Structural perfection of InGaAs/InP strained-layer superlattices grown by gas source molecular-beam epitaxy: A high-resolution x-ray diffraction study

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High-resolution x-ray diffraction (HRXRD) studies have been carried out to determine the structural perfection and periodicity for a number of high-quality InGaAs/InP strained-layer superlattices grown by gas source molecular-beam epitaxy. X-ray scans were carried out with a compact four-crystal monochromator resulting in a resolution of one molecular layer (~ 3 Å), which enables one to observe very small variations in the periodic structure. Sharp and strong higher-order satellite reflections in the XRD profiles were observed indicating smooth interfaces with well-defined modulated structures. Excellent computer simulated fits of the x-ray satellite pattern could be generated based on a kinematical XRD step model which assumes ideally sharp interfaces. Our results demonstrate that HRXRD in conjunction with the kinematical step model provides a powerful tool to evaluate the structural perfection of InGaAs/InP strained-layer superlattices.

INTRODUCTION

Recent advances in the gas source molecular-beam epitaxy (GSMBE) have led to the growth of InGaAs/InP quantum well structures of very high crystal quality.[1] Superlattices (SLs) have been grown with very thin wells, sharp interfaces, and well-defined periodic structures along with promising electronic and optical properties for device applications.[2,3] Characteristic for the GSMBE is its capability for excellent control of composition, lattice match, and layer thickness, which makes it possible to grow very closely matched SLs as well as strained-layer superlattices (SLSs) having positive or negative strain. In previous work on lattice-matched InGaAs/InP SLs grown by GSMBE on [100] InP, high-resolution x-ray diffraction (HRXRD) has proven to be an effective tool to evaluate their structural integrity.[4,5] The HRXRD spectra are analyzed with kinematical simulation based on a step model which assumes alternating layers with ideally sharp interfaces. In essence, the x-ray studies on GSMBE SLs demonstrated that kinematical simulation of HRXRD curves allows for very accurate determination of the periodic structure, including small structural modifications in the interfaces. This can be done with a precision of one molecular layer. With the thickness of the well small enough to accommodate the mismatch strain coherently, it is possible to grow either positively or negatively strained $In_xGa_{1-x}As$/InP SLSs by GSMBE spanning a wide range of the In concentration x. In the present study, kinematical simulation of the HRXRD curves has been carried out in order to determine the periodic structural parameters of a number of InGaAs/InP strained-layer superlattices which were grown on [100] InP with various degrees of strain in the InGaAs well. This method appears to be very useful in order to quantitatively determine the strain with the aim of exploring the relationship between strain and the optical and electronic properties of the quantum wells.[6,7]

RESULTS AND DISCUSSION

HRXRD was carried out using the x-ray geometry proposed by Bartels[8] and consisting of a compact four-crystal monochromator, the sample as the fifth crystal and an open-end detector. X-ray scans were taken along the [h00] direction in the vicinity of the (400) reflection with the diffractometer run in the θ–2θ mode. The x-ray scan of the (400) reflection is shown in Fig. 1 for three 10-period superlattices:

