Acta Cryst. (1986). A42, 539–545

X-ray Diffraction of Multilayers and Superlattices

BY W. J. BARTELS, J. HORNSTRA AND D. J. W. LOBEEK

Philips Research Laboratories, PO Box 80.000, 5600 *JA Eindhoven, The Netherlands*

(*Received* 3 *March* 1986; *accepted* 27 *May* 1986)

Abstract

Recursion formulae for calculating the reflected amplitude ratio of multilayers and superlattices have been derived from the Takagi–Taupin differential equations, which describe the dynamical diffraction of X-rays in deformed crystals. Calculated rocking curves of complicated layered structures, such as non-ideal superlattices on perfect crystals, are shown to be in good agreement with observed diffraction profiles. The kinematical theory can save computing time only in the case of an ideal superlattice, for which a geometric series can be used, but the reflectivity must be below 10% so that multiple reflections can be neglected. For a perfect crystal of arbitrary thickness the absorption at the center of the dynamical reflection is found to be proportional to the square root of the reflectivity. Sputter-deposited periodic multilayers of tungsten and carbon can be considered as an artificial crystal, for which dynamical X-ray diffraction calculations give results very similar to those of a macroscopic optical description in terms of the complex index of refraction and Fresnel reflection coefficients.

1. Introduction

X-ray diffraction theory for describing the reflection of X-rays at the surface of an infinitely thick absorbing perfect crystal has been known for some time. Prins (1930) introduced absorption as a complex attribute to the dynamical theory for non-absorbing crystals given by Darwin (1914) and Ewald (1917) (James, 1967; Pinsker, 1978). This was the first time that the characteristic asymmetric diffraction profile of an absorbing perfect crystal was described theoretically. Since then most of the theoretical and experimental effort has been devoted to the transmission or so-called Laue case of X-ray diffraction. Interesting subjects were the study of anomalous transmission and the understanding of the phenomenon of *Pendellösung* oscillations. The X-ray diffraction theory for crystals with a strain gradient perpendicular to the surface was developed by Takagi (1969) and Taupin (1964) in order to describe the diffraction of curved crystals and to calculate the contrast of dislocations visible in X-ray topographs. Their equations are only valid for a two-beam case and can easily be generalized for crystals whose reflection properties change with depth. This problem became more interesting after about 1970, because crystals were modified by epitaxy, ion implantation and diffusion for making electronic devices such as solid-state lasers and integrated circuits (Bartels & Nijman, 1978; Bartels, 1983). For understanding the X-ray diffraction phenomena of multilayers and superlattices (Segmüller, Krishna & Esaki, 1977; Kervarec, Baudet, Caulet, Auvray, Emery & Regreny, 1984), it is necessary to elaborate the dynamical theory for the Bragg case of X-ray diffraction.

Vardanyan, Manoukyan & Petrosyan (1985) described the dynamical diffraction of an ideal superlattice with Chebyshev polynomials of the second kind, whereas Speriosu & Vreeland (1984) used a geometric series of the kinematical theory. However, these solutions are not applicable to non-ideal superlattices. Kyutt, Petrashen & Sorokin (1980) used a semi-kinematical approach for calculating rocking curves of ion-implanted specimens. Halliwell, Lyons & Hill (1984) and Hill, Tanner, Halliwell & Lyons (1985) obtained an analytical solution to the Takagi–Taupin differential equations, which is useful for the computer simulation of rocking curves of multiple hetero-epitaxial layers. However, their solution is not applicable to the general case of an asymmetric reflection of a polar crystal and the relation with the Darwin–Prins formula for an infinitely thick absorbing perfect crystal is not clearly visible.

In this article we present the general solution for the dynamical reflection of an epitaxial layer of arbitrary thickness. From the Takagi–Taupin equations we derive a recursion formula, which is in a simple way related to the Darwin–Prins formula for an infinitely thick crystal. We have used the formula for calculating the diffraction satellites of a non-ideal superlattice.

2. Dynamical theory

In the dynamical theory the change of the amplitudes D_0 and D_H of the incident and the diffracted beam with the depth coordinate is described with a set of differential equations derived independently by Takagi (1969) and Taupin (1964). Taupin has combined the two equations for the Bragg case to give one differential equation for the amplitude ratio X, but has discussed only centrosymmetric reflections. The differential equation for the polar Bragg case can

