An Improved Deviation Parameter for the Simulation of Dynamical X-ray Diffraction on Epitaxic Heterostructures

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Abstract
X-ray diffraction rocking curves of a strained-layer superlattice structure have been measured at symmetric and asymmetric Bragg reflections and compared with simulated diffraction curves. The calculations are based on dynamical scattering theory. The experimental and theoretical curves exhibit a discrepancy with regard to the angular position of the higher-order satellite reflections, which can be removed by introducing a new expression for the deviation parameter in the dynamical diffraction theory. The improved deviation parameter extends the range of validity of the two-beam approximation, especially for asymmetric reflections with glancing exit geometry. Therefore, if the relaxation of strained-layer heterostructures is to be determined by comparison with simulated rocking curves, only the improved parameter should be used.

1. Introduction
During the last twenty years, high-resolution X-ray diffraction has become an important routine tool for the characterization of epitaxic layers of compound semiconductors (for a review, see Segmüller, Noyan & Speriosu, 1989). For single-layer structures, parameters such as the lattice mismatch, the chemical composition and the thickness of epitaxic layers can be easily determined by this non-destructive technique. For multilayer structures, however, the interference of X-rays scattered from different layers can result in complex diffraction curves, which cannot be evaluated directly. In these cases, a comparison of the measurement data with calculated diffraction curves is necessary to extract the information from the data. The determination of gradients of strain and chemical composition at heterointerfaces and the investigation of interface roughness also require simulations.

Both kinematic and dynamical theories have been used for simulating the diffraction of X-rays. The kinematical scattering theory is conceptionally simple and easy to implement as a computer program. It fails, however, to describe the Bragg reflections of layers with a thickness exceeding the extinction distance of the X-rays, since conservation of energy and multiple scattering of the X-rays are neglected.

In dynamical scattering theory, these effects are taken into account and there is no limitation with respect to the thickness of the crystal layers. Owing to the two-beam approximation, which is usually made in the dynamical equations, the solution is valid only in a small angular range near to the Bragg reflection under consideration. Nevertheless, dynamical simulation programs have been applied successfully to analyse diffraction curves from lattice-matched or nearly lattice matched heterostructures (Halliwell, Lyons & Hill, 1984; for a list of further references, see Segmüller, Noyan & Speriosu, 1989). As pointed out by Fewster & Curling (1987) and Wie (1989), the position of the Bragg peak of a thin layer can be shifted by interference with the nearby Bragg reflection of a thick layer or of the substrate. This interference effect is sensitively dependent on the phase difference of the scattered X-rays from both involved layers and will make a dynamical calculation necessary, even if all the epitaxic layers apart from the substrate are thin compared with the extinction distance.

Recently, new electronic and opto-electronic devices such as high-electron-mobility transistors and solid-state lasers were developed, which are based on thin strongly strained layers or strained-layer superlattices. Zaus, Schuster, Göbel & Reithmaier (1991) and Servidori, Cembali, Fabri & Zani (1992) observed that, for these types of heterostructures, the usual linear approximation for the so-called deviation parameter of the dynamical theory gives rise to incorrect angular positions for the Bragg reflections or satellite reflections of the simulated diffraction curve. They suggested that the original expression for the deviation parameter given by Taupin (1964) or a higher-order approximation of this expression should be used. The same modification was proposed by Möller (1991) in his study on II–VI semiconductor heterostructures.

In this paper, it is demonstrated that the deviation parameter given by Taupin should be applied only to symmetric Bragg reflections while for asymmetric reflections – especially with glancing exit – a new expression is required, which is presented for the first time.
2. Takagi-Taupin equation

Since the work of Halliwell, Lyons & Hill (1984), the dynamical theory developed by Takagi (1962, 1969) and Taupin (1964) for crystals with a strain gradient has become a standard method for the simulation of X-ray diffraction in epitaxic structures. For laterally homogeneous layers, the change of the reflected amplitude ratio $D_H/D_0$ of the diffracted and incident beams can be described by an ordinary differential equation (Barrels, Hornstra & Lobeek, 1986):

$$-i dX/dt = X^2 - 2\eta X + 1. \quad (1)$$

The complex quantities $X$, $T$ and $\eta$ are given by

$$X = (x_H/x_H)^{1/2}|\gamma_H/\gamma_0|^{1/2}D_H/D_0, \quad (2)$$

$$T = \pi C(x_Hx_H)^{1/2}t/|x_0\gamma_H|^{1/2}, \quad (3)$$

$$\eta = [-b(\theta - \theta_B) \sin 2\theta_B + \frac{1}{2}x_0(1 - b)] \times [|b|^{1/2}C(x_Hx_H)^{1/2}]^{-1}. \quad (4)$$

$X$ represents the normalized amplitude ratio, $T$ the normalized coordinate $t$ perpendicular to the crystal surface and $\eta$ the deviation parameter. $D_G$ is the electric displacement. The electric susceptibility $\chi_G$ is related to the structure factor $F_G$ of the crystal unit cell by $\chi_G = -\tau_e \lambda^2 F_G/(\pi V)$, where $\tau_e = e^2/4\pi\varepsilon_0 mc^2$ is the classical electron radius, $\lambda$ is the X-ray wavelength and $V$ the volume of the unit cell. $G \in \{0, H, \bar{H}\}$ is a reciprocal-lattice vector. $\gamma_0 = \sin(\theta_B - \varphi)$ and $\gamma_H = -\sin(\theta_B + \varphi)$ are the direction cosines of the incident and reflected beams with respect to the crystal-surface normal. The asymmetry factor $b = \gamma_0/\gamma_H$ is negative in the Bragg case. $C$ is the polarization factor, which is $1$ for $\sigma$ polarization and $|\cos 2\theta_B|$ for $\pi$ polarization.

