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In-plane and out-of-plane lattice parameters of [1 1 n] epitaxial strained layers

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Abstract

A procedure is proposed to determine the in-plane ($a_{||}$) and out-of-plane ($a_{\perp}$) lattice parameters of [1 1 n] epitaxial cubic strained layers by high resolution X-ray diffraction (HRXRD) rocking curves (RC). The common approach followed to obtain the lattice parameters from asymmetrical diffraction RC of [0 0 1] grown films, is extended to apply it to [1 1 n] grown layers. Epitaxial pseudomorphic Ge layers were grown on [0 0 1], [1 1 0], [1 1 1], [1 1 2], [1 1 3] and [1 1 4] GaAs substrates to analyze them by HRXRD. Reciprocal space maps (RSM) were also measured to obtain the lattice parameters of these samples. We observe an excellent agreement of the RC and RSM results, which demonstrates the validity of the suggested RC approach.

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Keywords: A1. High resolution X-ray diffraction; A1. Lattice parameters; A1. Substrates; B1. GeAs

1. Introduction

Heteroepitaxy is very important in the technology and science of semiconductors. Many electronic and optoelectronic devices have been developed with strained layer heterostructures. To estimate the degree of possible strain relaxation in these heterostructures it is important in particular to know the in-plane ($a_{||}$) and out-of-plane ($a_{\perp}$) lattice parameters of strained layers. These can be precisely determined by high resolution X-ray diffraction (HRXRD), following procedures described elsewhere [1,2]. However, most of the attention has been paid to [0 0 1] grown layers and the equations found in the literature to obtain both $a_{||}$ and $a_{\perp}$ from HRXRD rocking curves (RC) are readily applicable only to films grown on substrates with this orientation [1].

On the other hand, the usage of high index orientation substrates is more frequent in heteroepitaxy everyday, as an additional variable that modifies the properties of grown materials. For instance, the formation of InAs and $In_xGa_{1-x}As$ quantum dots is influenced by the orientation of the substrate and many experiments have been carried out on [1 1 7], [1 1 5], [1 1 4], [1 1 3] and [1 1 2] GaAs substrates [3,4]. On the other hand, [1 1 n] grown $In_xGa_{1-x}As/GaAs_{1-y}P_y$ and $GaAs_{1-y}P_y/GaAs$ quantum wells have exhibited photoluminescence dependence on growth direction [5,6]. Also, it has been reported the influence of growth direction on the zincblende to diamond transition of $(GaAs)_{1-x}(Ge_2)_x$ and $(GaAs)_{1-x}(Si_2)_x$ alloys grown on [1 1 0], [1 1 1], [1 1 2] and on [1 1 3] GaAs [7,8]. Thus, it is very important to follow a systematic procedure, to experimentally determine the lattice parameters of strained layers from HRXRD rocking curves, for other orientations besides [0 0 1].

In this work we present a study of strained Ge layers grown on GaAs. We chose these materials as a model heterostructure system with a lattice mismatch below 0.1%. We grew epitaxial strained Ge layers on [0 0 1], [1 1 0], [1 1 1], [1 1 2], [1 1 3] and [1 1 4] GaAs substrates. The

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in-plane and out-of-plane lattice parameters of these films were obtained from HRXRD RC for each growth direction, adapting the procedure usually followed for [0 0 1] grown layers to a [1 1 n] orientation [1]. Reciprocal space maps (RSM) are also used to determine the lattice parameters. A very good agreement is observed for these two methods, which validates the approach taken with the RC analysis.

2. Experimental conditions

Ge layers were epitaxially grown on [0 0 1], [1 1 0], [1 1 1], [1 1 2], [1 1 3] and [1 1 4] semi-insulating, epi-ready GaAs substrates, in a RF planar magnetron sputtering system with a base pressure better than 10^{-7} mbar. The sputtering agent was Ar (99.999%) maintaining a glow discharge to pulverize a 10 cm, water cooled Ge (99.999%) target at a sputtering pressure of 2×10^{-2} mbar. For each experiment $1\times1\,cm^2$ GaAs wafers of the five orientations were in-glued to a molybdenum block, which was introduced into the system through a load chamber. The substrate holder was placed 2 mm above a PBN heater, with target–substrates separation of 5 cm. Before each growth, the substrates were heated to 600 °C for 5 min to remove surface oxides, and then cooled to 550 °C, temperature at which the films were grown for 15, 30, 60 or 90 min. It has been previously found that strained layers of high structural quality can be obtained by RF sputtering using low RF power [7,8]. In this work, samples were grown at 50 W, which corresponds to a growth rate of 0.37 nm/s.