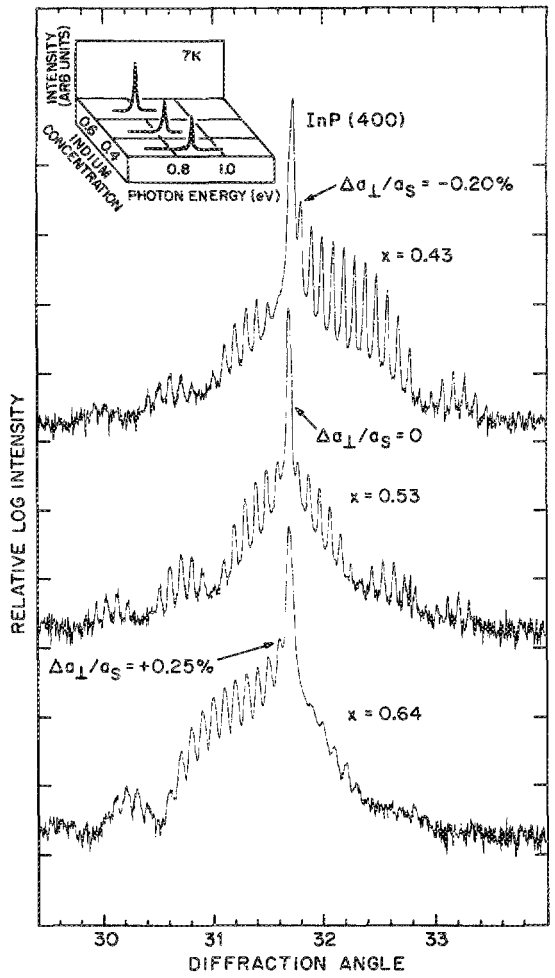

FIG. 1. X-ray diffraction scans of a lattice matched $x = 0.53$, and strained $In_xGa_{1-x}As$/InP superlattice. Inset shows 7-K photoluminescence spectra.

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a negatively strained ($x = 0.43$), a lattice-matched ($x = 0.53$), and a positively strained ($x = 0.64$) SL. The presence of very sharp and strong satellite intensities indicates that these SLSs maintain their structural integrity throughout the whole superlattice. This result is consistent with the low-temperature photoluminescence (PL) spectra (Fig. 1) which show sharp PL peaks up to room temperture.[6] While for the lattice matched SL the satellite intensities are symmetric ($+n$ vs $-n$) around the main (400) SL peak ($n = 0$), a strong asymmetry in the x-ray satellites around the (400) SL peak is characteristic for the SLSs, because of the strain modulation introduced by the accommodation of the large mismatch of the InGaAs wells with respect to the InP barriers. For negative strain as is the case for $x = 0.43$, the ($+n$) satellites become stronger than the ($-n$) satellites [Fig. 1(a)] while for positive strain this asymmetry is reversed as is demonstrated in Fig. 1(c) for the SLS with $x = 0.64$. Normally for zero-strained or weakly strained superlattices the period Λ and lattice mismatch can be directly determined from the x-ray scan[4,5] because the satellite intensities are fairly symmetric around the (400) SL peak. However, for the strongly strained superlattices this strain modulation causes the (400) x-ray satellite pattern to become asymmetric to the extent that the position of the (400) zero-order peak ($n = 0$) of the superlattice can no longer be identified unambiguously.

In order to identify the (400) SL peak and simultaneously determine the structural parameters, the x-ray satellite scans were computer simulated using a previously described kinematical step model which assumes ideally sharp interfaces. This model[9,10] permits calculation of the diffracted amplitude F of the structural periodicity of the superlattice along the [100] growth direction. The variable input parameters of the step model are the lattice spacings d_W and d_B between subsequent atomic layers and the number of molecular layers N_W and N_B in the InGaAs well (W) and InP barrier (B), respectively, where a molecular layer consists of one group III and one group V atomic layer. For alternating wells and barriers the diffracted amplitude F in the vicinity of the (400) reflection ($h = 4$) is given by[9]:

$$F(\mathbf{h}) = \sum_{N_{\mathrm{SL}}} \exp 2\pi i h N_{\mathrm{SL}} \Big((f_{W\mathrm{III}} + f_{W\mathrm{V}} e^{iQd_W}) \times \sum_{n=0}^{N_W - 1} e^{iQ2nd_W} + (f_{B\mathrm{III}} + f_{B\mathrm{V}} e^{iQd_B}) e^{iQ2N_W d_W} \times \sum_{n=0}^{N_B - 1} e^{iQ2nd_B} \Big), \quad (1)$$

where $Q = 2\pi h / d_{\mathrm{SL}} = 4\pi \sin\theta / \lambda$, and θ is the diffraction angle; $f_{W\mathrm{III}}, f_{W\mathrm{V}}$, etc. are the scattering factors for the group III and group V elements, respectively, calculated at the (400) diffraction angle θ, N_{SL} is the number of periods Λ in the superlattice and $N = N_W + N_B$. Once the variable parameters are extracted from the step model, the thickness of the well and barrier can then be calculated from the equations $t_W = 2d_W N_W$ and $t_B = 2d_B N_B$, and the corresponding lattices parameters from $a_\perp^W = 4d_W$ and $a_\perp^B = 4d_B$. The strain in the well is then given by the equation

TABLE I. Structural parameters of 10-well $In_xGa_{1-x}As/InP$ strained-layer superlattices grown by GSMBE.

