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Strain relief by periodic misfit arrays for low defect density GaSb on GaAs

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We demonstrate the growth of a low dislocation density, relaxed GaSb bulk layer on a (001) GaAs substrate. The strain energy generated by the 7.78% lattice mismatch is relieved by a periodic array of 90° misfit dislocations. The misfit array is localized at the GaSb/GaAs interface and has a period of 5.6 nm which is determined by transmission electron microscope images. No threading dislocations are visible. The misfits are identified as 90°, rather than 60°, using Burger's circuit analysis, and are therefore not associated with generation of threading dislocations. A low dislocation density and planar growth mode is established after only 3 monolayers of GaSb deposition as revealed by reflection high-energy electron diffraction patterns. Calculations corroborate the materials characterization and indicate the strain energy generated by the 7.78% lattice mismatch is almost fully dissipated by the misfit array. The low dislocation density bulk GaSb material on GaAs enabled by this growth mode will lead to new devices, especially in the infrared regime, along with novel integration schemes. © *2006 American Institute of Physics*.
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The Sb-bearing compounds offer a wide range of electronic band gaps, band-gap offsets, and electronic barriers along with extremely high electron mobility[1] and therefore enable a variety of extremely fast low-power electronic devices and infrared light sources.[2,3] Lattice-mismatched epitaxy of Sb-based materials on GaAs and Si substrates has attracted considerable attention due to the numerous advances in optoelectronic devices that can be enabled, including monolithically integrated lasers, detectors, solar cells, and transistors.[4] However, with the introduction of mismatch, the epilayer is limited to a critical thickness, beyond which the material relieves strain energy through misfit dislocations and often threading dislocations.[5] Vertically propagating threading dislocations are highly detrimental to device performance and, in materials with defect densities $>10^5$ cm^2, excessive carrier loss is caused through nonradiative recombination.[6] Researchers have attempted to mitigate these detrimental effects by bending the vertically propagating defects along strained interfaces using compositionally graded layers or selective area growth.[7,8] Compositionally graded metamorphic buffers have been demonstrated in AlGaAsSb on GaAs[9] and AlInSb on GaSb[10] to achieve mid-infrared (IR) and (IR) detectors and lasers.

Another approach to developing low dislocation density bulk material is to design a lattice-mismatched interface in which strain energy is solely relieved by laterally propagating (90°) misfit dislocations confined to the episubstrate interface.[11] The presence of a two-dimensional (2D) array misfit dislocations has been demonstrated in the growth of GaSb islands on GaAs.[12] The growth of thick GaSb layers on GaAs was previously believed to start as islands and then coalesce into a uniform layer. In these previous demonstrations, both 90° and 60° misfit dislocations were present.[13] While the predominant strain relief mechanism was believed to be the 90° misfits, the minority 60° misfits were shown to cause threading dislocations in the GaSb. The source of the 60° misfits is still unclear but attributed to one or more of the following factors—island coalescence, growth temperature, and the degree of the mismatch. Island coalescence, in which the {111} planes of adjacent islands merge, has been shown to cause 60° misfits. Supporting data include a strong correlation between island coalescence and the location of the 60° misfits. The growth temperature has been shown to be a strong factor in determining which type of misfit is produced, with GaSb grown at ~520 °C favoring 90° misfits and 560 °C favoring 60° misfits.[14,15] The lattice mismatch has also been shown to be of critical importance in the formation of 90° misfits. Low strain systems (<2%) have resulted in 60° misfits, moderate strain (3–4%) in mixed 90° and 60° misfits, and high strain (>6%) in pure 90° misfits.[16] The publications mentioned above are mostly studies of the misfit dislocations at the interface of thin layers of GaSb on GaAs using plane-view and side-view high-resolution transmission electron microscopy (HR-TEM). However, in device applications, the GaSb layer has to be much thicker (>100 nm). This makes it difficult to obtain HR-TEM images of the misfit dislocations at the interface. The use of high-resolution x-ray diffraction (HR-XRD) has been useful for characterizing the interface in these cases. A comprehensive HR-XRD study of GaSb on GaAs has been published by Babkevich *et al.*,[12,17] who documented the growth interface and the nature of the misfit dislocations under a variety of growth conditions and GaSb thicknesses. In our work, we have built on the results mentioned above to obtain growth conditions for the formation of 90° rather than 60° misfits, which seems to require balancing of strain energy with adatom migration and can be controlled through the optimization of lattice mismatch, Sb overpressure, and growth temperature.