All samples were measured by HRXRD in a MRD Philips diffractometer. RC were obtained with $K_{\alpha1}$ radiation of a Cu anode (1.540562 Å), operated at 35 kV–30 mA. All measurements were carried out in the (2 2 0) configuration of a Ge– four crystal Bartels monochromator [9]. The peak positions and the full width at half maximum (FWHM) of the RC were determined by least squares fits to Gaussian lineshapes. RSM were taken with a Ge two crystals analyzer also in the (2 2 0) configuration.

3. Lattice parameters

As a first approximation, it could seem straightforward to obtain the lattice parameters $a_{||}$ and $a_{\perp}$ using only a symmetrical diffraction to determine $a_{\perp}$ and then $a_{||}$ from the strain ratio $\lambda=\varepsilon_{\perp}/\varepsilon_{||}$ for each growth direction, calculated from the layer elastic constants and using $\varepsilon_{\perp}=(a_{\perp}-a_l)/a_l$ and $\varepsilon_{||}=\left(a_{||}-a_l\right)/a_l$ (where a_l is the bulk layer constant). This is the method commonly used for [1 1 n] grown strained layers, following the results of Anastassakis or Yang [10,11]. However, this approach has several important shortcomings that limit its applicability: first, it would only be correct assuming that both the layer bulk lattice parameter and the lattice constants were known quantities of well defined values. Clearly, this is not the case when the strained layer is an alloy and both the bulk lattice parameter and elastic constants are a function of the elemental composition. Another point to consider is that the elastic constants are not normally known with the same accuracy allowed by HRXRD for the lattice parameters, and in many cases they have to be estimated by a process of linear interpolation between the values known for the elements or familiar compounds. Hence, the uncertainties in the layer composition, in the linear extrapolation and that intrinsic in the known values of the parent elastic constants, add to what is considered an unsatisfactory derived value for $a_{||}$. In addition, in many cases the estimation of this elemental composition is one of the main purposes of the application of HRXRD in the first place.

In our case, the strained layer is Ge and the bulk lattice parameter is in fact a well known constant. We should note however, that as it has been previously observed, the lattice constant of Ge grown on GaAs can be influenced by Ga or As diffusion from the substrate to the grown film [12],

Table 1
Strain ratio λ of bisotropically strained cubic crystals for different growth directions

Growth direction	$\varepsilon_{\perp}/\varepsilon_{//}$
(0 0 1)	$-2C_{12}/C_{11}$
(1 1 0)	$-\left(\dfrac{C_{11}+3C_{12}-2C_{44}}{C_{11}+C_{12}+2C_{44}}\right)$
(1 1 1)	$-2\left(\dfrac{C_{11}+2C_{12}-2C_{44}}{C_{11}+C_{12}+4C_{44}}\right)$
(1 1 2)	$-\left[\dfrac{3(C_{11}-C_{12}+C_{44})(C_{11}+3C_{12}-2C_{44})+C^2}{3(C_{11}-C_{12}+C_{44})(C_{11}+C_{12}+2C_{44})-C^2}\right]$ $C\equiv C_{11}-C_{12}-2C_{44}$
(1 1 3)	$-\left[\dfrac{18(C_{11}-C_{12})(C_{11}+2C_{12})-4C_{44}(C_{44}-42C_{12}+\frac{17}{2}C_{11})}{9(C_{11}-C_{12})(C_{11}+2C_{12})+C_{44}(4C_{44}-34C_{12}+101C_{11})}\right]*$
(1 1 4)	$-\left[\dfrac{16(C_{11}-C_{12})(C_{11}+2C_{12})-C_{44}(31C_{11}-259C_{12}+2C_{44})}{8(C_{11}-C_{12})(C_{11}+2C_{12})+C_{44}(145C_{11}-31C_{12}+2C_{44})}\right]*$

which would make this approach inappropriate even for this heterostructure. In any case, we show in Table 1 the strain ratio λ for each of the studied growth directions. These equations are given in Ref. [10] for [0 0 1], [1 1 0], [1 1 1] and [1 1 2] orientations and were obtained for [1 1 3] and [1 1 4] following the procedure therein. We only use them to get a reference $a_{\perp}$ and angle position of fully strained layers in symmetric diffractions, but could prove useful in the study of strained layers for composition estimation by HRXRD if both the in-plane and out-of-plane lattice parameters were experimentally obtained. In this work, both $a_{||}$ and $a_{\perp}$ were determined from asymmetrical diffraction RC as described below.

