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Effect of graded buffer design on the defect structure in InGaAs/GaAs (111)B heterostructures

M. Gutiérrez [a], D. González [a], G. Aragón [a], M. Hopkinson [b,*], R. García [a]

[a] *Dpto. de Ciencia, de los Materiales e. Ingeniería Metalúrgica y Química Inorgánica, Universidad de Cádiz. Apdo. 40, Puerto Real, 11510 Cádiz, Spain*

[b] *Department of Electronic and Electric Engineering, University of Sheffield, Mappin Street, Sheffield S1 3JD, UK*

Abstract

In this work, the defective structure of InGaAs/GaAs (111)B has been studied, using different types of substrate misorientation and incorporating different types of graded buffer layers. The formation of deformation twins has been observed to be independent of misorientation direction, but with a distribution dependent on the substrate misorientation angle. Samples grown on 2° misoriented substrates showed long twins with the majority of them formed with only one {111} variant. The use of a step-graded structure achieved a threading dislocation (TD) density improvement, although it was not able to alter the density of plastic relaxation occurring through twins. Twin nucleation occurred at the surface, being controlled by the superficial step density and not by the relaxation sequence of the structure. In the perpendicular direction to the off-cut, the linearly graded layer structures showed a higher twin density and no misfit dislocations (MD) were observed. A diffraction pattern study indicated an epilayer tilt in the off-cut direction with respect to the substrate. This additional tilt, probably due to the introduction of dislocations with a preferential Burgers vector, produced a superficial step density increase and, therefore, strain relief occurred by twins in preference to MDs.

Keywords: InGaAs/GaAs (111)B; Transmission electron microscopy; Deformation twin; Step-graded buffer

1. Introduction

Bandgap engineering has been extensively used in InGaAs/GaAs heterostructures for high-speed optoelectronic device fabrication. Over the last few years, InGaAs/GaAs epilayers on the non-standard (111) substrate orientation have received great attention due to the possibility of using the internal piezoelectric field [1]. In addition, the use of pseudomorphic strained layers along directions other than (001) has the possible benefit of a larger critical layer thickness (CLT) for plastic relaxation. The 1.0–1.1 μm range for laser industrial applications can be covered by InGaAs/GaAs (111) heterostructures, which offer in addition a high efficiency, a low threshold current and tunability [2,3].

To obtain high quality InGaAs/GaAs (111) structures, two important problems must be overcome. Firstly, lattice defect formation due to misfit and secondly the poor quality of the surfaces. Until recent growth improvements, the occurrence of pyramidal shaped defects in structures grown on GaAs (111)B substrates was habitual [4,5]. The use of misoriented substrates and improved growth conditions has now allowed excellent surface quality to be achieved using conventional MBE [6]. In relation to lattice defects, very little bibliography exists regarding InGaAs/GaAs (111)B structures and, in addition, the results that are published often seem contradictory. The use of different substrate types; misoriented or not misoriented, as well as a wide variety of growth conditions, could explain this fact.

Initial studies by Mitchell and Unan [7], on $In_{0.1}Ga_{0.9}As$/GaAs superlattices grown on nominal (111) substrates, observed that plastic relaxation took place by means of a triangular misfit dislocation (MD) network along the $\langle 1\bar{1}0 \rangle$ directions with an isotropic distribution. Subsequently, Sacedón et al [8], using substrates misoriented 1° towards the $[\bar{2}11]$ direction, also reported a triangular MD network, but in this case, the

* Corresponding author.

E-mail address: marina.gutierrez@uca.es (M. Gutiérrez).

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distribution at the interface was very irregular. Large differences in the plastic relaxation percentage were shown, depending on the sample area studied. More recently, Edirishinge et al [9], carried out by transmission electron microscopy (TEM), study of single layers grown on substrates misoriented 2° towards $[2\bar{1}\bar{1}]$ and concluded that the samples presented two kinds of relaxation mechanisms. The first by the triangular network formation, as described earlier and a second one by deformation twin formation. In both cases, the defect distribution was strongly anisotropic. According to Edirishinge et al. [9], the particular substrate misorientation used in this case could be the explanation for the twin nucleation, as well as for the anisotropic defect distribution. Moreover, they observed that both the twin and dislocation densities increased with In content and layer thickness for the InGaAs/GaAs (111)B single epilayers.

