Surface Contrast in Two Dimensionally Nucleated Misfit Dislocations in InAs/GaAs(110) Heteroepitaxy

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Scanning tunneling microscopy has been used to study misfit-dislocation (MD) induced lattice distortion of the epilayer for InAs thin films grown on GaAs(110). Two-dimensional (2D) islands with regular size are observed in the first two monolayers. Interfacial MDs, identified in the images by an array of dark lines, appear following the coalescence of the 2D islands. The growth mode remains 2D for all coverages and the vertical contrast of these lines decreases with film thickness. The surface contrast can be explained only by classical elasticity theory if the properties of a thin InAs film with an exposed surface are considered. [S0031-9007(96)02167-9]

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Heteroepitaxial growth occurs when the chemical identity of the epitaxial layer differs from that of the substrate. The two materials may possess a parity in lattice parameter or a misfit which results in strained modes of growth. Small misfits can be accommodated by elastic distortion, but greater misfits lead to plastic deformation, or dislocations, in the strained layer [1]. The strained-growth mode of InAs on GaAs is particularly interesting as it depends strongly on the substrate orientation. For the (001) substrate, a transition in growth mode from two-dimensional (2D) to three-dimensional (3D) nucleation usually occurs some time *prior* to the incorporation of dislocations [2]. In contrast, reflection high-energy electron diffraction (RHEED) studies have shown that the formation of 3D nuclei is completely surpressed during growth on (110) [3,4] and (111)A surfaces [5]. In both cases, the InAs epilayer remains 2D even *after* strain relaxation. Since the lattice misfit ($\sim$7.1%) is common for all InAs/GaAs systems, the observed growth behavior cannot be explained by strain alone, but must derive from more *fundamental* grounds which are unique to each surface orientation.

Dislocations have traditionally been studied by transmission electron microscopy (TEM) [6]; however, scanning tunneling microscopy (STM) can generate complementary information at a more local level [7,8]. In highly mismatched heteroepitaxy, STM has a particular advantage in following the nucleation of dislocations in very thin films, since the morphology of fully strained material prior to the onset of the strain relief can be imaged [9] at a stage where no clear contrast is present in conventional TEM. Previous STM studies of semiconductor heteropitaxy have mainly centered on large-scale morphological features [10–13]. In a recent study of strain relief in metallic $CoSi_2$/Si [7], bright bands in STM topographs were associated with a surface distortion induced by the spatially extended strain field around the misfit dislocation (MD) cores. The contrast was found to be *independent* of the epilayer thickness and could be *partially* accounted for by classical elasticity theory. Unfortunately, TEM estimation of the vertical magnitude of the contrast distortion due to MDs in very thin films is extremely difficult [6], since a knowledge of the precise beam conditions and the elastic properties of the epilayer and substrate is required to estimate the *vertical* magnitude of surface distortion in the TEM data.

In this Letter, we provide a detailed STM study of the surface contrast during strain relief in InAs/GaAs(110) heteroepitaxy. The evolution of the MDs is monitored by a thickness-*dependent* surface contrast due to the strain field from the dislocation cores. The persistent 2D growth mode for all coverages facilitates the depth resolution and in turn enables the fine surface perturbation to be measured accurately and therefore allow comparison with elasticity theories.

The experiments were performed in a combined molecular beam epitaxy (MBE)/STM facility which has been described previously [14]. The epi-ready, $n+$ Si-doped, nonmisoriented GaAs(110) substrates were introduced to the vacuum system without any *ex situ* preparation and thermally cleaned at 300 °C. Following oxide removal at 630 °C, thin (10 ML) buffer layers of GaAs were grown at 500 °C and an As/Ga flux ratio of 10 [15]. After annealing, the substrate temperature was lowered to 420 °C for InAs deposition which was performed using an As/In flux ratio of 8. The nominal in flux was 5.6×10^{13} atoms cm^{-2} s^{-1}, as calibrated from RHEED specular beam intensity oscillations during InAs(001) homoepitaxy. Constant current STM images were obtained at room temperature using sample biases in the range $|V_s| = 2$–4 V and tunneling currents of $\sim$0.2 nA. The vertical resolution of the STM is $\sim$0.10 Å.