As we know the X-ray diffraction angle depends on the X-ray wavelength and the interplanar distance (d) that satisfy the Bragg condition. This distance will be different for symmetric and asymmetric RC and for each growth direction. In order to obtain the out-of-plane and in-plane lattice parameters from d, it is necessary to define a set of unitary cell vectors for each substrate orientation so we can determine the projection of d along these vectors.If we take the unitary cubic vectors as: $\langle 1, 0, 0\rangle$, $\langle 0, 1, 0\rangle$ and $\langle 0, 0, 1\rangle$ then for the $(1\,1\,n)$ orientation, a set of orthogonal unitary vectors would be [13]

$$\hat{x}_1 = \frac{1}{\sqrt{2}}\langle 1, \bar{1}, 0\rangle, \quad \hat{x}_2 = \frac{1}{\sqrt{2}\sqrt{n^2+2}}\langle n, n, \bar{2}\rangle,$$
$$\hat{x}_3 = \frac{1}{\sqrt{n^2+2}}\langle 1, 1, n\rangle. \tag{1}$$

Then $a_{\perp}$ would lie along $\hat{x}_3$, this parameter will correspond to the distance between an atom on a given [1 1 n] plane and

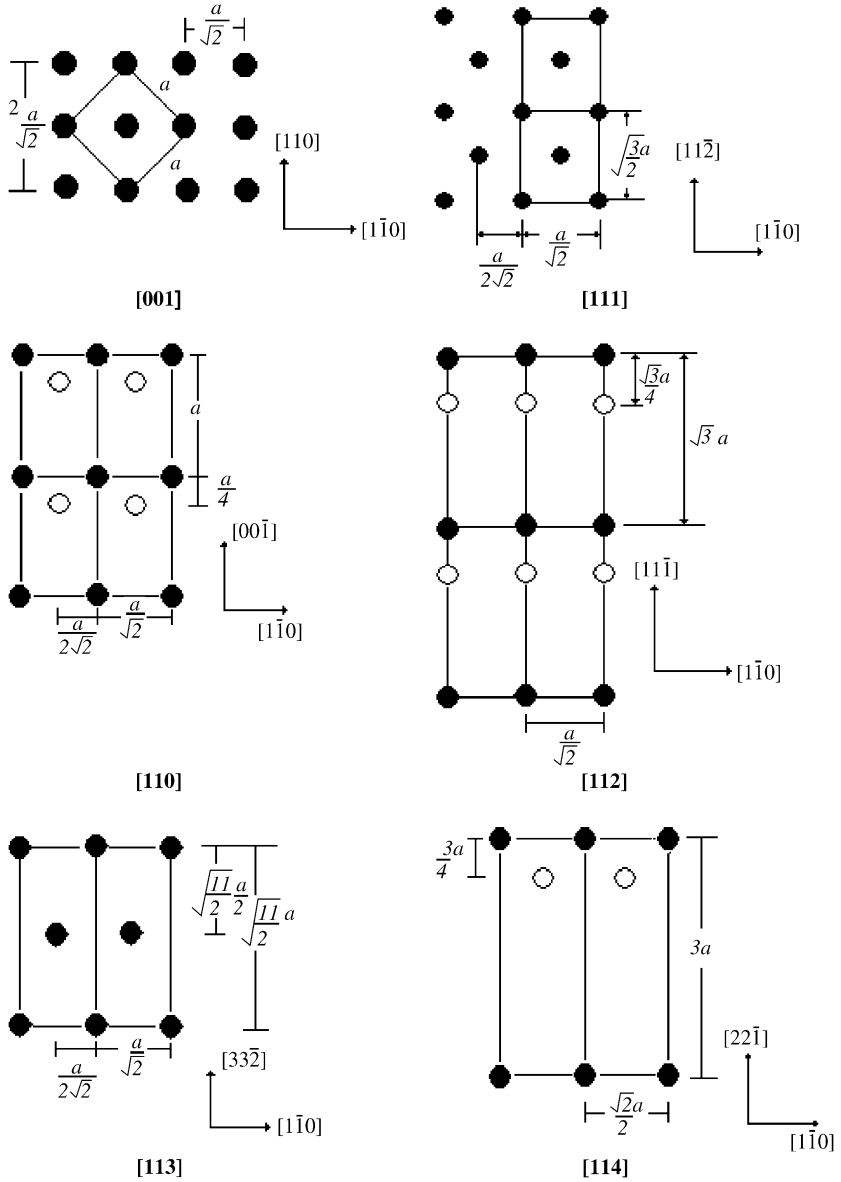

Fig. 1. Distribution of the atoms on surface parallel planes for different orientations. The in-plane lattice parameters are defined along the orthogonal vectors indicated by the arrows.

another atom exactly above it in one of the following [1 1 n] planes (4 atomic planes for [0 0 1], 2 planes for [1 1 0], etc.) and in general, two in-plane lattice parameters could be defined: $a_{||1}$ ($a_{||2}$) along $\hat{x}_1(\hat{x}_2)$. Fig. 1 shows the atomic arrangement of a [1 1 n] plane for a zincblende crystal. The inter-atomic distances and in-plane orthogonal vectors are also shown. During the HRXRD measurements there will be a different set of allowed reflections for each of these in-plane vectors. For instance, the reflections for a [1 1 2] grown zincblende crystal that can be measured in our difractometer are (1 1 3), (1 1 5), (2 2 4), (3 3 3), (3 3 5) and (4 4 4) for the in-plane vector $\langle 1, 1, \bar{1}\rangle$ and (2 2 4), (0 4 4) and (4 0 4) for $\langle 1, \bar{1}, 0\rangle$.