The goal of this contribution is a defect distribution study using different InGaAs graded buffer structures on GaAs (111)B substrates. Layers with graded composition have been shown to be a good tool for the reduction of threading dislocations (TD) in InGaAs/GaAs (001) heterostructures [10,11]. However, a systematic study of the graded composition effect does not exist, at present, for the other substrate orientations. To understand the formation of crystalline defects, it was necessary to establish design rules that allowed us to obtain buffer layers with high crystalline quality. We have then studied the substrate misorientation effect on the defect density in order to compare different buffer layer structure designs. Finally, step-graded and lineally graded epilayers were compared with a simple layer.

2. Experimental details

Three *pin* diode structures (A–C samples) were grown by MBE on different graded buffer structures (see Fig. 1). The *i*-region of the device structure consisted of 10 nm $In_{0.4}Ga_{0.6}As$ single quantum well, with 100 nm $In_{0.2}Ga_{0.8}As$ barriers either side. The n^+ region was formed by 300 nm $In_{0.2}Ga_{0.8}As$ doped with Si and the p^+ region by 300 nm of $In_{0.2}Ga_{0.8}As$ cap layer doped with Be. Electrical measurements on the *pin* device will be reported, elsewhere. The *pin* was grown on top of a buffer layer, which for the A and B samples consisted of three compositional steps, each with $\Delta x = 0.1$ and a layer thickness of 100 nm. These samples were grown on GaAs (111)B substrates misoriented 1 and 2° towards $[\bar{2}11]$ direction for the A and B sample, respectively. The C sample was similar to the B sample. It was grown on a substrate misoriented 2° towards the $[2\bar{1}\bar{1}]$ direction, but the buffer layer in this case consisted of a 100 nm linearly graded layer, where x varied between 0.0 and 0.3. Over this graded layer, an additional 100 nm layer with $x = 0.3$ constant composition was grown. To study the step number effect, three additional structures (D, E and F) were grown. Each of these structures had 500 nm of $In_{0.3}Ga_{0.7}As$ grown on different buffer structures. The D sample did not have buffer layer and it was used like reference, the E sample consisted of step-graded structure with two 200 nm steps and $\Delta x = 0.1$, and the F sample consisted of a step-graded structure with five 250 nm steps and $\Delta x = 0.05$. Samples D, E and F were grown on GaAs (111)B substrates misoriented 2° towards the $[2\bar{1}\bar{1}]$ direction.

The TEM study was achieved using a JEOL-1200 EX microscope. Sample preparation was carried out by mechanic thinning, followed by chemical etching (H_2SO_4–H_2O–H_2O_2 solution) for plan view observation (PVTEM) and by ion milling for cross sectional observation (XTEM).

3. Results and discussion

Deformation twin nucleation on GaAs (111)B has been associated with the use of substrates misoriented towards the $[2\bar{1}\bar{1}]$ direction [9]. However, the A and B samples, which were grown on substrates misoriented towards the $[\bar{2}11]$ direction, also revealed the presence of twins. However, there were distinct differences in the behaviour between them (see Fig. 2). In all the samples, the diffraction patterns were examined to check, if satellite spots due to twins were present. Sample A showed deformation twins distributed in the all three possible {111} variants. On the contrary, the twin distribution was anisotropic in sample B, with only one

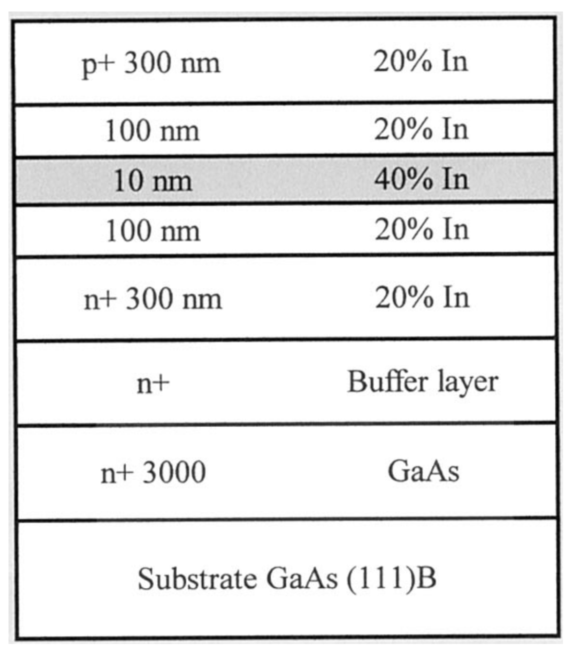

Fig. 1. Schematic diagram of the *pin* structure of samples A, B and C.

