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Metamorphic buffers and optical measurement of residual strain

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We show that the residual strain occurring in constant-composition metamorphic buffer layers of III–V heterostructures can be accurately predicted by the suitable design of the epitaxial structures and measured all optically by means of photoreflectance spectroscopy. This result allows one to single out the nonequilibrium models among those that have been proposed to predict strain relaxation. The resulting $\propto t^{-1/2}$ dependence of the residual in-plane strain on buffer thickness t can be used to design metamorphic buffers not only for 1.3–1.55 μm emitting quantum dot structures, but also for sophisticated graded-composition metamorphic structures for different classes of devices. © *2005 American Institute of Physics*. [DOI: 10.1063/1.2159106]

The engineering of physical properties of III–V semiconductor heterostructures often requires the use of epitaxial layers lattice mismatched to the substrate. For III–V-based devices, the substrate of choice is generally GaAs, since it is available as 6 in. diameter wafers and as a semi-insulating material. Moreover, as compared to InAs, InP, and GaSb, it is relatively less brittle, and has a much better structural quality, a more assessed technology, and lower cost.

In lattice-mismatched structures consisting of layers with a thickness in excess of the critical thickness (t_C) for plastic relaxation, misfit dislocation (MD) networks are formed. To this respect, metamorphic buffers (MBs) behave as a virtual substrate that can be designed in order to accomodate the lattice parameter of the topmost structure to that of the underlying substrate. MBs allow the reduction, by orders of magnitude, of the density of dislocations by confining them in definite regions of the structure, which can be kept apart from the active volume of the device. MBs may have constant or graded composition, either in a steplike or in a continuous way.[1–3] MDs can also give rise to threading dislocations that may reach the active region of the structure,[3,4] thus spoiling its physical properties. For these reasons MBs have been used to improve the performances of a number of device structures, such as HEMTs,[5] HBTs,[6] and multijunction solar cells.[7] Moreover, MBs have been usefully inserted in quantum dot (QD) structures where they act by reducing the lattice mismatch between confining layers (CLs) and QDs. It has been experimentally shown[8–10] and modeled[10] that, in such a way, the operation wavelength can be redshifted toward the 1.3–1.55 μm range, as a consequence of the reduced energy gap of InAs QDs grown on GaAs.

In this letter, we focus on constant-composition MBs in InAs/InGaAs QD structures and we demonstrate that: (1) By using MBs with a suitable composition and thickness, the strain of structures grown atop the buffers and some of their properties can be controlled; (2) the residual strain of MBs can be accurately measured all optically by means of photoreflectance (PR) spectroscopy in the spectral region of the fundamental energy gap; and (3) the strain of the structures can be accurately predicted by using the results of a class of models of strain relaxation (nonequilibrium models). The optical quality and the strain of the structures were also checked by spectroscopic ellipsometry through the energy position and line shape of interband transitions at critical points above the fundamental gap.

Knowledge of the dependence of residual strain on buffer thickness can be used to design MBs not only for long-wavelength-emitting QD structures, but also for the aforementioned devices. Moreover, the ascertained dependence can be used to reliably design more sophisticated graded-composition metamorphic structures, that may have further advantages as compared to constant-composition ones.

The investigated structures consist of InAs QDs with 3 monolayer coverage, grown by atomic layer molecular-beam epitaxy on (100) GaAs substrates; the QDs are embedded between $In_xGa_{1-x}As$ confining layers with x=0.15, 0.28, and 0.31. The lower CLs (LCLs) act as constant-composition MBs and—by means of the strain relaxation mechanism—their thickness t (20 nm$\leqslant t \leqslant$360 nm) is used to control their lattice parameter and the strain of the overlying QDs. The upper CL (UCL) is 20 nm thick for all samples and is assumed to be pseudomorphic to the LCL. Further details on the design and growth of structures are given in Ref. 10.

PR measurements were performed at near-normal incidence in the 0.8–1.5 eV range, with an energy step and spectral resolution of 1 meV, in the 80–300 K temperature range. Details on experimental apparatus and data analysis are reported elsewhere.[11] Ellipsometric spectra were taken at room temperature in the 1.4–5.0 eV range using a rotating polarizer SOPRA ellipsometer at two angles of incidence (70° and 75°) on pairs of identical samples with and without UCLs.

The ellipsometric results confirm the good structural and optical quality of the structures. In Fig. 1, we report the imaginary part ε_2 of the complex dielectric function of the

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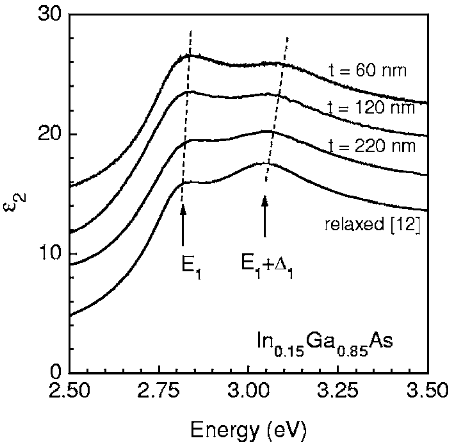

FIG. 1. Imaginary part of the complex dielectric function of $In_{0.15}Ga_{0.85}As$ LCL with different thicknesses and of fully-relaxed $In_{0.15}Ga_{0.85}As$ material (after data of Ref. 12) in the interband spectral region. Each curve is shifted vertically by 3 for clarity.