With the set of unitary vectors given above, the reciprocal space vectors set for the substrate and layer are:

$$\begin{aligned} \vec{A}_{1s} &= \frac{\hat{x}_1}{\sqrt{2}a_0}, & \vec{A}_{1l} &= \frac{\hat{x}_1}{a_{||1}}, \\ \vec{A}_{2s} &= \frac{\hat{x}_2}{\sqrt{2}(\sqrt{n^2+2})a_0}, & \vec{A}_{2l} &= \frac{\hat{x}_2}{a_{||2}}, \\ \vec{A}_{3s} &= \frac{\hat{x}_3}{(\sqrt{n^2+2})a_0}, & \vec{A}_{3l} &= \frac{\hat{x}_3}{a_{\perp}}, \end{aligned} \tag{2}$$

where a_0 is the bulk lattice constant of the substrate.

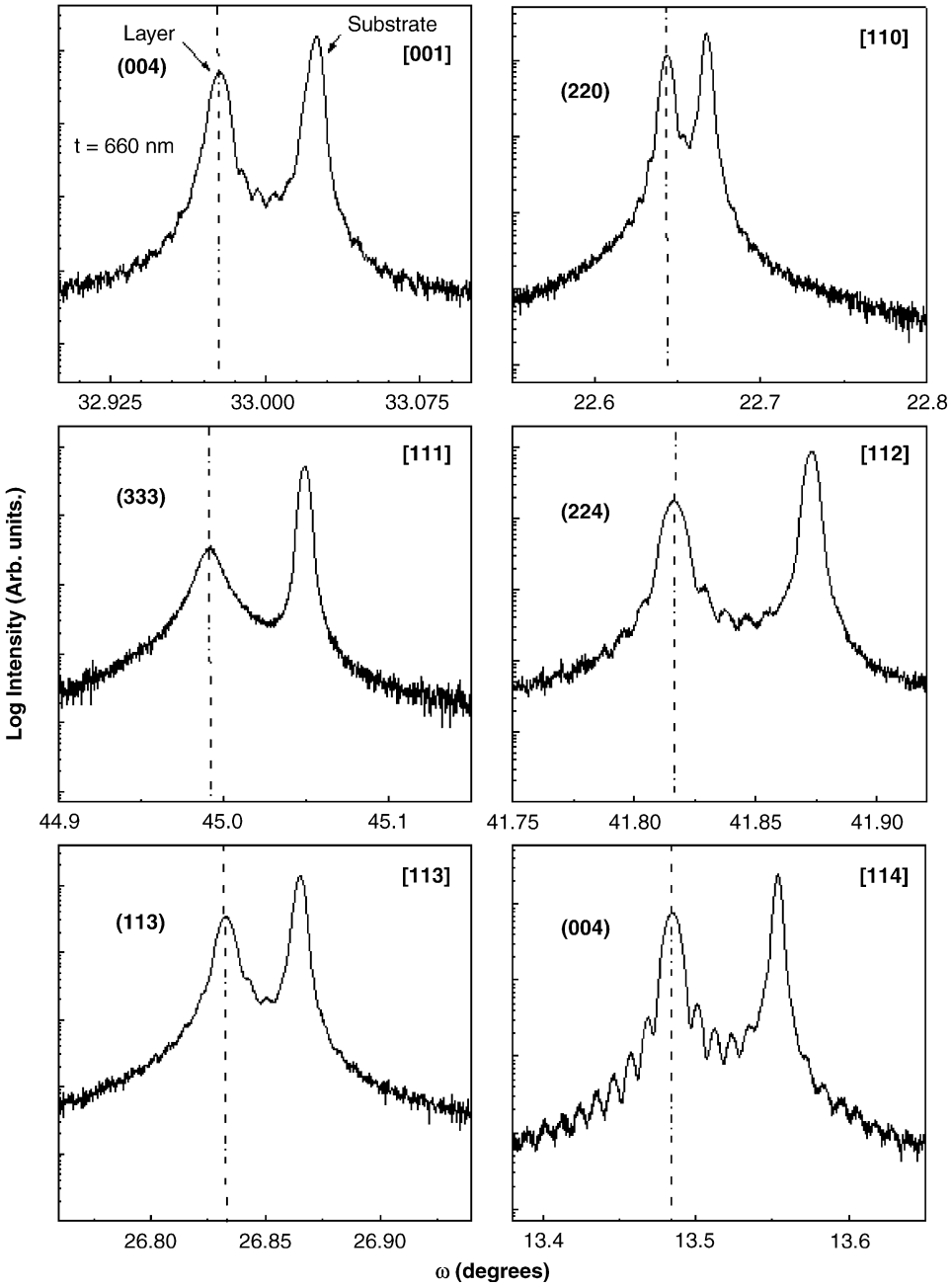

Fig. 2. Symmetrical diffraction rocking curves for the studied growth directions, except for (1 1 4).

