Anisotropic structural, electronic, and optical properties of InGaAs grown by molecular beam epitaxy on misoriented substrates

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We have investigated the structural, electronic, and optical properties of partially strain-relaxed In$_x$Ga$_{1-x}$As layers grown by molecular beam epitaxy on both misoriented and nominally flat (001) GaAs substrates. We find large anisotropies in bulk strain relaxation, interfacial misfit dislocation density, dark-line defect density, and electron mobility, as well as polarization anisotropy in cathodoluminescence for epilayers grown on misoriented substrates, in comparison with those grown on flat substrates.

Due to the lack of inversion symmetry in the zinc-blende lattice, orthogonal directions in III-V compound semiconductors are not equivalent. Thus, the orthogonal (110) dislocations ($\alpha, \beta$) and (001) surface steps ($A, B$) in these materials have different properties that affect the uniformity of processes such as epitaxial growth and strain relaxation. Anisotropies in the electrical and optical properties of these materials and devices fabricated in the [110] and [001] in-plane directions are often observed. Such asymmetries are usually associated with asymmetric strain relaxation, lattice defects, and/or surface morphologies, whose relative effects on electronic and optical properties in most cases are not understood. Complete correlations between asymmetric structural, electronic, and optical properties are lacking in the literature.

Anisotropic properties are also affected by epitaxial growth on misoriented substrates. The magnitude and direction of substrate misorientation have been found to affect electron mobility asymmetries in nearly lattice-matched modulation-doped AlGaAs/GaAs heterostructures, the degree of asymmetry in misfit dislocations formed during strain relaxation of In$_x$Ga$_{1-x}$As/GaAs interfaces, and the electron mobility and optical anisotropies of thick (~3 $\mu$m) In$_x$Ga$_{1-x}$As layers grown by metal vapor phase epitaxy. The exact mechanisms for each of these effects is not clear, and in each case, a complete investigation of the material properties was not undertaken. Therefore, in this letter, we have investigated the effect of substrate mismatch towards (011), on asymmetries in structural, electrical, and optical properties, for partially relaxed lattice- mismatched In$_x$Ga$_{1-x}$As layers grown on (001) GaAs by molecular beam epitaxy (MBE).

We emphasize comparisons between the structural, electrical, and optical properties of relatively thin layers (280 nm) with a low indium composition ($x=0.06$).

Samples were grown by solid-source MBE, with As$_4$/group III beam equivalent pressure ratios of 40 and growth rates of 0.9 $\mu$m/h. The sample structures consisted of 280 nm Si-doped ($N_d=10^{15}$ cm$^{-3}$) In$_{0.06}$Ga$_{0.94}$As on 500 nm undoped GaAs buffers grown simultaneously on semi-insulating (001)-oriented GaAs substrates (a) nominally flat ($\pm 0.05^\circ$) and (b) misoriented by 2$\pm 0.5^\circ$ towards the nearest (011) plane. The nominal substrate temperatures were $T_s=580$ °C for the growth of GaAs and $T_s=535$ °C for the growth of In$_x$Ga$_{1-x}$As.

Samples were characterized with x-ray rocking curves (XRC), cathodoluminescence (CL), and Hall measurements. XRC were measured with a high resolution x-ray diffractometer using CuK$_{\alpha1}$ radiation monochromated by four Ge(220) crystals. Symmetric (004) as well as asymmetric (224) rocking curves were recorded at several azimuthal angles to obtain the alloy composition, strain relaxation, and epilayer tilt. Scanning CL and linearly polarized cathodoluminescence (LPCL) measurements were performed with a modified JEOL 840-A scanning electron microscope. A rotatable linear polarizer was mounted in vacuo and a photomultiplier tube was used to measure the signal dispersed by a 0.25 m monochromator. An electron beam energy of 15 keV and a beam current of 10 nA was used to probe the sample which was cooled to 87 K. Resistivity and low field (0.1 T) Hall measurements were performed at room temperature and 77 K with six-arm Hall bars (200 X 800 $\mu$m) aligned along both the [110] and [101] directions. These were fabricated by standard photolithographic and lift off processes, with AuGe/Ni contacts deposited in vacuum and annealed at 450 °C.