$In_{0.15}Ga_{0.85}As$ LCLs in the 2.5–3.5 eV range, as derived from the analysis of the ellipsometric functions measured on samples without UCLs. The ε_2 spectra are obtained from numerical inversion assuming the structural model of the sample and keeping the dielectric functions of GaAs, InAs, and $In_{0.15}Ga_{0.85}As$ from literature.[12] The behavior of ε_2 spectra, as a function of the LCL thickness, obeys the predictions of strain effects on the interband dielectric function of ternary alloys.[12,13] The two clear peaks are related to the convolution of the E_1 and $E_1+\Delta_1$ interband critical point response. With decreasing the LCL thickness, we note a blueshift of the center of gravity of the E_1 and $E_1+\Delta_1$ peaks and an increase of the spin-orbit splitting Δ_1. In addition, the E_1 oscillator strength increases with respect to that of $E_1+\Delta_1$, as expected, due to the reduced coupling between the electronic states. Both of these are clear fingerprints of an increasing strain along the growth direction.[12]

In Fig. 2 room-temperature PR spectra in the region of the fundamental gap of $In_xGa_{1-x}As$ are reported for two typical samples with $x=0.15$ and different LCL thicknesses ($t > t_C \cong 43$ nm). The two PR features (E_0^{HH} and E_0^{LH}) can be related to the interband transitions from the heavy-hole (HH) and the light-hole (LH) valence bands, split by the residual strain in $In_{0.15}Ga_{0.85}As$ CLs.[14,15] The analysis of the PR spectra was carried out by using typical line shape models characterizing electromodulated signals in bulk semiconductor systems, and interpreted according to the Aspnes treatment.[16]

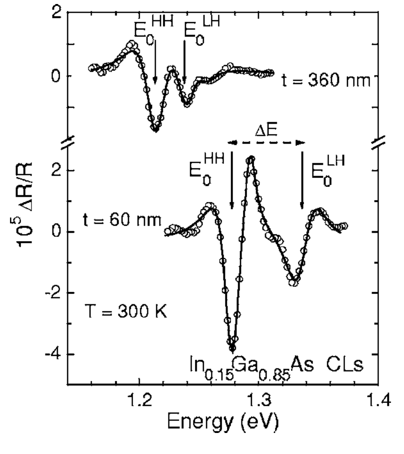

FIG. 2. PR spectra of $InAs/In_xGa_{1-x}As$ samples with $x=0.15$ and different LCL thicknesses. Evidence is given for the shift of the band gaps E_0^{HH} and E_0^{LH} and their splitting ΔE as induced by the CL residual strain. Arrows mark the transition energies derived from the best fit (solid line) to the experimental line shape (open circles).

Epitaxial $In_xGa_{1-x}As$ layers grown on (100) GaAs substrate are subject to a (100) biaxial stress, which can be decomposed into a hydrostatic and an uniaxial component. Both components affect the energy gaps and the second one splits the HH and LH valence bands by $\Delta E = E_0^{\mathrm{LH}} - E_0^{\mathrm{HH}}$. According to the deformation potential theory,[17,18] the resulting energy gap and splitting may be expressed in terms of the in-plane strain $\varepsilon = (a_0 - a_x)/a_x$ by:

$$E_0^{\mathrm{HH}} = E_0 + \delta E_H - \delta E_S/2, \quad \Delta E = \delta E_S - (\delta E_S)^2/2\Delta_0, \qquad (1)$$

where $\delta E_H = 2a\varepsilon\,(C_{11}-C_{12})/C_{11}$ and $\delta E_S = 2b\varepsilon\,(C_{11}+2C_{12})/C_{11}$; E_0 is the unstrained energy gap, a_0 and a_x are the GaAs and the free-standing $In_xGa_{1-x}As$ lattice parameters, while a and b are the hydrostatic and the shear deformation potentials, C_{ij} is the elastic stiffness constant, and Δ_0 is the spin-orbit splitting energy. The values of a and b, C_{ij}, and Δ_0 of the InGaAs alloys were obtained by linear interpolation between the end-binary materials GaAs and InAs.[14,20]

In epilayers with thicknesses exceeding t_C, partial strain relaxation occurs by means of plastic deformation[2,19] and the in-plane lattice parameter $a_x^{\parallel}$ of the partially relaxed $In_xGa_{1-x}As$ layer is related to the residual strain $\varepsilon_{\mathrm{res}}$ by $\varepsilon_{\mathrm{res}} = (a_x^{\parallel} - a_x)/a_x$, with $a_0 < a_x^{\parallel} < a_x$.

