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Anisotropic strain relaxation and surface morphology related to asymmetry in the formation of misfit dislocations in InGaAs/GaAs heterostructures

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Partially relaxed InGaAs/GaAs heterostructures with a small lattice mismatch (less than 1%), grown by metalorganic vapour-phase epitaxy have been studied by the transmission electron microscopy, atomic force microscopy as well as X-ray diffractometry. A regular network of 60° misfit dislocations formed at the (001) interface in two orthogonal ⟨110⟩ crystallographic directions has been revealed. A close correspondence between distribution of the interfacial misfit dislocations and undulating surface morphology in the form of a characteristic cross-hatch pattern has been observed. The structural analysis applied for the samples oriented either in $[\bar{1}10]$ or $[110]$ perpendicular directions, using reciprocal lattice mapping, revealed anisotropic strain relaxation, related to the asymmetry in the formation of α and β misfit dislocations along these both directions, respectively.

Key words: *misfit dislocation; strain relaxation; surface morphology; semiconductor heterostructure; InGaAs*

1. Introduction

Lattice mismatched InGaAs/GaAs heterostructures have found a wide range of technological applications in many novel optoelectronic and electronic devices. Investigations of such systems with a small lattice mismatch can be very instructive because they provide an invaluable information for understanding dislocation related strain relaxation mechanisms [1]. An elastic strain in epitaxial layers, 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 and their glide, provided that the layer

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thickness exceeds a certain critical value [2]. Both strain and misfit dislocations, usually accompanied by threading dislocations, can significantly affect electrical and optical properties of the epitaxial layers.

In heteroepitaxial III–V ternary compounds with a zinc-blende structure and a small lattice mismatch (less than 1.5%), the strain relaxation occurs primarily by the formation of a 2D network of 60° misfit dislocations, referred to as α and β, typically running in two orthogonal $\langle 110 \rangle$ crystallographic directions at the (001) interface [3]. The glide planes are the $\{111\}$ planes. By taking into account a different nature of the dislocation motion and the type of the atom located in the most distorted core position, four types of 60° dislocations can be distinguished [4]. The first two kinds of dislocations are called shuffle set dislocations if their motion is within two widely spaced $\{111\}$ planes, and the latter two are glide set dislocations if their motion is within two narrowly spaced $\{111\}$ planes. The dislocation core in the III(A)–V(B) compounds can consist of either A or B elements, therefore, the four types of dislocations, termed briefly A(g), B(g) and A(s), B(s), are indicated for glide set and shuffle set configurations, respectively. It was shown experimentally [5] that the mobile 60° misfit dislocations in III–V heterostructures are of the glide set. The α and β dislocation cores in the predominant glide set configurations are terminated by group V atoms and group III atoms, respectively. In the heterostructures grown under compressive strain conditions (e.g., $In_xGa_{1-x}As/GaAs$), α and β dislocations are oriented along the $[\bar{1}10]$ and [110] directions, respectively, while in heterostructures grown under tensile strain, the directions are reversed [2]. Different core structures of α and β misfit dislocations lead to significant differences in their dynamic activities and electronic properties. In fact, a distinct difference, depending on the kind of dopant impurities, between the glide velocities of both types of dislocations has been revealed experimentally in several III–V compound semiconductors [6, 7]. In undoped or n-type doped GaAs-based semiconductor crystals, the α dislocations have a higher glide velocity than the β dislocations while in p-type crystals, the situation is opposite. It manifests itself in the asymmetrical formation of both types of dislocations in $\langle 110 \rangle$ directions, resulting in the anisotropic misfit strain relaxation of the epitaxial layer [3, 8–11]. It is worth noting that the misorientation of the GaAs substrates can lead to the opposite results in strain relaxation comparing with those typically observed for the exactly (001)-oriented GaAs substrates, as it was reported in several papers [3, 12, 13].