Results from XRC measurements of both samples are presented in Table I. The sample grown on the nominally flat substrates relaxed 13$\pm$1% and 12$\pm$1% in the [110] and [001] directions, respectively. The anisotropy, $\sim 4\pm 8%$, is insignificant in comparison to the experimental error. Assuming that the in-plane compressive strain relaxes entirely via the edge component of 60° dislocation, the misfit dislocation density in each [110] direction is estimated as $D=(2\sqrt{2}\varepsilon/a)$, where $\varepsilon$ is the relaxed strain and $a$ is the epilayer lattice constant. Thus, the calculated dislocation density in the both [110] directions is 2.5$\pm 0.1\times 10^4$ cm$^{-1}$.

The sample grown on the misoriented substrate relaxed 8$\pm$1% and 20$\pm$1% in the [110] and [101] directions, a large anisotropy of $\sim 43\pm 7%$. The average relaxation, 14$\pm$1%, is slightly larger than that of the flat substrate. In this case, the
TABLE I. Strain relaxation data, electron mobilities $\mu$, and electron concentrations $[n]$ at room temperature and 77 K in both (110) directions, for 280 nm In$_{0.6}$Ga$_{0.4}$As layers grown simultaneously on nominally flat and misoriented (2° towards the (011) plane) (001) GaAs substrates.

<table>
<thead>
<tr>
<th>Substrate</th>
<th>Strain relaxation</th>
<th>$\mu$ (300 K) (10^3 cm^2/V s)</th>
<th>$[n]$ (300 K) (10^16 cm^-3)</th>
<th>$\mu$ (77 K) (10^3 cm^2/V s)</th>
<th>$[n]$ (77 K) (10^16 cm^-3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominally flat</td>
<td>[110]</td>
<td>13±1</td>
<td>4.4±0.1</td>
<td>6.7±0.1</td>
<td>5.0±0.1</td>
</tr>
<tr>
<td></td>
<td>[110]</td>
<td>12±1</td>
<td>4.5±0.1</td>
<td>6.7±0.1</td>
<td>5.0±0.1</td>
</tr>
<tr>
<td>Misoriented</td>
<td>[110]</td>
<td>8±1</td>
<td>4.3±0.1</td>
<td>7.1±0.1</td>
<td>4.9±0.1</td>
</tr>
<tr>
<td></td>
<td>[110]</td>
<td>20±1</td>
<td>5.0±0.1</td>
<td>7.9±0.1</td>
<td>3.7±0.1</td>
</tr>
</tbody>
</table>

calculated dislocation densities are 1.8±0.1 and 4.5±0.2×10^4 cm^-1 in the [110] and [110] directions, respectively.

Tilting of the epilayer with respect to the substrate is detected in both samples in proportion to the substrate offset, consistent with previous results. The tilt of the epilayer grown on the nominally flat substrate is 0.006° with an orientation 35° away from the [110] direction, revealing the original substrate offset orientation (not specified by the manufacturer). The tilt of the epilayer grown on the misoriented substrate is 0.017° with the same tilt orientation as the original substrate misorientation (tilted towards the [010] direction).

Typical CL images ($\lambda=869$ nm) of the samples grown on the flat and misoriented substrates are shown in Figs. 1(a) and 1(b). These pictures indicate a qualitative asymmetry in dark line defect densities in the sample grown on the misoriented substrate but not in the sample grown on the nominally flat substrate. LPCL spectra of both samples were taken with the analyzer rotated to detect emission of light with electric field perpendicular, $E_\perp$, and parallel, $E_\parallel$, to[110] detection orientations as a function of wavelength. Average values of $I_\parallel/I_\perp$ were measured from integrated LPCL spectra taken while the electron beam was rapidly scanning each region, approximately 100 $\mu$m^2. Average values of $I_\parallel/I_\perp$ for the sample regions displayed in Fig. 1 are 0.926 and 0.877, for the samples grown on the flat and the misoriented substrate, respectively.