In this letter, we demonstrate a highly periodic array of 90° misfit dislocation based growth of GaSb on GaAs to yield completely (>98%) relaxed and low dislocation GaSb bulk layers on GaAs. Furthermore, we show that the strain relief occurs within several monolayers (MLs) of the interface. The growth of the GaSb bulk on GaAs is performed

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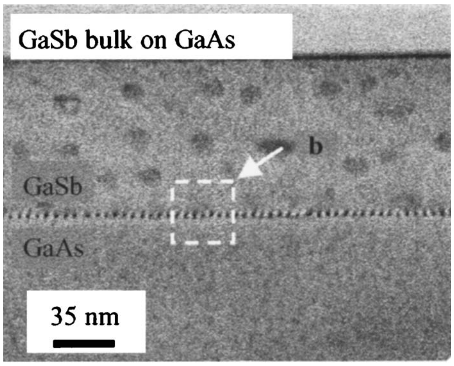

FIG. 1. Cross-sectional TEM image of 120 nm of GaSb on GaAs showing a highly periodic array of misfit dislocations at the GaSb layer and the GaAs substrate.

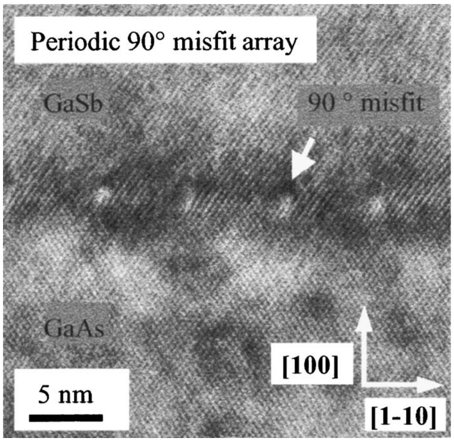

FIG. 2. HR-TEM image of the GaSb/GaAs interface showing a periodic 90° misfit array with a 56 Å spacing.

using a molecular-beam epitaxy reactor equipped with valved crackers for As and Sb sources. The GaAs substrate is deoxidized at 600 °C prior to the growth of 100 nm of GaAs at 560 °C to obtain a smooth surface. After completion of the homoepitaxy, the substrate temperature is reduced to 510 °C under constant As overpressure. Before the Sb growth is initiated, the As valve is closed allowing As adatoms to desorb leaving a Ga-rich surface. This process, confirmed by reflection high electron energy diffraction (RHEED) transition from an As-rich (2×4) to Ga-rich (4×2) surface, reduces As/Sb intermixing. Once the GaSb growth begins, the RHEED pattern resembles a 1×3 indicating that a thin film of GaSb forms on the surface. The pattern is difficult to analyze during the first few GaSb MLs. But, under optimized growth conditions, a clear 1×3 reconstruction pattern appears within the first 3–5 MLs indicating a planar growth mode of relaxed bulk material. Unoptimized parameters yield a spotty RHEED pattern with continued deposition that indicates a defective growth mode.

The misfit array and resulting bulk material have been studied carefully using low-resolution and HR-TEM bright-field images. Figure 1 shows the strain-relaxed low defect density GaSb (120 nm) buffer on GaAs and the GaSb/GaAs interface along the [1–10] direction. The bright spots in both images correspond to misfit dislocation sites.[18] The misfits are arranged in a highly periodic array and localized at the GaSb/GaAs interface. No threading dislocations or dark-line defects are detectable in the bulk and no misfit dislocations exist at any other location. The misfit separation, measured to be ~56 Å, corresponds to exactly 13 GaSb lattice sites and 14 GaAs lattice sites. Thus, every 14th Ga atom has a pair of dangling bonds (one going into and out of the image plane) to accommodate the larger Sb atom in the next (001) plane. An identical misfit array has also been noted in the GaSb/GaAs interface along the [110] direction.