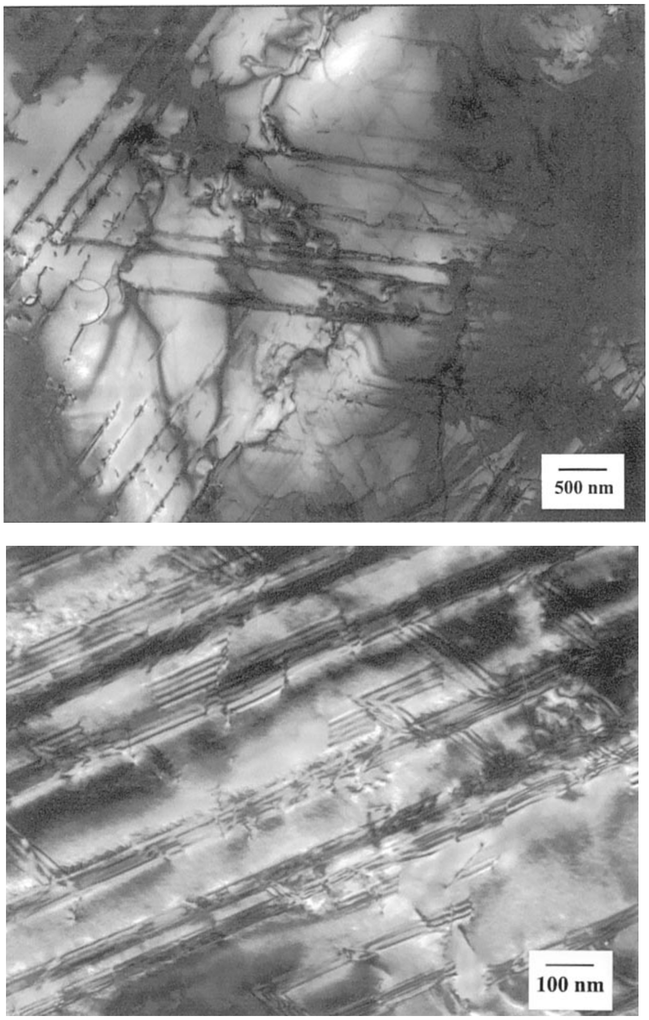

Fig. 2. Plan view micrograph (BF) with $g0\bar{2}2$ of sample A (a) and sample B (b).

twin variant favoured. In this case, large twins lying across the whole TEM area were observed. The other two variants had much smaller twins and these were observed to have a density almost one order of magnitude lower. In addition, the twin density observed on sample A was double (1×10^5 cm^{-1}) that of sample B. This fact motivated a study of the effect of the graded buffer layer design on defect density for the 2° misoriented substrate.

Fig. 3 shows a cross section micrograph of sample D using 220 bright field reflection. The $In_{0.3}Ga_{0.7}As$ layer shows both high TD and deformation twin densities. The deformation twins were present preferentially in one of the three possible {111} variants and had a density of 3×10^4 cm^{-1}. The average MD density at the interface was $2–3 \times 10^{-5}$ cm^{-1} comparable to that of Edirishinge et al [9]. In general, if the relaxation is near the saturated relaxation regime, a high increase of the TD density takes place [12].

In samples E and F, which have a buffer structure of two and five steps, respectively, the lattice misfit relaxation is carried out by steps to attempt modify the crystalline defect structure. For InGaAs/GaAs graded structures in the (001) orientation, a MD density profile proportional to the misfit gradient is observed [13]. As a consequence of this MD distribution along the epilayer, the upper layer of the graded structure is far from the saturated relaxation regime and has a lower MD density. Since the TD density has to be proportional to the MD density on the upper layer, a lower TD density was found at the surface on graded composition structures [10].

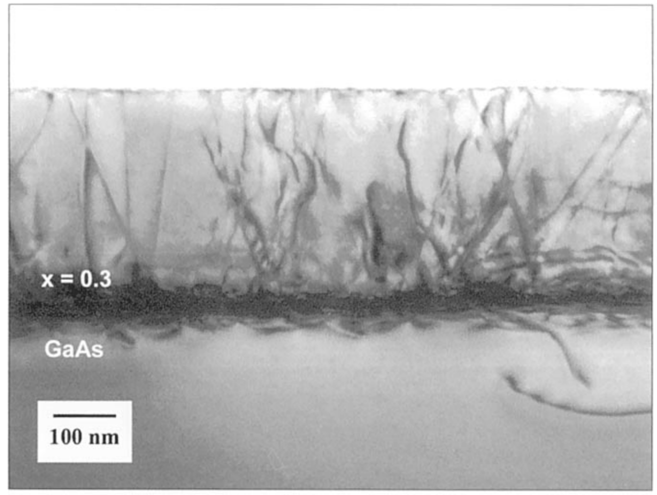

Fig. 3. Cross section micrograph (BF) with $g0\bar{2}2$ of sample D. The beam direction is $[0\bar{1}1]$.

