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The role of climb and glide in misfit relief of InGaAs/GaAs(111)B heterostructures

M. Herrera[a], M. Gutiérrez[a], D. González[a], G. Aragón[a], I. Izpura[b], M. Hopkinson[c,1], R. García

[a]Departamento de Ciencia de los Materiales e Ingeniería Metalúrgica y Química Inorgánica, Universidad de Cádiz, Apdo 40, Puerto Real, 11510 Cádiz, Spain
[b]Departamento de Ingeniería Electrónica, E.T.S.I. Telecomunicación, Universidad Politécnica de Madrid, Ciudad Universitaria s/n 28040 Madrid, Spain
[c]Department of Electronic and Electrical Engineering, University of Sheffield, Mappin Street, Sheffield S1 3JD, UK

Abstract

The plastic relaxation of InGaAs/GaAs(111)B quantum wells (QWs) is investigated. Critical layer thickness (CLT) models based on the theory of Matthews–Blakeslee have been applied, assuming that dislocations glide from the substrate. We have observed that when the In-content is above 0.25, a three-pointed star-shaped misfit dislocation (MD) configuration appears. A detailed analysis has shown that this configuration cannot originate from the glide of pre-existing dislocations. Instead, these MDs are generated by climb from an initial nucleus. A modified Matthews–Blakeslee model including an osmotic force component is proposed. The resulting revised CLT depends on the departure of the vacancy concentration from its equilibrium.

Keywords: Climb; Glide; Critical layer thickness; (111); InGaAs; Transmission electron microscopy; Molecular beam epitaxy

1. Introduction

There is considerable interest in GaAs-based optoelectronic components for optical fibre communication. InGaAs quantum well (QW) devices have already been successfully developed as pump lasers for rare earth-doped optical fibre amplifiers (0.98–1.02 μm). However, to access technologically important longer wavelengths a higher In-content is required. The critical layer thickness (CLT) for strain relaxation in InGaAs/GaAs(001) is rapidly exceeded for QW emission wavelength beyond 1 μm. However, a number of reports have suggested that InGaAs/GaAs(111)B strained layer epitaxy has the prospect of reaching a higher CLT than can be achieved for (001) substrates [1]. The higher CLT would allow for an increase in the In-content of strained QWs to access important wavelength ranges at, or beyond, 1.1 μm. The growth of InGaAs/GaAs(111)B has additional interest due to the possible device applications arising from the presence of a large piezoelectric field in such heterostructures [2].

We have studied the relaxation mechanism of InGaAs/GaAs(111)B QWs with relatively high In-content ($x > 0.25$). The existence of a new misfit dislocation (MD) configuration for such In-contents has been revealed by transmission electron microscopy (TEM) [3]. Plastic relaxation takes place through a polygonal network of MDs, which has its origin in a new MD source occurring through the formation of a three-pointed star-shaped configuration. The Burgers vectors of such a configuration are contained in the growth plane and this implies a higher misfit-relieving component than for the conventional 60° dislocation. The consequence of this is a reduction of the previous CLT estimates for high In-content InGaAs/GaAs(111)B QWs as has been previously reported [4].

These MDs which have in-plane Burgers vectors parallel to the growth plane can only develop a network when climb is also taking into account. By including an osmotic force component, a modified CLT can be derived which is the aim of this paper.

2. MD network in (001) and (111) GaAs substrates

Two types of MD networks are observed in InGaAs strained layers with In-contents below 0.2 on both (001) and (111)B GaAs substrates, respectively [5–7]. Both MD networks are similar and they are described as 60°-out MDs. The dislocation lines are along the, two or three, $\langle 110\rangle$ directions, reflecting the different crystal symmetry of the (001) and (111)B orientations, respectively. The Burgers vectors of these MDs are of the $1/2\langle 110\rangle$ type and are out of the growth plane. However, a different kind of MD network has been observed for $In_xGa_{1-x}As$/GaAs(111)B

[1] Present address: Marconi Optical Components, Caswell, Towcester, Northants NN12 8EQ, UK.

