Dislocation distributions and tilts in Al(Ga)InAs reverse-graded layers grown on misorientated GaAs substrates*

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Compositionally undulating step-graded Al(Ga)In_xAs ($x = 0.05$–0.52) buffers with the following InP layer were grown by metal–organic chemical vapor deposition (MOCVD) on (001) GaAs with a 15° miscut. The dislocation distribution and tilts of the epilayers were examined using x-ray rocking curve and (004) reciprocal space maps (RSM) along two orthogonal ⟨110⟩ directions. The results suggested that such reverse-graded layers have different effects on α and β dislocations. A higher dislocation density was observed along the [110] direction and an epilayer tilt of $-1.43°$ was attained in the [1-10] direction when a reverse-graded layer strategy was employed. However, for conventional step-graded samples, the dislocation density is normally higher along the [1-10] direction.

Keywords: Al(Ga)InAs reverse-graded layers, dislocation distribution, tilt

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1. Introduction

InP has long been widely accepted as a common material for many important devices utilized in telecommunications and high-speed electronics.[1] GaAs is chosen to be used as the substrate material in this case due to the increasing availability of its large-sized wafers and rapid improvement of the processing technology, which means higher device yield and lower costs. To achieve high-performance devices, it is often required to combine the materials with different lattice constants. The metamorphic technique which provides a promising way to break the limitation of lattice constants on materials has gained increasing attention.[2] Various metamorphic buffers are often grown with the composition of the compound changing linearly[3] or by steps,[4] and the application of graded buffers helps to reduce the threading dislocation density (TDD) which could otherwise degrade the performance of the devices. Among the used metamorphic buffer materials,[5–7] the Al(Ga)InAs alloy system is found to be quite efficient in achieving high performance in optoelectronic devices. Such performance is similar to or even better than what can be achieved in native InP-based devices. So it is believed that the Al(Ga)InAs is an ideal material used between different subcells as the intermediate transition layer in multijunction solar cells based on GaAs[8,9] or Ge substrates[10] mainly due to its relatively large band gap. The large bandgap along with its broad-ranged obtainable refractive index gives much potential for development offuture optoelectronic devices. To obtain high quality Al(Ga)InAs buffers, it is necessary to investigate and understand the properties of dislocations formed during the strain–relaxation process. Our experiments present that the dislocation distributions and tilts in [110] and [1-10] directions of the compositionally undulating Al(Ga)InAs differ from those of the conventional step-graded samples, which are attributed to the different effects of the reverse-graded layer on α and β dislocations.

2. Experiment

The growth of the metamorphic Al(Ga)InAs buffers was performed in an AIXTRON-200/4 metal–organic chemical vapor deposition (MOCVD) system with a horizontal reactor. Trimethylgallium (TMGa), trimethylindium (TMIn), trimethylaluminum (TMAl), and arsine (AsH_3) were used as the precursors and ultra high purity hydrogen (H_2) was used as the carrier gas. Si-doped GaAs wafers were used as the substrates and were (001)-oriented with a surface orientation of 15° off toward (111)A. The growth pressure was carefully controlled at 100 mbar and the V/III ratio was controlled to be in the range between 65 and 80. Inside the growth chamber, a temperature of 700 °C was maintained and the corresponding growth rates were measured to be between 0.6 nm/s and 0.7 nm/s. The band gap of the Al(Ga)InAs buffers was kept at about 1.5 eV by adjusting the Al, Ga, and In compositions.

Two types of structures were grown: (i) one with compositionally undulating step-graded buffers (sample A), and (ii) the other with conventional step-graded buffers (sample B). In sample A, a GaAs layer with 100 nm thickness was

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deposited first to smooth the surface, then a ten-layered metamorphic Al(Ga)InAs buffer of 180 nm with In composition step-graded from 0.05 to 0.52 was also deposited, followed by a 400-nm-thick $Al_{0.48}In_{0.52}As$ layer, and finally a 500-nm-thick InP cap layer was grown to cap this $Al_{0.48}In_{0.52}As$ buffer. A tensiled-strained Al(Ga)InAs reverse-graded layer of 100 nm thickness was inserted between the two adjacent step-graded buffers of which the reverse-strain was half of the preceding layer. Sample B was prepared in the same way and had the same total thickness as sample A, except that no reverse-graded Al(Ga)InAs intermediate layer was used and each of the Al(Ga)InAs layer was 280 nm thick instead. The schematic diagrams of the two samples have been given in Ref. [11].

