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Strain state in single quantum well GaAs/1ML-InAs/GaAs(100) **analysed by high-resolution** X**-ray diffraction**

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PACS. 61.10−i – X-ray diffraction and scattering.
PACS. 68.35−p – Solid surfaces and solid-solid interfaces.

Abstract. – The epitaxy-induced tetragonal strain in one monolayer of InAs buried in a GaAs(100) crystal is determined by measuring weak oscillations in X-ray reflectivity profiles. It is shown that the reflectivity of such heterostructure consists of a sinusoidal modulation of the usual rocking curve of a thick crystal. The oscillation period provides the distance of the buried layer from the crystal surface and the maximum positions in oscillations give the displacement induced by the buried layer. The vertical spacing between the In and As atom planes is found to be 1.64 ± 0.02 Å, which is consistent with an elastic behaviour.

Considerable efforts have been made to understand the electronic and structural properties of quantum wells such as GaAs/InAs/GaAs(100) [1]-[6], Si/SiGe/Si(100) [7], [8], CdTe/MnTe/CdTe(100) [9], [10] and CdTe/ZnTe/CdTe(100) [9]. The information on the atomic structure of the interface is essential to fully understand the electronic properties of such heterostructures. For ultrathin layers epitaxially strained in a host crystal, usually two contradictory strain models are used to evaluate the atomic displacements: the macroscopic elastic model and the model of the conservation of bond lengths. In the case of one monolyer of InAs laterally strained in GaAs(100), the elastic model leads to a perpendicular strain of 0.07 while the constant In-As bond length gives a value of 0.12, almost twice the previous one. Using the high-resolution transmission electron microscopy (HRTEM), Brandt *et al.* [2] indicated that the elastic theory breaks down in the limit of one monolayer (ML) of InAs. They found that the constant bond length model should be applied to this ultimate thin layer. This finding was supported by an *ab initio* total energy calculation by Shiraishi and Yamaguchi [1] and a valence-force field calculation on a surface layer by Massies and Grandjean [3]. Other experimental results

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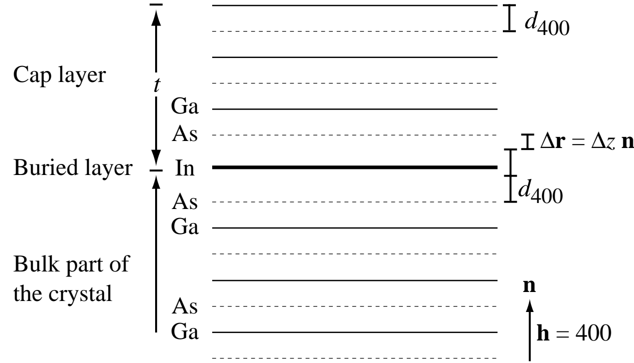

Fig. 1. – Schematic representation of one monolayer of InAs buried in GaAs(100) in the geometry for the reflection 400. The Ga, As and In atom planes are symbolised by solid and dashed lines. The normal **n** to the crystal surface and the reflecting vector **h** are parallel for this case. The displacement of the cap layer along the normal **n** is Δz, with respect to the bulk part of the crystal. The phase φ induced for the reflection 400 is equal to $\Delta z/d_{400}$, where d_{400} is the reticular distance.

indicated rather an elastic behaviour of one ML of InAs strained in GaAs. Using the X-ray standing waves (XSW), Giannini *et al.* [4] found that the In atom positions are consistent with the elastic model. This was confirmed by the work of Woicik *et al.* [6] for which both results from the XSW and extended X-ray absorption fine structure (EXAFS) experiments revealed an elastic behaviour of one ML of InAs. This point of view was supported by the calculation by Bernard and Zunger [5] using the density-functional theory in the local-density approximation. The present study proposes an experimental measurement of the strain in one ML of InAs buried in GaAs(100) using the high-resolution X-ray diffraction (HRXRD).

Theory. – An X-ray dynamical analysis in the case of a crystal containing an ultrathin buried layer can be found in ref. [11]. The main point of the analysis concerning the reflectivity is that the oscillations can be explained by a simple phase parameter φ. When the buried layer induces a displacement $\Delta\mathbf{r}$ of the cap layer with respect to the bulk part of the crystal (fig. 1), φ is defined by $\mathbf{h}\cdot\Delta\mathbf{r}$ with $\mathbf{h}$ the reflecting vector. If $F_{\mathbf{h}}$ is the structure factor for the bulk part of the crystal, a phase term should be added to the structure factor for the cap layer : $F_{\mathbf{h}}\exp[i2\pi\varphi]$. The phase φ and the thickness t of the cap layer entirely determine the reflectivity profile. It can be shown [11] that the reflectivity R is equal to the usual rocking curve for a thick crystal R_{thick} modulated by an oscillating term R_{osc}: $R = R_{\mathrm{osc}}R_{\mathrm{thick}}$. Out of the Bragg total reflection range, the reflectivity has a simple expression. The angular range of the total reflection is called the Darwin width ω_{DW}. For a thick crystal and a symmetric reflection, the rocking curve R_{thick} behaves as