The first term in the numerator of the deviation parameter $\eta$ describes the deviation of the incidence angle $\theta$ from the kinematic Bragg angle $\theta_B$ of the layer. The second term is a correction for refraction and absorption of the X-rays. In homogeneous layers, $\eta$ is constant and an analytical solution can be given for the differential equation (1). The amplitude ratio $X_t$ at the top of the layer is related to the amplitude ratio $X_0$ at the bottom by

$$X_t = \eta + (\eta^2 - 1)^{1/2}[(S_1 + S_2)/(S_1 - S_2)], \quad (5)$$

where

$$S_{1,2} = [X_0 - \eta \pm (\eta^2 - 1)^{1/2}] \exp[\mp iT(\eta^2 - 1)^{1/2}]. \quad (6)$$

For large $t$, this solution approaches the Darwin–Prins formula for the reflectivity of a semi-infinite crystal:

$$X_\infty = \eta - \text{sign}\{\text{Re}(\eta)\}(\eta^2 - 1)^{1/2}. \quad (7)$$

To obtain the reflected amplitude of a multilayer structure, we start with the Darwin formula for the substrate and add layer upon layer, using the recursion formula (5), until we arrive at the surface of the uppermost layer. Graded layers are subdivided into thin lamellae, which can be handled like homogeneous layers (Halliwell, Lyons & Hill, 1984). Finally, the reflectivity is given by

$$R = |y_H/y_0||D_H/D_0|^2$$

$$= |x_H/x_H||X|^2. \quad (8)$$

In (4), the angles $\theta$ and $\theta_B$ are measured with reference to the Bragg plane of the respective layer. As the Bragg angle and the inclination of the lattice planes may change from layer to layer according to the mismatch or the refractive index, it is convenient for the calculation to choose the Bragg plane of the substrate as a common plane of reference. The deviation from the Bragg condition can then be expressed by

$$\Delta \omega = \theta - \theta_{B,S} + \Delta \varphi - \Delta \theta, \quad (9)$$

where $\theta_{B,S}$ is the Bragg angle of the substrate, $\Delta \varphi$ the change of the inclination of the lattice planes and $\Delta \theta$ the change of the Bragg angle. To a first-order approximation in the mismatch components perpendicular and parallel to the substrate surface, $\Delta \varphi$ and $\Delta \theta$ are given by (Bartels & Nijman, 1978)

$$\Delta \varphi = [((\Delta d/d)_\perp - (\Delta d/d)_\parallel) \cos \varphi_S \sin \varphi_S, \quad (10)$$

$$\Delta \theta = -(\Delta d/d)_\parallel \cos^2 \varphi_S$$

$$+ (\Delta d/d)_\parallel \sin^2 \varphi_S \tan \theta_{B,S}, \quad (11)$$

where $\varphi_S$ is the inclination of the substrate lattice planes and $\theta_{B,S} - \varphi_S$ is the angle of incidence. This gives $\varphi_S > 0$ for glancing incidence and $\varphi_S < 0$ for glancing exit.

3. Experimental

The sample under investigation was a strained-layer multiple-quantum-well structure, grown by molecular-beam epitaxy on a (001)-oriented GaAs substrate. It consisted of ten periods of In$_x$Ga$_{1-x}$As/GaAs with nominal values of $t_{GaAs} = 100$ nm for the thickness of the GaAs layers, $t_{InGaAs}$ = 10 nm for the thickness of the In$_x$Ga$_{1-x}$As layers and $x = 0.20$ for the indium content. The thickness of a single In$_x$Ga$_{1-x}$As layer as well as that of the whole superlattice were chosen to be well below the critical value. The lattice mismatch was therefore expected to be accommodated by elastic strain. The high quality of the sample was confirmed by transmission electron microscopy, optical absorption spectroscopy and photoluminescence (Reithmaier, Höger, Riechert, Heberle, Abstreiter & Weimann, 1990).
No evidence of strain relaxation could be found by these techniques.

The X-ray measurements were carried out using a five-crystal high-resolution diffractometer with a 4 × Ge 044 monochromator (Zaus, 1992). The monochromator gives a nearly perfectly σ-polarized primary beam with a divergence of 5" in the scattering plane and a wavelength band of Δλ/λ = 2.2 × 10⁻⁵ (DuMond, 1937; Bartels, 1983). The goniometer, a modified Siemens D500 with a Harmonic-Drive differential gear, has a resolution of 25.000 steps per degree for the θ movement. A rotating anode (Siemens M18X) was used as an X-ray source for Cu Kα₁ radiation and an NaI scintillation counter as a detector.

The measurement of the GaAs 004 reflection is given in Fig. 1(a). In addition to the GaAs substrate reflection, the satellite reflections of the (In,Ga)As/GaAs superlattice can be seen from −26th to +13th order. (In this article, we use both ‘superlattice’ and ‘multiple quantum well’ as synonyms for a periodically layered epitaxic structure.) The main satellite reflection ‘0’ was identified by combining information from the GaAs 004 and GaAs 115 reflections (Zaus, Schuster, Göbel & Reithmaier, 1991). This reflection corresponds to the average unit cell of the epitaxic layers forming the superlattice (Kervarec, Baudet, Caulet, Auvray, Emery & Regreny, 1984). Therefore, it can be used to determine the average lattice mismatch of the superlattice parallel and perpendicular to the substrate surface.

The angular spacing of the satellite peaks in the measurement of the GaAs 004 reflection gives a superlattice period of tSL = 106.9 (10) nm. The influence of a small inclination between the surface and the (001) lattice planes of the superlattice can be estimated by the following relation between the period and the spacing of the satellites Δω,

\[ Δω = \frac{λ |γ_H|}{(t_{SL} \sin 2θ_B)} \]

which is valid in the neighbourhood of the substrate reflection. An inclination angle Δφ of the (001) lattice planes will give rise to a change of the direction cosine of the diffracted beam γH = −sin (θB + Δφ) and to a corresponding relative change of the period tSL by Δφ cot θB.

