(4) Is the active use of psi-zero triplets always advisable? Often, structures suffering by pseudotranslational symmetry show a bad psi-zero FOM, even for the correct solution. In this case, a phasing process that tries to improve the psi-zero FOM will hinder rather than favour the crystal structure solution. If structure factors are renormalized and triplet reliabilities are re-estimated by using the information on pseudotranslational symmetry as prior (Cascarano, Giacovazzo & Luić, 1987), then the psi-zero FOM is usually better and use of (12) works fine. In *SIR*92, in order to avoid the psi-zero contribution to (12) overcoming the contributions of the strong triplets and the negative quartets, we use a maximum of NLAR/3 weak reflections to construct psi-zero triplets (NLAR is the number of reflections used for constructing strong triplets). In this way, the active use of psi-zero triplets does not hinder the crystal structure solution also for CIME, CUIMID, ERICA, FEGAS, HOV1 and POCRO, which suffer from pseudotranslational symmetry.

Concluding remarks

The psi-zero triplets have thus far been considered as a tool for calculating a powerful figure of merit (Cochran & Douglas, 1957) for recognizing the correct phase set among numerous trial solutions. In a recent paper, Giacovazzo (1993) proposed their active use in the phasing process: in this paper, we describe the theoretical background necessary for a reasonable active use of the psi-zero triplets and the first applications of the method.

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X-ray Diffraction on Fibonacci Superlattices

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Abstract

The exact diffraction curve of the Fibonacci superlattice is calculated using the semi-kinematical approximation of dynamical X-ray diffraction. The properties of the discrete Fourier transform of quasiperiodically arranged layers are employed to derive explicit approximate formulae for the diffracted intensity and the angular positions of peaks. The exact and approximate curves are compared by a numerical simulation and a good agreement is found. The measurement of the diffraction curve was performed on the generalized Fibonacci superlattice built by stacked Fibonacci generations. This superlattice belongs to the same class of local isomorphism as the Fibonacci superlattice if both are infinitely thick. The explicit approximate formulae enabled the fitting of the structural parameters of the superlattice even in the low-resolution experimental set-up when the fitting of the whole measured diffraction curve was not possible.

1. Introduction

The Fibonacci lattice is a one-dimensional quasiperiodic structure with long-range order. The sequence of two building layers A, B forming the kth generation F_k of the Fibonacci lattice is given by the recurrent Fibonacci rule $F_k = F_{k-1}F_{k-2}$, starting with $F_0 = B$, $F_1 = A$. The infinite Fibonacci lattice is the limit of its generations $f = \lim_{k\to\infty} F_k = ABAABABAABAAB\ldots$

The intensity in diffraction experiments is in the first Born approximation proportional to the square of the modulus of the Fourier transform of the electron density. The quasiperiodic arrangement of the Fibonacci superlattice (FSL) results in self-similarity in the Fourier transform of its density (Steinhardt & Levine, 1987). The calculations of the discrete Fourier transform of point density arranged according to the Fibonacci rule were worked out earlier using different methods. The cut and projection method was established by Zia & Dallas (1985) and Elser (1986), the modulated phase method was presented by Levin & Steinhardt (1986). Severin (1989) pointed out the necessity of introducing two sublattices for a description of the diffraction properties of one class of quasicrystalline superlattices.

The development of molecular beam epitaxy (MBE) enables one to prepare high-quality semiconductor superlattices (SLs). They form artificial one-dimensional lattices due to their lateral translational symmetry. The Fibonacci superlattices, in which the layers alternate according to the Fibonacci rule, have already been prepared and their diffraction spectra have been measured (Merlin, Bajema, Clarke, Juang & Bhattacharya, 1985; Todd, Merlin, Clarke, Mohanty & Axe, 1986; Tapfer & Horikoshi, 1987; Terauchi *et al.*, 1988, 1990). Merlin *et al.* (1985) have found, in analogy with Levin & Steinhardt (1984), that, for the diffraction-curve peak position in reciprocal space, $k_{pq} = 2\pi(p + q/\tau)/d$ holds, where p, q are integers, $d = d_A + d_B\tau$ is the average layer thickness, d_A, d_B are thicknesses of layers A, B and $\tau = (5^{1/2} - 1)/2$ is the golden mean. Tapfer & Horikoshi (1987) determined, in accordance with the projection method (Zia & Dallas, 1985; Elser, 1986), the thicknesses of the building layers from the diffraction-curve peak positions. The influence of imperfect growth of the FSL has also been investigated numerically (Tapfer & Horikoshi, 1987) and the broadening of the peaks has been found.

