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X-ray double-crystal diffraction studies of GaInAsP/InP heterostructures[a) *]

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The lattice mismatch and the half-width of the rocking curves in GaInAsP epitaxial layers grown on (001) InP substrates have been determined by means of x-ray double-crystal diffractometry. The state of strain of GaInAsP epitaxial layers has also been investigated. The relaxed lattice constant of the epilayers in stress-free states has been found from observed lattice deformation using strain relations.

I. INTRODUCTION

There has been great interest in recent years on the quaternary III–V compound GaInAsP/InP epitaxial layers grown on (001) oriented InP substrates for a variety of applications in optoelectronic devices such as heterojunction lasers and photocathodes, etc.[1,2] The control of crystalline perfection, composition, layer thickness, and lattice match between the epitaxial layer and substrate are extremely important for the device properties.[3–6]

In this paper, x-ray double-crystal diffraction studies of epitaxial layers of GaInAsP grown by liquid phase epitaxy is presented. The experimentally determined mismatches and half-widths of rocking curves have given information on the perfection of the epitaxial layers. The relaxed lattice constants of the epitaxial layers in stress-free states was determined from observed lattice deformation using the strain relations.

II. EXPERIMENT

Mismatch and rocking curve measurements were made using a Rigaku x-ray double-crystal diffractometer. The first crystal used is a dislocation-free silicon crystal, Si(111). The Si(224) asymmetric reflection with CuK_{α_1} radiation was used to provide a highly parallel incident beam to the sample crystal. Epitaxial layers of GaInAsP were grown on (001) oriented InP substrates. The compostion (X,Y), wavelength, and thickness of the epitaxial layers are listed in Table I.

III. RESULTS AND DISCUSSION

A. Lattice deformation and mismatch between the epitaxial layer and substrate

GaInAsP epitaxial layers of high perfection may be grown on InP substrates when composition is adjusted properly. Otherwise, deformation from the layers and mismatches between the layer and substrate will occur, not only positively but also negatively. In this situation the same diffraction plane will produce a different peak, i.e., the shift of diffracted peak ΔW will occur from the substrate to the layer.

The difference ΔW includes two components $\Delta\theta$ and $\Delta\varphi$.[7–9] The difference in Bragg angle $\Delta\theta$ comes from the difference in the lattice plane spacing $\Delta d/d$ for the lattice plane of layer and substrate. The second component of ΔW is the difference $\Delta\varphi$ in the inclination with the surface of corresponding plane of layer and substrate. To describe the state of strain of epitaxial layer, $\Delta\theta$ and $\Delta\varphi$ should be obtained separately. For this purpose, ΔW is measured twice from the same reflection plane but with different geometry. In general, the two ways are converted into each other by rotating the sample 180° around the normal of the diffracting lattice planes. So we have one with $W_a = \theta + \varphi$ and another with $W_b = \theta - \varphi$. W_a and W_b are an angle of incidence of the x ray with crystal surface. θ is the Bragg angle and φ is the inclination of the diffraction lattice plane with the crystal surface.

The rocking curves for the (004), $(115)_a$, and $(115)_b$ diffraction are shown in Fig. 1.

For the peak separation of layer and substrate

$$\Delta W_a = W_a^L - W_a^s = (\theta_L - \theta_s) + (\varphi_L - \varphi_s), \quad (1)$$

$$\Delta W_b = W_b^L - W_b^s = (\theta_L - \theta_s) - (\varphi_L - \varphi_s), \quad (2)$$

we have

$$\Delta\theta = \theta_L - \theta_s = \tfrac{1}{2}(\Delta W_a + \Delta W_b), \quad (3)$$

$$\Delta\varphi = \varphi_L - \varphi_s = \tfrac{1}{2}(\Delta W_a - \Delta W_b), \quad (4)$$

since Bragg law

$$2d \sin\theta = \lambda, \quad (5)$$

so that

$$\Delta d/d = -(\cot\theta)\Delta\theta. \quad (6)$$

Assuming the apparent crystal system of the epitaxial layer is deformed tetragonally and $a^{\perp}$ and $a^{\parallel}$ are the lattice constants of the epitaxial layer perpendicular and parallel to (001) plane, respectively, a_s is the lattice constant of the

TABLE I. Parameters of the sample $Ga_{1-x}In_xAs_{1-y}P_y$.

