Depth profiles of perpendicular and parallel strain in a $GaAs_xP_{1-x}$/GaP superlattice

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Using double-crystal x-ray rocking curves, depth profiles of parallel and perpendicular strain were obtained in a $GaAs_{0.14}P_{0.86}$/GaP superlattice grown on a buffer layer on (100) GaP. Combining symmetric Fe $K_{\alpha 1}$ (400) and asymmetric Cu $K_{\alpha 1}$ (422) reflections, a constant parallel strain of 0.19% relative to the substrate was found throughout the superlattice and buffer layer. Relative to the substrate, the perpendicular strain was found to be 0.26% in the buffer, and 0.80% and -0.19% in the 176-Å-thick superlattice $GaAs_xP_{1-x}$ and GaP layers, respectively. The strain profiles indicate the buffer is $\sim 80\%$ decoupled from the substrate by misfit dislocations near the buffer/substrate interface, and the lattice misfit in the superlattice is elastically accommodated by the epitaxial structure with a small shift in the average lattice constant relative to the equilibrium superlattice structure.

Superlattices[1] are a class of epitaxial materials grown by periodic depth modulation of the composition. When the lattice parameters of the alternating layers are unequal, the modulation of the composition results in a modulation of the lattice parameter (i.e., strain). For strained-layer superlattices (SLS's) of good quality, the misfit strain is entirely accommodated by elastic deformation in the layers. The electrical and optical properties of semiconductor SLS's depend on the state of strain as well as on the composition modulation of the layers.[2]

Present growth procedures frequently incorporate a buffer or graded layer between the superlattice and the substrate.[3–5] Models of strain in the superlattice and buffer have evolved from measurements of dislocation densities,[3,4,6] and by ion channeling,[5,7] electrical,[8] and optical[4] property measurements. It is thought that if the buffer is sufficiently thick, the lattice mismatch between the buffer and substrate can be accommodated by misfit dislocations in the buffer layer. If a buffer composition close to the average composition of the superlattice is used, the lattice constant at the buffer surface can be set to minimize the elastic strain energy stored in the SLS. In this idealized case, the superlattice is decoupled from the substrate and the state of strain in the superlattice is determined entirely by the lattice mismatch, elastic properties, and thicknesses of the superlattice layers.

Double-crystal x-ray diffraction has also been used to obtain depth profiles of composition and superlattice strain in the direction perpendicular to the crystal surface.[9,10] However, x-ray rocking curves are also capable of providing depth profiles of strains in directions other than perpendicular to the surface.[11,12] In this letter we present rocking curve determinations of the depth profile of strain both perpendicular and parallel to the surface for a $GaAs_xP_{1-x}$/GaP superlattice. The results provide the first direct determination of the three-dimensional state of the strain in SLS and buffer layers.

The superlattice was grown by metal organic chemical vapor deposition (MOCVD) on a (100) oriented GaP substrate at 800 °C.[13] The superlattice consists of 30 alternating layers of GaP and $GaAs_xP_{1-x}$ with x near 0.14. A $GaAs_yP_{1-y}$ ($y \sim 0.07$) buffer layer was grown between the substrate and superlattice. For directions perpendicular and parallel to the (100) surface we define the strain in the layers relative to the substrate by

$$\epsilon^i = (a_f^i - a_s)/a_s, \tag{1}$$

where i corresponds to $\parallel$ or $\perp$, and a_f and a_s refer to the film and substrate lattice parameters, respectively. This definition of strain differs from the standard definition in elasticity theory where strain is defined relative to the lattice parameter of the free film rather than the substrate. From the equilibrium lattice parameter of the film, it is a simple matter to convert x-ray strain given by Eq. (1) to the strain of elasticity theory.

Double-crystal x-ray rocking curves were obtained using the Fe $K_{\alpha 1}$ (400) and Cu $K_{\alpha 1}$ (422) reflections. The symmetric (400) reflection is sensitive to $\epsilon^\perp$ only, while the asymmetric (422) reflection measures both $\epsilon^\perp$ and $\epsilon^\parallel$. For the (422) reflection with the incident beam at glancing angle $\theta_{inc} = 79°$, the sensitivity to $\epsilon^\parallel$ is five times greater than that to $\epsilon^\perp$. The x-ray beam was first collimated and rendered nearly monochromatic by the (400) reflection in ⟨100⟩ GaAs for the Fe $K_{\alpha 1}$ (400) reflection and by the (333) reflection in ⟨111⟩ Si for the Cu $K_{\alpha 1}$ (422) reflection. The divergence of the beam incident on the sample was less than 20 arcs. The spot size at the sample was limited by a set of slits to 0.5×1 mm or less. The incident beam intensity was 10^4–10^5 counts/s, depending on the reflection and spot size. Rocking curves (reflecting power versus angle) were measured with a microprocessor-controlled diffractometer. A detailed discussion of the application of x-ray analysis to superlattices will be given elsewhere.[14]