In this paper, we use the semi-kinematical approximation of the dynamical theory of X-ray diffraction to calculate the diffraction curves of FSLs. The direct approach is to calculate the diffraction amplitude layer by layer but we have found a simpler recurrent formula for it. With the modulated phase method (Levin & Steinhardt, 1986), another approximate formula for the diffraction amplitude is derived. Both formulae are compared with a numerical simulation. The fit of the experimental diffraction curve of a generalized FSL formed by stacked FSL generations using the derived formulae was employed to determine the structural parameters (thicknesses and lattice parameters) of the layers.

2. Theory

This section is organized as follows. Firstly, the method of diffraction-curve calculation within the semi-kinematical approximation is briefly presented. Then this exact approach is used to derive the recurrent formula for the diffraction amplitude of the FSL and the generalized FSL. The approximate approach is employed consequently to derive the explicit formula for the diffraction amplitude and for the angular positions of its maxima.

2.1. *Semi-kinematical approximation*

We briefly describe the formalism of the semi-kinematical approximation of dynamical X-ray Bragg diffraction. The response of a superlattice to incoming X-radiation is usually calculated on the basis of the Takagi theory (Takagi, 1969), which gives a fully dynamical recurrent formula for the diffraction curve of an ideal multilayered system (Bartels, Hornstra & Lobeek, 1986). For thin multilayers with the total thickness being smaller than the extinction length, the semikinematical approximation is valid (Speriosu, 1981). The diffracted amplitude $X = D_h/D_0$ [D_h and D_0 are the amplitudes of the electric induction of the diffracted and transmitted beams, respectively (Azaroff *et al.*, 1974)] for a system containing N layers, numbering them from the substrate to the vacuum as represented in Fig. 1, is expressed by the summation formula

$$X(\eta) = \exp(i\varphi_N)[X_{\text{sub}} + (iKC/2\gamma_h)\sum_{k=1}^{N} F_k \exp(-i\varphi_k)],$$
$$\varphi_k = \sum_{j=1}^{k} \phi_j. \qquad (1)$$

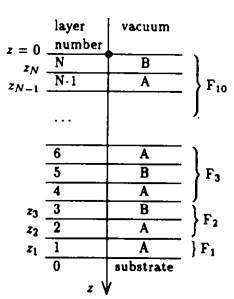

Fig. 1. Sketch of the superlattice. The measured generalized FSL built by stacked FSL generations from order $r = 1$ to order $s = 10$ is also shown.

In this formula, $F_k = \chi_{h,k} d_k \operatorname{sinc}(\phi_k/2)\exp(i\phi_k/2)$, the structure factor of the kth layer, where $\operatorname{sinc}(z) = \sin(z)/z$, $\phi_k = u_k d_k/\gamma_h$, the phase shift on the kth layer, $u_k(\eta) = u(\eta) + \gamma_h h_z \Delta c_k$, the wave vector departure on the kth layer, $u(\eta) = K\eta \sin 2\theta_B + \frac{1}{2}K\chi_0(1 - \gamma_h/\gamma_0)$, the wave vector departure on the substrate, which linearly depends on the angular departure $\eta = \theta - \theta_B$ from the exact Bragg angle θ_B, and the polarization factor $C = 1$ and $C = |\cos 2\theta_B|$ for σ and π polarizations, respectively.

