear compressibility is calculated by $\Delta a/a_0$. Closed squares in Fig. 4 represent data obtained from the (008) reflection, and closed circles represent data obtained from the (004) reflection, because the (008) reflection is in the blind area under low pressure. The compressibility of the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice changed remarkably when the compressibility of the GaAs substrate was 0.15% (about 5 kbar). The remarkable change of the compressibility indicates that the elastic anomaly exists in this $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ system. Although the symmetry of the superlattice in the high-pressure range has not been clarified, we suppose that the origin of the elastic anomaly was the monoclinic distortion from the buffer layer and the substrate. With increasing pressure, the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice changed from a partially relaxed to a fully relaxed state (free-standing). To estimate the anomalous parts of the compressibility, the compressibility in the high-pressure range is extrapolated to 0 kbar Fig. 4 (broken line). It is important that the compressibility of the superlattice at 0 kbar is not equal to zero. This behavior also indicates that the $In_{0.2}Ga_{0.8}As/GaAs$ superlattice on GaAs substrate is not an epitaxial cube-on-cube crystallography, and that the superlattice undergoes stress even under low pressure.

4. Discussion

From the X-ray measurements of the strained superlattice grown by MBE, we conclude that the lattice symmetry of the sample is monoclinic. This behavior is very similar to an $In_xGa_{1-x}As/GaAs$

single quantum well. Grundemann et al. [12] claimed that dislocations of $In_xGa_{1-x}As/GaAs$ systems were found to be asymmetrically distributed within the (001) interface plane. Along the dislocations lines, with the lattice planes showed an anisotropic tilting. If the misfit is too large, the misfit dislocations no longer form a rectangular array but rather form a random array. We clarified that asymmetrical lattice distortion exists even in the micrometer-order $In_{0.2}Ga_{0.8}As/GaAs$ superlattice. The anisotropy has its origin in the asymmetric density of the dislocations along the [110] and [$1\bar{1}0$] directions. The relations of the lattice constants are shown schematically in Fig. 5. The anisotropy and periodicity of the FWHM were explained by Grundemann et al. [12]. In brief, the plane orientations are distributed with Gausians with standard deviations σ_{110} and $\sigma_{1\bar{1}0}$ for tilting angles [110] and along [$1\bar{1}0$], leading to a statistical broadening of the layer peak by convolution with both distributions. It is obvious that for $\sigma_{110} = \sigma_{1\bar{1}0}$. Both the $(In_{0.2}Ga_{0.8}As)_7$ layers and the $(GaAs)_7$ layers are thin enough to keep the pseudomorphic interface, which cannot generate anisotropic dislocation. Thus the origin of the monoclinic structure of the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice is the strain from the buffer layer and the substrate.

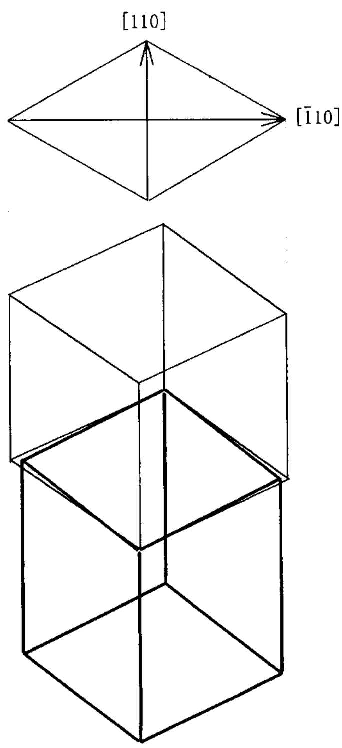

Fig. 5. Monoclinic distortion of the unit cell (projection onto the (001) plane) and monoclinic deformation of the unit cell of an epilayer grown on a cubic substrate.

We also found the elastic anomaly caused by the anisotropic dislocations lines from high-pressure X-ray measurements. In the low-pressure range, the crystal symmetry of the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice was deformed because of monoclinic distortion, and the compressibility of the superlattice showed a small change with increasing pressure. The stress of the monoclinic lattice distortion was larger than the additional hydropressure. Hence, the linear compressibility of the superlattice is different from that of the GaAs substrate. With increasing the hydropressure further, the stress from the additional hydropressure was larger than that of the monoclinic distortion. Therefore, the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice changed from a partially strained to a free-standing state, and the linear compressibility of the superlattice was nearly equal to that of the GaAs substrate. The anomaly of the compressibility jumped around 5 kbar. This is the experimental value of the stress of the anisotropic strain caused by the dislocations. These behaviors of the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice will be strongly dependent on the buffer layer and the substrate. For example, if the fully relaxed $In_xGa_{1-x}As$ buffer is used, the anomaly would be absent or become blurred, because the superlattice is not under the influence of anisotropic strain from the buffer layer and substrate.

5. Summary

From high-resolution X-ray diffraction measurements and high-pressure X-ray diffraction measurements of the $[(In_{0.2}Ga_{0.8}As)_7(GaAs)_7]_{250}$ superlattice, we conclude the following. (1) Anisotropic dislocations exist even in the micrometer-order strained superlattice. (2) Stress caused by the anisotropic lattice distortion is about 5 kbar. The lattice mismatch is accommodated by elastic strains in the low dislocation density. It is important to clarify the structural and elastic nature of the interface in superlattices with large lattice mismatch in order to produce novel superlattices.

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