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Structural Characterization of $Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.52}As$ Superlattices Grown by Molecular Beam Epitaxy

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We report detailed double-crystal X-ray diffraction measurements of MBE grown $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ superlattices lattice-matched to InP. Interpretation of the experimantal X-ray diffraction patterns yields information on the structural parameters of the constituent $Ga_xIn_{1-x}As$ and $Al_xIn_{1-x}As$ superlattice layers. It is shown that only a comparison between theoretical diffraction pattern and experimental data describes the characteristic structure of the superlattice accurately.

1. Introduction

Quantum well heterostructures and superlattices composed of III-V semiconductors play an important role for application in advanced photonic devices. The knowledge of chemical composition, elastic strain and thickness of the constituent layers is required to understand the characteristic optical transitions in $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ superlattice devices. Double-crystal diffractometry is frequently used to study the structural and geometrical parameters of heterostructures and superlattices. Unfortunately, for ternary compound superlattices only few data can be extracted directly from the experimental diffraction pattern. A comparison between theoretical and experimental diffraction pattern is thus required for a detailed description of the superlattice structure. We have performed the calculations of the theoretical diffraction pattern by applying a semikinematical approach of the dynamical theory of the X-ray diffraction for distorted crystals [1, 2].

2. Experimental

The X-ray diffraction measurements were performed with a computer-controlled double-crystal diffractometer in non-dispersive Bragg-geometry. An asymmetrically cut (100) Ge crystal was used for monochromizing and collimating the X-ray radiation. The investigated superlattices were grown in a molecular beam epitaxy system equipped with a continuously azimuthally rotating substrate holder. The $Ga_xIn_{1-x}As$ and $Al_xIn_{1-x}As$ layers were deposited lattice matched onto <100> oriented Sn-doped InP substrates at a temperature of 500 ^{o}C [3]. The superlattices consist of 10 periods of $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ double layers. The period length of different samples ranges from 20.4 to 21.2 nm, and the well width L_Z and the barrier width L_B are kept equal.

3. Results and Discussion

The X-ray diffraction patterns were recorded in the vicinity of the symmetric (200) and (400) reflections and of the asymmetric (422) and (440) reflections using $CuK\alpha_1$ radiation. Both symmetric

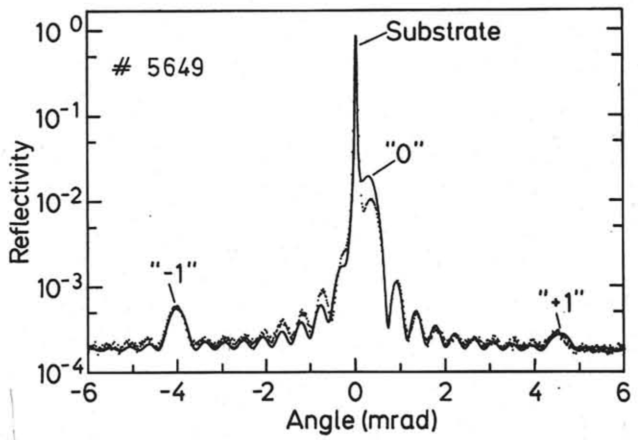

Fig. 1 $CuK\alpha_1$ (400) diffraction pattern of $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ superlattice on (100) InP with $L_Z = L_B = 10.6$ nm (.... experiment, ____ theory)

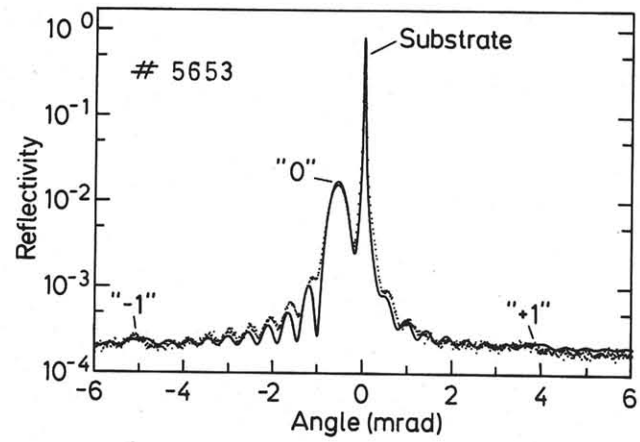

Fig. 2 CuKα_1 (400) diffraction pattern of $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ superlattice on (100) InP with $L_Z = L_B$ = 10.2 nm (.... experiment, ——— theory)