Fig. 4 shows a cross-sectional (XTEM) micrograph using 220 bright field reflection of sample E. We can observe that the TD density that has arrived at the surface is much smaller by comparison to sample D, used as a reference. MD are distributed in the buffer structure at the buried layer interfaces and the upper interface is free of MD. The MD density on the buried

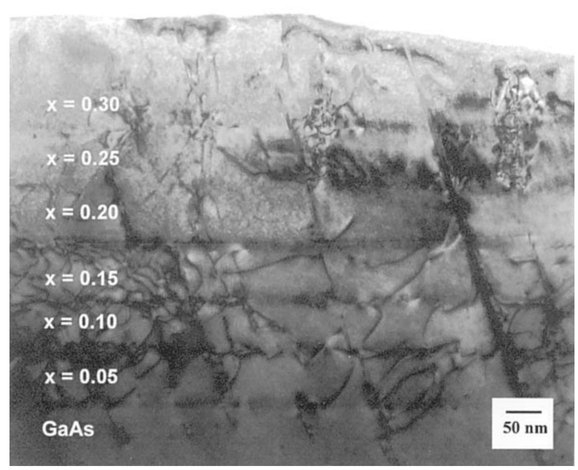

Fig. 4. Cross section micrograph (BF) from sample E with $g0\bar{2}2$. The beam direction is $[0\bar{1}1]$.

layers was 1.5×10^5 cm^{-1} for sample E and 4×10^4 cm^{-1} for sample F. The sum of the MD densities in whole structure was comparable to the reference sample D [9]. However, the TD density was lower by more than one order of magnitude compared with the single $In_{0.3}Ga_{0.7}As$/GaAs (111)B epilayer (sample D).

In step-graded structures, the relaxation first takes place in the buried layers during the growth [13] and we think the relaxation of a smaller lattice misfit should modify the deformation twin generation in some way. From [9], the twin density on the 150 nm $In_{0.3}Ga_{0.7}As$/GaAs (111)B single epilayer was 3×10^5 cm^{-1}. This result was one order of magnitude above that observed in the epilayer with an In content of $x = 0.1$ (2×10^4 cm^{-1}). Considering this, a deformation twin density of $2–3 \times 10^4$ cm^{-1} should be found on first $In_{0.1}Ga_{0.9}As$ layer of sample A (lattice misfit $f = 0.0071$). The growth of the second layer ($In_{0.2}Ga_{0.8}sAs$) will have occurred on top of an $In_{0.1}Ga_{0.9}As$ layer, in which plastic relaxation was close to the saturated regime. The lattice misfit of the $In_{0.2}Ga_{0.8}As$ layer that was grown over the practically relaxed $In_{0.1}Ga_{0.9}As$ layer should be close to $f = 0.0071$. If twin formation is proportional only to the lattice misfit, two possibilities would exist. In the first, new twins are generated with an average density of $2–3 \times 10^4$ cm^{-1} and their twin boundaries are located on the second interfaces. The total twin density at the surface is the sum of the twins coming from the first and second interface. In the second possibility, no twins are nucleated. The twins from the first interface experience an increase of the twin thickness as twins cross the different layers. Therefore, the twin density would have to be the same as a single layer with an In content equal to the first step. If the first possibility was true, the total twin density at the stepped structure surface should be around $6–9 \times 10^4$ cm^{-1} for a three-step sample. However, if the second possibility was true, the twin density would be $2–3 \times 10^4$ cm^{-1}, the same as for a single layer with $x = 0.1$. This effect would be much more evident in sample F, which contains six layers and the twin density in this case should be similar to a simple $In_{0.05}Ga_{0.95}As$/GaAs structure. In both cases, a reduction in the deformation twin density should be observed with regard to a $In_{0.3}Ga_{0.7}As$ single epilayer directly grown on GaAs (111)B (sample D).

Nevertheless, in samples D, E and F, the twins crossed the whole structure with the same density and with a dominant twin variant. Moreover, we can observe that most of twins are going into the substrate. This behaviour suggests that twins are nucleated at the surface and then grow downward towards the substrate, eventually going into it. According to the Pirouz model [14], twins are generated at surface steps by half loop partial dislocation nucleation. Therefore, the first half loop formation originated at a preferred step for the second half loop formation. In this way, the twin thickness increases whilst sufficient stress exists in the film.