Another characteristic effect associated with the presence of dislocations is undulating surface morphology with ridges and grooves parallel to the intersection of dislocation slip planes with the crystal surface, generally known as a cross hatch. The cross-hatch pattern is often observed in many lattice mismatched semiconductor heterostructures in partial relaxation conditions, e.g. SiGe/Si, InGaAs/GaAs, GaAsP/GaAs and the other III–V semiconductor systems [11, 14–20], where the ridges and grooves oriented along the $[\bar{1}10]$ and [110] directions on the surface are exhibited. Despite frequent observations of a cross-hatch surface morphology and proposals of several mechanisms describing the rise of this morphology, its origin is still controversial and unresolved.

One of the mechanisms proposed for cross-hatch development is an enhanced growth over strain relaxed regions due to fluctuations of composition in the epitaxial layer by the anisotropy of surface diffusion [14, 15]. As alternative explanations, surface undulations resulting primarily from generation of misfit dislocations and a glide process [11, 16–20] have been proposed. A very interesting model, explaining the cross-hatch pattern formation, has been recently put forward by Andrews et al. [21–23]. Within this model, the cross hatch is mainly attributed to the production of surface steps during plastic relaxation of the misfit strain and their subsequent elimination by a lateral mass transport.

In this paper, we report the results of studies of anisotropic strain relaxation and surface morphology related to the asymmetry in the formation of misfit dislocations at the interface of partially relaxed $In_xGa_{1-x}As/GaAs$ heterostructures with a small lattice mismatch.

2. Experimental

$In_xGa_{1-x}As$ epitaxial layers grown on the (001)-oriented GaAs substrates by means of metalorganic vapour-phase epitaxy (MOVPE) technique were investigated. The growth was performed in an atmospheric pressure MOVPE system, fitted with the AIX-200 R&D horizontal reactor made by AIXTRON. The organometallic group III precursors TMGa (trimethylgallium) and TMIn (trimethylindium) were transported by passing H_2 through bubblers and controlled by the pressure level in bubblers. AsH_3 was used as the arsenic source reactant. The structures consisted of a (001) oriented n^+-GaAs substrate, a 0.5 μm thick GaAs buffer layer doped with Si to a net donor concentration of about 2×10^{17} cm^{-3}, and of the $In_xGa_{1-x}As$ epitaxial layer, with a small indium content x, 7.7% (structure A) and 8.6% (structure B), and different thicknesses h_c, about 0.16 μm and 0.28 μm, respectively. The epitaxial layers were not intentionally doped but the background net doping concentration with donors revealed by C–V measurements was equal to about 10^{16} cm^{-3}. Due to the difference in lattice parameters between $In_xGa_{1-x}As$ layers and the GaAs substrate of about 0.55% and 0.62% for samples A and B, respectively, the epitaxial growth was performed under a compressive misfit strain. All the epitaxial layers were grown at the same temperature equal to 670 °C and different times in order to achieve the thicknesses just above the critical value, i.e. to obtain partially relaxed samples [24].

Structural properties of the partially relaxed $In_xGa_{1-x}As$ epitaxial layers were examined by means of high-resolution X-ray diffraction (HRXRD) measurements using a Philips Materials Research Diffractometer (MRD) equipped with a four-crystal Bartels Ge monochromator and Bonse/Hart analyser. The (220) reflection of a monochromator was used with $CuK_{\alpha1}$ radiation and triple-axis configurations were applied for recording 2D reciprocal lattice maps (RLMs).

The discrimination between two perpendicular $\langle110\rangle$ directions on the (001) surface of heterostructures was made by subjecting the samples to selective chemical etching in the HF:H_2SO_4:H_2O_2: (2:2:1) solution [25] diluted in 1:1 proportion in water, for 45 s at room temperature. This etching gives rise to a characteristic microrelief in the form of quasi-parallel grooves (with the heights equal to about 250 nm) on the (001) GaAs surface, oriented in $[\bar{1}10]$ direction (Fig. 1).