Λ (Å)	$\Delta a_\perp/a_\perp$ (%)	N_W	N_B	$\epsilon_\perp^W$ (%)	t_W (Å)	t_B (Å)	x(In)
528	−0.2	26	154	−1.4	75	452	0.43
540	0	27	157	0	79	461	0.53
517	+0.25	26	150	+1.5	77	440	0.64
316	−0.3	7	101	−5.0	20	296	0.15
326	−0.32	7	105	−5.7	19	308	0.10
429	+0.66	34	112	+2.7	102	328	0.72
573	−0.63	59	137	−2.2	169	405	0.37

$\epsilon_\perp^W = (a_\perp^W - a_\perp^B)/a_\perp^B$, where $a_\perp^B = a_{\mathrm{InP}} = 5.8687$ Å. From the strained-lattice parameter $a_\perp^W$, the relaxed value can be calculated by multiplying the strain $\epsilon_\perp^W$ with the quantity $c_{11}/(c_{11} + 2c_{12})$ using elastic theory[11]; from Vegard's law, the In concentration x can then be extracted. The results of the kinematical simulation of a number of SLSs are presented, together with the structural parameters obtained from this model, in Table I. Also listed are the period Λ which can be determined from the position of the satellite peaks and the perpendicular lattice mismatch $\Delta a_\perp/a_\perp$ which can be calculated from the difference of the main SL peak ($n = 0$) and the InP peak.[5] As an illustration, the simulated fit is shown in Fig. 2 for one of the three SLs of Fig. 1 ($x = 0.43$) with the structural input parameters listed in Table I, which also lists the fitted parameters of the other two SLs.

With the precision afforded by GSMBE it is possible to grow SLSs with very low In concentrations with the thickness of the well small enough to accommodate the large mismatch coherently. Two such examples of SLSs are shown in

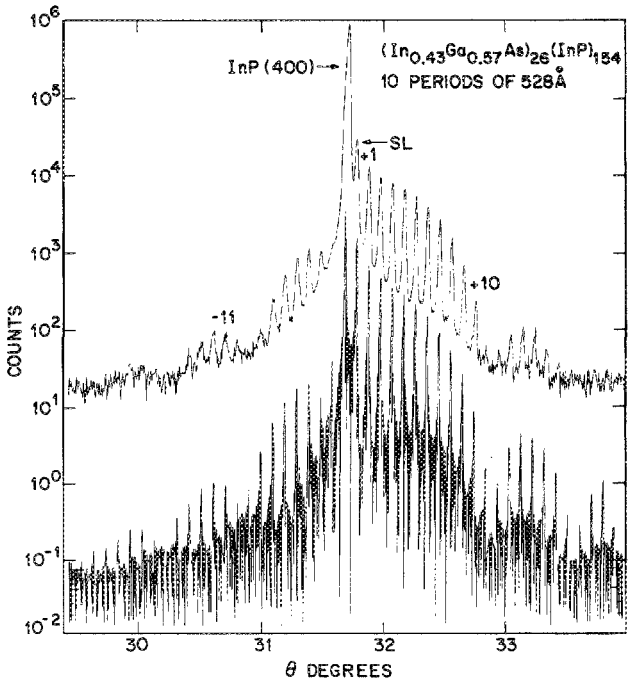
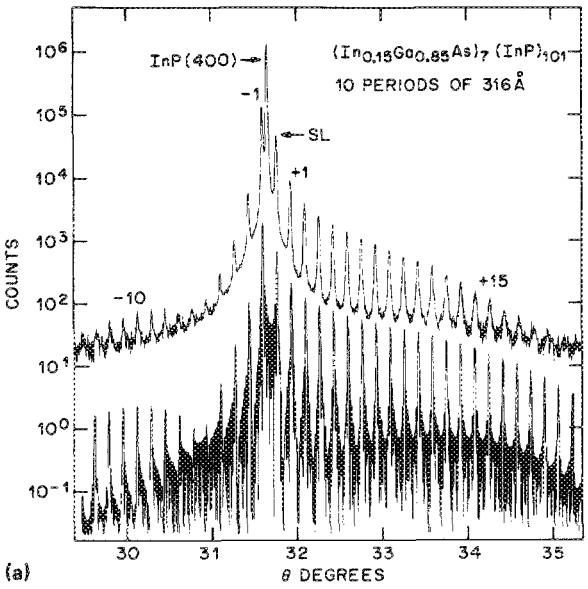