The polarization and energy dependence of luminescence provides information about the strain-induced splitting of the heavy-hole (hh) and light-hole (lh) valence bands at $k=0$. When the in-plane strain relaxation is isotropic, there is an in-plane biaxial stress, and no polarization of hh or lh excitonic emissions is expected for emission normal to the (001) plane. When the in-plane strain relaxation is highly anisotropic, the stress is approximately uniaxial with a stress relief along the relaxation direction. For a uniaxial stress along a (110) direction, the mixing of hh and lh characters in the strain-split bands is negligible, hh excitonic emission is totally linearly polarized perpendicular to the same (110) direction, and lh excitonic emission is partially linearly polarized parallel to the same (110) direction. For a (110) uniaxial compressive stress, the lh excitonic emission has the lowest energy. The increased deviation of $I_\parallel/I_\perp$ from unity for the sample grown on the misoriented substrate in comparison to that of the sample grown on the flat substrate is indicative of an increase in the density of regions of uniaxial stress, and an increase in strain relaxation anisotropy. Since the luminescence intensity is highest when $E_\parallel[110]$, it is expected that the regions of uniaxial compressive stress, and anisotropic strain relaxation, correspond to regions which have enhanced relaxation along [110], in agreement with the strain relaxation asymmetry determined by XRC.

The electrical properties of both samples are summarized in Table I. At room temperature, the sample grown on the flat substrate has equal electron concentrations and electron mobilities, to within experimental error, in both (110) directions. In the temperature range of our measurements, both GaAs and InAs are extrinsic, and we expect the electron concentration to remain constant with temperature. Thus, the observed reduction in electron concentration at 77 K in comparison to room temperature is an indication of acceptor-like electron traps in the material. This has been further confirmed by depth-dependent CL and PL measurements which indicate that there are deep-level states in this material.

![CL images](image_url)
Furthermore, photoconductivity measurements of similar samples suggest that the observed deep levels are acceptor-like. Finally, the mobility anisotropies for the sample grown on the flat substrate are negligible at room temperature and 77 K.

For the sample grown on the misoriented substrate, the electron concentrations are asymmetric at room temperature and symmetric at 77 K. The mobility anisotropies are significant, 15 ± 1% at room temperature and 77 K. Again, the reduced electron concentration at 77 K in comparison to that at room temperature is an indication of acceptor-like traps in the material. The presence of deep levels in this material has also been confirmed by the depth-dependent CL and PL measurements mentioned earlier. The anisotropy in electron concentration at room temperature suggests that there are different sets of scatterers acting in the two [110] directions, or an inhomogeneous distribution of traps in this material.

Electron mobility asymmetries of two-dimensional electron gases (2DEGs) confined in quantum-well structures have often been attributed to electron scattering from asymmetric distributions of misfit dislocations. In our case, this is not likely because the direction of highest electron mobility, [110], is also that of highest misfit dislocation density. Alternatively, one set of (110) misfit dislocations (or point defects associated with misfit dislocations) is electrically active. This would be consistent with the asymmetric electron concentration and may account for the reduced electron mobility in the [110] direction for both samples. However, the surface and interface depletion widths are approximately 100 and 20 nm. Thus, the region which contains carriers (electrons) is not located at the interface (as in the 2DEG case) but lies in a region between 10 and 200 nm above the interface. Thus, interfacial contributions to the bulk electron mobility may be insignificant.

The mobility asymmetry may be partly due to variations in residual strain, since the highest electron mobility is in the direction of greatest strain relaxation. Monte Carlo simulations of the effects of strain on electron transport in bulk InGaAs have indicated that the electron mobility of strain-free InGaAs will be higher than that of strained InGaAs, consistent with our asymmetry direction. However the magnitude of our asymmetry is much greater than that predicted in these simulations. An additional contribution may be electron scattering due to the piezoelectric effect. The zinc-blende lattice has one piezoelectric constant, $d_{14}$, which couples to shear (uniaxial) stresses. Thus, piezoelectric effects may contribute to the asymmetry in the presence of a nonzero uniaxial stress, which occurs when the in-plane strain relaxation is anisotropic.

In summary, we have studied the effect of substrate misorientation towards (011) on anisotropic structural, electronic, and optical properties of partially strain-relaxed In$_x$Ga$_{1-x}$As layers grown on GaAs (001) by MBE. Mobility measurements using Hall bars aligned along the [110] and [110] directions reveal an asymmetry in the bulk InGaAs electron mobility for the layer grown on the misoriented substrate. This asymmetry is correlated with an anisotropic bulk strain relaxation, an anisotropic CL dark-line defect density, and an optical polarization anisotropy.

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