The samples were analyzed by a high resolution x-ray diffractometer (HRXRD) that contains a 2 kW sealed x-ray tube of which the wavelength is 0.154 nm (Cu $K\alpha 1$). All the samples were mounted on a sample holder with 4 axes and each axis was controlled by a stepper motor. The full width at half maximum (FWHM) of the x-ray rocking curve (XRC) was measured to estimate the TDDs of the InP layer, and the tilts of the epilayers with respect to the substrate were characterized by the symmetric (004) reciprocal space mappings (RSMs).

3. Results and discussion

In III–V lattice-mismatched heteroepitaxy, eight dislocation slip systems can be activated and the metamorphic Al(Ga)InAs buffers relieve their strain mostly by formatting a misfit dislocation of $a/2\langle 110\rangle\{111\}$.[12] The burgers vectors of $a/2\langle 101\rangle$-type dislocations do not sit perfectly on their [110] or [1-10] line direction but are leaning off towards the [001] direction. These burgers vectors can be resolved into three parts, i.e., an edge component, a screw component both in $\langle 110\rangle$, and another tilt component in $\langle 001\rangle$. Ideally, if the nucleation of these dislocations on these slip systems is sufficiently random and isotropic, these components will cancel out and produce no net tilt. Otherwise, the surface normal of the epilayer will tilt away from [001]. Two types of 60° dislocations exist, i.e., [1-10] α and [110] β dislocations, both exist at compressively stressed interfaces, presumably with Ga- and As- as their dislocation cores, respectively. The difference in the core structures of α and β dislocations leads to a significant difference in their activation energy for nucleation, as well as for their movements, as shown in Table 1. Several research studies on n-type InGaAs grown on misoriented GaAs substrate have shown a higher density of β than α misfit dislocation.[13–15]

Table 1. The slip systems for 60° dislocations in III–V compressively strained zinc blende semiconductors.

Slip system	Line direction	Burgers vector	$\boldsymbol{b}_{\text{misfit}}$	$\boldsymbol{b}_{\text{screw}}$	$\boldsymbol{b}_{\text{tilt}}$	Slip plane	Dislocation type
1	[1-10]	$a/2$[01-1]	$a/4$[110]	$a/4$[-110]	$a/2$[00-1]	(111)	α
2	[1-10]	$a/2$[10-1]	$a/4$[110]	$a/4$[1-10]	$a/2$[00-1]	(111)	α
3	[1-10]	$a/2$[101]	$a/4$[110]	$a/4$[1-10]	$a/2$[001]	(-1-11)	α
4	[1-10]	$a/2$[011]	$a/4$[110]	$a/4$[-110]	$a/2$[001]	(-1-11)	α
5	[110]	$a/2$[011]	$a/4$[-110]	$a/4$[110]	$a/2$[001]	(1-11)	β
6	[110]	$a/2$[-101]	$a/4$[-110]	$a/4$[-1-10]	$a/2$[001]	(1-11)	β
7	[110]	$a/2$[-10-1]	$a/4$[-110]	$a/4$[-1-10]	$a/2$[00-1]	(-111)	β
8	[110]	$a/2$[01-1]	$a/4$[-110]	$a/4$[110]	$a/2$[00-1]	(-111)	β

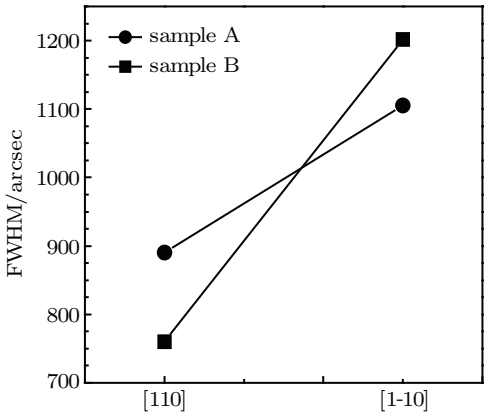


Fig. 1. FWHMs of the symmetric (004) rocking curves of samples A and B with the incident x-ray beam along the [110] and [1-10] directions.

In our experiments, the FWHMs of the symmetric (004) XRC for InP/Al(Ga)InAs buffers were measured using the x-ray incident along the two $\langle 110\rangle$ directions. Broadening of the FWHM corresponding to the x-ray beam along the [110] and [1-10] directions is observed, which is mainly induced by α and β dislocations, respectively.[16] Figure 1 shows that the FWHMs of (004) XRCs of sample A are larger than those of sample B in the [110] direction, while an opposite tendency is observed in the perpendicular direction. These results suggest that the α dislocation density in sample A is higher than that in sample B, while the β dislocation distribution has an opposite tendency in the two samples.