0108-7673/86/060539-07$01.50

be written as

$$-i\,\mathrm{d}X/\mathrm{d}T = X^2 - 2\eta X + 1, \quad (1)$$

where X, η and T are complex quantities given by

$$X = (F_{\bar{H}}/F_H)^{1/2}|\gamma_H/\gamma_0|^{1/2} D_H/D_0, \quad (2)$$

$$\eta = [-b(\theta-\theta_B)\sin 2\theta_B - \tfrac{1}{2}\Gamma F_0(1-b)] \times [|b|^{1/2} C\Gamma (F_H F_{\bar{H}})^{1/2}]^{-1}, \quad (3)$$

$$T = \pi C\Gamma (F_H F_{\bar{H}})^{1/2} t/\lambda |\gamma_0\gamma_H|^{1/2}, \quad (4)$$

where

$$\Gamma = r_e\lambda^2/\pi V, \qquad r_e = e^2/4\pi\varepsilon_0 mc^2, \qquad b = \gamma_0/\gamma_H. \quad (5)$$

T is determined by the crystal thickness t and the structure factor F_H of the reflection. The departure from the Bragg angle θ_B determines the deviation parameter η. The second part of the numerator of η corresponds to the refraction and absorption of the X-rays. In the Bragg case the direction cosines γ_0 and γ_H of the incident and the diffracted beam with respect to the surface normal are opposite in sign so that the asymmetry factor b is negative. The classical electron radius r_e is equal to $2{\cdot}818\times10^{-5}$ Å, λ is the X-ray wavelength and V is the volume of the unit cell. $C=1$ for perpendicular (σ) polarization and $C=|\cos 2\theta_B|$ for parallel (π) polarization of the incident beam.

The differential equation can be solved for layers of constant η and arbitrary thickness. This solution can also be used for sections for which η can be considered to be constant. The following recursion equation gives the relation between the amplitude ratio X_0 at the bottom of the layer and X_t at its top:

$$X_t = \eta + (\eta^2-1)^{1/2}[(S_1+S_2)/(S_1-S_2)], \quad (6)$$

where

$$S_1 = [X_0 - \eta + (\eta^2-1)^{1/2}]\exp[-iT(\eta^2-1)^{1/2}], \quad (7)$$

$$S_2 = [X_0 - \eta - (\eta^2-1)^{1/2}]\exp[iT(\eta^2-1)^{1/2}]. \quad (8)$$

The recursion formula we have obtained is the general solution for the dynamical reflection of an epitaxial layer of arbitrary thickness. The recursion process allows one to calculate rocking curves of complicated layered structures such as non-ideal superlattices on perfect crystals. For an infinitely thick crystal the equation reduces to the well known Darwin formula modified by Prins (1930) for absorption (Fingerland, 1971):

$$X_\infty = \eta \pm (\eta^2-1)^{1/2}, \quad (9)$$

where the sign to be selected is opposite to the sign of $\mathrm{Re}(\eta)$. The rocking curve of the crystal is given by the reflectivity P_H as a function of the deviation parameter η. For an asymmetric reflection we must take into account the change in beam cross section, so that the reflectivity P_H is given by

$$P_H = |b|^{-1} I_H/I_0 = |\gamma_H/\gamma_0||D_H/D_0|^2 = |F_H/F_{\bar{H}}||X|^2. \quad (10)$$

In the kinematical theory the influence of multiple reflections is neglected. For the differential equation this implies loss of the quadratic term, so that

$$-i\,\mathrm{d}X/\mathrm{d}T = -2\eta X + 1. \quad (11)$$

Integration of this equation gives the recursion formula

$$X_t = X_0\exp(-i2\eta T) + [1-\exp(-i2\eta T)]/2\eta, \quad (12)$$

which can also be written in a form comparable to that given by Speriosu & Vreeland (1984):

$$X_t = X_0\exp(-i2\eta T) + i\exp(-i\eta T)\sin(\eta T)/\eta. \quad (13)$$

Multiplication of the amplitude ratio X_0 with the exponential term corresponds to taking into account absorption and the change in phase when adding a section to the crystal. Thus, in the kinematical theory the amplitude ratios of different crystal parts occur separately.

The dynamical and kinematical theories are compared in Fig. 1 for the 004 Cu $K\alpha_1$ reflection of a structure consisting of four epitaxial $Ga_{1-x}Al_xAs$ layers of different thickness and composition x on a [001] GaAs substrate. The substrate surface is taken as the origin of the thickness scale in the depth profile.