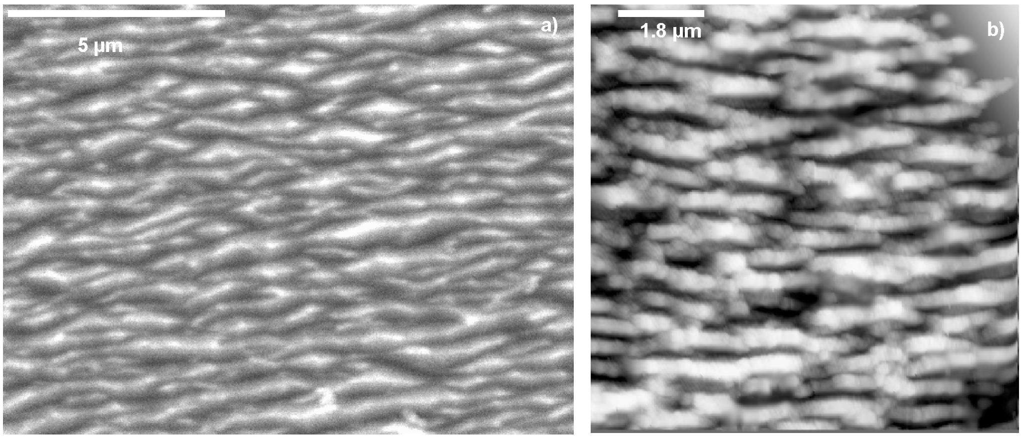

Fig. 1. Exemplary SEM (a) and AFM (b) images of a microrelief obtained by anisotropic chemical etching of the $In_{0.077}Ga_{0.923}As$/GaAs (structure A) surface

The surface morphology of the $In_xGa_{1-x}As$ epilayers was characterized by atomic force microscopy (AFM). The etched samples were also studied by scanning electron microscopy (SEM). Additionally, transmission electron microscopy (TEM) has been exploited to reveal the network of misfit dislocations at the heterostructure interface and the probable presence of threading dislocations in the epitaxial layer.

3. Results and discussion

3.1. Distribution of misfit dislocations and surface morphology

The distribution of misfit dislocations was obtained by the TEM method which allows a direct imaging of individual dislocations. In Figure 2, the cross-sectional TEM images of the both heterostructures are presented. In these images, one can see a clearly outlined interface between the epitaxial layer and the substrate, including a periodic array of misfit dislocations with an average spacing of 50 nm. However, no threading dislocations were observed in the heteroepitaxial layers, what means that the epilayer included less than 10^7 cm^{-2} of threading dislocations. Furthermore, an exemplary planar view TEM image of the $In_{0,086}Ga_{0,914}As$/GaAs heterostructure interface (structure B), shown in Fig. 3, revealed a regular 2D network of 60° misfit dislocations oriented in two orthogonal ⟨110⟩ crystallographic directions at the (001) interface, with a linear density of about 10^5 cm^{-1}.

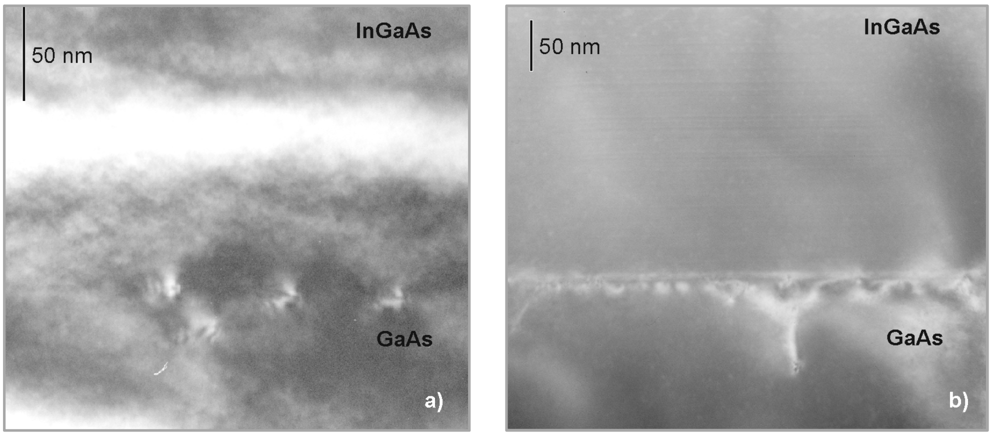

Fig. 2. TEM bright-field images showing the cross-sectional views of $In_xGa_{1-x}As$/GaAs heterostructures: a) structure A with $x = 0.077$, b) structure B with $x = 0.086$