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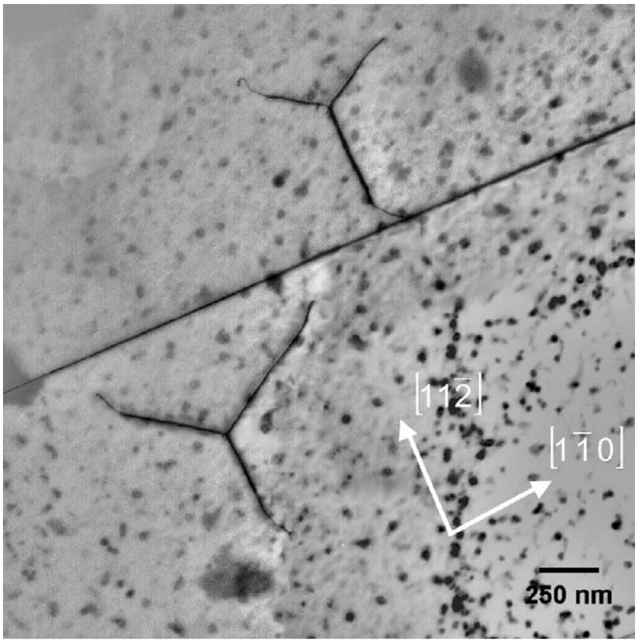

Fig. 1. Planar view 220 bright field TEM image showing a three-point star-shaped MD configuration in an InGaAs(111) QW with In-content 0.3 and thickness 10 nm.

heteroepitaxies with high In-contents ($x > 0.25$–0.30), as can be seen in Fig. 1 [3]. This new MD network has a three-pointed configuration and exhibits major differences compared to the previous dislocation type. In this case the MD lines lie parallel to the three $\langle 112 \rangle$ directions and although the Burgers vectors are also of the $1/2\langle 110 \rangle$ type, they are contained in the growth plane. These dislocations are described as 30°-in MDs and have a misfit-relieving component that is larger than the 60°-out type [3]. There is another large difference: the three-pointed star-shaped MD has arms of a finite length, while the classical MD arms have not. From a dislocation theory point of view, the three-pointed star-shaped MD has a glide plane within the growth plane, i.e. the (111) plane. As will be discussed in Section 3, this has major consequences for (111) strained layer heteroepitaxy.

In Fig. 2, Threading dislocations (TDs) in a cross sectional TEM image of an InGaAs(111)B QW sample sandwiched between two GaAs barriers are shown. From a $\mathbf{g}\cdot\mathbf{b}$ analysis, the TD arms have Burgers vectors of the $1/2\langle 110 \rangle$ type which are contained in the growth plane. These originate from three-pointed star-shaped MDs located at the QW interface [8]. In the same figure is shown a planar view TEM image of a double QW InGaAs(111)B sample with GaAs barriers. Three small isolated TD segments can be observed, which have a common origin at the InGaAs interface [9]. These images and other observations show that the three-pointed star-shaped dislocation configuration has three MD arms with each one ending with TD segments.

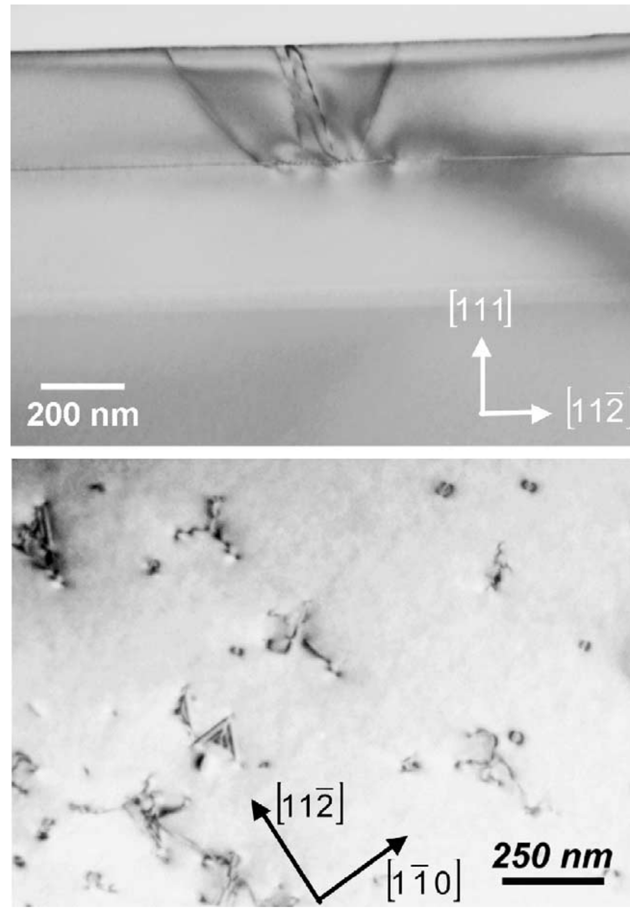

Fig. 2. (a) Cross sectional 220 bright field TEM image showing TDs in an InGaAs(111)B QW. A $\mathbf{g}\cdot\mathbf{b}$ analysis shows that the Burgers vectors are contained in the growth plane, the same Burgers vectors that for three-pointed star-shaped MDs. (b) Planar view 220 bright field TEM image of InGaAs(111)B double QWs. Three small TD segments are observed which originate from a common point.