And the reciprocal vector that locates a real space plane on the new basis is

$$\vec{H} = h'\vec{A}_{1s,l} + k'\vec{A}_{2s,l} + l'\vec{A}_{3s,l}. \quad (3)$$

Thus it can be easily seen that

$$\begin{bmatrix} h' \\ k' \\ l' \end{bmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ n & n & -2 \\ 1 & 1 & n \end{bmatrix} \begin{bmatrix} h \\ k \\ l \end{bmatrix}, \quad (4)$$

where $(h\,k\,l)$ are the Miller indexes on the cubic vector set and $(h'\,k'\,l')$ are the indexes referred to the unitary vectors of the $[1\,1\,n]$ orientation.

From the norm $\|\vec{H}\|$ the interplanar distance for the substrate and layer are, respectively,

$$d_s = \frac{\sqrt{2}\sqrt{n^2+2} * a_0}{\sqrt{(n^2+2)h'^2 + k'^2 + 2l'^2}},$$
$$d_l = \sqrt{\frac{1}{\frac{h'^2}{a_{\parallel 1}^2} + \frac{k'^2}{a_{\parallel 2}^2} + \frac{l'^2}{a_\perp^2}}}. \quad (5)$$

The angle between the $[1\,1\,n]$ sample surface and the measurement plane for the substrate (γ'_s) and layer $(\gamma'_l = \gamma'_s + \Delta\tau)$ can be obtained from the product $\vec{H}_{s,l} \bullet \vec{A}'_{3s,l}$

$$\cos\gamma'_s = \frac{2l'}{\sqrt{(n^2+2)h'^2 + k'^2 + 2l'^2}}$$
$$\cos(\gamma'_s + \Delta\tau) = \frac{l'}{a_\perp\sqrt{\frac{h'^2}{a_{\parallel 1}^2} + \frac{k'^2}{a_{\parallel 2}^2} + \frac{l'^2}{a_\perp^2}}}. \quad (6)$$

Here $\Delta\tau$ is the change in γ'_s of the cubic substrate due to strain.

And from Eqs. (5) and (6) and Bragg law the out-of-plane and in-plane lattice parameters are given by

$$a_\perp = \sqrt{n^2+2}\,\frac{a_0 \sin\theta'_s}{\sin(\theta'_s + \Delta\theta)}\,\frac{\cos\gamma'_s}{\cos(\gamma'_s + \Delta\tau)}, \quad (7)$$

$$a_{\parallel 1[1\ \bar{1}\ 0]} = \frac{\sqrt{2}a_0 \sin\theta'_s \quad \sin\gamma'_s}{2\sin(\theta'_s + \Delta\theta)\sin(\gamma'_s + \Delta\tau)},$$
$$a_{\parallel 2[n\ n\ \bar{2}]} = \frac{\sqrt{n^2+2}a_0 \sin\theta'_s \quad \sin\gamma'_s}{\sqrt{2}\sin(\theta'_s + \Delta\theta)\sin(\gamma'_s + \Delta\tau)}. \quad (8)$$

θ'_s is the Bragg angle of the substrate and $\Delta\theta$ is the difference between the Bragg angles of the layer and substrate. These expressions are the equivalent of Ref. [1] for [0 0 1] oriented cubic crystals adapted to a $[1\,1\,n]$ orientation. Both $\Delta\tau$ and $\Delta\theta$ are obtained from the measured RC of the usual glazing incidence ω^- and exit ω^+ geometries, as defined elsewhere [1,2].

$$\Delta\tau = \frac{\Delta\omega^- - \Delta\omega^+}{2}, \quad \Delta\theta = \frac{\Delta\omega^- + \Delta\omega^+}{2}. \quad (9)$$

4. Results

Fig. 2 shows typical HRXRD RC of strained Ge layers on GaAs for each of the studied growth directions and for 30 min of growth (660 nm of layer thickness). All the diffraction profiles are from symmetrical reflections except for the [1 1 4] sample, since only asymmetrical reflections can be measured in our diffractometer for this substrate orientation. The substrate and layer peaks are easily seen

