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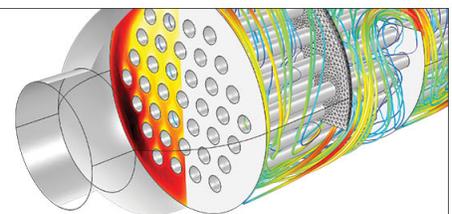
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Incoherent interface of InAs grown directly on GaP(001)

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We report molecular beam epitaxial growth of InAs on GaP(001), which has the largest lattice mismatch (11%) among all the arsenides and phosphides. Reflection high-energy electron diffraction and high-resolution transmission electron microscopy were used to optimize the growth and characterize the epilayer. It is found that the growth mode can be controlled by the surface V/III ratio: three-dimensional and two-dimensional layer-by-layer growths under As-stable and In-stable conditions, respectively. In both cases, a regular network of pure edge-type (90°) misfit dislocations with a spacing of 4 nm was formed directly at the heterointerface, which corresponds to 85% of degree of strain relaxation. The epilayers grown under In-stable conditions have relatively smooth surfaces with low threading dislocation densities. This is owing to the fact that the interface misfit dislocations were exclusively of the edge-type which have no threading component and which relieve strain most effectively. The results demonstrate the ability to control the growth mode as well as the misfit dislocation nucleation type. © 1996 American Institute of Physics. [S0003-6951(96)05033-4]

Recently there has been an increased interest in compound semiconductor device structures made of materials which are not lattice matched to commonly available substrate materials. As a result, much effort was devoted toward developing epigrowth techniques for minimizing the propagation of dislocations, required for strain relief in mismatched systems, into the epilayers used for the active devices. This effort has produced a variety of specific techniques, including linearly graded¹⁻⁵ or step graded^{6,7} procedures. In both procedures, the gliding of 60° (mixed) misfit dislocations is the dominant strain relaxation mechanism.^{1,6} However, there are two major disadvantages. First, these techniques produce a rough “cross-hatch” patterned surface which is not suitable for devices with submicron features.^{1,7} Such cross-hatch patterns are speculated to be associated with the 60° dislocation which could produce a step on the surface due to its out-of-plane Burgers vector.⁵ Second, these techniques are generally not suitable for systems with lattice mismatch greater than 3% as the buffer layer thickness also increases proportionally.

Direct growth has also been investigated for systems with various amounts of lattice mismatches. It is found that for the systems with moderated lattice mismatch such as GaAs/Si, the coexistence of both 60° and pure edge-type (90°) misfit dislocations is observed.^{8,9} The resulting epilayers usually have high densities of bulk defects larger than 10^{12} cm^{-2} . It is recognized that these bulk defects, including stacking faults and threading dislocations, originate from sources such as 60° misfit dislocations.^{8,9} While 90° dislocations can relieve strain most effectively at the interface without any threading component, 60° misfit dislocations are highly active sources for the generation of threading dislocations. Therefore, it is desirable to have a heterointerface with primarily 90° dislocations. It has been observed that extremely large mismatches favor the nucleation of 90° dislocations. For example, Otsuka *et al.* investigated the CdTe/GaAs system with a 14% mismatch.¹⁰ In addition, Bourret

and Fuoss's work on GaSb/GaAs suggested that pure edge-type dislocations could be created and thus a highly relaxed epilayer is produced.¹¹ In this letter we have chosen to examine this effect using the largest possible mismatch available in our molecular beam epitaxy (MBE) system: the growth of InAs on GaP(001) with a 11% mismatch.

InAs epilayers of 25 nm thickness were grown by solid-source MBE on (001)-oriented GaP substrates. The growth of phosphides was achieved by a valved-phosphorus cracker.¹² Reflection high-energy electron diffraction (RHEED) was used to monitor the surface morphology as well as the growth rate and surface V/III ratio. The quality of the GaP buffer layer is critical to the growth of InAs as indicated by RHEED and transmission electron microscopy (TEM) observations. Surface oxide was desorbed at 660°C . GaP buffer layers were grown at 600°C . A streaky (2×4) RHEED pattern was observed during the growth of the 200-nm-thick GaP buffer layer. The growth rate for InAs is 0.7 monolayers (ML) per second. The growth parameters for InAs, i.e., temperatures and V/III ratios, were varied over a wide range to optimize growth conditions. The V/III ratio here, different from the beam flux ratio, is defined as the incorporation ratio of group-V and -III constituents. It is measured by the RHEED intensity oscillation induced by In and As on a separate InAs surface. Our optimized growth temperature is 350°C . At higher temperatures ($450\text{--}500^\circ\text{C}$), interfacial reaction between InAs and GaP appeared to occur as protrusions highlighted with moiré fringes were seen in the GaP buffer layer at the heterointerface. No 90° dislocations were observed at the heterointerface and the resulting layers were highly defective. Similar results have been reported in the InAs/GaAs system.¹³

