Atomic-scale imaging of strain relaxation via misfit dislocations in highly mismatched semiconductor heteroepitaxy: InAs/GaAs(111)*A*

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Strain relaxation in InAs/GaAs(111)*A* heteroepitaxy has been studied on the atomic scale by scanning tunneling microscopy. The coalescence of small islands and the formation of a dislocation network are identified at the critical layer thickness (CLT), and no three-dimensional growth is observed, even beyond the CLT. The atomic displacement around the threading segments and the strain fields induced by the misfit dislocations are both identified. The measured density of the misfit dislocations indicates that the strain is not fully relaxed at the CLT, but is instead gradually relieved with the additional growth of InAs. [S0163-1829(97)03503-0]

The influence of strain on the epitaxial growth of lattice mismatched systems is a subject of significant current interest both from a fundamental understanding of crystal growth mechanisms and also the technologically important requirement for the growth of materials with compositionally abrupt interfaces and defect free layers. Provided that the lattice mismatch is not too large, the initial layers are strained elastically so that pseudomorphic two-dimensional (2D) growth occurs up to some critical layer thickness (CLT). Beyond this point, the strain energy is reduced by nucleation and propagation of dislocations at the interface between the two materials.[1] Transmission electron microscopy (TEM) has been the primary technique used for identifying misfit dislocations. However, scanning tunneling microscopy (STM) offers a unique atomistic perspective of the strain relaxation processes in highly mismatched heteroepitaxy. Previous STM studies of misfit dislocations have been restricted to metal systems.[2–6]

STM studies of strain relaxation in semiconductor heteroepitaxy have largely focused on morphological aspects,[7–9] and only two groups have reported on strain relaxation in ultrathin films by misfit dislocations. One was with the EuTe/PbTe system[10] based on large scale imaging of surface steps, while the other concerned the observation of a strain field caused by a dislocation in Si/Ge.[11] The strain field results in the displacement of lattice positions on the subangstrom scale so that their imaging by STM is often obscured by larger scale effects. These include the formation of three-dimensional (3D) islands as a result of total surface energy minimization of strained layers and/or strain-induced modification of step barriers.[12] Their size is at least two orders of magnitude larger than the displacement, so its practical observation is difficult in view of the dynamic imaging range required. A second possibility is the existence of a surface reconstruction which may result in a surface corrugation with a depth of more than one angstrom. In addition, the presence of phase boundaries further degrades the identification of dislocations in the STM image.

The heteroepitaxy of InAs on GaAs(111)*A* is an ideal system for the study of dislocations by STM. In contrast to the (001) surface, the growth mode remains 2D for all InAs coverages despite the larger lattice mismatch ($\sim$7.2%).[13] In addition, the InAs surface exhibits a (2×2) reconstruction and a corrugation of only 0.2 Å. We have therefore used STM to study the strain relaxation during the early stages of heteroepitaxy in this system. The strain field induced by the misfit dislocations, located at the interface, has been resolved at the atomic scale.

A purpose-built STM/molecular beam epitaxy growth system was used for imaging the grown surfaces.[14] InAs films of different thicknesses were grown at 450 °C with a growth rate of 0.077 ML/s, and an As/In flux ratio of 15. A

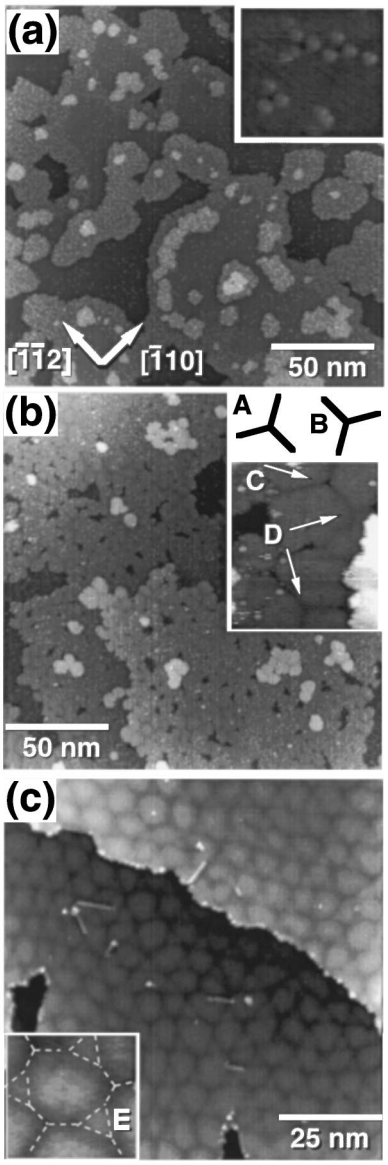

FIG. 1. STM surface topographs of GaAs(111)*A* after the growth of (a) 0.5 ML, (b) 2 ML, and (c) 5 ML of InAs obtained with sample voltages of -1.5–-3.5 V, and tunneling currents of 0.08 − 0.2 nA. The inset in (a) shows a magnified image of a decorated region displaying local (3×3) structures adsorbed on the surface. The inset in (b) shows two possible types of *junction* on the same surface while the dashed line in (c) shows the position of the misfit dislocations.