Careful examination of the atomic lattice surrounding the misfits using very HR-TEM, as in Fig. 2, allows the identification of misfits and analysis of strain relief. Completing a Burger's circuit around one misfit dislocation indicates that the Burger's vector lies along the interface and identifies the misfit as 90° type. Measurement of the GaAs substrate and GaSb bulk lattice constants within 4 MLs of the interface yield $a_o=0.398$ nm and $a_o=0.430$, respectively, which are equivalent to the published values along [1–10] and indicate complete strain relaxation.

Most of the strain energy generated by the GaSb/GaAs lattice mismatch is dissipated by the misfit array at the interface. In the following paragraph, we calculate and compare the strain energy areal density E_ε, with the energy density dissipated from a 2D misfit array, E_d'. The strain energy density, E_ε, is found using $E_\varepsilon=\varepsilon^2 Bh=0.182\,62 J/m^2$, where $\varepsilon_\parallel=a_s-a_f/a_f$ and $B=2\mu_f(1+\nu)/(1-\nu)$.[6] In these equations, $\varepsilon_\parallel$ is the in-plane strain, B is a constant, $h=0.38$ nm is thickness of the strained material measured from transmission electron microscopy (TEM), $a_s=0.565\,325$ nm, is the in-plane lattice constant of the GaAs substrate, $a_f=0.609\,593$ nm is the lattice constant of the relaxed GaSb film, $\mu=2.4\times10^{10}$ N/m^2 is the GaSb shear modulus, $\nu=0.31$ is GaAs Poisson's ratio, $f=|a_s-a_f|/a_s=0.07831$ is the GaSb/GaAs lattice mismatch, and $b=a_f/\sqrt{2}=0.431\,05$ nm is the Burger's vector along the [1–10] direction in GaAs substrate. The dislocation energy per unit area dissipated by a 2D misfit array is calculated as $E_d'=E_d/S=0.184\,99$ J/m^2, where $E_d\approx\mu_f b^2/4\pi(1-\nu)^6$ is energy per unit length of a single edge dislocation. The misfit spacing, S, can be derived theoretically by $S=b/f=5.504\,70$ nm which agrees very well with $S=5.56$ nm measured from TEM images. A comparison of values for $E_\varepsilon=0.182\,62 J/m^2$ and $E_d=0.184\,99$ J/m^2 for a film thickness of $h=0.38$ nm indicates that the misfit dislocations relieve 98.5% of the strain energy generated by the GaSb/GaAs lattice mismatch at the growth temperature and allow fully relaxed bulk GaSb growth.

The presence of low dislocation densities under optimized growth conditions for thicker GaSb layers (>100 nm) can be verified using KOH etch-pit measurements on the epilayer. The study involves three samples with 3100 nm of GaSb grown on GaAs at growth temperatures of 480, 510, and 540 °C. These wafers were then etched in 20% KOH solution and roughly 100 nm of the epilayer is removed in each case. The etch-pit density results show that the sample grown at 510 °C had the lowest defect density of 7×10^5 defects/cm^2. The 480 °C sample had the highest decoration density of defects/cm all the samples grown. These values provide an upper limit for the defect density numbers and corroborate well with the defect densities measured through TEM. However, for the sample grown at 510 °C, the TEM images did not show any threading dislocations.

