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Misfit strain anisotropy in partially relaxed lattice-mismatched InGaAs/GaAs heterostructures

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Abstract
Partially relaxed InGaAs/GaAs heterostructures with a small lattice mismatch have been studied by means of atomic force microscopy and high-resolution x-ray diffractometry. Additionally, electron-beam induced current in a scanning electron microscope and transmission electron microscopy have been employed to investigate misfit dislocations formed at the (001) heterostructure interface. The measurements revealed a direct correlation between the surface cross-hatched morphology and the arrangement of interfacial misfit dislocations. The reciprocal lattice mapping and the rocking curve techniques employed for the samples aligned with either the [$\bar{1}$10] or the [110] crystallographic direction perpendicular to the diffraction plane revealed anisotropic misfit strain relaxation of the InGaAs layers. This anisotropy results from an asymmetry in the formation of the α and β types of misfit dislocations oriented along the [$\bar{1}$10] and [110] directions, respectively, which differ in their core structures. The misfit strain anisotropy causes a distortion of the unit cell of the layer and lowers its symmetry to orthorhombic.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Investigation of semiconductor heterostructures with a small lattice mismatch can be very instructive for understanding dislocation relaxation mechanisms occurring in heteroepitaxial layers [1]. In such heterostructures a strain in the epitaxial layer, resulting from a difference in lattice parameters between the substrate and the layer, can be released by the formation of misfit dislocations at the interface, provided the thickness of the layer exceeds a critical value.

The misfit dislocations are associated with threading dislocations which propagate through the epitaxial layer up to the surface.

In heteroepitaxial systems of III–V compound semiconductors with zinc-blende structure, grown on (001)-oriented substrates, orthogonal arrays of 60° misfit dislocations lying along two different ⟨110⟩ crystallographic directions are formed at the interface, which differ in their core structures. In the predominant glide set configuration the two dislocation types, referred to as α and β, consist of extra half-planes terminated in a row of group V and group III atoms, respectively, in the dislocation core. Owing to different core structures the α and β dislocations are expected to differ in their dynamic and electronic properties. In fact, a distinct difference, dependent on dopant impurities, between the glide velocities of the two types of dislocations in several III–V compound semiconductors was revealed [2]. This difference causes an asymmetry in the formation of the two types of misfit dislocations resulting in an initially anisotropic relaxation of epitaxial layers [3–5].

On the other hand, the presence of a misfit dislocation network at the interface often results in a characteristic undulating morphology, known as cross hatch, of the heterostructure surface. This morphology occurs in many lattice-mismatched semiconductor systems including SiGe/Si and various III–V compound heterostructures [6–12]. The understanding of such a surface relief formation is important for the fabrication of low-dimensional devices based on those systems, which exhibit atomically smooth but mesoscopically rough surfaces and are not compatible with planar integrated-circuit technologies. Despite several mechanisms that have recently been proposed to describe the cross-hatch development its origin remains still controversial and unresolved [13].

The aim of this paper is to study the origin of the surface cross-hatched morphology and the misfit strain anisotropy in partially relaxed InGaAs/GaAs heterostructures with a small lattice mismatch and their correlations with the interfacial misfit dislocations.

2. Experimental details

We investigated two types of InGaAs/GaAs heterostructures, which were grown by molecular beam epitaxy (MBE) on (001)-oriented n-type GaAs substrates, misoriented by 2° towards the (011) plane, with etch pit density (EPD) of about 2×10^4 cm^{-2}. Each heterostructure contained 1 μm thick, beryllium doped, p-type InGaAs layer grown at a temperature of 530 °C on a silicon doped n-type GaAs buffer layer, grown at 600 °C, to form a p–n junction near the interface. Two investigated structures differed by an indium content in the InGaAs layer, which amounted to 2.2% in the structure called A and 2.7% in the structure called B, as determined by energy dispersive spectrometry (EDS) in a scanning electron microscope. The InGaAs layers were grown under compressive misfit stress resulting from the lattice mismatch between GaAs and the ternary compound, which was below 0.2% in the both structures. The layer thickness of 1 μm exceeded a little the critical value for misfit dislocation formation in the both structures, so they were partially relaxed.