Sample No.	$84\text{-}4\text{-}B_2$	$84\text{-}5\text{-}B_6$	$84\text{-}4\text{-}B_3$	$84\text{-}5\text{-}B_7$	$84\text{-}5\text{-}B_2$	$84\text{-}5\text{-}B_8$
X	0.083	0.266	0.250	0.275	0.305	0.358
Y	0.155	0.472	0.531	0.585	0.658	0.790
(m)	1.005	1.176	1.225	1.275	1.344	1.452
(m)	2.0	1.75	1.5	1.5	1.0	2.0

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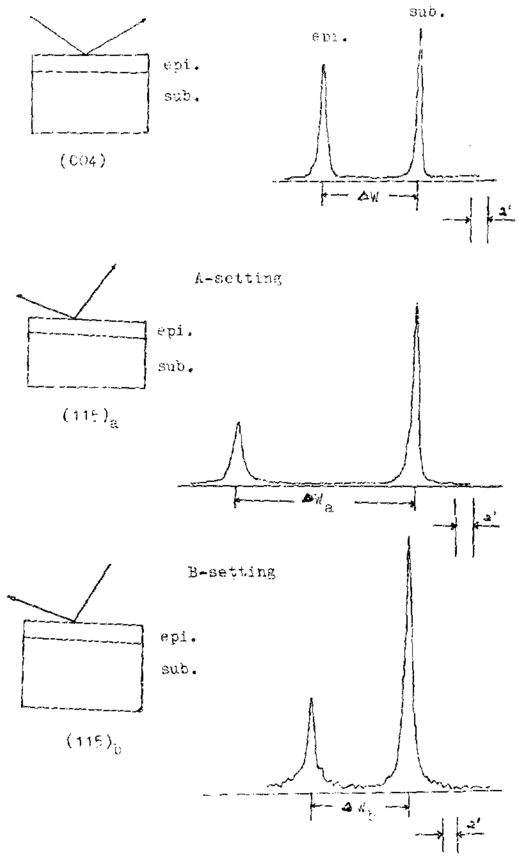

FIG. 1. Rocking curves for the (004), $(115)_a$, and $(115)_b$ setting reflections.

substrate. The following relations are presented. Then we have

$$\Delta a^{\perp} = a^{\perp} - a_s, \tag{7}$$

$$\Delta a^{\parallel} = a^{\parallel} - a_s. \tag{8}$$

For the lattice plane spacing of epitaxial layer of tetragonal structure,

$$d = \left(\frac{h^2 + k^2}{a^{\parallel 2}} + \frac{L^2}{a^{\perp 2}}\right)^{-1/2}. \tag{9}$$

Differentiating Eq. (9), we get

$$\frac{\Delta d}{d} = \frac{h^2 + k^2}{h^2 + k^2 + L^2}\left(\frac{\Delta a^{\parallel}}{a_s}\right) + \frac{L^2}{h^2 + k^2 + L^2}\left(\frac{\Delta a^{\perp}}{a_s}\right). \tag{10}$$

According to the crystallographic principle

TABLE III. The results of parameters.

Sample	$(a/a)_{\rm rel}$ 10^3	a_L (Å)	$\varphi(m)$	V (Å^3)
84-5-B_6	−2.40	5.8547	7.81	200.68
84-4-B_3	−2.04	5.8568	10.72	200.92
84-4-B_2	−1.44	5.8603	11.38	201.26
84-5-B_7	−1.33	5.8610	16.44	201.33
84-5-B_8	−0.82	5.8640	20.00	201.64
84-5-B_2	0.40	5.8711	81.99	202.38

$$\cos\varphi = d_{h_1k_1L_1} d_{h_2k_2L_2}\left(\frac{h_1h_2 + k_1k_2}{a^{\parallel 2}} + \frac{L_1L_2}{a^{\perp 2}}\right), \tag{11}$$

differentiating Eq. (11) and considering the condition

$$(a^{\perp} - a^{\parallel})/a_s \ll 1, \tag{12}$$

we then get

$$\Delta\varphi = \cos\varphi \sin\varphi\left(\frac{\Delta a^{\perp}}{a_s} - \frac{\Delta a^{\parallel}}{a_s}\right). \tag{13}$$

In combination with Eqs. (6), (10), and (13), we obtain

$$\Delta a^{\perp}/a_s = (\tan\varphi)\Delta\varphi - (\cot\theta)\Delta\theta, \tag{14}$$

$$\Delta a^{\parallel}/a_s = -(\cot\varphi)\Delta\varphi - (\cot\theta)\Delta\theta. \tag{15}$$

The corresponding measured and calculated values of the above parameters are shown in Table II.

From these results it is seen that the relation $\Delta a^{\perp}/a_s \gg \Delta a^{\parallel}/a_s$ has shown the lattices of all epitaxial layers are tetragonally deformed due to the interfacial stresses. The result of $\Delta a^{\parallel}/a_s \simeq 0$ implies that the lattice parameters of the epitaxial layers parallel to the interfaces equal to that of the substrate. This suggests that there are no misfit dislocations at the interface.

B. Determination of relaxed lattice constant and curvature

It was shown that when the thickness of an epitaxial layer is negligible as compared with that of the substrate, the relation between lattice constant $\Delta a^{\perp}/a_s$ in oriented (001) direction with strained state and relaxed value $(\Delta a/a)_{\rm rel}$ can be represented as follows[10]:

$$\frac{\Delta a^{\perp}}{a_s} = \left(1 + \frac{2\nu}{1-\nu} + \frac{8\nu}{1-\nu} - \frac{t_L}{t_s}\right)\left(\frac{\Delta a}{a}\right)_{\rm rel}. \tag{16}$$

The Poisson's ratio[11] is

TABLE II. Deformation of GaInAsP epitaxial layer grown on (001) InP substrate.