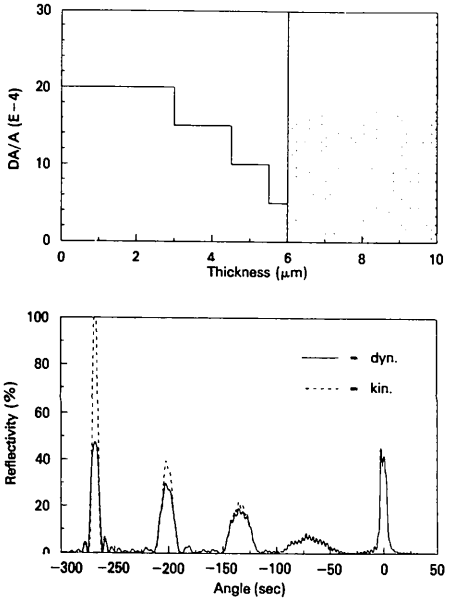

Fig. 1. Comparison of 004 Cu $K\alpha_1$ X-ray diffraction profiles calculated with the dynamical and kinematical theories for a four-layer structure on a [001] GaAs substrate. Depth profile with perpendicular lattice mismatch *versus* total layer thickness is shown in the upper drawing.

The reflection of the GaAs substrate is chosen as origin of the angle scale. The reflectivity of the layers increases with thickness, while the reflection width decreases. Interference fringes are visible, which can be correlated with layer thickness or distance. Below 10% reflectivity the two curves almost coincide, but above this limit the difference increases progressively. Hence, the kinematical approximation is allowed only if the reflectivity is below 10% so that multiple reflections can be neglected.

3. Recursion formulae

The dynamical recursion formula given in the preceding section can be written in two other interesting forms. For this purpose we first determine the reflected and transmitted amplitude ratios X_R and X_T of a thin crystal that is added to a substrate to make the final combination of epitaxial layer and substrate. The process is illustrated in Fig. 2. The amplitude ratio X_R of the reflected beam of a thin crystal can be obtained from (6) by making $X_0=0$. Substitution of

$$\alpha = T(\eta^2-1)^{1/2}, \tag{14}$$

$$Q=(\eta^2-1)^{1/2}\cos\alpha + i\eta\sin\alpha \tag{15}$$

results in

$$X_R = i\sin\alpha/Q. \tag{16}$$

The transmissivity as a function of crystal thickness is given by (Bonse & Graeff, 1977)

$$P_T=\exp[-(\mu t/2)(|\gamma_0|^{-1}-|\gamma_H|^{-1})]|X_T|^2, \tag{17}$$

where μ is the linear absorption coefficient and the amplitude ratio X_T is given by (Bonse & Graeff, 1977)

$$X_T=(\eta^2-1)^{1/2}/Q. \tag{18}$$

After substitution, (6) can be rewritten in the form

$$X_t=[X_R-X_0(X_R^2-X_T^2)]/(1-X_0X_R). \tag{19}$$

When X_T approaches zero the reflectivity of the system is determined by X_R alone.

In combining the crystal parts in Fig. 2, the incident beam of the lower part is replaced by the transmitted beam of the upper part. Owing to multiple reflections the amplitude ratios will vary, but can be expressed in the original values X_T, X_R and X_0, so that:

$$Z=X_T+YX_R, \quad X_t=X_R+YX_T, \quad Y=X_0Z. \tag{20}$$

Elimination of Y and Z results in (19), which can also be derived by realizing that the multiple reflections make an infinite geometric series with $X_0X_T^2$ as the first term and common ratio X_0X_R (Vardanyan, Manoukyan & Petrosyan, 1985). The complex quantity Q in X_R and X_T can be written as

$$Q=(\sin^2\alpha+\eta^2-1)^{1/2}\exp(i\varphi), \tag{21}$$

where

$$\varphi=\arctan[\eta\tan\alpha/(\eta^2-1)^{1/2}]. \tag{22}$$

Then (19) takes the form (Vardanyan & Manoukyan, 1982)

$$X_t=[X_R+X_0\exp(-i2\varphi)]/(1-X_0X_R). \tag{23}$$

The expression for the 'phase angle' φ illustrates that in the dynamical theory the phase relation between X_0 and X_R is not very simple. Only for very small layer thickness t may we replace the phase factor by $\exp(-i2\eta T)$.

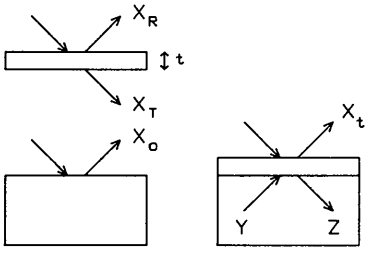

Fig. 2. In the recursion process a thin layer of thickness t is added to a substrate so that the reflected amplitude ratio at the surface changes from X_0 to X_t.