The investigated samples were subjected to anisotropic chemical etching in $HF:H_2SO_4:H_2O_2$ (2:2:1) solution [14] in order to distinguish between the nonequivalent ⟨110⟩ crystallographic directions on the (001) face of the heterostructures. Additionally, an ultrasonic-vibration aided etching in CrO_3–HF aqueous solution [15] was used to reveal the terminations of threading dislocations at the surfaces of the structures.

A systematic study of the surface morphology of both the InGaAs/GaAs heterostructures was performed using atomic force microscopy (AFM), which provides a powerful technique for microscopic surface roughness measurements. Structural properties of partially relaxed InGaAs layers were investigated by analysis of x-ray diffraction (XRD) results obtained by

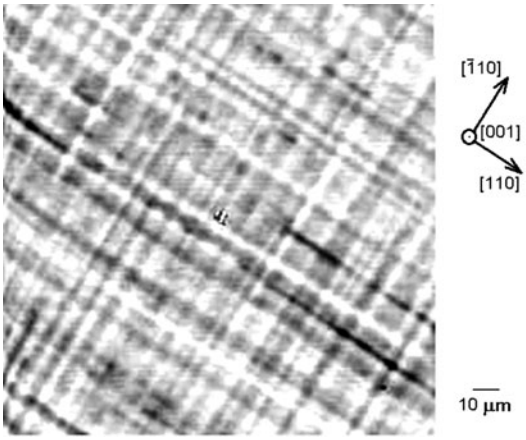

Figure 1. Distribution of misfit dislocations at the interface of $In_{0.027}Ga_{0.973}As/GaAs$ heterostructure (structure B) revealed by means of the EBIC technique in a scanning electron microscope.

means of a high-resolution x-ray diffractometer equipped with a parabolic x-ray mirror and four-bounce Ge 220 monochromator at the incident beam and a three-bounce Ge analyser at the diffracted beam. Additionally, electron-beam induced current (EBIC) in a scanning electron microscope and transmission electron microscopy (TEM) have been employed to reveal misfit dislocations formed at the heterostructure interface. The samples for TEM analysis were prepared by means of mechanical polishing followed by low-angle and low-energy ion milling to a thickness of electron transparency.

3. Results and discussion

3.1. Misfit dislocations and surface morphology

A regular network of 60° misfit dislocations aligned along two orthogonal $\langle 110 \rangle$ directions at the (001) interface was revealed by means of the EBIC technique utilizing the p–n junction situated near the interface. It is shown in figure 1, where the misfit dislocations are visible as dark lines owing to the enhanced recombination rate of electron–hole pairs generated by an electron beam (for a mechanism of the EBIC contrast formation see [16]). That network of misfit dislocations has also been revealed, under higher resolution, by means of TEM, which allows direct imaging of individual dislocations. It is shown in figure 2, which presents a plan view of the heterostructure interface.

We observed a larger density, by a factor of about 30%, of misfit dislocations of the β-type, aligned along the [110] direction, as compared to that of α dislocations, aligned along the [$\bar{1}$10] direction, which was in contradiction to earlier results [3–5]. The reason for this is, most probably, the p-type doping of the epitaxial layers, in which the glide velocity of β-type dislocations is higher than that of α-type dislocations [2]. In contrast, the glide velocity of α-type dislocations exceeds that of β-type dislocations in undoped and n-type GaAs crystals. Another possible contribution to the asymmetry in the misfit dislocation density, namely the substrate miscut, should be excluded in our case, since the miscut towards the (011) plane gives rise to the same shear stress resolved on the glide planes of both the α and β dislocations, as calculated by Goldman *et al* [4].