Theoretical rocking curves were obtained using a kinematical model of diffraction in epitaxial layers with diffraction in the substrate treated using dynamical theory.[11] The structure factor and normal absorption coefficient were calculated from the approximate composition and tabulated

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atomic scattering values.[15] Although the structure factor of GaP is different from that of $GaAs_{0.14}P_{0.86}$, the average composition was used for the superlattice layers. While the modulation of the structure factor does in general affect the rocking curve, in the present case its influence is much lower than that of the strain modulation.[14] Rocking curves were calculated using the nominal number of superlattice periods (15) and assuming that each period consists of layers A and B, each with its own thickness and $\epsilon^{\perp}$ and $\epsilon^{\parallel}$ values. The presence of a buffer layer of arbitrary thickness and strain gradients was also allowed. The strain distribution was varied through a systematic trial-and-error procedure[11] until a good fit to the experimental curves was obtained. Good agreement between measured and calculated curves determines the average superlattice periodicity and strain, as well as the strain in the buffer layer, to a precision of about $\pm 2\%$.[11] The amplitude of the superlattice strain modulation and the relative layer thickness should be accurate to within 5%.

Figure 1 shows experimental (dashed line) and calculated (solid line) rocking curves. The angle $\Delta\theta$ is shown relative to the Bragg angle of the substrate peak. The abscissa is shown at significantly higher magnification for Fig. 1(b) than 1(a), because of the narrower intrinsic diffraction widths and satellite structure for the (422) reflection. The calculated curves are the plane wave, planar structure solutions convolved with Gaussians with standard deviations of 45 and 20 arcs for Figs. 1(a) and 1(b), respectively. Although in Fig. 1(b) the predicted narrow oscillations for the (422) reflections were not resolved experimentally, the envelopes of the curves are in agreement. The broadening of the narrow oscillations implies small undulations in atomic planes and/or fluctuations in the local value of strain. Although lateral variations in strain and undulations in crystal planes affect the results of Fig. 1(b) much more than Fig. 1(a), both rocking curves imply undulations of less than 1 arcmin.

Final results for the depth profile of the strain corresponding to the rocking curves of Fig. 1 are given in Table I. The Fe $K_{\alpha 1}$ (400) reflection determined the values of the perpendicular strain and layer thickness for the buffer and superlattice. The $\epsilon^{\perp}$ values in the $GaAs_xP_{1-x}$ and GaP layers were found to be uniform throughout the SLS. The $\epsilon^{\perp}$ in the buffer is also uniform throughout most of the buffer layer thickness, with the transition region (where $\epsilon^{\perp}$ drops to zero at the interface with the substrate) confined to less than 10% of the buffer layer thickness. The values of $\epsilon^{\perp}$ obtained with the Fe $K_{\alpha 1}$ (400) rocking curve were used together with the Cu $K_{\alpha 1}$ (422) rocking curve to obtain the depth profile of $\epsilon^{\parallel}$. The large $\epsilon^{\parallel}$ indicates that, to a significant extent, the buffer and superlattice are crystallographically decoupled from the underlying substrate. The uniformity of $\epsilon^{\parallel}$ versus depth suggests that the decoupling has occurred by misfit dislocations originating in a narrow region ($<0.1\,\mu$m) of the buffer near the substrate consistent with previous studies.[6] From the measured parallel strain of 0.19% we may estimate, for example, $\sim 5\times 10^4$ misfit dislocations of type $b = 1/2\ \langle 011\rangle$ along a unit length of line in the plane of growth, or a total of $\sim 10^5/\text{cm}^2$ in the transition region near the buffer/substrate interface.

TABLE I. Profiles of perpendicular and parallel strain in buffer and superlattice. Strain is defined with respect to the substrate [see Eq. (1)].

	Thickness (Å)	$\epsilon^{\perp}$ (%)	$\epsilon^{\parallel}$ (%)
Superlattice[a]			
$GaAs_xP_{1-x}$ layers	176	0.80	0.19
GaP layers	176	−0.19	0.19
Buffer	10 000[b]	0.26	0.19

[a] Number of periods = 15.

[b] Value assuming same structure factor as for SLS. Angle lap and chemical stain results suggest a thicker buffer layer ($\sim 1.7\,\mu$m) suggesting a lowering of the structure factor for the buffer layer possibly due to point defects.