Here we report two sets of heterostructures grown at 350°C under different V/III ratios. The InAs epilayer of the first sample (sample A) and the second sample (sample B) were grown under As-stable and In-stable conditions, respectively. The RHEED patterns of sample A become spotty immediately, indicating three-dimensional (3D) growth, after the deposition of 2 ML and remains so until the end of the growth [Figs. 1(a) and 1(b)]. The As_4/In beam flux ratio

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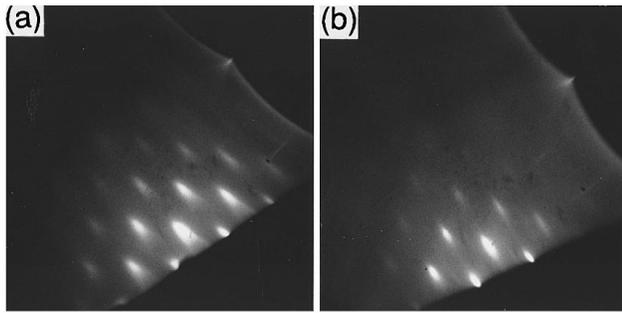


FIG. 1. RHEED patterns taken during the deposition of (a) 2 ML and (b) 25 nm of InAs on GaP under As-stable conditions. The spot patterns are indicative of island growth.

used for sample A was 10. For sample B, the growth mode was two-dimensional (2D) throughout the entire growth of InAs as the RHEED patterns taken after 2 ML and 25 nm depositions are streaky as shown in Figs. 2(a) and 2(b), respectively. The As_4/In beam flux ratio in this case was 5. It has been calibrated that the surface V/III incorporation ratio under such beam fluxes is less than unity at 350 °C. This was further verified by the fact that the RHEED patterns of sample B were In-stable (4×2) during growth and changed into As-stable (2×4) several seconds after the growth was terminated.

Cross-sectional transmission electron microscopy (XTEM) was conducted on the samples along both $[110]$ and $[\bar{1}\bar{1}0]$ orientations. A JEM 2000 EX electron microscope equipped with an ultrahigh resolution pole piece was used at an operating voltage of 200 kV. No significant difference was found in the two perpendicular $\langle 110 \rangle$ directions in terms of dislocation structures and densities. Figures 3(a) and 3(b) are the bright-field and high-resolution images of 25-nm-thick InAs epilayers grown on GaP(001) under As-stable conditions, respectively. The surface appears undulated with amplitudes up to 40 nm, consistent with the observed spotty RHEED pattern. Clusters of stacking faults or threading dislocations that have reached the epilayer surface were observed in the valleys. It is evident that island growth and subsequent coalescence had occurred. Unlike the InAs island/GaAs^{14,15} interface where a mixture of 60° and 90° dislocations were distributed in a wide band of 1 nm around the interface, a series of 90° dislocations with an equal spacing of 4 nm located directly at the heterointerface are observed as shown in Fig. 3(b). These 90° dislocations are not formed by the reaction of two 60° dislocations. They are proposed to be spontaneously generated at the interface within the first two monolayers. Direct incorporation of sessile 90° dislocations into the edge of the growing island has also been reported by LeGoues *et al.* on Ge islands/Si(001) grown at low temperature.¹⁶ The resulting island are almost fully relaxed.