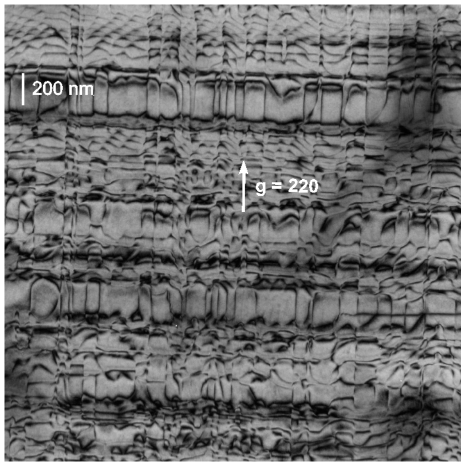

Fig. 3. An exemplary TEM image showing a network of misfit dislocation at the interface plane of the $In_{0.086}Ga_{0.914}As$/GaAs heterostructures (structure B)

A detailed analysis of the planar view image (Fig. 3) showed that about 38% more misfit dislocations running along [$\bar{1}$10] (α-type dislocations) were detected as compared to those along perpendicular [110] direction (β-type dislocation). It is in good agreement with the previous results [8–10] but it contradicts the recent results by Yastrubchak et al. [11]. The difference can be explained by the use of p-doped layers investigated by the authors [11], in which the glide velocity of β-type dislocations is higher than that of α-type ones, in contrast to the undoped or n-type doped GaAs -based heterostructures, used in this communication, where the α-type dislocations have a higher glide velocity in comparison to that of β-type ones [6, 7].

The studies of surface morphology have also been performed for all investigated heterostructures by atomic force microscopy (AFM), prior to chemical etching. The most pronounced surface morphology was observed for the structure B with $x = 0.086$, showing a well-defined cross-hatch pattern in the form of ridges and grooves oriented along two perpendicular $\langle 110\rangle$ directions on the (001) epitaxial layer surface (Fig. 4).

The average peak-to-peak spacings between the ridges along the $[\bar{1}10]$ direction were equal to 2.1 μm and those along [110] – 3.2 μm. The undulations were equal to about 2 nm peak-to-valley amplitude. As was mentioned earlier, such a cross-hatch morphology is often observed in many semiconductor heterostructures with a lattice mismatch, such as SiGe/Si, InGaAs/GaAs, and other III–V semiconductor systems [11, 14–20], grown on (001)-oriented or slightly misoriented substrates. It is widely accepted that a cross-hatch pattern reproduces a network of underlying interfacial misfit dislocations, as a consequence of their local strain fields. A direct comparison of misfit dislocation distribution obtained by TEM with the results of AFM has confirmed these findings. A linear density of misfit dislocations estimated from AFM measurements of surface undulations was equal to about 10^4 cm^{-1} but we observed about 37% higher density of α misfit dislocations, running along $[\bar{1}10]$ direction, than β misfit dislocations along [110] direction.

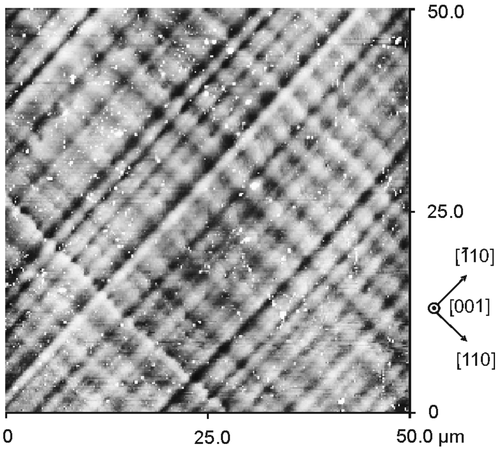

Fig. 4. AFM image (50×50 μm^2) of the $In_{0.086}Ga_{0.914}As$/GaAs (structure C) surface morphology showing a well defined cross-hatch pattern