Since the substrate miscuts toward (111)A, α dislocations tend to be formed all along the [1-10] directions, being parallel to each other; while β dislocations do not, those on (1-11) planes tend to cross those on (-111).[17] Parallel dislocations can act as a long wall of stress field, blocking the movement of other dislocations, but nonparallel dislocations do not have

this behavior. So α dislocations at the interface can effectively hinder the gliding of β dislocations, while β dislocations have no significant effect on α dislocations. Since the line direction of α dislocation rotates 90° when the stress state changes from compression to tension, the major axis of relaxation will rotate accordingly and the reverse-graded layers with tensile strain slow α dislocation glide due to the block effect of β dislocations. Under this case, an energetically favorable way to relief strain is in the form of α threading dislocations, which leads to higher α TDDs in sample A, while the Al(Ga)InAs reverse-graded layers exert an inverse impact on β dislocations, which promotes the β dislocation to glide in the interface to reduce β TDDs.

Figures 2 and 3 show the typical (004) RSM pictures of samples A and B along the [110] and [1-10] directions, respectively. In the RSM pictures, the tilt angle θ can be calculated by $\tan(\theta) = |\Delta Q_x|/\left(4/a_{\text{sub}} + Q_{\text{cap}} - Q_{\text{sub}}\right)$,[18] where ΔQ_x is the peak splitting between the epilayer and the substrate, a_{sub} is the substrate lattice constant, and Q_{cap} and Q_{sub} are 6.92 nm^{-1} and 7.08 nm^{-1} in Q_z, respectively. As shown in Fig. 2, the tilt of the InP cap layer in sample A along the [110] direction is calculated to be +0.67°, and the InP tilt with respect to the substrate is +1.22° in sample B, which is larger than that in sample A, where "+" represents that the tilt is in the direction to the miscut with the substrate.

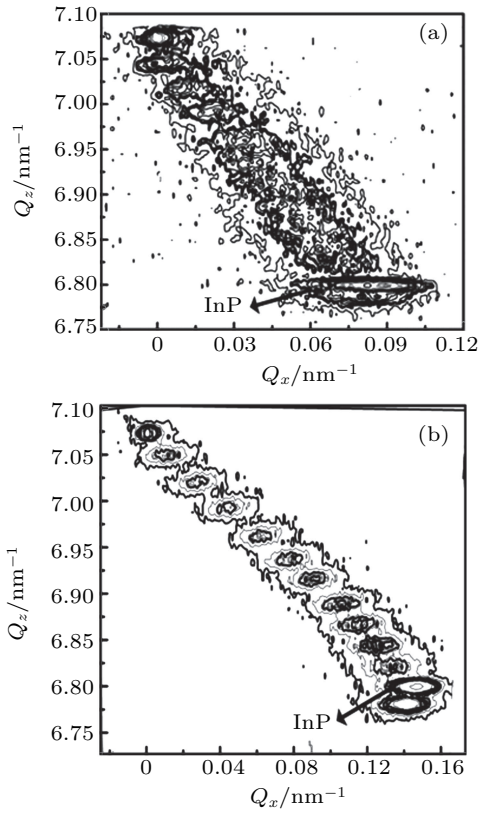


Fig. 2. Symmetric (004) RSM of (a) sample A and (b) sample B with projection of the incident beam on (001) surface along the [110] direction.

It is proposed that there are two possible mechanisms for this tilt in the epilayer. The first one is due to the surface steps formed as a result of the substrate miscut, the second one is due to the formation of an array of dislocations whose tilt components all point perpendicularly toward the interface. The size of such tilt of InP layer grown on 15°-miscut substrate is predicted to be 0.58° using Nagai's model. This model bases purely on the size of the substrate miscut,[19] our experimental value, however, gives a higher value than this prediction. Therefore, it is believed that the second mechanism proposed is the predominant factor causing such tilt.

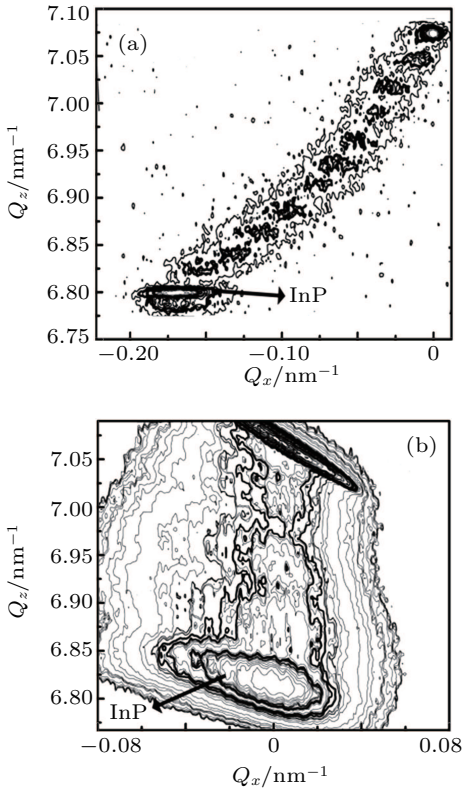


Fig. 3. Symmetric (004) RSM of (a) sample A and (b) sample B with projection of the incident beam on (001) surface along the [1-10] direction.