3. Glide and climb force of 30° MDs

The three-pointed star-shaped dislocation configuration described earlier is undergone mechanical forces due to the lattice misfit stress of a strained layer. The force **F** per unit length of a dislocation is given by the Peach–Koehler equation:

$$\mathbf{F} = (\boldsymbol{\Sigma}\cdot\mathbf{b}) \times \mathbf{l} \tag{1}$$

where $\boldsymbol{\Sigma}$ is the lattice mismatch stress tensor, **b** the Burgers vector and **l** is the unit vector of the dislocation line. If **m** denotes the unit vector normal to the glide plane and **n** denotes the unit vector normal to **l** and lying in the glide plane, then the glide and climb components can be written as [10]:

$$\mathbf{F}_{\text{glide}} = [(\boldsymbol{\Sigma}\cdot\mathbf{b}) \times \mathbf{l}]\cdot\frac{\mathbf{l}\times(\mathbf{b}\times\mathbf{l})}{|\mathbf{b}\times\mathbf{l}|} = \boldsymbol{\Sigma}\cdot\mathbf{b}\cdot\mathbf{m} \tag{2}$$

$$\mathbf{F}_{\mathrm{climb}} = [(\boldsymbol{\Sigma}\cdot\mathbf{b})\times\mathbf{l}]\cdot\frac{(\mathbf{b}\times\mathbf{l})}{|\mathbf{b}\times\mathbf{l}|} = \boldsymbol{\Sigma}\cdot\mathbf{b}\cdot\mathbf{n} \tag{3}$$

For the (111) substrate orientation, the lattice mismatch stress tensor is taken as:

$$\boldsymbol{\Sigma} = Mf\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{4}$$

where M is the biaxial modulus and f is the lattice misfit. By applying Eqs. (2) and (3) to the (111) orientation and taking into account the fact that the Burgers vectors are contained in the (111) plane, it is calculated that the glide force is null and climb force is $1/2Mfb$ for the three-pointed star MDs. By extending Eqs. (2) and (3) to TDs coming from three-pointed star-shaped MDs, a null glide force and a value of $3/2Mfb$ for the climb force is obtained. This means that the three-pointed star-shaped dislocation configuration grows by climb and not by glide, i.e. 30° MD segments are developed by the climb movement of their TD arms. This would explain why a finite size is observed for isolated three-pointed star-shaped MDs.

4. The role of climb in CLT

Following the Matthews–Blakeslee formulation of CLT [11], for the case of dislocation climb the balance of forces can be written as:

$$\mathbf{F}_{\mathrm{line}} = \mathbf{F}_{\mathrm{climb}} + \mathbf{F}_{\mathrm{osmotic}} \tag{5}$$

where $\mathbf{F}_{\mathrm{line}}$ is the line tension of the MD [11], $\mathbf{F}_{\mathrm{climb}}$ is the mechanical force (the Peach–Koehler force given in Eq. (3)) and $\mathbf{F}_{\mathrm{osmotic}}$ is the osmotic force [12] on the moving dislocation. Eq. (5) can be written as:

$$\frac{Gb^2(1-\upsilon\cos^2\theta)}{4\pi(1-\nu)}\ln\left(\frac{\alpha h}{b}\right) = \left\{[(\boldsymbol{\Sigma}\cdot\mathbf{b})\times\mathrm{l}]\cdot\frac{(\mathbf{b}\times\mathbf{l})}{|\mathbf{b}\times\mathbf{l}|} \mp \frac{kT}{\Omega}\ln\left(\frac{c}{c^0}\right)(\mathbf{b}\times\mathbf{l})\cdot\frac{(\mathbf{b}\times\mathbf{l})}{|\mathbf{b}\times\mathbf{l}|}\right\}h \tag{6}$$

where G is the shear modulus, ν the Poisson ratio, θ the angle between Burgers vector and dislocation line, α the dislocation core, k the Boltzmann constant, Ω is the point defect volume and c and c^0 are the point defect concentrations during epitaxial growth and at equilibrium, respectively. The minus and plus signs are for vacancy and interstitial movement, respectively. Concerning G and ν, Anan's approximation [13] was used instead of Colson's one [14].