We determined the strain all optically from the measured valence bands splitting ΔE by using Eqs. (1). As an example, for the $x=0.15$ samples, the ΔE value varies monotonically from 64 to 24 meV with increasing t from 20 to 360 nm. It is worth noting that, according to Eq. (1), the value of residual strain of CLs could be deduced by the shift of the energy gap $\Delta E_0 = E_0^{\mathrm{HH}} - E_0$, which is linearly related to the strain. However, this approach has drawbacks: (a) It requires the knowledge of E_0 as a function of x, with an accuracy of a few meV, which is generally not available,[14,15] and (b) it is directly affected by the uncertainty in the composition x of the epitaxial layers via the E_0 value. For these reasons, we propose using the information derived from the valence-band splitting ΔE, which does not depend on the absolute energy values and is less affected by the composition.

In Fig. 3, we show the $\varepsilon_{\mathrm{res}}$ values in structures with LCL thicknesses ranging from 20 to 360 nm and different compositions x. The PR measurements were also performed on some samples without UCL and dots. From the comparison of these spectra to the corresponding ones with UCL, only negligible variations have been observed in the parameter values of E_0^{HH} and E_0^{LH} transitions, confirming that UCLs are pseudomorphic to LCLs. The uncertainty of the PR estimate of the residual strain runs from 2×10^{-4} to 3×10^{-4} in the $x=0.15-0.31$ range and is due both to composition fluctuations and to PR transition energies accuracy (±1 meV) to the same extent.

In the case of InGaAs epitaxial layers grown on GaAs substrates, two phenomenological relationships were put forward to describe the partial relaxation of compressively strained layers with uniform composition and thickness larger than t_C. They are $\varepsilon_{\mathrm{res}} \propto t^{-n}$, with $n=1/2$ (Ref. 20) or $n=1$ (Ref. 2). Figure 3 unarguably shows that the experimen-

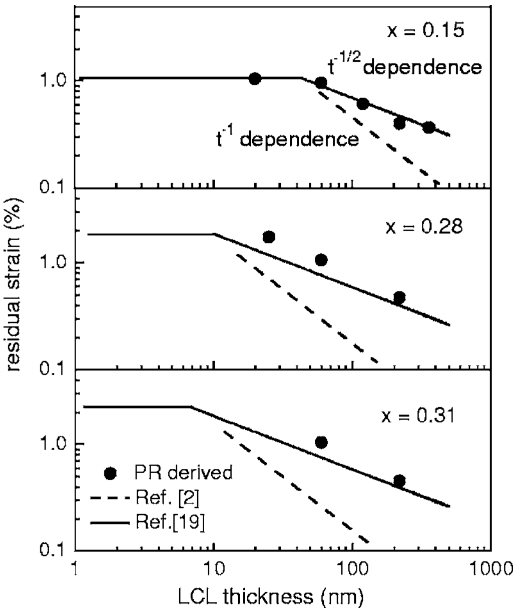

FIG. 3. PR-determined residual strain values (dots) of the CLs in $InAs/In_xGa_{1-x}As$ QD structures of different composition x and different LCL thickness t, [as compared to the results of Ref. 2 and Ref. 19 models (lines)]. Horizontal lines represent the pseudomorphic regimes.

tal results point to a $t^{-1/2}$ dependence of ε_{res} instead of a t^{-1} one. The $n=1/2$ dependence has been interpreted on the basis of the so-called nonequilibrium models of strain relaxation (energy-balance and nucleation models, described in Refs. 21 and 19, respectively). On the other hand, the t^{-1} dependence is the result of equilibrium models that take into account the thermodynamic equilibrium between a rectangular grid of MDs and the strained epitaxial layer.[22,23] The $n=1/2$ dependence has been observed also in other mismatched systems, such as AlGaSb/GaAs.[24] It is interesting to note (see Fig. 3) that the experimental value corresponding to a pseudomorphic layer ($x=0.15$, $t=20$ nm) falls exactly on the theoretical segment representing the pseudomorphic regime.

In conclusion, we have shown that: (a) The lattice parameter of metamorphic buffers can be designed by exploiting the strain relaxation process; this in turn allows one to control the strain of the structures grown atop buffers and, then, their properties; (b) PR is an efficient tool to measure the residual strain of epilayers, with accuracy comparable to that of x-ray diffraction[24] and Rutherford backscattering;[20] and (c) the strain relaxation obeys the predictions of nonequilibrium models, such as that proposed in Ref. 19. In addition, these results are of great interest for the engineering of both QD structures for long-wavelength operation and advanced heteroepitaxial structures, where graded-composition MBs gain advantages over the constant-composition counterparts,[1] in regard to the distribution of dislocations far from the active region of the structures.

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