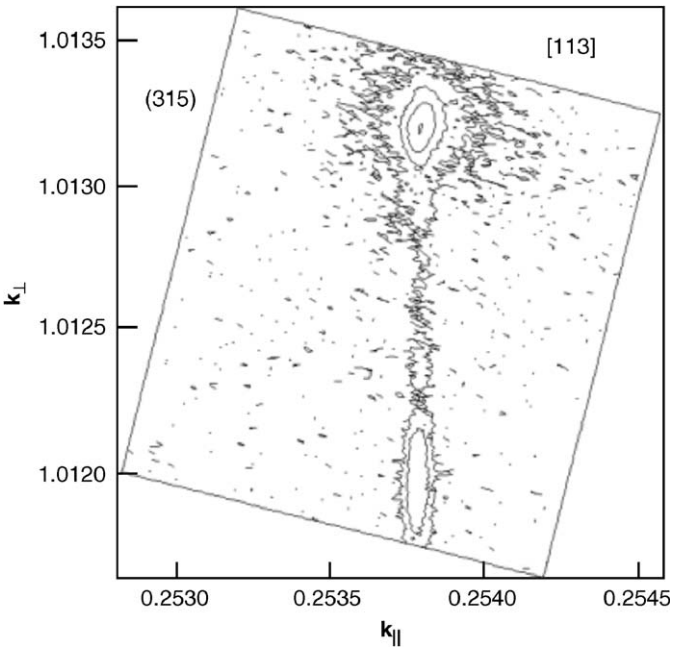

Fig. 3. Reciprocal space map of a 330 nm pseudomorphic Ge layer, grown on GaAs (1 1 3) around the asymmetrical diffraction (3 1 5). The graph axes are in reciprocal lattice units (1/Å).

Table 2
Measured asymmetrical diffractions and transformed indexes and angles for each growth direction

Growth direction	Asymmetrical difractions $(h\,k\,l)$	Indexes on the new axes $(h'\,k'\,l')$	θ's (degrees)	γ' (degrees)
(1 1 0)	(6 2 0) (2 6 0)	(0 4 8) (0 $\bar{4}$ 8)	59.5369	26.565
(1 1 1)	(5 1 3) (1 5 3)	(4 0 9) ($\bar{4}$ 0 9)	53.684	28.5608
(1 1 2)	(4 0 4) (0 4 4)	(4 0 12) ($\bar{4}$ 0 12)	50.4385	30
(1 1 3)	(3 1 5) (1 3 5)	(2 2 19) (2 $\bar{2}$ 19)	53.7346	14.4583
(1 1 4)	(4 0 4) (0 4 4)	(4 4 2 0) (4 $\bar{4}$ 2 0)	50.4399	33.5573

for each sample. The vertical dotted line shows the layer peak position of a pseudomorphic Ge layer on GaAs, as obtained from elastic theory (Table 1). All the grown layers are fully strained, as will be proved lately by the in-plane lattice parameters. Furthermore, the curves show Pendellösung fringes, which are characteristic of high structural quality layers. The layer lattice parameters were obtained following the procedure described above for each growth direction. The asymmetrical reflections used for each orientation, and the angles θ'_s and γ'_s are shown in Table 2. Using these values and the experimental angular separations of Eq. (9), we get the lattice parameters using Eqs. (7) and (8). The parameters were also determined from RSM.

In order to obtain the lattice parameters from RSM, it is necessary to decompose the $\langle h,k,l\rangle$ vector associated to the measured diffraction planes, along the orthonormal reciprocal space vectors (1). For instance, if an asymmetrical (2 2 4) space map is measured, for a [0 0 1] oriented sample, this reciprocal space vector is

$$\langle 2,2,4\rangle = 2\langle 1,0,0\rangle + 2\langle 0,1,0\rangle + 4\langle 0,0,1\rangle$$
$$= 2\sqrt{2}\hat{x}_{\langle 1,1,0\rangle} + 4\langle 0,0,1\rangle,$$