4. Experimental parameters

The calculation of rocking curves requires the specification of the complex variables η and T for each crystal section. The deviation parameter η contains the departure from the Bragg angle, which is related to the spacing and orientation of the lattice planes in a given section. When the refraction correction $\Delta\theta_0$ is written as

$$\Delta\theta_0=(\tfrac{1}{2}\Gamma F_0'/\sin 2\theta_B)[1+|\gamma_H/\gamma_0|], \tag{24}$$

we can specify the departure from the Bragg angle in each section as

$$\Delta\omega=\theta-\theta_B-\Delta\theta_0-\Delta\omega_\perp-\Delta\omega_\parallel, \tag{25}$$

where θ_B is the Bragg angle of the substrate and $\Delta\omega_\perp$ and $\Delta\omega_\parallel$ contain the change in Bragg angle and lattice-plane orientation due to the components of lattice mismatch perpendicular and parallel to the substrate surface given by (Bartels & Nijman, 1978)

$$\Delta\omega_\perp=-(\Delta a/a)_\perp[\cos^2\varphi\tan\theta_B+\cos\varphi\sin\varphi], \tag{26}$$

$$\Delta\omega_\parallel=-(\Delta a/a)_\parallel[\sin^2\varphi\tan\theta_B-\cos\varphi\sin\varphi]. \tag{27}$$

These formulae have been written for the case where $(\theta_B-\varphi)$ is the angle of incidence so that $|\gamma_0|=\sin(\theta_B-\varphi)$. Reversal of the asymmetry of the reflection is taken into account by reversing the sign of the angle φ for the inclination of the lattice planes. The components of lattice mismatch can be determined from the measured differences in Bragg angle $\Delta\theta$ and

lattice-plane orientation $\Delta\varphi$ with respect to the substrate according to (Bartels, 1983)

$$(\Delta a/a)_\perp = \Delta\varphi \tan\varphi - \Delta\theta \cot\theta_B, \quad (28)$$

$$(\Delta a/a)_\parallel = -\Delta\varphi \cot\varphi - \Delta\theta \cot\theta_B. \quad (29)$$

The relaxed lattice mismatch can be obtained after taking the anisotropic elastic deformation of the crystal lattice of the layer into account (Hornstra & Bartels, 1978):

$$(\Delta a/a)_{\text{relax}} = \varepsilon_\parallel/(\varepsilon_\parallel - \varepsilon_\perp)[(\Delta a/a)_\perp - (\Delta a/a)_\parallel] + (\Delta a/a)_\parallel, \quad (30)$$

where $\varepsilon_\parallel$ and $\varepsilon_\perp$ are the parallel and perpendicular strains of the layer. The ratio $\varepsilon_\parallel/(\varepsilon_\parallel - \varepsilon_\perp)$ depends on the orientation of the crystal lattice and can be expressed in the elastic constants of the material.

Structure factors are complex owing to the complex atomic scattering factors and, in addition, for the general case of a polar crystal, the spatial arrangement of the atoms in the unit cell can make the real and imaginary components of the structure factor of a reflection complex as well. Cole & Stemple (1962) have introduced parameters κ, p and s such that

$$(F_H F_{\bar{H}})^{1/2} = |F'_H|(1-\kappa^2+i2p)^{1/2}, \quad (31)$$

$$|F_H/F_{\bar{H}}| = (1+\kappa^2+2s)/[(1-\kappa^2)^2+4p^2]^{1/2}, \quad (32)$$

where $\kappa = |F''_H/F'_H|$. In the case of centrosymmetric reflections $s=0$ and $p=\kappa$ so that the square root in (31) is replaced by $(1+i\kappa)$ and the ratio of (32) is unity. The linear absorption coefficient μ can be obtained from tabulated X-ray cross sections and is related to F''_0 by

$$\Gamma F''_0 = \lambda\mu/2\pi. \quad (33)$$

A comparison between observed and calculated diffraction profiles of a laser structure consisting of four epitaxial layers grown by liquid-phase epitaxy on a [001]-oriented InP substrate is shown in Fig. 3. The rocking curve has been measured with a high-resolution X-ray diffractometer equipped with a germanium four-crystal monochromator (Bartels, 1983). The divergence of 5″ of the (σ) polarized incident beam has been taken into account by applying a corresponding smoothing function to the calculated profile. After the growth of a 2 μm thick layer of InP with zero lattice mismatch, a quaternary $In_{1-x}Ga_xAs_yP_{1-y}$ layer was grown for which the perpendicular lattice mismatch changes linearly with thickness due to compositional variation. The third layer is InP contaminated with a small amount of gallium so that the lattice constant is somewhat smaller than that of the substrate. The fourth layer is a quaternary layer for which the perpendicular lattice mismatch is constant first and then varies again linearly. The depth profile is the result of trial and error fitting of the observed and calculated profiles. The complicated interference pattern occurs because of the small average lattice mismatch of the layers so that their reflection profiles nearly coincide with the substrate reflection.