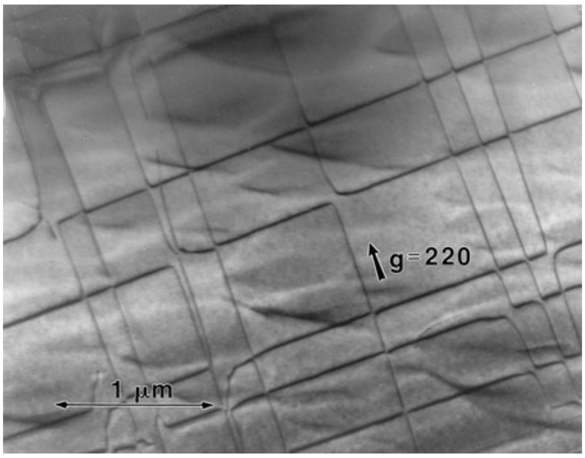

Figure 2. TEM bright field image of misfit dislocations at the interface of the same heterostructure as in figure 1.

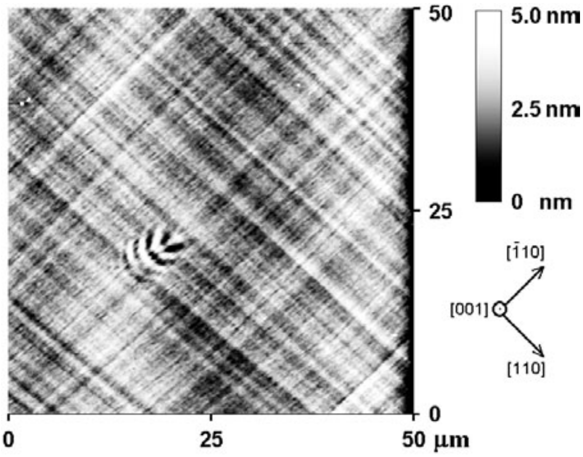

Figure 3. Surface morphology of the same heterostructure as in figures 1 and 2 revealed by AFM showing a well-defined cross-hatch pattern reproducing the network of misfit dislocations. A characteristic feature visible on the structure surface reveals an outcrop of a threading dislocation.

A typical surface morphology of structure B measured with AFM is shown in figure 3. It reproduces the network of misfit dislocations in the form of a well-defined cross-hatch pattern, with undulations, of about 2 nm peak-to-valley amplitude, running along two perpendicular $\langle 110 \rangle$ directions, on the (001) surface of the structure. A characteristic feature visible on the surface reveals an outcrop of a threading dislocation lying on a (111) plane inclined to the surface by an angle of 55°. This ascription of the feature to a threading dislocation has been confirmed by chemical etching revealing dislocation etch pits.

Similar results obtained for structure A display a smaller density of misfit dislocations but a larger density of the terminations of threading dislocations at the surface. These findings indicate a smaller degree of misfit strain relaxation in the layer with lower In content, and confirm the mechanism of misfit strain relaxation proposed by Matthews and Blakeslee [17], which dominates in low-misfit systems [1]. According to this mechanism, the formation of interfacial misfit dislocations occurs from pre-existing threading dislocations, originating from the substrate, by bending them and gliding on inclined slip planes, driven by the misfit stress, to the interface.

Our present observations, which evidence almost one-to-one correspondence between the structure of misfit dislocations at the interface and the cross-hatch surface morphology, clearly demonstrate that the cross-hatch development is a consequence of misfit dislocation formation. It is in agreement with the models in which the undulations result primarily from misfit dislocation generation and glide processes [6, 8, 9, 11]. Alternative explanations of the surface relief formation, as originating from composition fluctuations in the layer of ternary compound due to anisotropic surface diffusion [7, 10], should be excluded in view of our results.