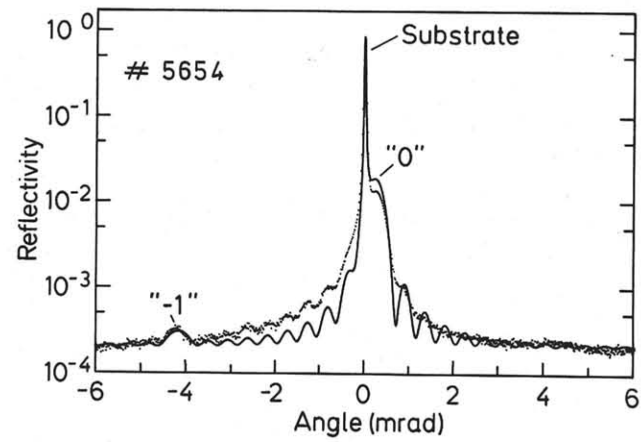

Fig. 3 CuKα_1 (400) diffraction pattern of $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ superlattice on (100) InP with $L_Z = L_B$ = 10.2 nm (.... experiment, ——— theory)

and asymmetric diffraction data yield the average lattice strain perpendicular, $\bar{\varepsilon}_{zz}$, and parallel, $\bar{\varepsilon}_{xx}$, to the (100) substrate surface. The lattice strains $\bar{\varepsilon}_{zz}$ and $\bar{\varepsilon}_{xx}$ are correlated with the angular distances $\Delta\Theta_I$ and $\Delta\Theta_{II}$ between the substrate diffraction maximum and the main epitaxial layer peak ("0"-peak) by the equation

$$\begin{pmatrix} \bar{\varepsilon}_{zz} \\ \bar{\varepsilon}_{xx} \end{pmatrix} = \begin{pmatrix} A_I & B_I \\ A_{II} & B_{II} \end{pmatrix}^{-1} \begin{pmatrix} \Delta\Theta_I \\ \Delta\Theta_{II} \end{pmatrix} \qquad (1)$$

with

$$A_{I,II} = \cos\alpha_{I,II} * [\cos\alpha_{I,II} * \tan\Theta_{I,II} + \sin\alpha_{I,II}] \qquad (2)$$

$$B_{I,II} = \sin\alpha_{I,II} * [\sin\alpha_{I,II} * \tan\Theta_{I,II} - \cos\alpha_{I,II}]$$

and

$$\bar{\varepsilon}_{zz} = (\bar{d}_e^{\perp} - d_s) \;/\; d_s$$
$$\bar{\varepsilon}_{xx} = (\bar{d}_e^{\parallel} - d_s) \;/\; d_s \qquad (3)$$

The indices I and II hold for symmetric and asymmetric reflections, respectively. Here, $\bar{d}_e^{\perp}$ and $\bar{d}_e^{\parallel}$ are the average interplanar spacings of the epitaxial layer perpendicular and parallel to the crystal surface, while d_s is the interplanar spacing of the substrate crystal, respectively. Θ_I and Θ_{II} are the kinematic Bragg angles, and α_I and α_{II} the angles between crystal surface and reflection planes I and II. The evaluation of our experimental diffraction data reveals that the superlattice is not misoriented with respect to the substrate crystal and that $\bar{\varepsilon}_{xx} = 0$ for all samples, i.e. the lattice spacing parallel to the crystal surface in the constituent $Ga_xIn_{1-x}As$ and $Al_xIn_{1-x}As$ layers and in the InP substrate crystal are the same. Hence it follows that the lattice strain in the $Ga_xIn_{1-x}As$ and $Al_xIn_{1-x}As$ epilayers perpendicular to the crystal surface is a measure of their mole fraction x. The relation between elastic strain and chemical composition in the $Ga_xIn_{1-x}As$ layers is given by

$$x = \frac{1}{a_{GaAs} - a_{InAs}} * [a_{InP}(1 + \frac{2c_{12}}{c_{11}+c_{12}}\varepsilon_{zz}) - a_{InAs}] \qquad (4)$$

where c_{11} and c_{12} are the elastic stiffness constants of the epilayer material. For the $Al_xIn_{1-x}As$ layers the lattice constant a_{GaAs} in Eq. (4) must be replaced by that of a_{AlAs}.

Figures 1 - 4 show the experimental (dotted line) and the best theoretically fitted diffraction patterns (solid line) in the vicinity of the symmetrical (400) CuKα_1 reflection. From the theoretical diffraction pattern we obtain the thickness as well as the lattice strain of the individual epilayers. The chemical compositions are determined by using Eq. (4). The measured and computed structural data are summarized in TABLE I. It is shown that for all samples $L_Z = L_B$, as adjusted by the growth conditions. The lattice mismatch perpendicular to the (100) growth surface for the tetragonal distorted epilayers on InP are $< |2.8*10^{-3}|$, i.e. the lattice mismatch in these samples is smaller than in the AlAs/GaAs system.