5. Reduced parameters

The complex quantities η and T describe for each crystal section the departure from the Bragg angle and the layer thickness in relation to the strength of the reflection expressed by the complex structure factor. Often it is convenient to use reduced real parameters as introduced by Zachariasen (1945) for non-polar crystals. A layer thickness of about twice the extinction depth t_{ext} results in saturation of the reflectivity:

$$t_{\text{ext}} = \lambda|\gamma_0\gamma_H|^{1/2}/\pi C\Gamma|F'_H|. \quad (34)$$

A non-reflecting layer with a thickness equal to the absorption depth t_{abs} reduces the reflectivity of the substrate by a factor e, where

$$t_{\text{abs}}^{-1} = \mu[|\gamma_0|^{-1} + |\gamma_H|^{-1}]. \quad (35)$$

After these definitions the complex quantities η and T can be written as

$$\eta = (y+ig)/(1+i\kappa), \quad T = (1+i\kappa)A, \quad (36)$$

where

$$y = \pi t_{\text{ext}} \sin 2\theta_B \Delta\omega/\lambda|\gamma_H|, \quad A = t/t_{\text{ext}}, \quad (37)$$

$$g = -t_{\text{ext}}/4t_{\text{abs}}, \quad \kappa = |F''_H/F'_H|. \quad (38)$$

Extinction and absorption are competing processes

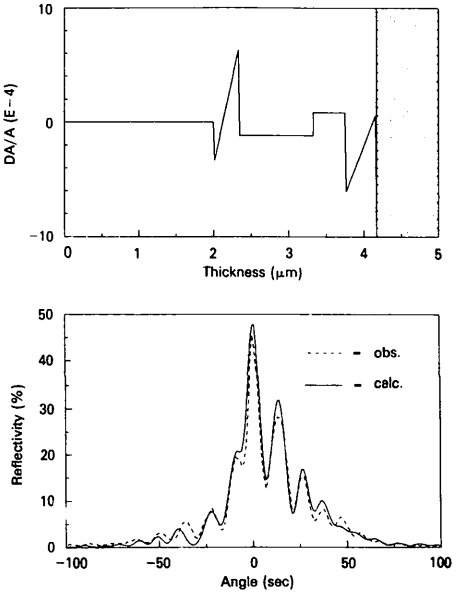

Fig. 3. Comparison of observed and calculated X-ray diffraction profiles of the 004 Cu $K\alpha_1$ reflection of a laser structure grown on [001] InP. Depth profile with perpendicular lattice mismatch *versus* total layer thickness.

and at the center of the reflection, defined as $y=0$, the reflectivity of a crystal is nearly independent of κ so that it is to a good approximation determined by the factor g alone. Some formulae of practical use can be derived when we confine the case to symmetrical reflections of non-polar crystals. The reflection, absorption and transmission for a crystal of arbitrary thickness fulfilling the Bragg condition are related by

$$P_R + P_A + P_T = 1. \tag{39}$$

Writing

$$Q_0 = (1+g^2)^{1/2}\cosh[A(1+g^2)^{1/2}] - g\sinh[A(1+g^2)^{1/2}], \tag{40}$$

we obtain from (16) and (18)

$$P_R = \sinh^2[A(1+g^2)^{1/2}]/Q_0^2, \tag{41}$$

$$P_A = -2g\sinh[A(1+g^2)^{1/2}]/Q_0, \tag{42}$$

$$P_T = (1+g^2)/Q_0^2. \tag{43}$$

In deriving these formulae a rather unexpected result appeared. For a crystal of arbitrary thickness fulfilling the Bragg condition there is a relation between absorption and reflection given by

$$P_A = -2gP_R^{1/2} = (t_{ext}/2t_{abs})P_R^{1/2}. \tag{44}$$

The percentages of reflection, absorption and transmission for a reflecting crystal as a function of the thickness are shown in Fig. 4 for $g=-0{\cdot}25$ and $t_{ext}=3\mu$m. The transmission of a non-reflecting crystal has also been plotted and is given by

$$P_E = \exp(-\mu t/\sin\theta) = \exp(-t/2t_{abs}). \tag{45}$$

6. Superlattices

A regular repetition of a given sequence of layers of a perfect crystal will give superlattice diffraction satellites. Often the reflectivity of the satellites is below

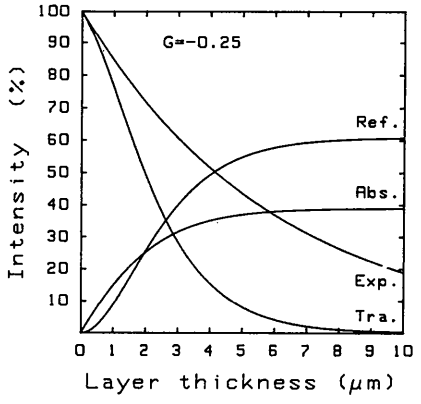

Fig. 4. Reflection, absorption and transmission of a reflecting crystal *versus* thickness. For comparison the exponentially decreasing incident beam is given for the non-reflecting crystal.