Recently, Andrews *et al* [13] proposed a model explaining the formation of cross-hatch surface morphology, in which steps are primarily produced at the layer surface during plastic relaxation of the misfit strain, which are subsequently eliminated by lateral mass transport. This model requires the contribution of many misfit dislocations gliding on different slip planes to form a single undulation ridge. In our investigations we could directly compare results obtained with the AFM and EBIC methods. This comparison shows, in essence, the one-to-one correspondence between the contrasts given by these two methods. It has been observed that the surface of the structure exhibits waviness, which correlated spatially with the positions of the underlying misfit dislocations. This means that each undulation ridge reflects either an individual misfit dislocation or a bundle of a few closely spaced dislocations. This result rather excludes the Andrews' model for our case, i.e. for heterostructures with a small lattice mismatch and the layer thickness which only slightly exceeds the critical value for misfit dislocation formation. On the contrary, our findings are in accordance with the conclusions of Albrecht *et al* [9] and Chen *et al* [11] that locally increased growth rate at the strain relaxed surface above individual misfit dislocations leads to the formation of the undulation ridges.

3.2. Misfit strain relaxation

Misfit strain anisotropy in partially relaxed InGaAs layers has been investigated by means of XRD using the reciprocal lattice mapping and the rocking curve techniques for the symmetrical 004 and asymmetrical 444 reflections of Cu Kα_1 radiation. The measurements were performed at 27 °C for two sample positions, with the [$\bar{1}$10] and [110] directions perpendicular to the diffraction plane. The relaxed lattice parameters were calculated assuming Vegard's rule.

Figures 4 and 5 show the combined reciprocal lattice maps (RLMs) obtained using the 444 reflection where the vertical axis corresponds to the component of the reciprocal lattice vector perpendicular to structure surface (parallel to the [001] direction) and the horizontal axis corresponds to the vector component, lying in the diffraction plane, parallel to the surface, either along the [$\bar{1}$10] (denoted a) or the [110] (denoted b) direction. The vertical and diagonal dotted lines denote the RLM peak positions calculated for pseudomorphic and fully relaxed layers, respectively. For both the heterostructures investigated the RLM peaks of InGaAs layers are situated between the two lines, showing that the structures are partially relaxed. Structure B, with the larger In content, displays a larger degree of misfit strain relaxation (figure 5). In both structures the relaxation is anisotropic, being larger along the [$\bar{1}$10] direction with respect to that along the [110] direction.

These findings are confirmed by the results of the rocking curve measurements, which show the lowest value of full-width at half-maximum (FWHM) of the rocking curve for the diffraction plane parallel to the [$\bar{1}$10] direction and the highest FWHM value for the orthogonal configuration, as presented in table 1. Furthermore, the values of FWHM measured for

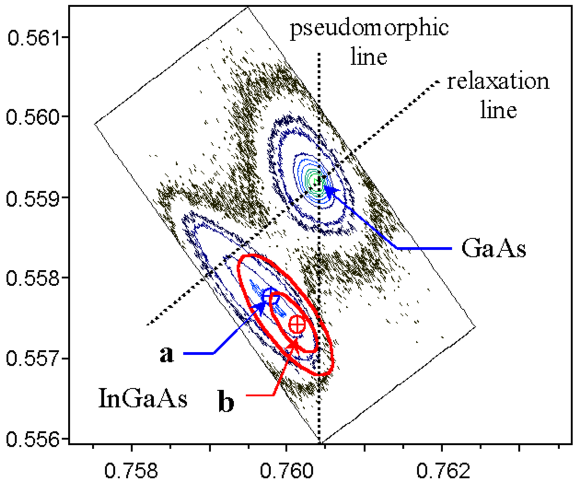

Figure 4. Combined RLM of the $In_{0.022}Ga_{0.978}As/GaAs$ heterostructure (structure A) for the 444 reflection where the vertical axis is in the [001] direction and the horizontal axis is either along the $[\bar{1}10]$ (denoted a) or along [110] (denoted b) direction. The units are in $\lambda/2d$, where $\lambda = 1.5406$ Å and d is lattice spacing of (444) planes.