The angular deviation between the surface and the (001) lattice planes of the substrate was determined by four measurements of the GaAs 004 reflection to be less than 0.01 (1)°. Between measurements, the sample was rotated by 90° in the plane of the wafer and the surface normal was realigned using a laser beam reflected from the surface of the sample.

Similarly, the tilt angle between the (001) lattice planes of the substrate and the superlattice was checked by measuring the angular distance between the main satellite and the GaAs 004 substrate reflection for four different azimuths of the sample (Tanner, Miles, Peterson & Sacks, 1988). We obtained 0.000 (1)° for the tilt angle and (Δd/d) ⊥ = 2.19 (3) × 10⁻³ for the perpendicular component of the average lattice mismatch. In summary, it can be said that, for the sample under investigation, the inclination angle between the surface and the (001) lattice planes of the superlattice is negligible for the determination of the period.

Green, Tanner, Turnbull, Barnett, Emeny & Whitehouse (1991) have observed highly anisotropic misfit dislocation densities in partially relaxed (In,Ga)As/GaAs layers. Therefore, we have determined the parallel component of the average lattice mismatch (Δd/d) || separately from the asymmetric 224, 224, 224 and 224 reflections. Each reflection was measured with both glancing incidence and glancing exit geometry. The four values for the mismatch parallel to the [110] and [110] directions vary from 1.4 × 10⁻⁵ to 2.5 × 10⁻⁵, which is slightly below the error of this technique (3 × 10⁻⁵).

In the following, asymmetric scattering geometries are denoted by an index ‘−’ for glancing incidence or ‘+’ for glancing exit. Fig. 2(a) shows a typical measurement of the GaAs 224, reflection. The minima of intensity between the satellites are less pronounced than for the 004 reflection. This can be explained in part by the fact that the asymmetric reflection was measured without a slit in front of the detector. Furthermore, the influence of the divergence of the primary beam is stronger for the glancing exit geometry, because the angular distance between the satellite reflections is smaller for this scattering geometry.
4. Failure of the conventional deviation parameter

In Figs. 1(c) and 2(c), simulated diffraction curves of the 004 and 224-reflections of the superlattice are shown, which have been calculated with the algorithm described in §2. The parameters used in the calculation are \( a_{\text{GaAs}} = 5.6533 \) Å for the lattice parameter of GaAs, \( t_{(\text{In,Ga})\text{As}} = 9.2 \text{ nm} \) and \( t_{\text{GaAs}} = 97.7 \text{ nm} \) for the thickness of the epitaxic layers, \( x = 0.187 \) for the In content and \( (\Delta d/d)_{\perp} = 0.0257 \) for the perpendicular lattice mismatch of the (In,Ga)As layers. The parallel mismatch and the tilt angle between the surface and the (001) lattice planes have been assumed to be zero.

From the simulation of the 004 reflection (Fig. 1), we find that at least the substrate and the two satellites with highest intensity have to be calculated by dynamical theory as their reflectivity is above 0.1. A comparison of dynamical and kinematical simulation gives maximum reflectivities of \( R_{\text{dyn}} = 0.222 \) and \( R_{\text{kin}} = 0.264 \) for the +first-order satellite and \( R_{\text{dy}n} = 0.105 \) and \( R_{\text{ki}n} = 0.114 \) for the +second-order satellite.

The measured (a) and simulated (c) diffraction curves of the 004 reflection are in good agreement with respect to the positions of the satellites in the neighborhood of the substrate reflection. This was expected owing to our choice of period and mean lattice mismatch of the superlattice. The simulation parameters for curve (c) have not been optimized with respect to the satellite intensities and a considerably improved fit of the intensities could be obtained if chemical grading at the interfaces is taken into account, assuming a different width for the GaAs/(In,Ga)As and the (In,Ga)As/GaAs interfaces (Zaus, 1992).

A closer examination reveals that the satellites of the simulated curve at the low-angle side are shifted slightly to the left (see the –21st-order satellite indicated in Fig. 1). The amount of the shift increases with the distance from the main satellite. This deviation cannot be explained by an error in the determination of the period because the satellites on the high-angle side, above 33.3°, also show a small shift to the left with respect to the measurement (not visible on the scale of Fig. 1). By additional simulations, the possibility that the satellite shift is caused by a tilt angle between the surface and the (001) lattice planes of the order of 0.01° was ruled out.

The deviation is even more striking for the GaAs 224+ reflection (Fig. 2). Owing to the asymmetric scattering geometry – the incidence angle is 77.1°, the exit angle is 6.6° – the spacing of the satellites is smaller than that at the 004 reflection. If we use the order of the satellites as a common scale for the comparison, we find that the shift of the –14th-order satellite is about 1.5 periods whereas, for the 004 reflection, the shift of the –21st-order satellite only amounts to 0.1 periods. The deviation between measured and calculated satellite positions is also clearly visible on the high-angle side of the 224+ reflection.

In contrast to the situation for the 224+ reflection, there is good agreement between the satellite positions of the measured and the simulated diffraction curve over the whole range of measurement for the 224+ reflection with glancing incidence. Thus, the deviation is also seen to be dependent on the scattering geometry.

The fact that the satellite reflections in the simulation are shifted indicates that the phase factors \( \exp \left[ \pm IT \left( \eta^2 - 1 \right)^{1/2} \right] \) in the solution of the Takagi-Taupin equation (6) are not correct for large values of the deviation parameter \( \eta \), i.e. far from the Bragg reflection of the respective layer. Owing to the linear dependence of the deviation parameter on \( \theta \), the distance between the satellites is approximately constant with regard to \( \theta \), while it is actually constant with regard to the reciprocal-space coordinate \( q_{\perp} \) perpendicular to the crystal surface. For symmetric scattering geometries, \( q_{\perp} \propto \sin \theta \). According to Taupin (1964), the first part of the numerator of \( \eta \) is obtained by setting

\[
2(\sin \theta - \sin \theta_B) \sin \theta_B \approx (\theta - \theta_B) \sin 2\theta_B. \tag{13}
\]

The deviation parameter defined by using the original, more exact, expression on the left side of (13) will be called \( \eta' \). With \( \eta' \), a perfect fit of the satellite positions can be obtained in the case of the 004 reflection (Fig. 1b) (Zaus, Schuster, Göbel & Reithmaier, 1991). The parameters for the superlattice are the same as for simulation (c) but the Bragg angle \( \theta_B \) and the inclination...
angle $\varphi$ for each layer is calculated directly from the dimensions of the unit cell. The linear approximations for $\Delta \varphi$ and $\Delta \theta$, (10) and (11), have not been used, since they are not exact enough for layers with a mismatch of 0.0257.