streaked (2×2) reflection high-energy electron diffraction pattern was maintained throughout the growth regardless of the InAs layer thickness. The absence of transmission diffraction features is consistent with the lack of 3D islands.[13]

STM images of the (111)*A* surface after the growth of 0.5, 2, and 5 ML InAs films are shown in Fig. 1. Two sizes of island (5–20 nm and 50–200 nm) characterize the surface after 0.5 ML deposition [Fig. 1(a)]. The large islands were also observed on the GaAs(111)*A* surface before the deposition of InAs. Small bright features decorate the small islands and the perimeters of the larger islands, which detailed STM observation with atomic resolution [the inset of Fig. 1(a)] revealed to consist of three atoms forming an isolated 1.2×1.2 nm triangle. These features disappear in empty state images suggesting that they are three As atoms forming a local (3×3) structure adsorbed on the surface. In contrast, the central region of the larger islands is undecorated. The decorated and undecorated regions correspond to strained InAs and unstrained GaAs surfaces, respectively. While some part of InAs growth occurs in a step flow mode propagating from the larger islands, there is also a contribution from 2D nucleation in the form of small islands.

With increasing deposition, the adsorbed regions increase in size at the expense of the undecorated regions and the surface becomes a fully strained InAs film at 1 ML coverage. With an additional 1 ML of InAs, the inner parts of the large islands maintain the same characteristic of a strained surface while the outer parts develop a different feature [Fig. 1(b)]. These appear as partially coalesced islands, each 5–10 nm in diameter. The boundary between any two *coalesced islands* displays a dark contrast band with a depth of ~0.5 Å, a value considerably smaller than the actual 1 ML step height of 3 Å. In addition, the characteristic (2×2) reconstruction is uninterrupted over this dark band. The implication is that it is not an actual gap between two islands, but rather is associated with the strain field induced by misfit dislocations at the heterointerface.[15] The same observation has also been reported for $CoSi_2$/Si (Ref. 16) and Si/Ge.[11] This suggests that the InAs layer starts to relax by forming misfit dislocations at a thickness between 1 ML and 2 ML, without forming 3D islands and that the first stage of dislocation formation proceeds by the coalescence of small, initially coherent, 2D islands. This mechanism of dislocation formation by island coalescence has also been observed with the Si/Ge system,[11] although there the islands are higher than for the InAs/GaAs(111)*A* system considered here.

When three islands coalesce to form three short misfit dislocations between each island pair, a 1 ML deep hole is formed at the center of the islands. With increasing InAs coverage, the hole reduces its size by additional growth, and the three dislocations for each island pair extend and meet to form a *junction*. At 2 ML [Fig. 1(b)], two different features can be seen at the junction. One is a small hole about 1 ML deep (labeled *C*), and the other has a contrast of 0.8 Å (*D*) which is deeper than the dislocation. This is not a real hole, but can be assigned to a *dislocation node*. The misfit dislocations are in $\langle 11\bar{2}\rangle$ directions and can form two differently directed junctions (labeled *A* and *B*). Hole *C* is predominantly observed for junction *A* and the dislocation node *D* occurs at junction *B*. At higher InAs thicknesses, a third feature appears at the junction [Fig. 1(c)]. This is a small triangle formed by three dislocation lines, each side of which is aligned in $\langle 110\rangle$ directions and the contrast gives a depth of 0.5 Å (*E*). This feature is only seen for junction *A* and the number of previously observed holes decreases. This suggests that the triangle is formed after the hole is filled by new material, and its formation is preferred to the unstable dislocation node at junction *A*. In contrast, the dislocation node at junction *B* appears stable, as no triangles are observed.