If the buffer layer was totally decoupled from the substrate then the $\epsilon^{\perp}$ and $\epsilon^{\parallel}$ values would be equal to each other and would correspond to the equilibrium lattice constant as defined by Eq. (1). For the case of (100) oriented layers and isotropic in-plane strain, the perpendicular and parallel strains are related by

$$\epsilon^{\perp} = (1 + 2C_{12}/C_{11})\,(a_0 - a_{\text{GaP}})/a_{\text{GaP}} - \epsilon^{\parallel} 2C_{12}/C_{11}, \qquad (2)$$

where the layer $\epsilon^{\perp}$, $\epsilon^{\parallel}$ are referenced to the GaP substrate [Eq. (1)], C_{11} and C_{12} are the elastic constants[16] and a_0 the unstrained lattice constant of the layer. For the $GaAs_yP_{1-y}$ buffer layer we obtain $a_0 = 5.463$ Å; which from Eq. (1) corresponds to $\epsilon^{\perp} = \epsilon^{\parallel} = 0.23\%$. Thus the buffer layer contains a small residual coherency strain of $\Delta\epsilon^{\parallel} = (0.23 - 0.19) = 0.04\%$. Also by Vegard's law for alloyed semiconductors we may infer a composition $y = 0.061 \pm 0.003$, which is close to the nominal value of 0.07. From the $\epsilon^{\perp}$ and $\epsilon^{\parallel}$ values in the SLS we may similarly determine an equilibrium lattice parameter $a_0 = 5.4560$ Å for the $GaAs_xP_{1-x}$ layers, which corresponds to $x = 0.14 \pm 0.01$; independent Rutherford backscattering measurements gave a consistent value of $x = 0.16 \pm 0.02$. One can verify this procedure by applying it to the superlattice GaP layers for which the relaxed unit cell should be identical to the substrate. For the GaP layers, Eq. (2) yields $a_0 = 5.4504$ Å compared to the bulk value of 5.4512 Å. The difference corresponds to an error of -3×10^{-4}, which is

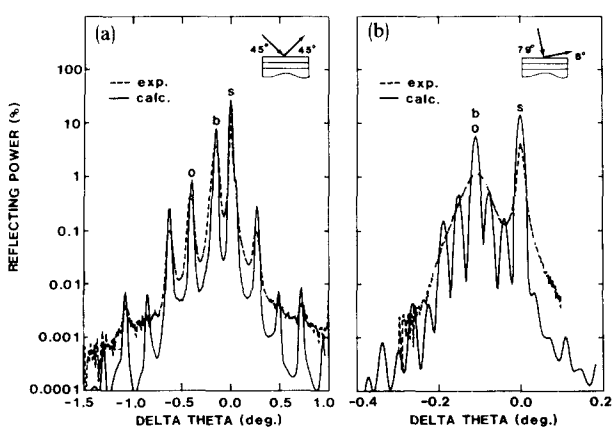

FIG. 1. Measured (dashed line) and calculated (solid line) rocking curves corresponding to the (a) Fe $K_{\alpha 1}$ (400) reflection and (b) Cu $K_{\alpha 1}$ (422), $\theta_{\text{inc}} = 79°$. The substrate, buffer and zero order superlattice peaks are indicated by s, b, and 0, respectively; in (a) the superlattice + 1 order peak falls under the buffer peak.

probably due to a misorientation of $\sim 1°$ in the $\langle 100 \rangle$ axis of the substrate.

The equilibrium value for the in-plane lattice constant of the SLS can be calculated under the conditions of the superlattice floating free of the buffer and substrate.[2] This corresponds to the minimum stored energy in the superlattice, and using the above composition values we obtain an equilibrium $\epsilon^{\parallel} = 0.25\%$. This in-plane strain is larger than the observed $\epsilon^{\parallel}$ of 0.19% and indicates that a small, cumulative component of compressive stress is stored in the SLS. This offset is produced by the slightly lower than ideal lattice constant at the buffer surface, and arises from the residual coherency strain in the buffer and the slightly lower ($y = 0.061$ vs 0.07) than optimal As concentration in the buffer layer. We suggest that such effects may be important factors in the stability of SLS structures under the growth of thick layers or in subsequent device applications.

In summary, we have used x-ray rocking curves to measure the depth profiles of perpendicular and parallel strain in a $GaAs_xP_{1-x}/GaP$ superlattice. The technique is simple, rapid, nondestructive and unmatched in its ability to obtain strain profiles with high precision. The nonzero parallel strain in buffer and superlattice layers provides direct evidence for the hypothesis that the epitaxial structure is crystallographically decoupled from the underlying substrate. The strain decoupling occurs in a narrow region at the buffer/substrate interface. The combined values of parallel and perpendicular strains provide a detailed description of the state of elastic strain of the structure. A discussion of the degree of decoupling for different buffer layer conditions, as well as comparisons with other techniques, will be given later in a detailed report. We may conclude that the x-ray rocking curve method is a powerful tool to determine the complete state of strain of strained-layer superlattices.

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