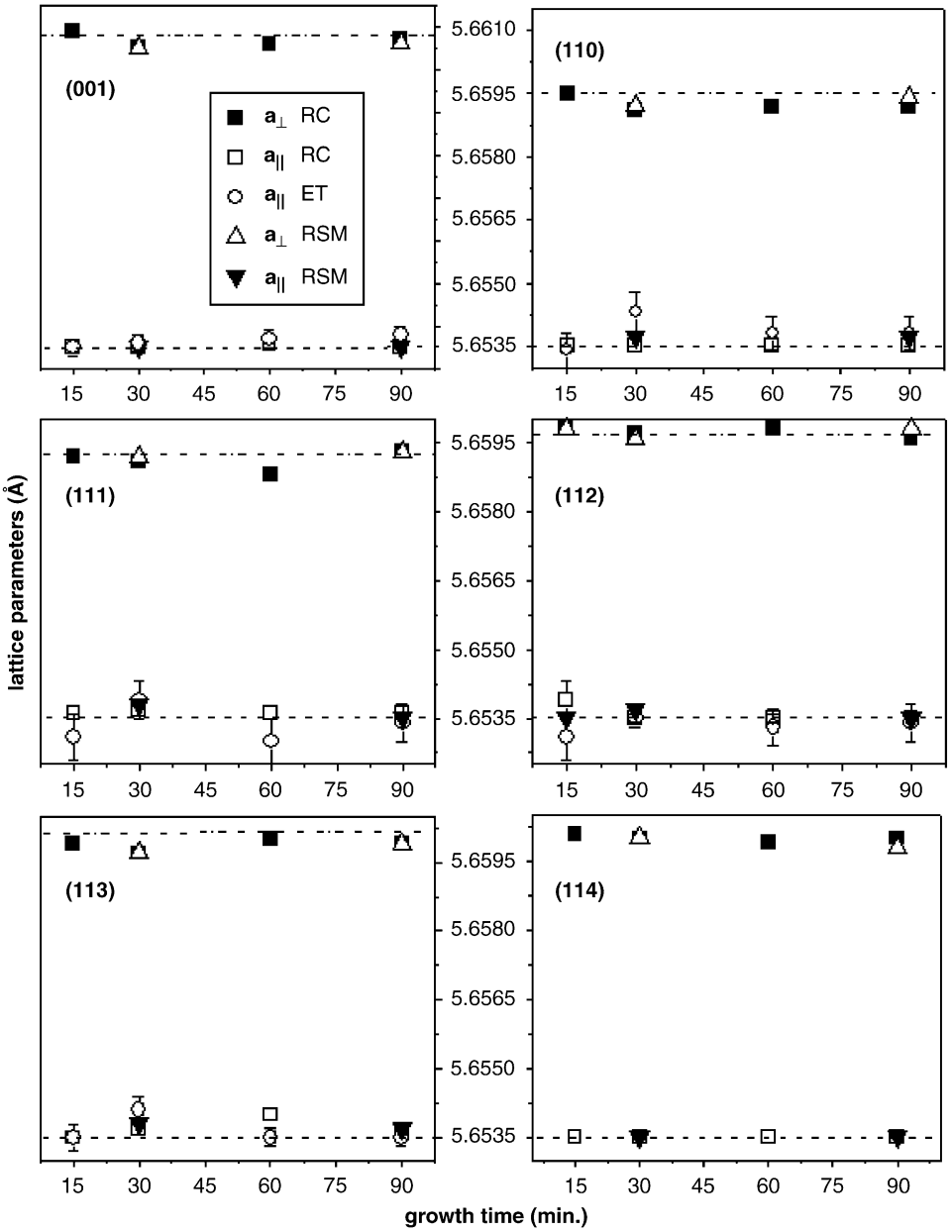

Fig. 4. In-plane and out-of-plane lattice parameters of strained Ge layers on GaAs as determined by high resolution X-ray diffraction, using rocking curves (RC), elastic theory (ET) and reciprocal space maps (RSM).

Table 3
In-plane and out-of-plane lattice parameters of a 660 nm Ge strained layer grown on GaAs, determined by elastic theory (ET), rocking curves (RC) and reciprocal space maps (RSM).

Growth direction	$a_\perp$(Å) (PM)	$a_{\|\|}$(Å) (ET)	$a_\perp$(Å) ±0.0001 (RC)	$a_{\|\|[1\,\bar{1}\,0]}$ (Å) ±0.0001 (RC)	$a_{\|\|[n\,n\,\bar{2}]}$ (Å) ±0.0001 (RC)	$a_\perp$(Å) ±0.0001 (RSM)	$a_{\|\|}$(Å) ±0.0001 (RSM)
(0 0 1)	5.6608	5.6536	5.6605	5.6535	5.6535	5.6605	5.6535
(1 1 0)	5.6596	5.6543	5.6592 (4.0016)	5.6535 (3.9976)	5.6535 (5.6535)	5.6592	5.6537
(1 1 1)	5.6592	5.6538	5.6591 (9.0802)	5.6537 (3.9978)	5.6537 (6.9244)	5.6592	5.6538
(1 1 2)	5.6597	5.6535	5.6597 (13.8637)	5.6535 (3.9976)	5.6535 (9.7921)	5.6596	5.6537
(1 1 3)	5.6601	5.6541	5.6597 (18.7710)	5.6537 (3.9978)	5.6537 (13.2592)	5.6597	5.6538
(1 1 4)	—	—	5.6600 (24.0136)	5.6535 (3.9976)	5.6535 (16.9605)	5.6599	5.6535

The first column (PM) gives the out-of-plane lattice parameter of a pseudomorphic Ge layer on GaAs for each growth direction.

where $\hat{x}_{\langle 1,1,0\rangle}$ is a unitary vector along $\langle 1,0,0\rangle + \langle 0,1,0\rangle$, and the reciprocal space points coordinates for the substrate and layer are $\left(2\sqrt{2}/a_0, 4/a_0\right)$ and $\left(2\sqrt{2}/a_{||}, 4/a_\perp\right)$, respectively.