We have attempted further studies of the interface growth mode using atomic force microscope (AFM) images and RHEED. As noted above, the RHEED pattern transforms

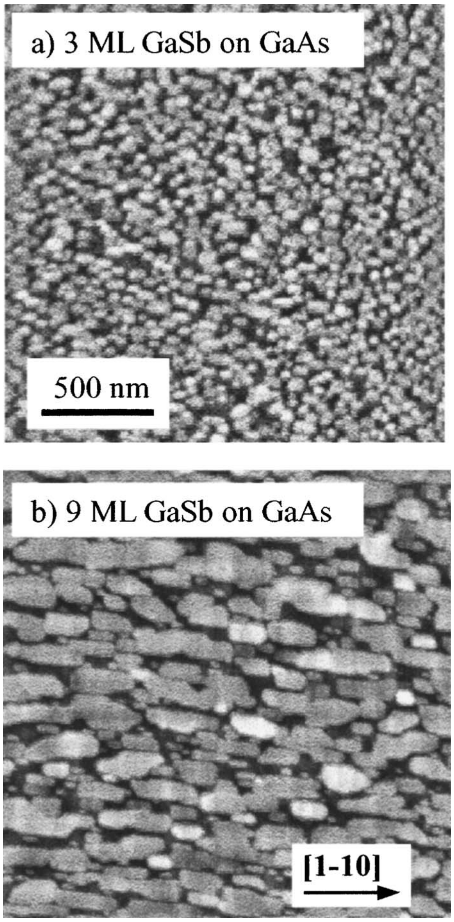

FIG. 3. AFM images of the growth of GaSb on GaAs after (a) 3 ML deposition and (b) 9 ML deposition, showing formation of islands that are elongated along the [1–10] direction.

from a 2×4 to a 1×3 reconstruction within the first 3 MLs of GaSb deposition on GaAs as the As-terminated surface yields to the Sb-terminated surface. However, if the growth is terminated and the substrate temperature reduced after only a few MLs, i.e., at 3 or 9 MLs, the 1×3 reconstruction transforms into a spotty RHEED pattern indicating a island formation. Figure 3 shows AFM images of [Fig. 3(a)] 3 ML and [Fig. 3(b)] 9 ML GaSb deposition on GaAs. The 3 ML deposition results in slightly elongated [1–10] islands that are 6 nm in height, 120 nm length, and 80 nm width with fairly uniform size distribution. The 9 ML deposition leads to larger highly elongated islands with a large variation in island size. Average dimensions are 10 nm in height, 450 nm length, and 120 nm width. The island formation, driven by residual strain, is likely enabled in this growth scenario by the increased adatom migration time allowed after the growth is terminated.

Figures 4 shows a cross-section TEM image of a GaSb island on the sample with 9 ML deposition, cleaved along the [1–10] direction. The image clearly shows the presence of misfit dislocations at the GaSb/GaAs interface. From the low-resolution image, the dislocation separation is measured to be ~50–60 nm. The island is 10 nm high and 50 nm long and bound by the {111} plane. No threading dislocations are observed in this particular island or in numerous other islands. Defective islands are also visible, in low density, on this surface. These defective islands have no misfit dislocations at the interface and appear more dome-shaped rather than crystallographic. The contrast of these two islands indicates the importance of the misfits in enabling this high quality growth mode.

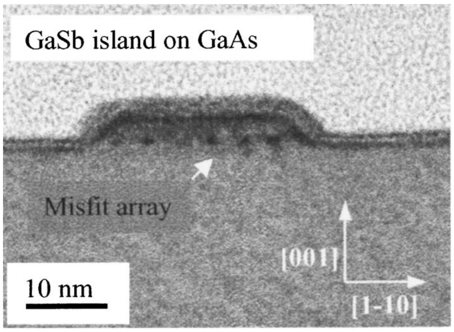

FIG. 4. Cross-sectional TEM image of a GaSb island on GaAs resulting from 9 ML deposition of GaSb with strain relieving misfit dislocations that can be observed at the interface.

In conclusion, we have demonstrated that a periodic array of 90° misfit dislocations can be formed under specific growth parameters to fully relieve strain energy in a highly strained system such as GaSb on GaAs. Our calculations indicate that the misfit dislocation array dissipates the majority 98.5% of strain energy due to the 7.78% lattice mismatch. The growth mode after only 3 MLs of deposition appears planar from observation of RHEED. However, with sufficient surface migration, Ga and Sb adatoms will migrate to form island ensembles in response to the small residual strain. Finally, the low dislocation density, strain-relieved bulk material enabled by this growth mode will lead to new devices, especially in the infrared regime, along with novel integration schemes.

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