In spite of this success with the 004 reflection, approximation (13) is not the reason for the strong shift of the satellite positions in the simulation of the 224+ reflection. This can be confirmed by a simulation of the 224+ reflection, using the same modifications as for the 004 reflection (not shown in Fig. 2). In the simulation, the spacing of the satellites over the small angular range of 0.3° is approximately constant and equal to 0.0095° whereas, in the measurement (Fig. 2a), the distance between the satellites increases with the incidence angle $\theta$ from 0.0075° at the -14th-order satellite to 0.0105° at the +9th-order satellite.

The error caused by (13) increases with $|\theta - \theta_B|$. Therefore, contrary to our observation, the approximation should have a stronger effect on the simulation of the 224+ reflection, where the angular range of the measurement is larger by a factor of $\sqrt{b} \approx 8.5$ compared with the 224+ reflection.

Recently, Möller (1991) and Servidori, Cembali, Fabri & Zani (1992) suggested that the expansion (13) should be extended to the second order in $|\theta - \theta_B|$. From the argument above, it is clear that this modification does not help either; however, we will return to this issue later, when the properties of the improved deviation parameter are discussed.

5. New deviation parameter

It should be noted that, for homogeneous layers, the solution of the Takagi-Taupin equation and of the Ewald-Laue formulation of the dynamical scattering theory are identical (Taupin, 1964). Therefore, if we approximate the inhomogeneous layers in the calculation by stacks of homogeneous lamellae, the two theories will give the same results. We will use this fact to derive the new deviation parameter $\eta^*$ within the framework of Laue’s theory. The result will then be transferred to the Takagi-Taupin equation.

5.1. Angle of exit

In two-beam approximation, the dynamical equations for the amplitudes of the electric field† in the crystal can be written as (Batterman & Cole, 1964)

\[
\begin{align*}
[(k_H^2 - k^2)/K^2]E_H & = C_{\chi_H}E_0 + \chi_0E_H, \\
[(k_0^2 - k^2)/K^2]E_0 & = \chi_0E_0 + C_{\chi_0}E_H,
\end{align*}
\]  

where the longitudinal components of the field, which are of the order $O(\chi_H)$, have been neglected. As the wave field in the crystal has the form of a Bloch function, the wave vectors $k_0$ and $k_H$ of the incident and diffracted waves in the crystal are related by

\[ k_H = k_0 + \mathbf{H}, \]

$\mathbf{H}$ being the reciprocal-lattice vector of the Bragg reflection. $K = 2\pi/\lambda$ is the magnitude of the vacuum wave vector. In the following, we will consider only $\sigma$-polarized radiation so that the polarization factor is $C = 1$.

The secular equation of the linear equation system (14) gives the dispersion relation

\[ (k_0^2 - k^2)(k_H^2 - k^2) = K^4\chi_H\chi_0, \]

where

\[ k = nK \]

is the ‘mean’ magnitude of the wave vector inside the crystal and $n = (1 + \chi_0)^{1/2}$ is the mean refractive index of the crystal. In the conventional theory (von Laue, 1960), the solution of the dispersion equation is needed close to the Bragg reflection only, so each of the factors on the left side of (16) may be approximated by

\[ k_G^2 - k^2 \approx 2k(k_G - k). \]

Thereby, the dispersion equation is reduced to second degree in $k_0$. The two solutions lost by this approximation can be neglected unless the scattering geometry is extremely asymmetric (Farwig & Schürmann, 1967). Only after this approximation and the subsequent solution of the equation is the relation between the wave fields inside and outside the crystal established.

In contrast to this conventional line of reasoning, we will take into account the orientation of the crystal surface before (16) is reduced to an equation of second degree. The scattering geometry is shown in Fig. 3. The wave vectors of the incident and diffracted waves in vacuum are denoted by $\mathbf{K}_0$ and $\mathbf{K}_H$, respectively. The wave vectors in the crystal are marked by an index $i$ as a reminder of the fact that the dispersion equation has several solutions. For corresponding waves inside and outside the crystal, the components of the wave vectors parallel to the surface are equal, so we have, by (15),

\[ \mathbf{K}_i = (\mathbf{K}_H^i)^\parallel = (\mathbf{K}_0^i)^\parallel + \mathbf{H}^\parallel = \mathbf{K}_0^\parallel + \mathbf{H}^\parallel, \]

for all values of $i$. The angle of exit $\theta_H + \varphi$ of the diffracted wave in vacuum is therefore given by

\[ \cos(\theta_H + \varphi) = \cos(\theta - \varphi) - 2\sin\theta_B\sin\varphi. \]

For symmetrical Bragg reflections, where $\varphi = 0$, this
relation reduces to the well known ‘law of reflection’ \( \theta_H = \theta \). In the asymmetric Bragg case, we find that, for an X-ray beam incident at an angle of \( \theta_B - \varphi \), the angle of exit of the diffracted beam is \( \theta_H + \varphi \).