FIG. 2. X-ray scan of the (400) reflection of a 10-well strained-layer $In_{0.43}Ga_{0.57}As/InP$ superlattice with simulation of fit in lower part.

Fig. 3 for nominal In concentrations $x = 0.13$ and 0.075 and a well thickness ~ 20 Å. The very strong asymmetry in the x-ray satellite patterns reveals a very large negative strain $\epsilon_{\perp}^{W}$ as a result of the much lower In concentration in the well. Despite the large lattice mismatch, these SLSs retain their structural perfection, as judged by the sharpness and intensity of satellites and the excellent simulated fits. The fact that excellent computer-simulated fits can be obtained with the kinematical step model, which assumes ideally sharp interfaces, implies that the interfaces in the GSMBE SLSs are indeed extremely smooth and their periodicity is very well defined. Previous work on single quantum-well structures grown by the same method and studied by photoluminescence (PL) show single well-defined PL peaks for layers as thin as 5 Å.[12] The results of this work are consistent with the PL results in that layers of varying thickness, such as may occur with other methods,[13] are not seen .

During a recent study[14] on the relationship between critical layer thickness and electrical characteristics in strained $In_xGa_{1-x}As/InP$ quantum wells, SLSs were grown by GSMBE with the nominal well thickness varying from 40 to as high as 200 Å, while the nominal In composition was kept at $x = 0.37$ and 0.74. Sharp and intense x-ray satellite spectra were measured as shown in Fig. 4 for a low



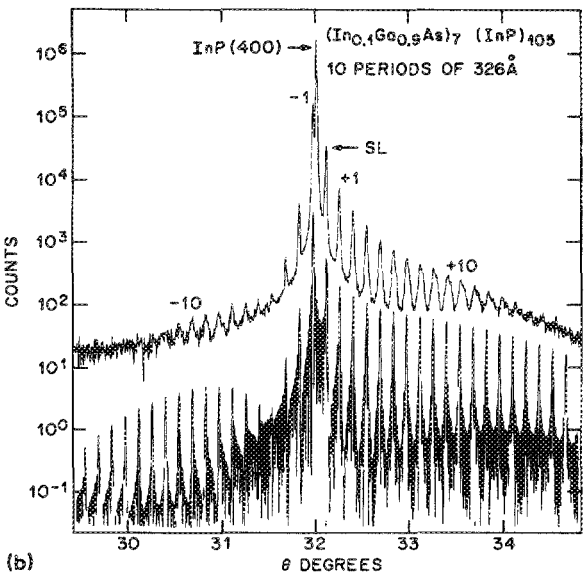
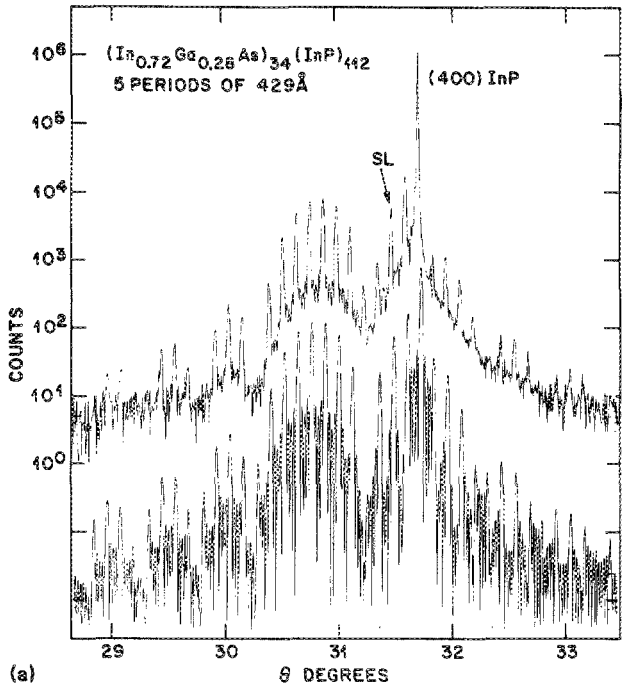