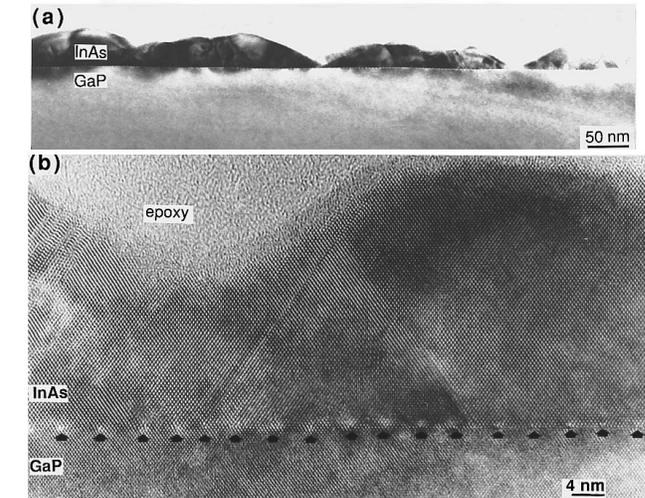


FIG. 3. $\langle 011 \rangle$ cross-sectional (a) bright field and (b) HRTEM images of a 25-nm-thick InAs epilayer grown on GaP under As-stable conditions showing 3D islanding and a regular array of 90° misfit dislocations (arrowed) right at the heterointerface. Stacking faults are observed at the joint of two islands, indicating island coalescence.

As expected from the streaky RHEED patterns, the sample grown under In-stable conditions has a relatively smooth surface without grooves or valleys under TEM observations as shown in Fig. 4(a), consistent with a layer-by-layer 2D growth mode. The 25-nm-thick InAs epilayer appears clean with very few defects detected. No threading dislocations were observed. A couple of stacking faults are present in the interfacial region, but the density is relatively low considering the mismatch is 11%. Figures 4(b) and 4(c) are a high resolution TEM (HRTEM) image and a selected area diffraction pattern (SADP) taken from the InAs/GaP

interface area. Figure 4(b) is a high resolution TEM (HRTEM) image revealing an incoherent interface with a series of 4 nm-spaced 90° misfit dislocations (arrowed). Figure 4(c) is an electron diffraction pattern taken from the interface area indicating a strain relaxed InAs epilayer in perfect epitaxial relationship with GaP.

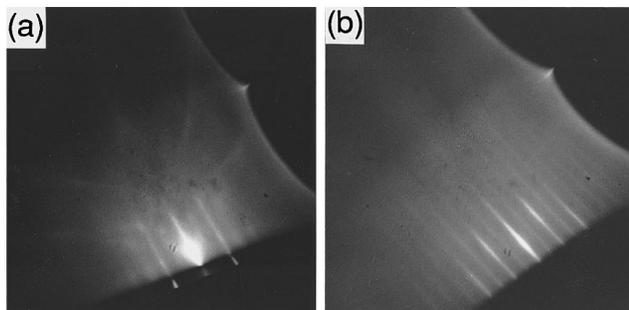


FIG. 2. RHEED patterns taken during the deposition of (a) 2 ML and (b) 25 nm of InAs on GaP under In-stable conditions. The streaky patterns are indicative of planar growth.

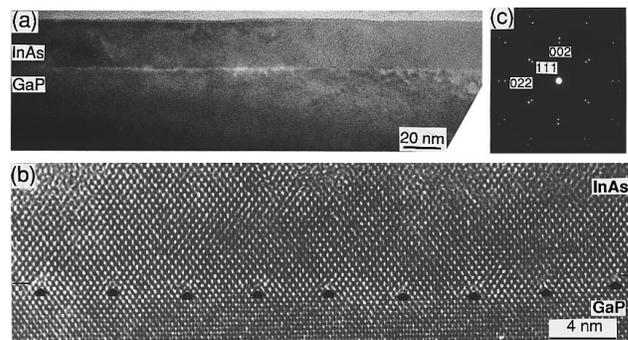


FIG. 4. $\langle 011 \rangle$ XTEM micrographs of a 25-nm-thick InAs epilayer grown on GaP under In-stable conditions: (a) a HRTEM image showing that the epilayer has a relatively smooth surface with very few defects detected, (b) a HRTEM image revealing an incoherent interface with a series of 4 nm-spaced 90° misfit dislocations (arrowed), (c) an electron diffraction pattern taken from the interface area indicating a strain relaxed InAs epilayer in perfect epitaxial relationship with GaP.