In the case of InGaAs/GaAs(111)B, InGaAs QWs on GaAs substrates are grown under compressive stress. This means an extra half plane of MDs and TDs is introduced, orientated towards the substrate. If TDs are absorbing vacancies, this implies that the extra half plane reduces its size. This is equivalent to the movement of TDs. A 30°-in MD increases its length when its corresponding TD arm moves by climb. This is the driving force for the growth of the three-point star-shaped MDs. Considering the stress tensor $\boldsymbol{\Sigma}$ (Eq. (4)), a Burgers vector $\mathbf{b}$ parallel to the growth plane and a dislocation line corresponding to the TD directions, Eq. (6) can be written as:

$$\frac{h}{b} = \frac{\mathrm{G}(1-\upsilon\cos^2\theta)\ln\left(\frac{\alpha h}{b}\right)}{4\pi(1-\upsilon)M\left[f - \frac{kT}{M\Omega}\ln\left(\frac{c}{c^0}\right)\right]\frac{\sqrt{3}}{2}} \tag{7}$$

The expression obtained for the (111) CLT is essentially the classical Matthews–Blakeslee one, but the main consequence of including climb is the apparition of an effective lattice mismatch given by:

$$f' = f - \frac{kT}{M\Omega}\ln\left(\frac{c}{c^0}\right) \tag{8}$$

This means that the climb of TDs due to excess vacancies during the epitaxial growth is equivalent to a MD with a misfit-relieving component equal to $\sqrt{3}/2$ in a strained layer with a modified lattice misfit equal to f'. The value of f' is dependent on the deviation of the vacancy concentration with respect to equilibrium.

The CLT due to climb, versus the In-content for InGaAs(111)B QWs for several vacancy deviations (c/c^0) is shown in Fig. 3 where M and G value of 55.28 and 200.19 GPa for an InGaAs alloy has been taken, respectively. The CLT due to glide of 30°-in MDs is also shown for comparison. As shown in Fig. 3, a vacancy deviation of between 10^2 and 10^3 has an important influence on the CLT for In-contents in the range 0.2–0.4. Another important consequence can be derived from Eq. (8): for a given vacancy deviation, there exists a critical In-content below which the CLT is not dominated by climb, but instead is due to the glide of 60°-out MDs:

$$x < x_{\mathrm{cr}}^{c/c^0} = \frac{\frac{kT}{M\Omega}}{0.071}\ln\left(\frac{c}{c^0}\right) \tag{9}$$

where $f = 0.071x$ has been taken (0.071 is the lattice mismatch between InAs and GaAs).

From previous experimental studies [3], we can make an estimation of the likely value for the vacancy deviation. For InGaAs(111)B QWs with an In-content of 0.3, the CLT is around 10 nm. This experimental CLT is in agreement with a value of c/c^0 equal to approximately 250 as can be seen in Fig. 3. In the same Fig. 3, a proposed CLT for InGaAs/GaAs(111)B QWs is added. There are two competing relaxation mechanisms: the glide of 60°-out dislocations and the climb of 30°-in ones. The former is dominant for In-contents below 0.3 and the latter is dominant for contents above 0.3.