The change in the angle of exit with \( \theta \) can be obtained by implicit differentiation of (20):

\[
d\theta_H/d\theta = \sin(\theta - \varphi)/\sin(\theta_H + \varphi) = -b. \tag{21}
\]

5.2. Reflected amplitude ratio in the crystal

For the following considerations, we define two vectors \( \mathbf{k}_0 \) and \( \mathbf{k}_H \) (Fig. 4). If the crystal is replaced by an amorphous medium with the same mean refractive index \( n \), the vector \( \mathbf{k}_0 \) will be the wave vector of the refracted incident wave. Its components parallel and perpendicular to the surface are

\[
\begin{align*}
\mathbf{k}_0^\parallel &= K \cos(\theta - \varphi), \\
\mathbf{k}_0^\perp &= K [\sin^2(\theta - \varphi) + \chi_0]^{1/2} \\
&= K \Gamma_0.
\end{align*}
\tag{22}
\]

\( \mathbf{k}_H \) is the corresponding wave vector for the refracted diffracted wave, therefore we have

\[
\begin{align*}
\mathbf{k}_H^\parallel &= K \cos(\theta_H + \varphi), \\
\mathbf{k}_H^\perp &= -K [\sin^2(\theta_H + \varphi) + \chi_0]^{1/2} \\
&= K \Gamma_H.
\end{align*}
\tag{23}
\]

\[\xi_G = \xi_G(x) - k, \tag{27}\]

we obtain, for the components perpendicular to the surface,

\[
\begin{align*}
k_0^\perp &= \left[ k_0^2 - (k_0^\parallel)^2 \right]^{1/2} \\
&= \left[ (k + \xi_0)^2 - K^2 \cos^2(\theta - \varphi) \right]^{1/2} \\
&= K \left( \Gamma_0^2 + 2k\xi_0/K^2 + \xi_0^2/K^2 \right)^{1/2}, \tag{28}\end{align*}
\]

and

\[
\begin{align*}
k_H^\perp &= -K \left( \Gamma_H^2 + 2k\xi_H/K^2 + \xi_H^2/K^2 \right)^{1/2}. \tag{29}\end{align*}
\]

Furthermore, we have, by (15) and Fig. 3,

\[
k_H^\perp = k_0^\perp + H = k_0^\perp - 2K \sin \theta_H \cos \varphi. \tag{30}\]

The two tie points \( A^{(1)} \) and \( A^{(2)} \) will now be treated separately. First, we consider \( A^{(1)} \), which is the tie point

\[
\begin{align*}
&\Gamma_0 \text{ and } \Gamma_H \text{ are the direction cosines of } \mathbf{k}_0 \text{ and } \mathbf{k}_H \text{ with} \\
&\text{respect to the surface normal directed into the crystal.}
\end{align*}
\]

The factors on the left side of the dispersion relation can now be written as

\[
k_G^2 - k^2 = (k_G^\perp - k_G^\parallel)(k_G^\perp + k_G^\parallel). \tag{26}\]

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\end{align*}
\]
for the wave field with Poynting vector directed into the crystal. (For larger angles of incidence, when the tie points in Fig. 4 lie to the left of the gap of the dispersion surface, \( A^{(1)} \) will become the upper tie point and \( A^{(2)} \) the lower.) We exclude extremely asymmetric geometries, so that

\[
\theta - \varphi \gg \theta_e \quad \text{and} \quad \theta_H + \varphi \gg \theta_e,
\]

(31)

where the critical angle of total reflection \( \theta_e = (-\chi_0)^{1/2} \) is typically smaller than 0.5°. Then, \( \xi_0 / K \) is of the order of \( |\chi_0| \approx 10^{-5} \) and, since \( k / k' \approx 1 \), the expression for \( k_0' \) can be approximated by

\[
k_0' \approx K(\Gamma_0 + \xi_0 / K\Gamma_0).
\]

(32)

Using the factorization (26) and substituting the expressions for the vector components (23), (25), (30) and (32), we obtain for the dispersion equation

\[
(\xi_0 / K\Gamma_0)(2\Gamma_0 + \xi_0 / K\Gamma_0)(\delta + \xi_0 / K\Gamma_0) \times (2\Gamma_H + \delta + \xi_0 / K\Gamma_0) = \chi_{H}\chi_{H},
\]

(33)

where we have introduced the abbreviation

\[
\delta = \Gamma_0 - \Gamma_H - 2\sin \theta_B \cos \varphi.
\]

(34)

The dynamical Bragg angle, which differs from the kinematic Bragg angle \( \theta_B \) by a small correction for refraction, can be determined from the condition \( \Delta \theta = 0 \). Expanding the square roots contained in \( \Gamma_0 \) and \( \Gamma_H \) linearly in \( \chi_0 \) and the sine functions linearly in the correction \( \Delta \theta = \theta - \theta_B \), we find, in agreement with James (1967, p. 426),

\[
\Delta \theta = (-\chi_0/2\sin 2\theta_B)(1 + |\gamma_H / \gamma_0|).
\]

(35)

In the neighbourhood of the Bragg reflection, both \( \xi_0 / K\Gamma_0 \) and \( \delta \) are small compared with \( \Gamma_0 \) and \( \Gamma_H \); therefore, we may neglect these terms in the second and fourth factors on the left side of (33). The solution of the resulting quadratic equation is given by

\[
(\xi_0 / K\Gamma_0)_{1,2} = \frac{1}{2} \left[ -\delta \pm \left( \delta^2 + \frac{\chi_{H}\chi_{H}}{\Gamma_0\Gamma_H} \right)^{1/2} \right].
\]

(36)

According to our definition of \( A^{(1)} \), we must take the minus sign for incidence angles smaller than the Bragg angle \( \delta < 0 \) and the plus sign for larger angles \( \delta > 0 \). By means of the dynamical equations (14), the factorization (26) and (23) and (32), the amplitude ratio for the wave field belonging to \( A^{(1)} \) can now be expressed by

\[
E_{H}^{(1)} / E_{0}^{(1)} = \left\{ -\Gamma_0\delta \pm \left[ (\Gamma_0\delta)^2 + \chi_{H}\chi_{H}\Gamma_0 / \Gamma_H \right]^{1/2} \right\} / \chi_{H}.
\]

(37)

A similar consideration can be applied to the tie point \( A^{(2)} \) (see Appendix A). Excluding the sign of the square root, the formula for the amplitude ratio (A.4) is the same as for tie point \( A^{(1)} \).