FIG. 3. X-ray scan of the (400) reflection of a 10-well strained-layer $In_xGa_{1-x}As/InP$ superlattice: (a) $x = 0.13$, (b) $x = 0.075$; simulation of fit in bottom part.



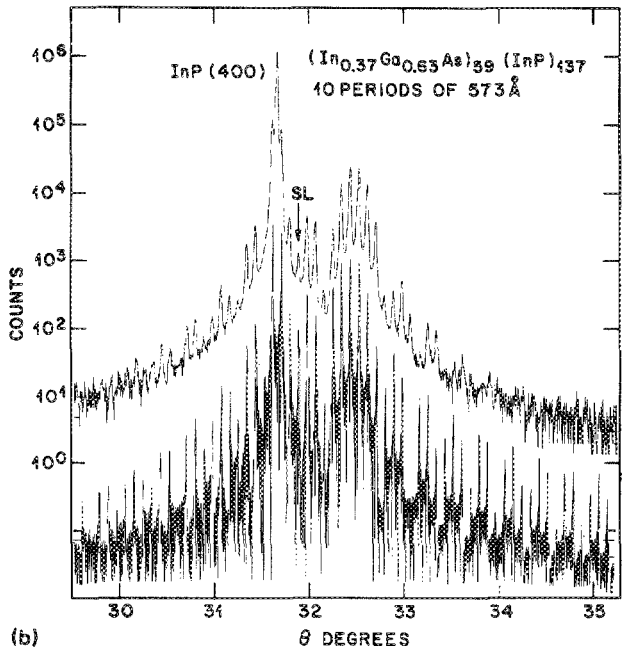


FIG. 4. X-ray scan of the (400) reflection of a 5- and 10-well strained-layer $In_xGa_{1-x}As/InP$ superlattice: (a) 100 Å—well, $x = 0.74$ (b) 200 Å—well, $x = 0.37$.

and high In concentration SLS. Both SLSs were at least partly relaxed by the networks of misfit dislocations as judged from the electrical measurements.[14] Since the electrical measurements are sensitive to a very small amount of relaxation, on the order of 4%, these SLSs maintained most of their structural perfection. It should be noted that the large strain in the relatively thick wells results in very pronounced maxima and minima in the x-ray satellite structure of these two SLSs. In the other SLSs the large strain is accommodated in much thinner wells resulting in a more gradual decrease of the satellite intensities; this is, in particular, so for the two SLSs shown in Fig. 3, where a very large strain of $\sim -5\%$ is accommodated in very thin wells of ~ 20 Å. In either case, despite the large strain or thick wells, these SLSs retain their structural integrity, as judged by the sharpness and intensity of the satellites and the excellent simulated fits.

CONCLUSION

Our results demonstrate that HRXRD curves of GSMBE superlattices can be computer simulated in great detail by using a kinematical step model which assumes a series of alternating layers with ideally sharp interfaces. The successful application of this x-ray method is strongly enhanced by the fact that GSMBE superlattices can be grown with extreme precision and a large degree of structural perfection resulting in a very accurate assessment of the periodic structure and the strain in strained-layer superlattices.

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