interface region, respectively. Both the HRTEM image and the SADP show the formation of a single-phase zincblende InAs epilayer in perfect epitaxial relationship with GaP. The shapes of the diffraction spots are rounded without streaks, indicating a good crystalline quality. The InAs epilayer is strain-relaxed as its diffraction spots are separated from those of GaP. The actual degree of strain relaxation was measured by HRTEM and plan-view TEM as shown later. HRTEM revealed an incoherent interface with equally spaced misfit dislocations of pure edge type. No other phase or misoriented grains were found. Most dislocations can be clearly identified as their images show highly localized cores, indicating that dislocation lines are exactly normal to the image plane. Interfacial Burgers vector circuits around each defect give an apparent projected edge type displacement vector of $1/2[110]$ or $1/2[\bar{1}10]$ which are parallel to the interface. Since the dislocation lines are perpendicular to the image, they are of the pure edge type. Furthermore, each dislocation shown in Fig. 4(b) has extra lattice fringes along both $\{111\}$ planes, having a symmetrical image with respect to the $[001]$ axis.^{8,9} This further confirms that all the misfit dislocations are of the pure edge type. The average spacing between two parallel misfit dislocations is approximately 4.1 ± 0.1 nm, corresponding to 9.4% strain relaxation and 85% (=9.4%/11.1%) of degree of strain relaxation in the InAs epilayer with respect to the substrate.

Atomic force microscope (AFM) and plan-view TEM were performed to further support the aforementioned observations. AFM line traces of the samples grown under As- and In-stable conditions showing the surface peak-to-trough heights are in the range of 5–7 and 120–150 Å, respectively. Plan-view TEM images of the sample grown under In-stable conditions exhibit cross-grating moiré fringes, indicative of strain relief as they are a pattern of interference fringes from two overlapped crystals with different lattice constants. The $\{220\}$ fringes taken under $g = \{220\}$ two-beam conditions have a measured spacing of about 2.13 nm. The theoretical parallel moiré fringe spacing is given by the expression, $D = |g_{\text{InAs}} - g_{\text{GaAs}}|^{-1}$. Hence the predicted parallel moiré fringes spacing (assuming a fully relaxed InAs film) for $\{220\}$ reflections is 1.93 nm. This corresponds to 88% of degree of strain relaxation, consistent with the estimation by HRTEM.

Our results demonstrate the ability to control the growth mode as well as the misfit dislocation nucleation type in the InAs/GaP system. The control of surface morphology by the cation to anion flux ratio seen here has been reported in InAs/GaAs system and the mechanism has been investigated.^{17–19} It is proposed that In-stable surface imposes kinetic limitations to the migration of In adatoms and forces layer-by-layer nucleation, thus acting as a virtual surfactant. The significance of the sole existence of the 90° dislocations in our system is that they are more beneficial to mismatched growth than the 60° dislocations which were commonly seen in graded-type mismatched heterostructures. Since $\{001\}$ planes are not easy glide planes in the zincblende structures, the 90° misfit dislocations whose Burgers vectors lie on the $\{001\}$ plane are not expected to move by gliding under normal condition. It is also unlikely that these dislocations will propagate toward the epilayer

surfaces. Furthermore, the 90° dislocations are energetically favorable since they are most effective at accommodating the lattice mismatch. As a result, the InAs epilayer grown on GaP under In-stable conditions is almost fully relaxed with very little threading dislocations propagating to the surface.

The potential applications of this heterostructure are long wavelength detectors and lasers and small band gap electronic devices. The GaP substrate has an advantage of being transparent and a better thermal conductor than GaAs, InP, and InAs. It is also conceivable that this technique can be applied to other heterostructures with comparable lattice mismatches, such as InGaSb/GaP. In our InAs/GaP sample grown under In-stable conditions, the partially relaxed InAs epilayer has an in-plane lattice constant of 5.9673 Å, corresponding to the lattice constant of $\text{In}_{0.8}\text{Ga}_{0.2}\text{As}$ or $\text{In}_{0.8}\text{Al}_{0.2}\text{As}$. The former, with a band gap energy of 0.5 eV, is of great interest for optoelectric and electronic device applications. Therefore, this strained 25-nm-thick InAs with a low defect density could be used as a template or a “superstrate” for the growth of InGaAs/InAlAs heterostructures with a high indium mole fraction. The growth and fabrication of small bandgap devices based on $\text{In}_{0.8}\text{Ga}_{0.2}\text{As}/\text{InAs}/\text{GaP}$ are currently under investigation.

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