$$R_{\mathrm{thick}} \approx \frac{1}{8(\Delta\theta-\Delta\theta_0)^2/\omega_{\mathrm{DW}}^2}$$

for angles $|\Delta\theta-\Delta\theta_0| \gg \omega_{\mathrm{DW}}$. $\Delta\theta$ is the angular departure from the exact Bragg angle θ_{B} and $\Delta\theta_0$ the angular shift due to the refraction. The oscillating term R_{osc} is

$$R_{\mathrm{osc}} \approx 1 + 4\sin^2(\pi\varphi) - 4\sin(\pi\varphi)\sin\left(2\pi\frac{\Delta\theta-\Delta\theta_0}{\omega_{\mathrm{S}}} + \pi\varphi\right),$$

where $\omega_{\mathrm{S}} = \lambda/2t\cos\theta_{\mathrm{B}}$ and it is the oscillation period according to the Scherrer formula. It is obvious that the cap layer thickness t can be determined from the oscillation period ω_{S}, exactly

as for the case of a thin film. From the positions of maxima (and minima) in reflectivity, the phase φ, thus the displacement vector $\Delta\mathbf{r}$, is obtained. For φ ranged in $[0, \pi]$, for instance, the position of the M-th maximum $\Delta\theta_{\rm M}$ is given by: $(\Delta\theta_{\rm M} - \Delta\theta_0)/\omega_{\rm S} + \varphi/2 = M - 1/4$. X-ray reflectivity profiles thus constitute a direct and simple method to measure the displacement induced by an ultrathin buried layer. Besides the above qualitative considerations, a full dynamical treatment [11] namely for the region near the Bragg total reflection allows to affine the calculated oscillation shape with respect to the experimental one. For the present study, the dynamical treatment was used.

Experiment. – The heterostructures were grown by molecular beam epitaxy. The growth procedure was described in a previous work on similar heterostructures analysed by X-ray standing waves [4]. The present study concerns two samples where one monolayer of InAs was grown at 480 °C (Sample A) and at 420 °C (Sample B) on GaAs(100) substrates. The 1 ML-InAs was further capped by a layer of GaAs, about 900 Å thick. The amount of In atoms actually deposited was evaluated within a range of 8% from the nominal monolayer, according to the previous work [4]. The HRXRD experiments were performed at the beamline D25B of the DCI storage ring at the LURE (Orsay, France). The experimental set-up consists of a double-crystal diffractometer in the nondispersive (+, −) geometry. The first crystal is a Si-monolithic grooved four-reflection (+, −) monochromator where the third reflection is asymmetric [12]. Two monochromators of 400 and 220 reflections were used for measurements with GaAs 400 and 220 reflections, respectively. Concerning the detection of the reflectivity, a wide dynamical range of at least $1 - 10^4$ was needed, since both Bragg peak and weak oscillations far from the Bragg angle should be recorded. For the present case, a logarithmic scale range was used for the recording.

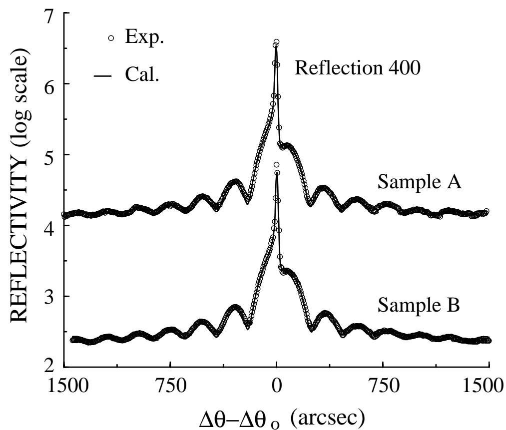

Fig. 2

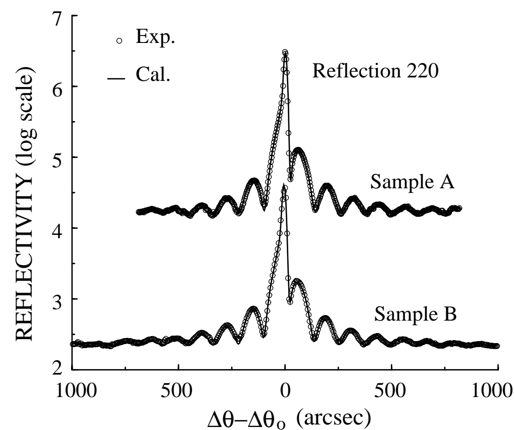

Fig. 3

Fig. 2. – Experimental and calculated reflectivity curves for the samples A and B. The experimental data were obtained at wavelength 1.62 Å with the reflection 400. The baseline of the curves for the sample A is vertically shifted to enhance visibility.