The STM images presented in Fig. 1 demonstrate the appearance of the growing InAs layer as the coverage is increased from the pseudomorphic regime [Fig. 1(a)] through the various stages of relaxation [Figs. 1(b)–1(d)]. Below 1 ML, the InAs appears to grow via 2D island nucleation with a smaller contribution from a step-flow mode [Fig. 1(a)]. A high density of islands ($\sim 10^{11}$ cm^{-2})

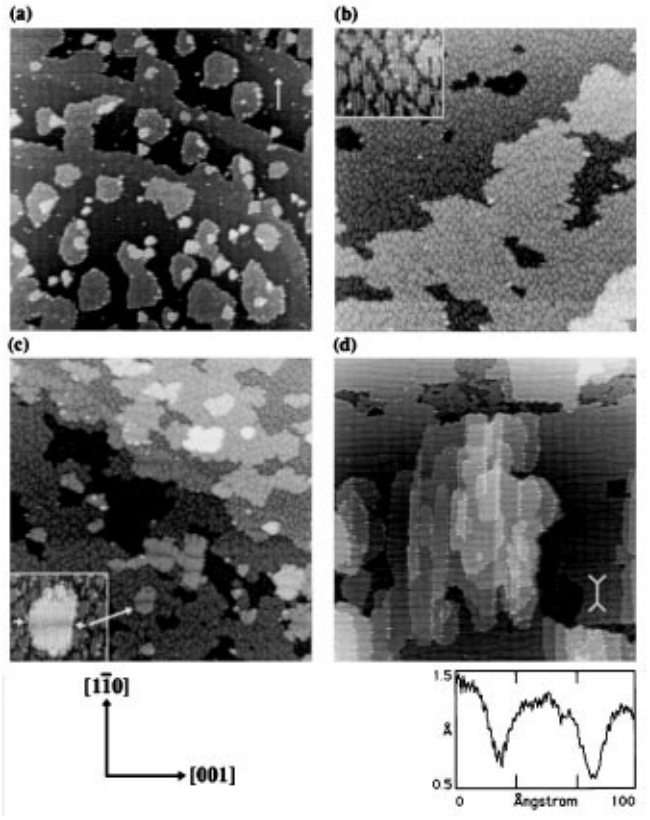

FIG. 1. Filled-states STM images of InAs on GaAs(110) for the following coverages: (a) 0.5 ML, (b) 2 ML, (c) 3 ML, (d) 5 ML. The inset in (b) highlights the morphology of "fractured" islands, while the inset in (c) shows the minimum island size needed for nucleation of a MD beyond the critical thickness. The plot below (d) shows the surface profile of MDs taken at the vertical white bar. Image sizes: (a),(d) $(200\ \text{nm})^2$, (b),(c) $(100\ \text{nm})^2$.

is observed, many possessing sections of bilayer (4 Å) height, a characteristic of GaAs(110) homoepitaxy [15]. A small difference in image contrast, equivalent to just 0.3 Å, allows the identification of strips of InAs $\sim$ 150 Å wide decorating the residual steps on the nominally singular GaAs substrate [arrow in Fig. 1(a)].

The next characteristic development of the strained layer occurs at 2 ML [Fig. 1(b)]. Within the single exposed InAs layer, 1 ML-deep trenches eventually form a network of very small InAs islands. The uniformity in the size of these islands is striking (mean area = 494 Å^2, standard deviation = 310 Å^2), and they are all only a single monolayer (2 Å) in height. The island size was not affected by extended annealing at the deposition temperature.