For InAs coverages >3 ML, the entire surface is covered by the relaxed regions and no holes are observed even at junction *A*, and only the large islands 50–200 nm in size were present. A typical STM image obtained for a 5 ML InAs film is shown in Fig. 1(c). At this InAs thickness the

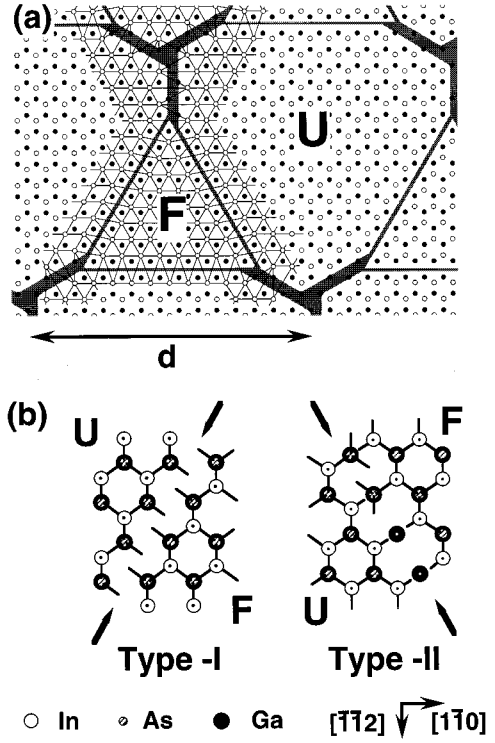

FIG. 2. (a) A model for the atomic structure at the InAs/GaAs(111)*A* interface. Open (closed) circles show the position of Ga(In) atoms just below (above) the interface. *F* and *U* indicate faulted and unfaulted interfaces, respectively. Gray lines and bands display the positions of partial and perfect dislocations. The thin solid line is a guide to the eye for the trigonal lattice formed by the In atoms. (b) The atomic structures of two possible partial dislocations. The shaded circle shows an As atom at the interface. The solid lines and arrows indicate chemical bonds and the position of dislocations, respectively.

misfit dislocations form a periodic network. The adsorbed arsenic which was observed on the strained InAs layer [Fig. 1(a)] is not present on the relaxed surface. This suggests that As adsorption is activated by the strain in InAs layers. The dislocation network disappears completely after 20 ML deposition presumably because the strain field is screened by a layer of this thickness.

Since the dislocation network is not a simple hexagonal structure (i.e., a honeycomb structure), the interface must contain a proportion of partial dislocations. Partial dislocations occur at the boundary of faulted and unfaulted domains and the interface must also contain stacking faults. Figure 2(a) shows a possible model for the atomic arrangements at the InAs/GaAs(111)*A* interface. The sides of the triangles at junction *A* form partial dislocations giving rise to stacking faults at the InAs/GaAs interface. Upon completion of a single-crystal relaxed InAs epilayer, both the dislocations and stacking faults are buried at the interface.

A similar network structure has been reported for misfit dislocations in sputtered PtNi alloys[5] and for the surface atomic arrangement at domain walls in Ag/Pt(111) heteroepitaxy.[3] In both cases, trigonal stacking faults of different size were observed at both junctions *A* and *B*. For InAs/GaAs(111)*A*, only junction *A* has a trigonal stacking fault, suggesting an energetic difference in triangle formation

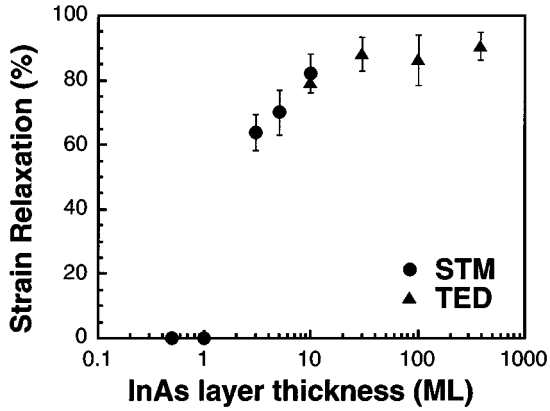

FIG. 3. Strain relaxation calculated from STM images and TED patterns as a function of InAs layer thickness. The error bars indicate the standard deviation obtained statistically at several different positions on the same surface.

at the two junctions. This may occur if the formation energy of the dislocation node is higher for the triangle at junction *A* than at junction *B*. The transformation from a dislocation node to the triangle of a stacking fault bounded by partial dislocations needs only the displacement of atoms along the (111)*A* interfaces. Once hole *C* is filled, the dislocation node evolves quickly to form triangle *E* when this energetic condition is satisfied. The formation energy of a triangle at junctions *A* and *B* is expected to be different as the formation energy of the dislocation nodes at these junctions should be slightly different, due to the structure of their corresponding partial dislocations. Three partial dislocations referred to as type-I form a triangle at junction *A* and three referred to as type-II form one at junction *B* [Fig. 2(b)]. There are two possibilities for the type-II structure, one involving an As vacancy (lower arrow) and the other without the vacancy (upper arrow). For both cases, the line density of dangling bonds along the dislocation is 1.5 times higher in type-II than type-I, suggesting a higher formation energy for the type-II dislocation.