When the substrate surface normal is misorientated toward (111)A, the miscut changes the effective misfit Burgers vector of α dislocations and the resolved shear stress (RSS) which is expected to dominate both the nucleation and glide processes on (111) and (-1-11) slip planes. The activation energy for dislocation nucleation is inversely proportional to the RSS, while the dislocation glide velocity is directly proportional to the RSS.[11] The tilts along [110] in epilayers of the two samples, as shown in Fig. 2, suggest that the four different 60° $a/2\langle 110\rangle$ $\{111\}$ slip systems of α dislocations are not equally activated during the strain relaxation process of Al(Ga)InAs metamorphic buffers.

Based on the nucleation-limited model by LeGoues,[20] in which neither dislocation–dislocation interaction nor multiplication are taken into account, the tilt angle θ can be related

to the number of α dislocations as shown below:

$$\frac{N_{\alpha(111)}}{N_{\alpha-\text{total}}} = \frac{1}{2}\left(1 + \frac{b_{\text{misfit}}}{b_{\text{tilt}}}\frac{\tan\theta}{\varepsilon}\right), \quad (1)$$

where ε represents the relieved strain, which is found to be 3.8%, $N_{\alpha(111)}$ is the number of α dislocations in the (111) slip planes, $N_{\alpha-\text{total}}$ is the total number of α dislocations in both (111) and (-1-11) slip planes, and $b_{\text{tilt}} = a_e/2$ and $b_{\text{misfit}} = a_e\sqrt{2}/4$ are the Burgers vector of misfit dislocations and threading dislocations, respectively. Calculating from Eq. (1), roughly 60.8% of α dislocations are on the (111) slip planes in sample A, while 69.8% of α dislocations are on the (111) slip planes in sample B, which means that the tilt is quite sensitive to the metamorphic buffer structure. α dislocations in the (111) slip planes typically require lower energy for nucleation but experience higher force during gliding compared with those in the (-1-11) plane.[14,21] Another tilt is found along the [110] direction, which is the result of the imbalance in the dislocation density between the (111) and (-1-11) planes. However, for sample A, the tilt has a smaller size of 0.67° compared to 1.22° of sample B, primarily attributed to the Al(Ga)InAs reverse-graded layers with tensile strain. The Al(Ga)InAs reverse-graded layers as discussed above slow α dislocation glide, and the effect on α dislocations in the (111) planes which experience higher glide force is obvious. During the strain relaxation process, α dislocations in the (111) planes are first generated at the step edges. Eventually, by gliding, the total net tilt component of α dislocations in sample A are brought down.

In the case of Al(Ga)InAs multilayers grown on GaAs substrates with misorientation toward (111)A, no tilt is observed in the [1-10] direction. However, a large tilt of $-1.43°$ inverse direction to the substrate miscut is obtained in the [1-10] direction in sample A as shown in Fig. 3(a). In contrast, the (004) plane of sample B only tilts by $< 0.1°$ in the [1-10] direction, which is almost parallel to the substrate. It seems that the Al(Ga)InAs reverse-graded layers decrease the nucleation activation energy of β dislocations with tilt along [00-1] in (-111) slip planes and more β dislocations generate in the (-111) slip planes than the (1-11) slip planes. The total tilt components could not be canceled out and a negative tilt is generated in the [1-10] direction to relax the strain. In Fig. 3(b), the mosaic spread of sample B is seen in the Q_z direction associated with the GaAs substrate through the Al(Ga)InAs step-graded buffers, which is correlated with more β dislocations than those in sample A[21] and the results of RSM and the FWHM of (004) XRCs are in good agreement.

4. Conclusion

InP/Al(Ga)InAs buffers with reverse-graded buffers were grown by MOCVD on GaAs substrates with 15° miscut toward (111)A. The effects of the reverse-graded layers on the anisotropic properties of dislocation density and tilts of metamorphic have been investigated. In the [110] direction, the reverse-graded layers tend to relieve the strain in the form of α TDDs and promote α dislocations to uniformly distribute in (111) and (-1-11) slip planes to reduce the epilayer tilt. In contrast, the elastic strain is relieved not only through misfit dislocations in the reverse-graded buffers, but also through the lattice tilting and eventually reduces β TDDs in the [1-10] direction.

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