For InAs thicknesses between 3 and 5 ML, STM images show that some of the InAs nuclei are not broken into small islands, but instead possess an intact surface layer [Fig. 1(c)]. A peculiar quality of these nuclei is the presence of a subtle depression along the [001] direction, which gives a vertical contrast of about 0.5 Å, a value substantially less than the 2 Å step height for a monolayer on the (110) surface [see inset in Fig. 1(c)]. These islands expand and coalesce with further InAs deposition and the surface at 5 ML coverage is smooth and characterized by an array of parallel *dark* bands [Fig. 1(d)].

The appearance of the dark bands (>3 ML) coincides with the relaxation of the InAs film, as monitored by measuring the separation of any two integral order rods in the RHEED pattern. Between 3 and 5 ML, the data exhibit a very rapid transition from the lattice constant of GaAs to that of InAs (Fig. 2). After deposition of 5 ML of InAs, there is an $\sim$86% relaxation in the [1$\bar{1}$0] direction accompanied by only a very small change in the orthogonal [001] direction. Previous TEM studies of InAs films grown on GaAs(110) have shown that strain relaxation is strongly anisotropic and thickness dependent [16]. Strain relief occurs first in the [1$\bar{1}$0] direction with the formation of 90° perfect MDs lying in the [001] direction at the heterointerface. This is followed at higher coverages by relaxation in the orthogonal [001] direction through the formation of 60° type dislocations with a [1$\bar{1}$0] orientation.

A plan-view TEM micrograph of the 5 ML InAs/GaAs sample is shown in Fig. 3 and confirms the regular network of MDs with Burgers vector, $\mathbf{b} = (1/2)a_0\,[1\bar{1}0]$ ($a_0 = 6.054$ Å), lying at the interface. The MD features observed in TEM have a remarkable resemblance to the dark bands shown in Fig. 1(d) in terms of both spacing and line direction. As both measurements agree well with the average separation expected for 90° MDs in InAs/GaAs ($\sim$60 Å), it can be concluded that the dark bands in the STM image are also associated with 90° MDs. In addition, since these bands which develop during

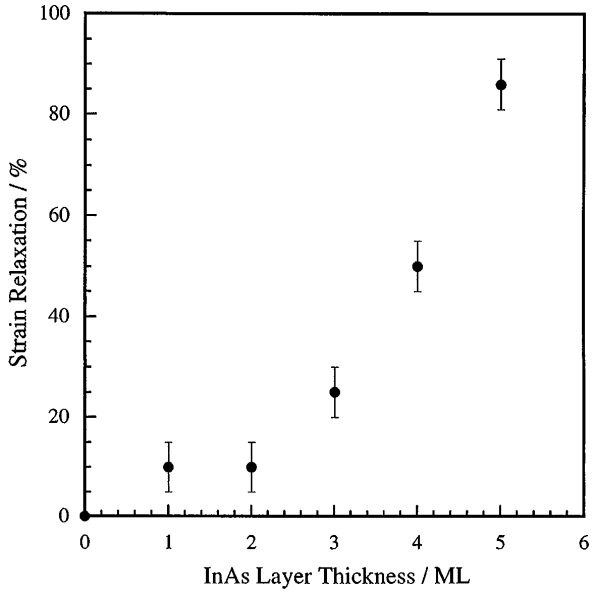

FIG. 2. The strain relaxation as measured by the separation of first order rods in the RHEED pattern as a function of InAs coverages. The transition from the lattice constant of GaAs (0%) to that of InAs (100%) is mot pronounced between 3–5 MLs.