10% and in the case of an ideal superlattice the kinematical theory can save considerable computing time, because we can apply a geometric series for calculating the diffraction pattern in this case. For the amplitude ratio of the first period of a two-layer sequence (12) gives

$$X_p = [1-\exp(-i2\eta_1 T_1)]/2\eta_1\exp(i2\eta_2 T_2) + [1-\exp(-i2\eta_2 T_2)]/2\eta_2. \tag{46}$$

The absorption and the change in phase due to one period is described with

$$\varphi = \eta_1 T_1 + \eta_2 T_2, \tag{47}$$

so that the amplitude ratio for an ideal superlattice of N_p periods is given by

$$X_{SL} = X_0\exp(-i2\varphi N_p) \times X_p[1-\exp(-i2\varphi N_p)]/[1-\exp(-i2\varphi)]. \tag{48}$$

The angular distance $\Delta\omega_p$ of diffraction satellites is inversely proportional to the superlattice period t_p, *viz*

$$\Delta\omega_p = \lambda|\gamma_H|/t_p\sin 2\theta_B. \tag{49}$$

Vardanyan, Manoukyan & Petrosyan (1985) have described the Bragg diffraction of an ideal superlattice with Chebyshev polynomials of the second kind, but computation of these polynomials is rather complicated and requires more time. However, the solutions given above are not useful for non-ideal superlattices. In this case the dynamical recursion formula (6) can be applied.

A comparison between observed and calculated diffraction profiles of ideal and non-ideal superlattices is shown in Fig. 5. The superlattices are composed of 47 periods of about 100 Å AlAs and 700 Å GaAs and the layers were grown by metalorganic vapour-phase epitaxy on [001] GaAs substrates. The observed profiles are 002 Cu $K\alpha_1$ reflections measured with the high-resolution X-ray diffractometer (see § 4). For both calculated profiles we have used the dynamical recursion formula (6). The computing time was 20 s on the IBM 3081 computer for an angular resolution of 1″ in the given angular range. We used a value of 2·2μm for the extinction depth of AlAs, which is slightly larger than the theoretical value of 1·8μm. In case (*a*) the period was 817 Å; case (*b*) is a non-ideal superlattice where the period varied linearly from 985 to 860 Å, as deduced from trial and error fitting of the profiles. For such a 10% variation of the superlattice period, the width of the diffraction satellites increases progressively with the order.

7. Optical theory for multilayers

Sputter-deposited periodic multilayers of tungsten and carbon are used as soft X-ray monochromators.

Insight into their reflecting properties has been obtained with Cu $K\alpha_1$ radiation where the Bragg angle is about 1° for an artificial period of 50 Å. Lee (1981) used the characteristic matrix method from the optical theory of thin films (Born & Wolf, 1980) as a macroscopic description of the Bragg reflection of periodic multilayers. He obtained a solution with Chebyshev polynomials of the second kind, but this solution is only suitable when the system is exactly periodic. For non-periodic multilayers an optical recursion formula is more useful (Underwood & Barbee, 1981). The important parameter in the macroscopic description is the complex index of refraction given by

$$n = 1 - \delta - i\beta. \tag{50}$$

The parameters δ and β are related to the real and imaginary parts of atomic scattering factors used in calculations of structure factors. Multilayers have large d spacings, so the contribution of f_0 to the atomic scattering factor can be approximated by the atomic number Z. With the number density N_a of these atoms, δ and β are given by (Underwood & Barbee, 1981)

$$\delta = (N_a r_e \lambda^2/2\pi)(Z + f'), \tag{51}$$

$$\beta = (N_a r_e \lambda^2/2\pi) f'' = \mu\lambda/4\pi, \tag{52}$$

where f' and f'' are the corrections to atomic scattering factors due to resonance and absorption.

The optical recursion formula for multilayers is given by

$$X_t = [r + X_0 \exp(-i2\varphi)]/[1 + rX_0 \exp(-i2\varphi)], \tag{53}$$

where r is the Fresnel reflection coefficient for σ or π polarization at the top of a layer (Born & Wolf, 1980) and X_0 and X_t are the reflected amplitude ratios at the bottom and the top of this layer. The phase difference φ across layer j of thickness t can be related to the angle of incidence θ at the surface of the multilayer so that

$$\varphi = (2\pi/\lambda) t n_j \sin\theta_j = (2\pi t/\lambda)(n_j^2 - \cos^2\theta)^{1/2}. \tag{54}$$