5.3. Boundary conditions and recursion formula

The relation between the wave fields in the crystal and in vacuum is established by the continuous boundary conditions for the field amplitudes at the upper and the lower surface of the crystal (James, 1967, p. 427). The amplitude ratio \( (E_H / E_0)(t) \) at the upper surface can be expressed as a function of the ratio \( (E_H / E_0)(0) \) at the lower surface of the crystal, where \( t \) is the thickness of the crystal slab. We shall skip the straightforward algebra. The result can be obtained from (2)–(6) if the following substitutions are made:

\[
\gamma_0 \rightarrow \Gamma_0, \quad \gamma_H \rightarrow \Gamma_H, \quad -b(\theta - \theta_B) \sin 2\theta_B \rightarrow \Gamma_0 \delta. \quad (38)
\]

(39)

(Furthermore, the difference between the electric field \( E \) and the electric displacement \( D \) is neglected.) In summary, \( \eta \) has to be replaced by

\[
\eta^* = \Gamma_0 \delta / (|\Gamma_0 / \Gamma_H|^{1/2}C(\chi_{H}\chi_{H})^{1/2}).
\]

(41)

By substitutions (38) and (39), the refraction of the X-rays at the interface between crystal and vacuum is taken into account. Since we have excluded extremely asymmetric scattering geometries, these corrections are small and can be neglected – apart from the refraction corrections of \( \delta \), which cause an angular shift of the Bragg reflection and must be kept in first order in \( \chi_0 \):

\[
\delta = \gamma_0 - \gamma_H - 2\sin \theta_B \cos \varphi \\
+ \frac{1}{2}\chi_0(1 - b) \rightarrow \Delta \theta.
\]

(42)

By this approximation, the computation time is reduced.

The transfer of the results of this derivation to the Takagi-Taupin theory can also be justified by a more fundamental approach, starting from the system of partial differential equations (18) given by Takagi (1969). If the argument of §5 is applied to these equations by analogy, we will arrive at the Takagi-Taupin equation (1), modified by the substitutions (38)–(40).

6. Final form of the new deviation parameter and comparison with the experiment

The simulations in Figs. 1(b) and 2(b) have been calculated using the definitions (2)–(3), the recursion formulae (5)–(7) and the following form of the deviation parameter \( \eta^* \):

\[
\eta^* = \gamma_0(\gamma_0 - \gamma_H - 2\sin \theta_B \cos \varphi) + \frac{1}{2}\chi_0(1 - b) \times \left[ (|b|^{1/2}C(\chi_{H}\chi_{H})^{1/2})^{-1} \right].
\]

(43)
\( \gamma_0 = \sin(\theta - \varphi) \) is now dependent on the incidence angle. \( \gamma_H = -\sin(\theta_H + \varphi) \) can be determined by (20). Note that \( \gamma_0 \) and \( \gamma_H \) also appear in the definitions of \( X \) and \( T \), (2) and (3). As in §2, \( \theta_B \) is the kinematic Bragg angle and \( \varphi \) is the inclination angle of the lattice planes of the layer.

Figs. 1 and 2 demonstrate that a perfect fit of the satellite positions is obtained for both the 004 and the 224\(_+\) reflections. It should be noted that the intensity of the satellites is also influenced by the choice of the deviation parameter, as can be seen from a comparison of the -6th-order satellite and the neighbouring satellites of curves (b) and (c). Furthermore, if we compare the simulations of the 224\(_+\) reflection, Figs. 2(b) and (c), with respect to the envelope of the satellites below 41.8°, we will find a significant shift of the envelope maximum. For the 004 reflection, the shift of the envelope maximum at 32.2° is hardly visible.

In the neighbourhood of the maximum, the shape of the envelope is mainly determined by the structure factor of the In\(_x\)Ga\(_{1-x}\)As layers, since the Bragg condition for In\(_x\)Ga\(_{1-x}\)As is satisfied about this incidence angle, whereas the scattering intensity contributed by the GaAs layers is rather negligible. The shift of the envelope maximum corresponds therefore to a shift of the In\(_x\)Ga\(_{1-x}\)As layer peak in the simulation of a single strained In\(_x\)Ga\(_{1-x}\)As layer (Figs. 5 and 6).

### 7. Discussion of the new deviation parameter

If we compare the angular dependence of the new deviation parameter \( \eta^* \) (43) with that of \( \eta \) and \( \eta' \), we may concentrate on the term \( \gamma_0 - \gamma_H - 2\sin\theta_B\cos\varphi \). The variation of the refraction correction in \( \eta^* \) is small compared with the variation of the first part of the numerator. The factor \( \gamma_0/|b|^{1/2} \) will cancel out when \( \eta^* \) is multiplied by the thickness \( T \) to give the phase factors \( \exp[\mp iT(\eta^*|^2 - 1)^{1/2}] \).

Using (21) and its derivative, we expand

\[
\begin{align*}
\sin(\theta - \varphi) + \sin(\theta_H + \varphi) - 2\sin\theta_B\cos\varphi \\
= \Delta\theta - \sin(2\theta_B) \\
+ \frac{1}{2}(\Delta\theta)^2 \left( \frac{\cos2\theta_B}{\sin(\theta_B + \varphi)} - \frac{\sin^2(\theta_B - \varphi)}{\sin^3(\theta_B + \varphi)} \right) \\
+ O(\Delta\theta^3)
\end{align*}
\]

in Taylor series in the neighbourhood of \( \theta = \theta_B \). For \( \eta' \), a similar expansion up to second order in \( \Delta\theta \) can be obtained from (4) and (13):

\[
2(\sin\theta - \sin\theta_B)\sin\theta_B/\sin(\theta_B + \varphi) \\
= \Delta\theta - \sin2\theta_B \\
+ \frac{1}{2}(\Delta\theta)^2(-2\sin^2\theta_B)/\sin(\theta_B + \varphi) \\
+ O(\Delta\theta^3).
\]

We find that the two expansions are equal to first order of approximation in \( \Delta\theta \) (and coincide to this order with the angular dependence given by \( \eta \)). Therefore, all deviation parameters lead to the same diffraction curves in the small angular range around the Bragg reflection, where multiple scattering has a great influence on the reflectivity.