To relax fully the InAs epilayer, i.e., to make the epilayer form a zinc-blende lattice with an average lattice constant $\sim$7.2% larger than the substrate, the period of the network [labeled *d* in Fig. 2(a)] has to be $\sim$6.0 nm. The average spacing between the centers of two neighboring hexagons seen in the STM images is larger than this, suggesting that the InAs layer is not fully relaxed and Fig. 3 shows the amount of strain relaxation calculated from the average spacing. It is clear that beyond the CLT of 1–2 ML's, the strain is gradually relieved up to about 10 ML. Transmission electron diffraction (TED) measurements have also been performed for several of the InAs/GaAs(111)*A* samples with thicker InAs layers. The amount of strain relaxation obtained from the shift in the transmission diffraction spots is also plotted in Fig. 3 and very good agreement exists between the STM and TED data obtained from the 10 ML InAs sample.

No study of strain relaxation is complete without discussing the threading segments of the misfit dislocations. These surface terminating segments can be resolved by STM and appear as bright spots with a dark shadow [Fig. 4(a)]. The magnified image in the vicinity of one spot [Fig. 4(b)] shows a phase boundary (indicated by a closed arrow) in the

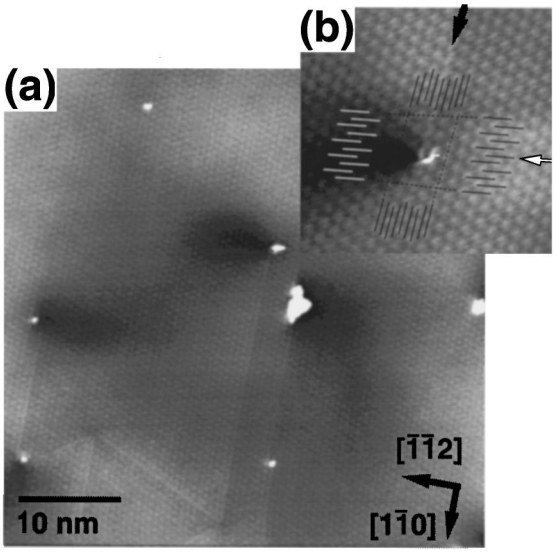

FIG. 4. STM surface topographs of a 20-ML-thick InAs layer on GaAs(111)*A*. (b) shows a magnified image of the same surface as (a) in the vicinity of one bright spot. See text for a discussion of the alignment of In atom rows indicated by the solid lines in (b).

(2×2) reconstruction running in the $[1\bar{1}0]$ direction, terminated by the bright spot. Solid lines on the figure indicate atomic rows of surface In atoms in two orthogonal directions, $[\bar{1}10]$ and $[\bar{1}\bar{1}2]$, based on a vacancy-buckling model.[17,18] The angle between them is not 90° in the image because of residual thermal drift. It can be clearly seen that one atomic row (indicated by the open arrow) is terminated by the bright spot, and the left-hand side of the phase boundary is displaced upwards (in $[\bar{1}10]$) by a surface lattice constant of 0.4 nm, but no displacement in $[\bar{1}\bar{1}2]$ is apparent indicating that the spot is indeed a threading dislocation with Burgers vector $\frac{1}{2}[\bar{1}10]$. This result coincides with that for one of the perfect misfit dislocations in our model [Fig. 2(a)].

Plan-view TEM images of InAs/GaAs(111)*A* samples confirm the presence of threading dislocations as projected lines in the transmission image, indicating that the dislocation are not normal to the (111)*A* surface. Their angle from the normal to the surface calculated from the average length of the line in the TEM image was $51°\pm8°$. Similarly, the accompanying shadow with a depth of about 0.5 Å in the left hand side of the threading dislocation in Fig. 4(b) can be assigned to the strain field induced by a threading segment moving towards the surface.

In conclusion, the precise control of 2D growth of InAs on GaAs(111)*A* has enabled the initial stages of strain relaxation to be viewed at the atomic scale. The early stage of relaxation is the formation of misfit dislocations at the boundaries of coalescing strained islands. The misfit dislocations form a trigonal network with anisotropy between $[1\bar{1}0]$ and $[\bar{1}10]$ maintaining the threefold rotational symmetry of the (111)*A* surface. The strain is gradually relieved with increasing InAs thickness and no 3D islands are formed. Detailed STM imaging of the threading segments allows the Burgers vectors of the dislocations to be identified.

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