A typical RSM is shown in Fig. 3. The diffraction of the substrate and layer are easily observed for this [1 1 3] grown layer around a (3 1 5) reflection. The layer diffraction is elongated along the growth direction due to the layer thickness (330 nm), but along the in-plane axis the width of this diffraction is smaller than that of the substrate, evidencing the high structural quality of the layer. The decomposition of ⟨3, 1, 5⟩ using Eq. (1) for this orientation gives

$$\langle 3,1,5\rangle = \langle 1,\bar{1},0\rangle + \frac{1}{11}\langle 3,3,\bar{2}\rangle + \frac{19}{11}\langle 1,1,3\rangle = 2\sqrt{\frac{6}{11}}\hat{x}_{\hat{x}_1+\hat{x}_2} + \frac{19}{\sqrt{11}}\hat{x}_3,$$

where $\hat{x}_{\hat{x}_1+\hat{x}_2}$ is a unitary vector along $\hat{x}_1 + \hat{x}_2$, thus, the expected coordinates of the substrate point in reciprocal lattice units are $\left(2\sqrt{6/11}/a_0, 19/\sqrt{11}a_0\right)$ that is, (0.2612714, 1.013304) Å^{-1}. The layer lattice parameters were determined from the center of the film diffraction coordinates $\left(2\sqrt{6/11}/a_{||}, 19\sqrt{11}a_\perp\right)$ shifted accordingly to the measured substrate coordinates. RSM were also used for the other growth directions to obtain the lattice parameters.

Fig. 4 shows the lattice parameters for each growth direction and different layer thickness. The horizontal lines indicate the values of GaAs lattice constant 5.6535 Å (bottom) and $a_\perp$ for a fully strained Ge layer on GaAs (top) as obtained from the ratios λ of Table 1 and Ge bulk lattice constant 5.6577 Å.(For Ge $C_{11} = 12.87$, $C_{12} = 4.77$ and $C_{44} = 6.67$ [$\times 10^{11}$ dyn/cm^2]). As we can see, Ge layers are pseudomorphically grown on GaAs for all the substrate orientations, and as expected, the in-plane parameters obtained only from symmetrical diffractions an elastic theory (ET) show the largest deviation from both the lattice constant of the substrate and $a_{||}$ as obtained from RC and RSM. We show a comparison of the obtained values in Table 3 for the 660 nm (30 min) film. The first parameter column, gives the expected out-of-plane lattice parameter of a pseudomorphic (PM) Ge layer on GaAs for each growth direction. The second column (ET) is $a_{||}$ as obtained from elastic theory using just a symmetric diffraction, the bulk Ge lattice constant and the ratios λ of Table 1. As we mentioned before, there was not a measurable symmetric reflection for the [1 1 4] orientation. The next three columns show the parameters: $a_\perp$, $a_{||[1\,\bar{1}\,0]}$ and $a_{||[n\,n\,\bar{2}]}$ determined from asymmetrical RC and following Eqs. (4) to (9) above. The values in parentheses are the parameters as obtained directly from (8) and (9) and give the distances marked in Fig. 1. The other values above them are the equivalent lattice parameters of a [0 0 1] strained layer. The last two columns show $a_\perp$ and $a_{||}$ determined from RSM. Comparing the parameter values, it can be seen that those obtained from ET show the highest difference, in particular the [1 1 0] and [1 1 3] layers, which would apparently exhibit a degree of relaxation on layers that we know from RSM are fully strained. On the other hand, the values obtained from RC and RSM compare extremely well, all the differences are within the experimental uncertainty of 1×10^{-4} Å. Considering that RSM give an immediate picture of the strain status and that accurate values for the lattice parameters can be obtained from their analysis independently of orientation, it is evident that the approach followed to determine the lattice parameters from RC is correct and accurate.

In summary, we propose a procedure to experimentally determine both the in-plane and out-of-plane lattice parameters of [1 1 n] epitaxial strained layers from HRXRD rocking curves. The heterostructure Ge/GaAs is used as a model system, due to its small lattice mismatch, to study the validity of this approach. We conclude that accurate values for the lattice parameters are obtained

from [1 1 n] strained layers rocking curves when compared to the results of a more general but more time consuming option such as reciprocal space mapping. Thus, we believe this procedure should prove useful in the strain analysis and composition estimation by HRXRD of more complex cubic heterostructures.

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