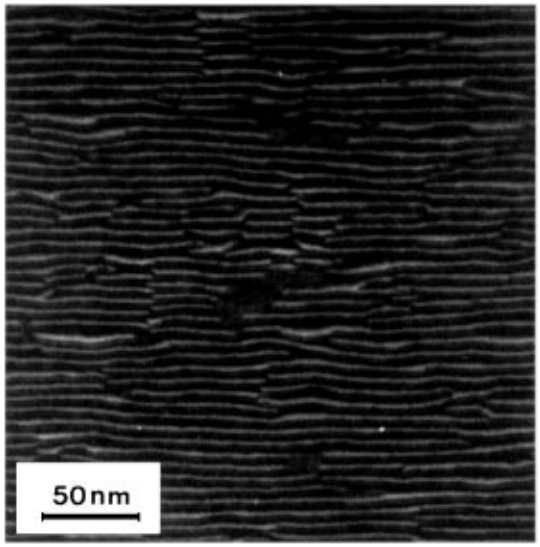

FIG. 3. A plan-view TEM dark field image of the 5 ML InAs sample taken at $g = [2\bar{2}0]$. The 90° MDs are seen as light contrast lines. The TEM specimen was prepared by chemical jet thinning from the substrate side, and examined at 200 kV. Image size is ~200 nm × 200 nm.

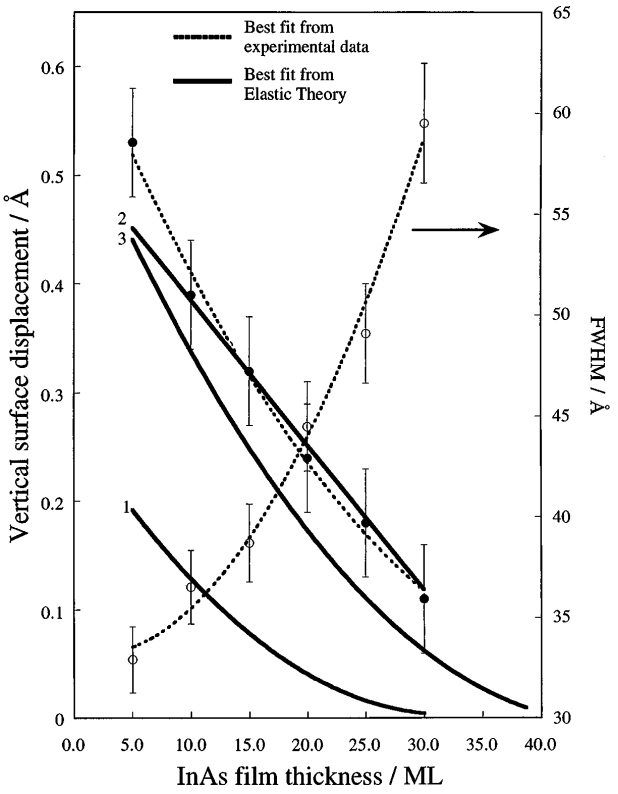

FIG. 4. Vertical displacement (*filled circle*) and FWHM (*open circles*) of the dark bands associated with MDs as measured by STM as a function of film thickness. Also shown are the displacement values calculated from simple elasticity theory (1) and the modified versions with (2) a *linear* thickness-dependent ν_{epilayer} and (3) a *free* surface and ν_{epilayer} and μ_{epilayer} variables.

the 3–5 ML stage are relatively shallow (see surface profile in Fig. 1), the depressions detected by STM are likely to be related to the strain field of the buried MDs. In this compressively strained system, missing planes of atoms exist in the epilayer above dislocation lines and produce a *negative* contrast in the surface image.

It is clear from the STM images that there is a striking relationship between the surface structure at 2 ML deposition and the evolution of the dislocation network from 3 ML thickness. The uniformity in size of the small 2D InAs islands [Fig. 1(b)] must be an effect that best accommodates elastically the compressive strain in the film. Coalescence of these islands leads to incorporation of short MD segments [Fig. 1(c)] and the absence of any threading segment linking the surface with the MDs implies that the dislocation is located directly below the surface atomic plane, i.e., in the second InAs layer.

The question remains as to whether the image contrast measured by STM is a lattice distortion induced by the MDs, or whether there is some electronic contribution to the magnitude of the measured contrast. The dimensions of the dark bands can be measured directly from the STM images as a function of InAs coverage (Fig. 4). In contrast to previous studies on $CoSi_2/Si$ [7], the vertical dimension of the bands *changes* with film thickness, *decreasing* from 0.55 Å at 5 ML to 0.10 Å at 30 ML. There is a concomitant increase in the full width at half maximum (FWHM) of the dark bands from 33 to 59 Å for the same range of film thickness. It should be noted that it is difficult to established any correlation between the increase in the FWHM and the decrease in the contrast of dark bands as the values of the FWHM are too close to that of the average separation of the MDs (~60 Å).