The second-order terms of both expansions become large for Bragg reflections with glancing exit geometry, where \( \sin(\theta_B + \varphi) \) is small. This agrees with our observation that the difference between the measurement and the simulation using the conventional deviation parameter \( \eta \) is most striking for the GaAs 224\(_+\) reflection. For that reflection with \( \theta_B = 41.88 \) and \( \varphi = -35.26^\circ \), the coefficient of \( \frac{1}{2}(\Delta\theta)^2 \) in the expansion of \( \eta' \) has a numerical value of -7.7, while the corresponding term in the expansion of \( \eta^* \) is -619.4. In a distance of

---

**Fig. 5.** X-ray diffraction curve of a single In\(_{0.187}\)Ga\(_{0.813}\)As layer of 9.2 nm thickness on a GaAs substrate (GaAs 004 reflection, Cu \( K_{\alpha1} \)): simulation using the conventional deviation parameter \( \eta \) (dashed line) and the new deviation parameter \( \eta^* \) (solid line).

**Fig. 6.** X-ray diffraction curve of a single In\(_{0.187}\)Ga\(_{0.813}\)As layer of 9.2 nm thickness on a GaAs substrate (GaAs 224\(_+\) reflection, Cu \( K_{\alpha1} \)): simulation using the conventional deviation parameter \( \eta \) (dashed line) and the new deviation parameter \( \eta^* \) (solid line).
\( \Delta \theta = 0.15^\circ \) from the Bragg reflection, the relative change of the deviation parameter induced by the second-order correction is 0.0015 for \( \eta' \) and 0.13 for \( \eta^* \). Thus, the second-order term will contribute a noticeable correction only if the improved deviation parameter is used.

As is shown in Appendix B, \( \eta^* \) is exactly proportional to the reduced scattering vector \( |q| \) for the whole range of incidence angles, not just approximately in a small interval around the Bragg reflection like \( \eta' \). This is used in Appendix C to demonstrate that, for incident beams far from the Bragg condition, there is a smooth crossover from the solution of the Takagi-Taupin equation with the new deviation parameter to the reflected amplitude of the kinematic theory.

8. Concluding remarks

In this paper, the necessity of the new deviation parameter has been demonstrated with the example of a strained-layer superlattice but it is also necessary for the simulation of single strained layers. As can be seen from the formula for the reflected amplitude ratio (C.6), the diffracted intensity is calculated for points in reciprocal space that lie on a line perpendicular to the crystal surface. The satellite reflections of a superlattice will be distributed along such lines, even if there is a tilt between the surface and the (001) lattice planes of the substrate crystal (Neumann, Zabel & Morkoč, 1988). For thin crystal layers, the distribution of the diffracted intensity around reciprocal-lattice points can be represented by so-called ‘truncation rods’ (Andrews & Cowley, 1985; Robinson, 1986), which are perpendicular to the crystal surface as well. In that case, the relation between incidence angle and exit angle \( 2\theta \) may also be derived from a simple Ewald construction.

On a relative scale, the shift of the layer reflection caused by using the improved deviation parameter instead of the conventional one is large for asymmetric Bragg reflections with glancing exit (Fig. 6), small for symmetric reflections (Fig. 5) and negligible for asymmetric reflections with glancing incidence. Since the peak position is also sensitively dependent on the layer mismatch parallel and perpendicular to the surface, the choice of the deviation parameter will be crucial for an exact determination of the composition and relaxation of the layer. This subject will be discussed in more detail in a future paper.

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APPENDIX A

Reflected amplitude ratio for \( A^{(2)} \)

In the case of the tie point \( A^{(2)} \), the square root in expression (29) for \( k_H^0 \) is approximated by

\[
 k_H^0 \simeq K(\Gamma_H + \xi_H/K\Gamma_H) \tag{A.1}
\]

as \( |\xi_H/K| \ll 1 \). The dispersion equation takes the form

\[
 (\xi_H/K\Gamma_H)(2\Gamma_H + \xi_H/K\Gamma_H)(\delta - \xi_H/K\Gamma_H) \\
 \times (2\Gamma_0 - \delta + \xi_H/K\Gamma_H) = -\chi_H\chi_H. \tag{A.2}
\]

If we set \( 2\Gamma_H + \xi_H/K\Gamma_H \simeq 2\Gamma_H \) and \( 2\Gamma_0 - \delta + \xi_H/K\Gamma_H \simeq 2\Gamma_0 \), the solutions of the quadratic equation are

\[
 (\xi_H/K\Gamma_H)_{1/2} = \frac{1}{2} \left[ \delta \mp \sqrt{\left( \delta^2 + \frac{\chi_H\chi_H}{\Gamma_0\Gamma_H} \right)^{1/2}} \right], \tag{A.3}
\]

where the plus sign must be selected for incidence angles smaller than the Bragg angle \( \delta < 0 \) and the minus sign for larger angles \( \delta > 0 \). The amplitude ratio for the tie point \( A^{(2)} \) is now given by

\[
 \frac{E_H^{(2)}}{E_0^{(2)}} = \left\{ -\Gamma_0 \delta \mp \left[ (\Gamma_0\delta)^2 + \chi_H\chi_H\Gamma_0/\Gamma_H \right]^{1/2} \right\}/\chi_H. \tag{A.4}
\]

APPENDIX B

Geometrical comparison of the deviation parameters

In Fig. 7, the deviation parameters \( \eta^* \) and \( \eta' \) are illustrated in reciprocal space. The distance \( H\bar{Q} \) is the same for the two scattering geometries; therefore, the angles of incidence and exit in Figs. 7(a) and (b) are interchanged with respect to their magnitudes.