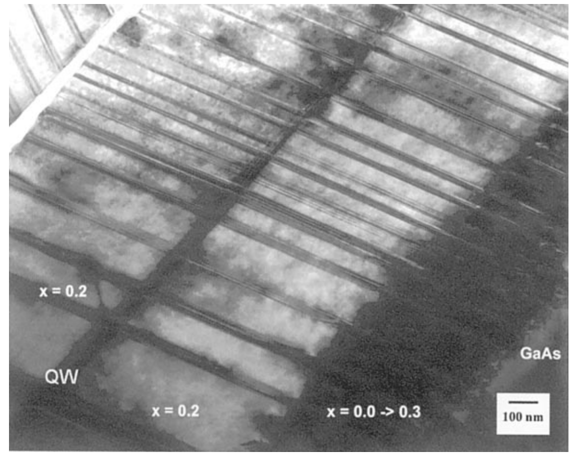

Fig. 5. Cross section micrograph (BF) from sample C with $g0\bar{2}2$. The beam direction is $[0\bar{1}1]$. We can observe an increase in the twin density but no MD are present.

We have observed that the twin density does not diminish by using graded buffer layers, which is contrary to our expectations if twin formation is proportional only to the lattice misfit. Although some twin boundaries were observed at different buffer layer interfaces, the greater part of them crossed whole structure towards the substrate. No change was observed in the twin thickness into different layers of the structure. The similar total MD density in all buffers samples also infers that the twin density did not change. Therefore, the stepped composition growth was not able to unbalance the competition between twin and MD relaxation. The proportion of plastic relaxation between twins and MD remained the same in all the layers. Although the improved MD distribution at different interfaces leads to a smaller TD density at the surface, the step-graded buffer structures did not improve the twin density with regard to the single layer.

From the results we have obtained it would be possible to think that the growth of graded composition structures could never modify the twin structure of InGaAs/GaAs (111)B epilayers. However, sample C showed a twin density one order of magnitude (2.1×10^5 cm^{-1}) higher than the rest of the samples studied (see Fig. 5). Moreover, MDs were not observed on this cross-sectional direction. Consequently, it was obvious that the linearly graduated layer growth had unbalanced the plastic relaxation of the structure, being in this case mainly by deformation twin formation. The sample also has a remarkable XTEM diffraction pattern rotation in relation to the other samples. The epilayer diffraction pattern showed a greater than 6° rotation in the off-cut substrate misorientation with regard to the substrate diffraction pattern. We think this epilayer inclination would produce a larger step density at the surface that, firstly, intensifies the twin formation and secondly, decreases the MD plastic relaxation.

The diffraction pattern rotation can be associated with epilayer tilt due to noncompensation of MD populations with different Burgers vector tilt components [15,16]. The tilt is due to the prevalence of one specific MD population that has the same Burger vector. It has been reported on graded layers that MD multiplication mechanisms are predominant and they generate large identical MD populations [17,18]. As a consequence, the tilt of the linearly graded structure with the same final composition was notably superior to the constant composition epilayer [19]. In sample C, the activation of the MD multiplication mechanism in the two $\langle 1\bar{1}0 \rangle$ directions where no twins were observed would explain the high tilt observed in the off-cut direction and, therefore, the increase in the twin density to the detriment of MD's. Further work is required to determine the properties of this tilt and its influence on twin formation.

In summary, the use of linearly graded buffer layers is effective in misoriented InGaAs/GaAs(111)B structures to eliminate threading dislocations (TD), but not twins. It is likely that the use of smaller substrate misorientations is required to obtain devices without any defects that cross the structure.

4. Conclusions

This work reveals that the use of oppositely misoriented substrate orientations does not modify the structure and formation of deformation twins considerably, but that they are modified by the change of the misorientation degree. Samples grown on 2° misoriented substrates showed a twin formation anisotropy, with large twins perpendicular to the off-cut direction. The comparison between different step-graded structures, grown on 2° misoriented substrates, shows there is no change in the plastic relaxation proportion between twin and MD. A TD density improvement is achieved, but a similar twin density is always obtained at the surface. This fact confirms that the twin formation depends mainly on the superficial step density and much less on the plastic relaxation sequence. However, on linearly graded structures in the $[01\bar{1}]$ direction, plastic relaxation only occurs through twins and not through MD. An epilayer tilt increase in the off-cut misorientation, probably due to the formation of a large MD population of the same Burgers vector, could explain this effect.

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