Although classical elasticity theory can be used to calculate the vertical displacement produced by interfacial MDs for a semiinfinite epilayer above a semi-infinite substrate [17], it is clearly not applicable to the very thin films in which we observe the MDs, as illustrated in Fig. 4 by comparing experimental data with calculations using the bulk Poisson ratio ($\nu_{\text{epilayer}} = 0.3$) for the InAs film (plot 1). We have therefore introduced empirically a thickness-dependent ν_{epilayer}, in which a value of 0.5 is used for the thinnest film (5 ML) [17]. The deformability of the film is assumed to decrease *linearly* with film thickness up to 45 ML, above which the bulk value of 0.3 is used (plot 2). Recent photoemission studies have indeed shown that the bulk band structure of InAs on GaAs(110) is not fully developed until the film thickness reaches ~100 Å (50 ML) [4]. It is not clear whether the apparent agreement with the thickness dependent ν_{epilayer} model for film thickness greater than 10 ML is fortuitous, or whether this is the point at which a bulk value of ν_{epilayer} is a reasonable approximation.

An alternative analysis takes into account both ν_{epilayer} and the shear modulus, μ_{epilayer}, as well as the *finite-size*

effect (free surface) of the epilayer [18]. This treatment was originally applied to explain the results of the contrast observed in the tensilely strained (-1.2%) $CoSi_2$/Si(111) system and it can be extended to compressively strained ($+7.1\%$) InAs/GaAs(110) for two reasons. First, both $CoSi_2$/Si(111) and InAs/GaAs(110) have only surface-bond relaxations with no complications due to additional stress induced by a surface reconstruction. Second, from the sense of the contrast, the lattice protrusion of the epilayer in the tensilely strained system should correspond to the lattice depression in our compressively strained InAs/GaAs. The degrees of lattice mismatch between the two systems influence the density of MDs during strain relief and therefore the value of μ_{epilayer}. The variation (from 50% to 200%) in μ_{epilayer} has been shown to account for *at least* 10% of the surface contrast [18].

Once the epilayer is fully relaxed in the $[1\bar{1}0]$ direction [19], the elastic properties remain important. The *correlation* between the density of MDs and the magnitude of the surface contrast [18] suggests that the contrast for the InAs/GaAs system can be reparametrized by taking into account the difference in the lattice constants of $CoSi_2$ and InAs epilayers (13%). Although we cannot formally justify these adjustments, the corrected plot (3) shown in Fig. 4 follows very *closely* the trend of the data even for thicknesses where the thickness dependent ν_{epilayer} model breaks down.

Additional STM measurements were carried out to investigate any possible *electronic* contribution to the surface contrast. No measurable influence on the surface contrast was found either by imaging in the filled/empty-state mode, or by varying the magnitude of the tunneling resistance (V/I). Further, spectroscopic mode studies did *not* reveal any electronic states that are localized to the regions containing the dislocations [20].

In conclusion, we have used STM to investigate the nucleation of MDs via the coalescence of small 2D islands in InAs/GaAs(110) heteroepitaxy. The surface contrast as measured by STM due to the presence of the dislocations depends on the InAs film thickness. A good estimate of this contrast can be obtained using a modified classical elasticity theory that takes into consideration the properties of a thin film with an exposed surface.

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[19] At this coverage relaxation in the orthogonal [001] direction is less than 15%. Strain relief in this direction becomes apparent in STM images of thicker InAs films and appears as a series of bright lines oriented in the $[1\bar{1}0]$ direction. A few examples can be seen in Fig. 1(d) for the 5 ML thick InAs film; these are half-loop dislocations in the form of surface slip traces.
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