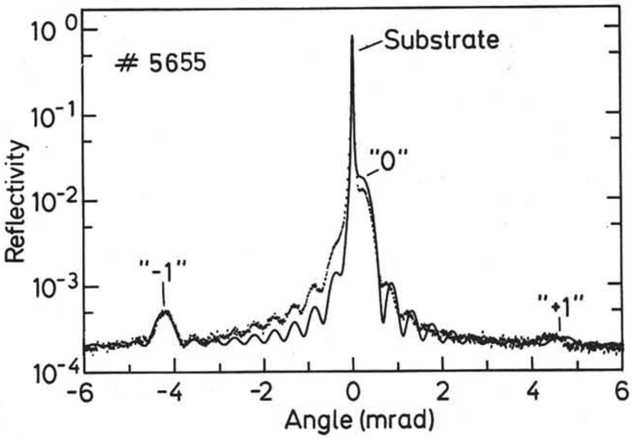

Fig. 4 CuKα (400) diffraction pattern of $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ superlattice on (100) InP with $L_Z = L_B$ = 10.2 nm (....experiment, ——theory)

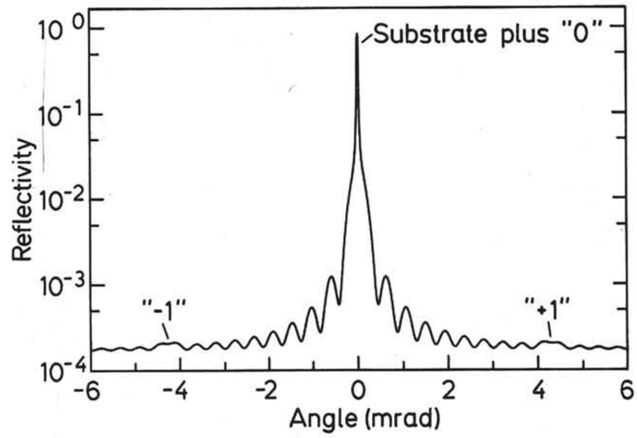

Fig. 5 Theoretical diffraction pattern of a perfectly lattice-matched $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ superlattice on (100) InP [CuKα_1 (400) reflection]

TABLE I Structural parameters of the four different $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ superlattices determined from the diffraction patterns shown in Figs. 1 - 4 .

Sample No.	Thickness of $Ga_xIn_{1-x}As$ layers (nm)	Thickness of $Al_xIn_{1-x}As$ layers (nm)	Average lattice mismatch of superlattice $\bar{\varepsilon}_{zz}$ (x 10^{-4})	Lattice strain in $Ga_xIn_{1-x}As$ layers $\bar{\varepsilon}_{zz}$ (x 10^{-4})	Lattice strain in $Al_xIn_{1-x}As$ layers $\bar{\varepsilon}_{zz}$ (x 10^{-4})	Mole fraction x of $Ga_xIn_{1-x}As$ layers	Mole fraction x of $Al_xIn_{1-x}As$ layers
5649	10.6	10.6	- 4.5	+ 6.0	- 15.0	0.464	0.487
5653	10.2	10.2	+ 9.4	9.5	9.3	0.462	0.470
5654	10.2	10.2	- 4.0	0.0	- 8.0	0.468	0.482
5655	10.2	10.2	- 3.5	7.0	- 14.0	0.464	0.486

The Pendellösung fringes observed between the main diffraction peaks and the satellite peaks "-1" and "+1" demonstrate the excellent thickness and composition homogeneity perpendicular and parallel to the crystal surface.

Finally Fig. 5 shows a theoretical diffraction pattern for a perfect lattice-matched $Ga_{0.468}In_{0.532}As/Al_{0.477}In_{0.523}As$ superlattice with $L_B = L_Z$ = 10.6 nm. It should be noted that the satellite peaks "-1" and "+1" have almost disappeared. This finding is in contrast to that observed in strained layer superlattices, where a strain periodicity produces strong satellite peaks. The low intensity and the Pendellösung fringes in Fig. 5 are caused only by the periodicity of the structure factors in the superlattice. A weak intensity of the satellite peaks is also observed if the lattice strains of the $Ga_xIn_{1-x}As$ and $Al_xIn_{1-x}As$ layers are of the same magnitude, which occurs in sample 5653 (see Fig. 2 and TABLE I).

Acknowledgement

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