One can notice that the distribution of misfit dislocations at the interface, obtained by the analysis of a planar view TEM image, exhibits the same asymmetry. These results can prove almost one-to-one correspondence between the arrangement of interfacial misfit dislocations obtained by TEM and the cross-hatch surface morphology, observed by AFM. However, it is worth noting that in this case, each undulation cannot be associated only with an individual misfit dislocation but with a bunch of few closely spaced dislocations, for which a superposition of strain fields can evoke a single undulation. A planar view TEM image (Fig. 3) showing a nonuniform distribution of misfit dislocations in each of the $\langle 110\rangle$ directions confirms these findings. It can explain a significantly lower density (about one order of magnitude) of misfit dislocations estimated from AFM observations in comparison to TEM. This is in agreement with the model proposed by Andrews et al. [21-23]. In this model, the formation of a single undulation requires a contribution of a group of misfit dislocations gliding on different slip planes. In contrast, higher [17] or the same [11] densities of misfit dislocations with reference to their real densities observed by TEM sometimes can be obtained by means of AFM. Nevertheless, the AFM technique can be still an effective tool for measuring the asymmetric formation of misfit dislocations at the interface of the partially relaxed epitaxial layers with a small lattice mismatch and small thicknesses, just above the critical value, but the estimation of the dislocation density can be incorrect.

3.2. Anisotropic misfit strain relaxation

The anisotropy of misfit strain relaxation in partially relaxed $In_xGa_{1-x}As/GaAs$ heterostructures has been investigated by means of XRD by recording and analyzing 2D reciprocal lattice maps (RLMs) for (224) asymmetrical reflections. The measurements were performed at room temperature, with the sample oriented either in $[\bar{1}10]$ or $[110]$ crystallographic directions perpendicular to the X-ray diffraction plane [26].

Figure 5 shows asymmetrical (224) RLMs obtained for the structures A and B. The horizontal axis corresponds to the reciprocal lattice vector in the diffraction plane, parallel to the surface of the heterostructure, either along $[\bar{1}10]$ or the $[110]$ crystallographic direction while the vertical axis corresponds to the reciprocal lattice vector perpendicular to the surface, i.e. along $[001]$ direction. From the sizes and positions of reciprocal lattice peaks one can get information on crystal imperfections, like point defects and dislocations as well as changes of lattice parameters of the epilayer unit cell due to strain relaxation.

The vertical and diagonal dotted lines denote the RLM peak positions expected for the case of fully strained (pseudomorphic) and fully relaxed layers, respectively. The RLM peaks located at the intersection of both lines correspond to the GaAs substrates while the other distinctly scattered peaks correspond to individual $In_xGa_{1-x}As$ epilayers. In Figure 5, the epilayer RLM peaks for all investigated heterostructures are located between these two lines. This means that all the structures are partially relaxed, and, moreover, this relaxation is strongly anisotropic, being larger along the $[110]$ direction than along the $[\bar{1}10]$ direction. These findings confirm the results obtained by TEM and AFM, and discussed in the previous subsection. A higher misfit strain relaxation observed along the $[110]$ direction is in agreement with a higher density of α misfit dislocations running in the $[\bar{1}10]$ direction at the interface and causing a larger relaxation of the layers along the perpendicular direction. The structure A exhibits a smaller strain relaxation. It is almost fully strained along $[\bar{1}10]$ direction but partially relaxed along the $[110]$ direction. This feature can explain the fact that we did not manage to detect any distinct cross-hatch pattern on the surface of this structure. On the other hand, the structure B exhibits a larger strain relaxation in both ⟨110⟩ directions, therefore the cross-hatch surface morphology is clearly visible (Fig. 4) for this structure.