For the special pair of wave vectors \( \bar{P}_10 \) and \( \bar{P}_{1H} \) in Fig. 7(a), the Bragg condition is satisfied exactly but generally the scattering vector

\[
 K_H - K_0 = \bar{P}_2\tilde{Q} - \bar{P}_2\tilde{0} = 0\tilde{H} + \tilde{H}\bar{Q} \tag{B.1}
\]

differs from the reciprocal-lattice vector by the reduced scattering vector \( H\bar{Q} \). If refraction effects are neglected, the magnitude of \( H\bar{Q} \) is

\[
 H\bar{Q} = K(\gamma_0 - \gamma_H - 2\sin \theta_B \cos \varphi) \\
 \simeq K\delta. \tag{B.2}
\]

Therefore, \( H\bar{Q} \) represents the difference that appears in the numerator of \( \eta^* \) (43). (For the reduced scattering vector \( \bar{q} \) belonging to the refracted wave vectors \( \bar{k}_0 \) and \( \bar{k}_H \) within the crystal, the relation \( |\bar{k}_H - \bar{k}_0 - 0\tilde{H}| = K\delta \)
holds exactly. However, for the sake of simplicity, we will neglect refraction in this section.)

In a similar way, the deviation parameter \( \eta' \) is represented by the line

\[
\overline{HR} = 2K(\sin \theta - \sin \theta_B) \sin \theta_B / \sin (\theta_B + \varphi). \tag{B.3}
\]

This relation can be proved by projecting the line \( \overline{HT} = 2K(\sin \theta - \sin \theta_B) \) onto \( \overline{HS} \) and then onto \( \overline{HR} \).

The line \( QR \) represents the difference between the conventional and the new deviation parameter.

The same argument can be applied to the scattering geometry with glancing exit (Fig. 7b). Elementary geometrical considerations (Zaus, 1992) show that the arcs \( QT \) in Figs. 7(a) and (b) are the same size. In both cases, the line \( QR \) is obtained by projecting the arc \( QT \) onto the straight line \( HQ \) in the direction normal to the straight line \( P_1H \). The different lengths of \( QR \) for glancing incidence and glancing exit are caused only by the angle between the straight line \( HQ \) and the direction of projection, which is \( \theta_B + \varphi \) in the former case and \( \theta_B - \varphi \) in the latter.

Symmetrical Bragg reflections stand out because the straight lines \( 0H \) and \( HQ \) coincide as do the three points \( Q, R \) and \( T \). In this case, \( HQ \) and \( HR \) will be identical and simulations using \( \eta^* \) and \( \eta' \) will give virtually the same rocking curves. (A small, usually negligible, difference is caused by the refraction correction, which is angular dependent for \( \eta^* \) but not for \( \eta' \).)

**APPENDIX C**

**Crossover to kinematic scattering theory**

If the influence of multiple scattering can be neglected, the dynamical amplitude ratio must change into the corresponding kinematic expression. Bartels, Hornstra & Lobeek (1986) studied the crossover to kinematic scattering theory by writing the recursion formula (5) as

\[
X_t = \frac{[X_R + X_0 \exp(-2i\phi)]}{1 - X_0X_R}. \tag{C.1}
\]

Here, \( X_R \) is the reflected amplitude ratio for a thin crystal, which can be obtained from (5) by making \( X_0 = 0 \), and

\[
\phi = \arctan \left\{ \eta^* \tan \left[ T(\eta^{*2} - 1)^{1/2}\right]/(\eta^{*2} - 1)^{1/2} \right\} \tag{C.2}
\]

is the 'dynamical phase angle'. With this phase angle, the reflected amplitude ratio of a thin crystal may also be written as

\[
X_R = i \exp(-i\phi) \sin \phi/\eta^*. \tag{C.3}
\]

For an incident beam far from the Bragg condition (|\( \eta^* \)| \( \gg 1 \)) or for a layer that is thin compared with the extinction distance (|\( T \)| \( \ll 1 \)), the phase angle (C.2) reduces to the kinematical expression \( \phi = \eta^*T \).

In kinematical calculations, multiple reflections between the crystal layer and the layers underneath can be neglected (|\( X_0X_R \)| \( \ll 1 \)) (Vardanyan, Manoukyan & Petrosyan, 1985); therefore, the reflected amplitude ratio is given by the recursion formula

\[
X_t = i \exp(-i\eta^*T) \sin(\eta^*T)/\eta^* + X_0 \exp(-2i\eta^*T). \tag{C.4}
\]
This corresponds to the equation given by Speriosu (1981) for the kinematic simulation of diffraction curves of epitaxic heterostructures.

As is shown in Appendix B, the new deviation parameter $\eta^*$ is proportional to the reduced scattering vector $\vec{q} = \vec{k}_H - \vec{k}_0 - \vec{H}$. If we write the phase angle $\eta^* T$ as

$$\eta^* T = \frac{1}{2} \vec{q}_\perp \cdot t = \frac{1}{2} N \vec{q}_\perp \cdot a,$$

where $a$ is the height of the crystal unit cell and $N$ the number of unit cells in the direction of $\vec{q}_\perp$, the reflected amplitude ratio $X_R$ of a thin layer will take the following form, which is well known from kinematic scattering theory

$$X_R = \frac{\pi C(x_H x_H)^{1/2} a \sin \left( \frac{1}{2} N \vec{q}_\perp \cdot a \right)}{\lambda (\gamma_0 |\gamma_H|)^{1/2} \frac{1}{2} \vec{q}_\perp \cdot a} \exp \left( -i \frac{1}{2} N \vec{q}_\perp \cdot a \right).$$

In the denominator of the amplitude ratio, we find the term $\frac{1}{2} \vec{q}_\perp \cdot a$ instead of $\sin \left( \frac{1}{2} \vec{q}_\perp \cdot a \right)$, which would be the general solution. This is a consequence of the two-beam approximation in the Takagi–Taupin theory.

References