The first medium in the recursion process is the infinitely thick substrate where at the bottom $X_0 = 0$. Recursion proceeds from bottom to top for each layer taking the double phase difference into account. The final value of the amplitude ratio X_t at the top of the multilayer gives the reflectivity as $P = |X_t|^2$. Non-correlated and correlated interface roughness can be taken into account by multiplying the Fresnel reflection coefficient r at every interface or the final value

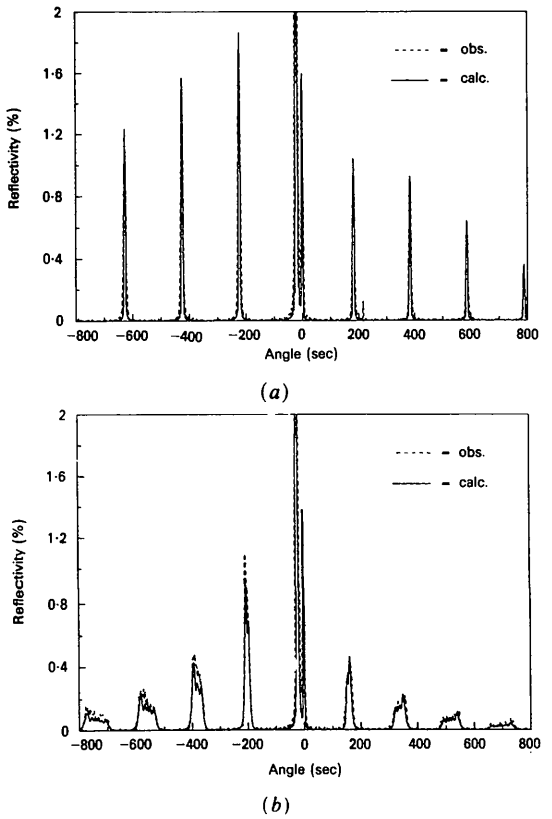

Fig. 5. Observed and calculated 002 Cu $K\alpha_1$ X-ray diffraction profiles of a [001] GaAs substrate covered with (*a*) an ideal superlattice with period 817 Å and (*b*) a non-ideal superlattice with a linear variation of about 10% in the period.

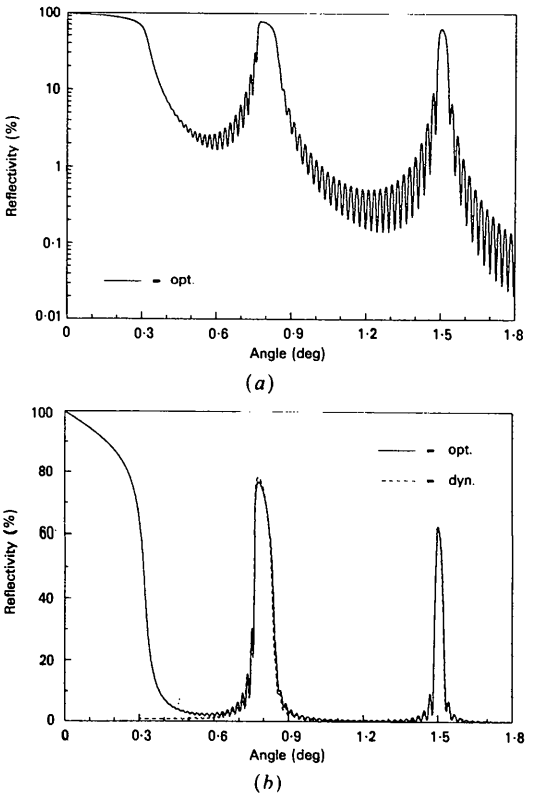

Fig. 6. Comparison of optical and dynamical theory for a Cu $K\alpha_1$ reflection of a tungsten and carbon multilayer with 30 periods of 60 Å: (*a*) logarithmic scale, (*b*) linear scale.

of X_t at the surface of the multilayer by a Debye-Waller factor.

When a multilayer is exactly periodic we can consider the structure as an artificial crystal and calculate the diffraction profile with the formalism of the dynamical theory. For a rectangular composition profile, the complex structure factors which are used in the expressions for η and T are given by (Underwood & Barbee, 1981)

$$\Gamma F_0 = 2(\bar{\delta} + i\bar{\beta}), \tag{55}$$

$$\Gamma(F_H F_{\bar{H}})^{1/2} = 2[\delta_1 - \delta_2 + i(\beta_1 - \beta_2)] \times \sin(m\pi d_1/d)/m\pi, \tag{56}$$

where $\bar{\delta}$ and $\bar{\beta}$ are weighted average values and d_1/d is the volume fraction of the heavy element in a two-layer sequence. Fig. 6 shows Cu $K\alpha_1$ reflection profiles on a logarithmic and a linear scale calculated with the optical and the dynamical theory for a multilayer with 30 periods of 60 Å composed of 15 Å tungsten and 45 Å carbon. Both theories take into account multiple reflections and are in this sense dynamical. However, it must be remembered that the Takagi-Taupin theory is essentially a two-beam theory, which can describe only one reflection at a time and is not valid in the region of total reflection below about 0·3°. This explains the small differences between the two profiles.