Sample No.	W_a (rad) 10^3		W_b (rad) 10^3		θ(rad) 10^3		(rad) 10^3		d/d 10^3	d/d 10^3	a/a 10^3	a/a 10^3
	(004)	(115)	(004)	(115)	(004)	(115)	(004)	(115)	(004)	(115)	(004)	(115)
84-5-B_6	3.14	5.75	3.14	3.08	3.14	4.415	0	1.325	−5.09	−4.73	−5.10	−0.047
84-4-B_3	2.71	4.85	2.69	2.69	2.70	3.77	0.01	1.08	−4.37	−4.03	−4.34	−0.22
84-4-B_2	1.90	3.40	1.90	1.94	1.90	2.67	0	0.73	−3.08	−2.86	−3.06	−0.28
84-5-B_7	1.72	3.19	1.72	1.72	1.72	2.455	0	0.735	−2.79	−2.63	−2.83	−0.032
84-5-B_8	1.12	1.96	1.12	1.05	1.12	1.505	0	0.455	−1.81	−1.61	−1.74	−0.004
84-5-B_2	−0.528	−0.94	−0.528	−0.518	−0.528	−0.729	0	−0.211	0.86	0.78	0.84	0.035

TABLE IV. The half-widths of peaks.

Sample	84-4-B$_2$	84-5-B$_6$	84-4-B$_3$	84-5-B$_7$	84-5-B$_2$	84-5-B$_8$
HW (s) of (004) reflection	76.5	43.4	62.8	38.7	46.1	38.8

$$\nu = C_{12}/(C_{11} + C_{12}). \quad (17)$$

When the composition of the epitaxial layer is not known, we assume that the elastic constant of the substrate may be used approximately for that of the layer. The elastic constant of III–V compounds were given in Ref. 11.

In our experiment

$$t_L/t_s = \sim 2\text{–}6 \times 10^{-3}.$$

t_L and t_s are the thickness of the layer and substrate, respectively. Therefore,

$$(\Delta a/a)_{\text{rel}} = \left(\frac{1-\nu}{1+\nu}\right)\frac{\Delta a^\perp}{a_s} = \frac{C_{11}}{C_{11}+2C_{12}}\frac{\Delta a^\perp}{a_s} = 0.47(\Delta a^\perp/a_s). \quad (18)$$

Relaxed constant of epitaxial layer can be obtained as follows:

$$a_L = a_s[1 + (\Delta a^\perp/a)_{\text{rel}}]. \quad (19)$$

Furthermore, the radius of curvature of the sample can be given[10]:

$$\varphi = \frac{C}{(\Delta a/a)_{\text{rel}}}\frac{t_s^2}{6t_L}, \quad (20)$$

where C denotes the function of the elastic constant of both compounds equal to 1 when these constants are assumed to be identical.

The results of the parameters discussed above are listed in Table III.

C. The half-widths of peaks in rocking curve

We also measured the half-widths of the rocking curve using slow scanning as shown in Table IV. One of the typical rocking curves was shown in Fig. 2. The half-widths of the x-ray rocking curves for the quaternary epitaxial layers have been regarded as the values being representative of crystal quality of the whole epitaxial layers. It was found that half-widths were changed very much from crystal to crystal. They depend on perfection of epitaxial layer, depth profile of composition in the layer, the machine function, and so on.

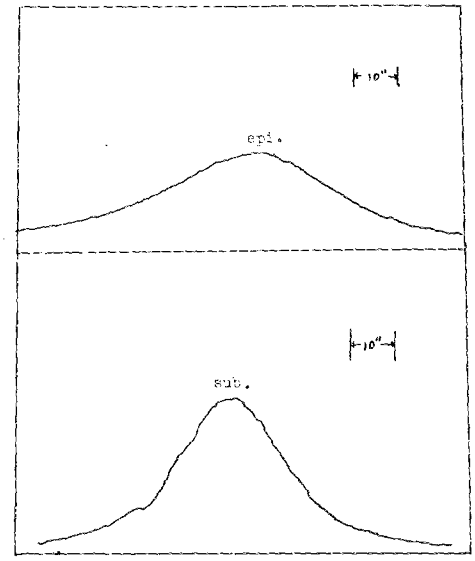

FIG. 2. Rocking curves of slowly scanning for (115) setting. Sample No. 84-5-B$_6$.

IV. CONCLUSIONS

It has been shown that x-ray diffractometry is a powerful technique to study the state of strain and stress in the quaternary GaInAsP system. The results of the experiments show that tetragonal deformation in the epitaxial layers has happened, i.e., $\Delta a^\perp/a_s \gg \Delta a^\parallel/a_s$. The relaxed constant of epitaxial layer can be obtained using correction factor. The experimental results also agree with the calculated results. The method is simple, fast, and nondestructive.

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