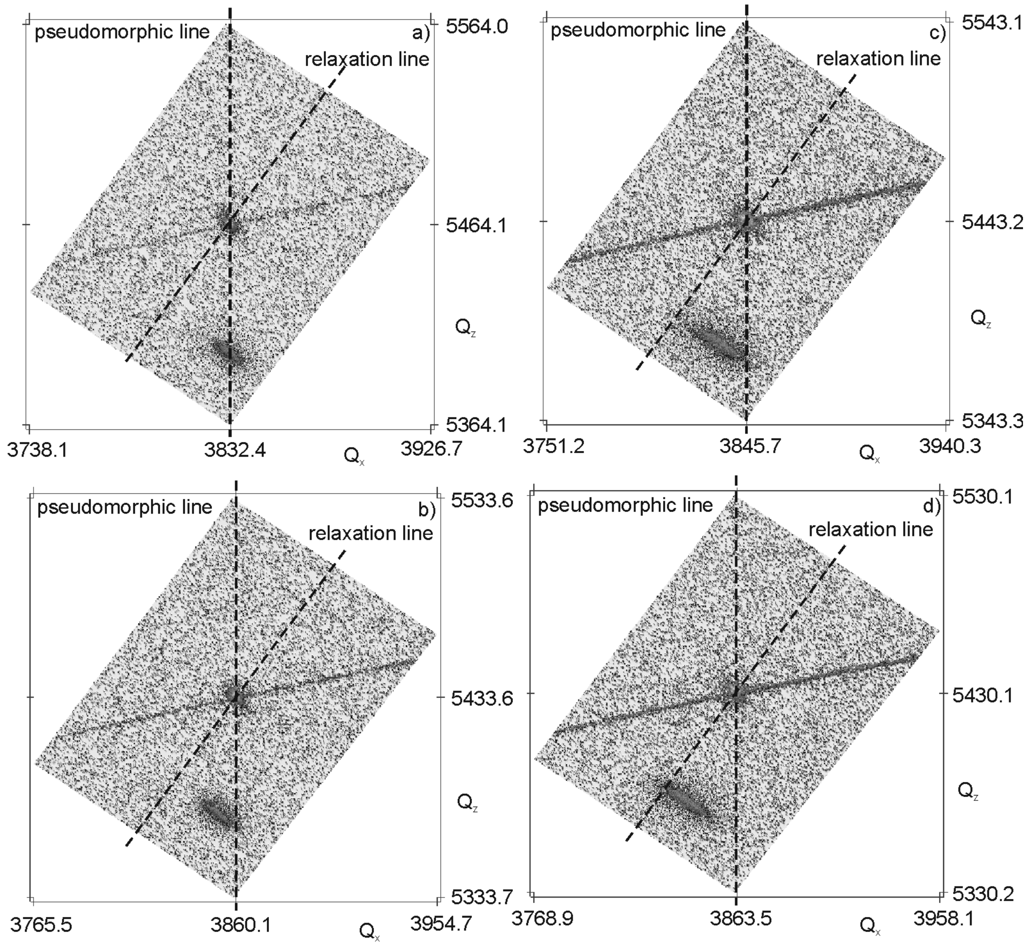

Fig. 5. The RLMs for the asymmetric (224) reflection of the $In_xGa_{1-x}As/GaAs$ heterostructures: a, b) structure A with $x = 0.077$, c, d) structure B with $x = 0.086$. The vertical axis is in the $[001]$ direction and the horizontal axis is either along $[\bar{1}10]$ (a, c) or $[110]$ (b, d) crystallographic directions. The RLM units are in $\lambda/2d$, where $\lambda = 1.540597$ Å and d is the lattice spacing of (224) planes

4. Conclusions

TEM, AFM and XRD techniques have been successfully employed for studying both anisotropic strain relaxation and surface morphology, related to the asymmetry in the formation of interfacial misfit dislocations of the partially relaxed $In_xGa_{1-x}As/GaAs$ heterostructures with a small lattice mismatch and grown by MOVPE. TEM investigations revealed a regular network of 60° misfit dislocations of α and β type, running along two orthogonal $\langle 110 \rangle$ crystallographic directions at the (001) interface of the heterostructure. This network was also reproduced on the surface, as a well-defined cross-hatch pattern, observed by AFM. A distinct anisotropy of strain relaxation along two orthogonal $\langle 110 \rangle$ directions in the (001) plane has been detected by means of XRD investigations. It was in good agreement with the asymmetry observed in the formation of interfacial misfit dislocations. A higher glide velocity of α dislocations along $[\bar{1}10]$ direction in undoped InGaAs epitaxial layers resulted in a higher density of misfit dislocations of this type in the $[\bar{1}10]$ direction and a larger misfit strain relaxation in these layers along the perpendicular $[110]$ direction.

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