The authors thank H.F.J. van 't Blik for the growth of superlattices and B.A.H. van Bakel for the growth of epitaxial layers on InP.

References

BARTELS, W. J. (1983). *J. Vac. Sci. Technol.* B1, 338-345.

BARTELS, W. J. & NIJMAN, W. (1978). *J. Cryst. Growth*, **44**, 518-525.

BONSE, U. & GRAEFF, W. (1977). *X-ray Optics*, edited by H.-J. QUEISSER, pp. 93-143. Berlin: Springer-Verlag.

BORN, M. & WOLF, E. (1980). *Principles of Optics*. Oxford: Pergamon Press.

COLE, H. & STEMPLE, N. R. (1962). *J. Appl. Phys.* **33**, 2227-2233.

DARWIN, C. G. (1914). *Philos. Mag.* **27**, 315-333, 675-690.

EWALD, P. P. (1917). *Ann. Phys. (Leipzig)*, **54**, 519-597.

FINGERLAND, A. (1971). *Acta Cryst.* A**27**, 280-284.

HALLIWELL, M. A. G., LYONS, M. H. & HILL, M. J. (1984). *J. Cryst. Growth.* **68**, 523-531.

HILL, M. J., TANNER, B. K., HALLIWELL, M. A. G. & LYONS, M. H. (1985). *J. Appl. Cryst.* **18**, 446-451.

HORNSTRA, J. & BARTELS, W. J. (1978). *J. Cryst. Growth*, **44**, 513-517.

JAMES, R. W. (1967). *The Optical Principles of the Diffraction of X-rays*. London: Bell.

KERVAREC, J., BAUDET, M., CAULET, J., AUVRAY, P., EMERY, J. Y. & REGRENY, A. (1984). *J. Appl. Cryst.* **17**, 196-205.

KYUTT, R. N., PETRASHEN, P. V. & SOROKIN, L. M. (1980). *Phys. Status Solidi A*, **60**, 381-389.

LEE, P. (1981). *Opt. Commun.* **37**, 159-164.

PINSKER, Z. G. (1978). *Dynamical Scattering of X-rays in Crystals*. Berlin: Springer-Verlag.

PRINS, J. A. (1930). *Z. Phys.* **63**, 477-493.

SEGMÜLLER, A., KRISHNA, P. & ESAKI, L. (1977). *J. Appl. Cryst.* **10**, 1-6.

SPERIOSU, V. S. & VREELAND, T. JR (1984). *J. Appl. Phys.* **56**, 1591-1600.

TAKAGI, S. (1969). *J. Phys. Soc. Jpn*, **26**, 1239-1253.

TAUPIN, D. (1964). *Bull. Soc. Fr. Mineral. Crystallogr.* **87**, 469-511.

UNDERWOOD, J. H. & BARBEE, T. W. JR (1981). *Appl. Opt.* **20**, 3027-3034.

VARDANYAN, D. M. & MANOUKYAN, H. M. (1982). *Phys. Status Solidi A*, **69**, 475-482.

VARDANYAN, D. M., MANOUKYAN, H. M. & PETROSYAN, H. M. (1985). *Acta Cryst.* A**41**, 212-217.

ZACHARIASEN, W. H. (1945). *Theory of X-ray Diffraction in Crystals*. New York: Wiley.

Acta Cryst. (1986). A**42**, 545-552

Dynamical Diffraction Calculations for RHEED and REM

BY LIAN-MAO PENG AND J. M. COWLEY

Department of Physics, Arizona State University, Tempe, AZ 85287, *USA*

(*Received* 3 *January* 1986; *accepted* 27 *May* 1986)

Abstract

The multislice formulation of the many-beam dynamical diffraction theory has been applied to the Bragg case of electron diffraction for the extended surface of a perfect crystal and also for a crystal surface with a surface step. The wavefunctions within and outside the crystal have been calculated and used to derive the standing-wave pattern in the top atomic layers of the crystal, the intensities of the reflection high-energy electron diffraction (RHEED) pattern and the contrast of the reflection electron microscopy (REM) image. Calculations made for the diffraction of 19, 40 and 80 keV electrons from (111) surfaces of Pt and Au demonstrate the channeling of electrons under the conditions of surface resonance, the perturbation of the standing-wave field in the crystal by a one-atom-high surface step and the REM contrast

0108-7673/86/060545-08$01.50