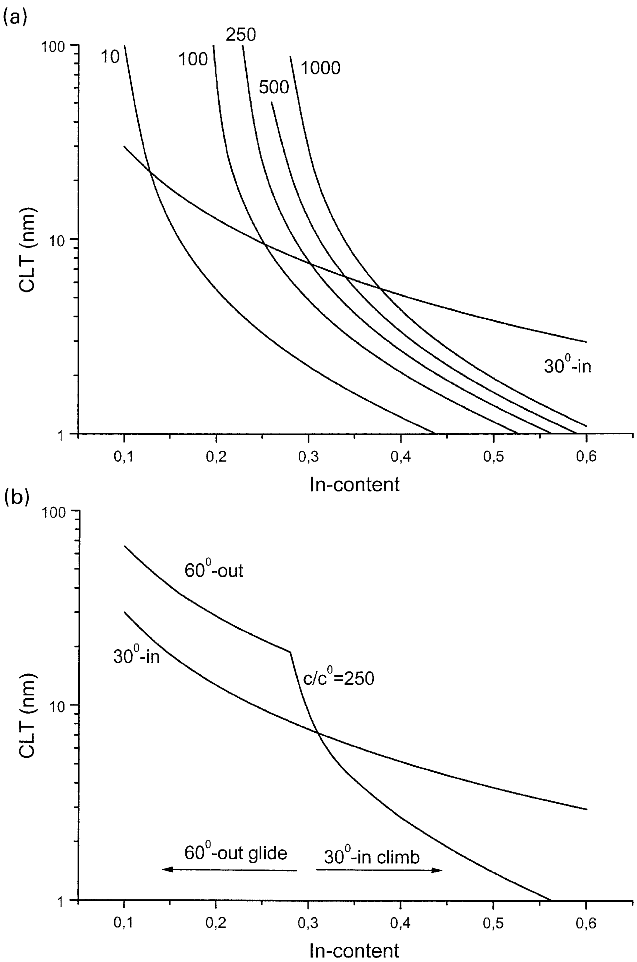

Fig. 3. (a) CLT due to climb for the three-pointed star-shaped MD for several vacancy deviations. (b) A representation of the InGaAs/GaAs(111)B CLT. The two dominant plastic relaxation mechanisms are shown. A value of 250 for the vacancy deviation has been assumed.

5. Discussion

In the last section, a CLT due to dislocation climb operating at relatively high In-content was introduced. A climb mechanism acts when a defect point deviation from equilibrium exists. When beam equivalent pressures of gases are calculated for the typical fluxes used in MBE, the growth occurs at a very large supersaturation, such that a marked deviation from equilibrium is to be expected [15]. Furthermore, a point defect concentration, which depends on the doping and stoichiometry of the growth conditions, has been proposed [16]. However, no reliable experimental data on point defect concentration for MBE growth are available [17]. At any case, note that at high growth temperatures, as vacancy concentrations exceeding 10^{18} cm^{-3} have been observed [17], while in As-rich, low temperature (200–350 °C) MBE, similar concentrations of Ga vacancies have been seen [18]. Due to the typically low arsenic overpressure used in MBE, the dominant point defects are As vacancies.

The concentration of vacancies can be written as:

$$c = c^0 \exp\left(-\frac{Q}{kT}\right) \tag{10}$$

where Q is the energy of vacancy formation. So, the vacancy concentration increases with the growth temperature. Furthermore, it has been also proposed that a compressive strain field in a strained layer such as InGaAs/GaAs(001) can lower the energy of vacancy formation [19]. This has the effect of increasing the vacancy concentration available for the climb to proceed.

The effect of impurities Si and Be on the creation of Ga vacancies in GaAs grown by MBE has been studied by positron annihilation [20]. A Ga vacancy concentration of $\sim 10^{19}$ cm^{-3} in Be-diffused GaAs and an equilibrium Ga vacancy concentration of $\sim 10^{17}$ cm^{-3} has been reported [20]. This implies a concentration deviation, c/c^0, $\sim 10^2$, a similar value to that estimated in the last section.

The concentration of vacancies in high quality MBE grown undoped GaAs (001) is expected to be low ($<10^{16}$ cm^{-3}). However, there exists, to our knowledge, no equivalent information on the typically vacancy concentrations in GaAs(111)B epitaxial layers. We may speculate that the use of relatively high As overpressures in the growth of the (111)B may give rise to an increased concentration of Ga vacancies compared to (001). In addition, we cannot rule out the role of doping in the InGaAs/GaAs(111)B samples we have studied. In these samples [3], the QW is within a p–i–n structure composed of Si-doped and Be-doped GaAs layers of 300 nm thickness and with a 2×10^{18} cm^{-3} doping level in each case. The TD arms of three-pointed star-shaped MD are located in the Be-doped GaAs layer. It is well known that there is a strong increase in the concentration of As vacancies (V_{As}^{+}) in the presence of oppositely charged acceptor atoms. In this case a migration of vacancies towards dislocations would be expected to occur. A high vacancy concentration intrinsic to the (111)B samples or a high vacancy concentration in the doped layers, or a combination of the two, might be expected to provide a mechanism whereby the three-point star-shaped MD grows by the climb of its TD arms.

6. Conclusion

Plastic relaxation of InGaAs/GaAs(111)B QWs is investigated for high In-contents. A Matthews–Blakeslee CLT model assuming the glide of pre-existing dislocations predicts a CLT larger than experimentally observed. A detailed Peach–Koehler force analysis of the three-pointed star-shaped MD configuration has revealed that this develops by climb during epitaxial growth due to a vacancy excess. A CLT based on Matthews–Blakeslee, but including an additional osmotic force component for InGaAs/GaAs(111)B QWs is derived. An explanation for the observed MD networks in InGaAs/GaAs(111)B QWs is proposed. One network ($x < 0.25$) is developed by the glide of 60°-out dislocations and another one ($x > 0.25$) occurs by the climb of 30°-in dislocations assisted by a vacancy supersaturation which is promoted by a high misfit stress level. Further studies are needed to determine the role of point defects in (111) epitaxial growth.

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