Fig. 3. – Experimental and calculated reflectivity curves for the samples A and B. The experimental data were obtained at wavelength 1.40 Å with the reflection 220, *i.e.* with the reflecting planes making an angle of 45 degrees with the surface.

Table I. – *Values of the effective thickness $t_{\mathbf{h}}$ and the phase parameter $\varphi_{\mathbf{h}}$ measured from the reflectivity profiles. The values of the thickness t and the displacement Δz are deduced from the previous ones as follows: $t = t_{400} = t_{220}/\sqrt{2}$ and $\Delta z/d_{400} = \varphi_{400} = 2\varphi_{220}$.*

	Reflection **h**	Effective thickness $t_{\mathbf{h}}$ (Å)	Thickness t (Å)	Phase $\varphi_{\mathbf{h}}$	Displacement Δz (Å)
Sample A	400	926 ± 10	926 ± 10	0.32 ± 0.02	0.45 ± 0.03
	220	1300 ± 15	919 ± 11	0.15 ± 0.05	0.42 ± 0.14
Sample B	400	915 ± 10	915 ± 10	0.32 ± 0.02	0.45 ± 0.03
	220	1290 ± 15	912 ± 11	0.17 ± 0.05	0.48 ± 0.14

Results. – The HRXRD experiments were carried out using two types of reflections, 400 and 220. With the reflection 400, the reflecting planes are parallel to the surface. Thus the thickness t_{400} measured from the reflection 400 is directly equal to the cap layer thickness t. The phase φ_{400} measured corresponds to $\Delta z/d_{400}$, with Δz the displacement normal to the crystal surface and d_{400} the reticular distance. The geometry used for 220 reflections is the so-called inclined symmetric geometry [13]. If the incidence plane is defined by the one containing the incident wave vector and the reflecting vector $\mathbf{h}$, the normal to the crystal is out of the incidence plane with an angle, 45 degrees for the present case. The reflection in the incidence plane is still a symmetric one. The effective thickness t_{220} measured from the reflection 220 is equal to $\sqrt{2}t = \sqrt{2}t_{400}$ and the phase φ_{220} to $\Delta z/\sqrt{2}d_{220} = \varphi_{400}/2$. Thus the reflection 220 allows a cross-checking of the measurements of t and Δz. Figures 2 and 3 show the experimental reflectivity profiles obtained with the samples A and B using the reflections 400 and 220, respectively. These profiles can be precisely calculated within the theoretical framework indicated above. The profiles from the samples A and B are very similar. It seems that the difference in the growth temperature does not modify the strain resulted in the monolayer of InAs. The oscillation period observed with the reflection 220 is shorter than the one with the reflection 400. Taking into account the difference of the wavelengths used for both reflections, the ratio of $\sqrt{2}$ between the periods is found for each sample. The positions of the maxima (and minima) in reflectivity profiles with respect to the Bragg peak are different, as can be observed in figs. 2 and 3, namely with the oscillations near the Bragg peak. This is directly related to the difference between the phases φ_{400} and φ_{220}. The results deduced from the experimental data are summarised in table I. The values determined from the reflection 400 are more accurate than the ones from 220, because the accuracy is inversely proportional to the oscillation period which is shorter for 220. Taking into account all the measurements, the displacement Δz normal to the crystal surface is found to be 0.45 ± 0.03 Å. The vertical spacing between the In atoms plane and the nearest As ones is equal to $d_{400} + \Delta z/2$ and its value is then 1.64 ± 0.02 Å.

Conclusion. – The present HRXRD result is fully consistent with those deduced from the XSW [4], [6] and EXAFS [6] experiments, disagreeing with the HRTEM observations [2]. It strongly promotes the fact that one ML of InAs buried in GaAs(100) still has an elastic behaviour. However, it is difficult to generalise this result to other types of heterostructures. The breakdown of the elastic model in ultimate thin layers remains a question to elucidate. The point is to know whether the harmonic approximation in the elastic theory still holds or not for the strain induced by a particular epitaxy and with the types of atoms implied in the heterostructure. To this end, experimental measurements and theoretical calculations on

other types of heterostructures, namely Si/SiGe/Si(100) and CdTe/MnTe or ZnTe/CdTe(100), should provide indications on the key parameters which characterise a possible departure from the elastic behaviour in ultrathin layers.

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