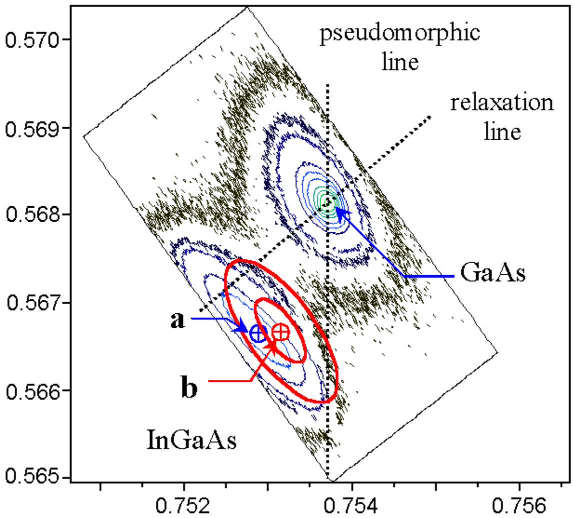

Figure 5. The same as in figure 4 for the $In_{0.027}Ga_{0.973}As/GaAs$ heterostructure (structure B).

structure A, with smaller degree of the misfit strain relaxation, are larger than those measured for the more relaxed structure B.

The XRD results are in agreement with the observed higher density of β misfit dislocations lying along the [110] direction at the interface, which produce a larger relaxation of the layers along the perpendicular $[\bar{1}10]$ direction. The misfit strain anisotropy causes a distortion of the unit cell of the layer and lowers its symmetry to orthorhombic with base lattice vectors **a**, **b** and **c** lying, respectively, along the [110], $[\bar{1}10]$ and [001] crystallographic directions of the zinc-blende structure. Lattice parameters calculated from the RLM results for the both heterostructures investigated are presented in table 1.

Table 1. Values of the FWHM of the 004 rocking curve measured along two orthogonal ⟨110⟩ directions and the lattice parameters a, b and c along the [110], [$\bar{1}$10] and [001] crystallographic directions, respectively, calculated from the RLMs measured at 27 °C.

	FWHM (arcsec)		Lattice parameters		
Sample	Along [$\bar{1}$10]	Along [110]	a (Å)	b (Å)	c (Å)
InGaAs layer A	200	300	3.999 59	4.000 01	5.670 98
InGaAs layer B	180	250	4.000 65	4.000 99	5.670 97
GaAs substrate	35	39	3.997 61	3.997 61	5.653 48

4. Summary and conclusions

TEM and EBIC investigations of the arrangement of misfit dislocations in InGaAs/GaAs heterostructures with a small lattice mismatch revealed a regular network of 60° misfit dislocations of α and β type aligned along two orthogonal ⟨110⟩ directions at the (001) interface. That network of misfit dislocations has been also reproduced in a form of a well-defined cross-hatch pattern on the surface of the structures, as revealed with the AFM technique. The observed correlation of the surface morphology with the interfacial misfit dislocations clearly demonstrates that the cross-hatch pattern results primarily from misfit dislocation generation.

Systematic study, by means of high-resolution x-ray diffractometry, of the misfit strain in partially relaxed InGaAs layers revealed a distinct anisotropy of the strain relaxation along two orthogonal ⟨110⟩ directions in the (001) plane. This anisotropy results from the observed asymmetry in the formation of two types of misfit dislocations. Higher glide velocity of the β dislocations in p-type InGaAs epitaxial layers, grown on GaAs under compressive misfit stress, results in a larger density of β misfit dislocations aligned along the [110] direction at the interface. This causes the layers to exhibit a larger relaxation along the perpendicular [$\bar{1}$10] direction with respect to that along the [110] direction. As a result, the unit cells of the layers exhibit neither cubic nor tetragonal, but orthorhombic symmetry. The misfit strain anisotropy is larger in the heterostructure with a lower In content, which underwent a smaller relaxation of the misfit strain.

Acknowledgments

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