The parameters of the SL are as follows. The kth layer thickness and lattice parameter are d_k and c_k, the relative lattice mismatch with respect to the lattice parameter c of the substrate is $\Delta c_k = (c_k - c)/c$, all in the direction perpendicular to the crystal surface. The angle between the diffracting plane and the crystal surface is ω, the direction cosines of diffracted and transmitted beams are γ_h and γ_0. The Fourier coefficients of susceptibilities are χ_0, $\chi_{h,k}$, the wave vector transfer in the perpendicular direction is $h_z = -2K\cos\omega\sin\theta_B$, the wave-vector length in vacuum is $K = 2\pi/\lambda$. The reflectivity of the crystal is then $R(\eta) = |\gamma_H/\gamma_0||X(\eta)|^2$.

In (1), it is useful to introduce the quantity

$$\mathcal{F} = \sum_{k=1}^{N} F_k \exp(-i\varphi_k), \tag{2}$$

which will be referred to as the structure–geometric factor (SGF). The total diffraction amplitude $X(\eta)$ of the SL is given by the sum of the diffraction amplitude of the multilayer $(iKC/2\gamma_h)\mathcal{F}(\eta)$ and the diffraction amplitude of the substrate $X_{\text{sub}}(\eta)$ (dynamically calculated Darwin-curve amplitude) multiplied by a factor of the phase shift on the layers. The Darwin curve is very narrow and the diffraction intensity profile is caused mainly by the diffraction from the multilayer. Therefore, only the angular dependence $\mathcal{F}(\eta)$ will be of interest.

2.2. *Exact approach*

In this section, we use the standard approach to derive an exact recurrent formula for SGF of the multilayer where the sequence of building layers A, B forms the kth generation F_k of the FSL grown up from the substrate. We denote their thicknesses by d_A, d_B, lattice parameters by c_A, c_B *etc.* From (2) and from the recurrent definition of FSL, one can derive the following recurrent formula for the SGF of the kth FSL generation:

$$\mathcal{F}_k = \mathcal{F}_{k-2} + \mathcal{F}_{k-1}\exp(i\Phi_{k-2}), \tag{3}$$

where the first two SGFs are given by the structure factors of the building layers: $\mathcal{F}_0 = F_B\exp(-i\varphi_N)$, $\mathcal{F}_1 = F_A\exp(-i\varphi_N)$. The phase $\Phi_{k-2} = \phi_A f_{k-1} + \phi_B f_{k-2}$ is expressed by means of the Fibonacci numbers f_k: $f_1 = 0, f_2 = 1, f_k = f_{k-1} + f_{k-2}$. With this formula, we can calculate the reflectivity curve numerically. Since the coefficient $\exp(i\Phi_{k-2})$ in the recurrent formula (3), linear in F_k, depends non-linearly on the generation index k, we cannot find an explicit non-recurrent formula for $\mathcal{F}_k$ as well as for the positions of the maxima of the SGF. We do this by another method in the following section.

If one treats the generalization of the FSL built up as the sequence of stacked successive FSL generations from the rth to the sth generations, as for a specific example shown in Fig. 1, then the exact structure–geometric factor is found to be expressed by the sum of the SGF of FSL generations:

$$\mathcal{F}_{r,s}^{\text{gen}} = \sum_{k=r}^{s} \mathcal{F}_k \exp\{i[\phi_A(f_{s+3} - f_{k+3}) + \phi_B(f_{s+2} - f_{k+2})]\}. \tag{4}$$

This formula is more complicated than that of a simple FSL generation. It can be shown, however, that both FSL and a generalized FSL (assuming they are infinitely thick) belong to the same class of the local isomorphism (Steinhardt & Levin, 1987) (any arbitrary large surroundings of any point in one SL can be found in the second SL), therefore both SLs exhibit the same diffraction spectrum.

In particular, the 12th generation of FSL and the generalized FSL with $r = 1$, $s = 10$ have almost the same thickness, therefore, we expect their diffraction curves to coincide although they are not infinite. This was confirmed by the numerical calculation using (3) and (4). Their common diffraction curve is shown in Fig. 2. The dense set of the diffraction peaks due to the quasiperiodic arrangement is clearly visible.

2.3. *Quasicrystalline approach*

In the previous section, we found an exact recurrent formula (3) for the SGF of the FSL. This formula cannot

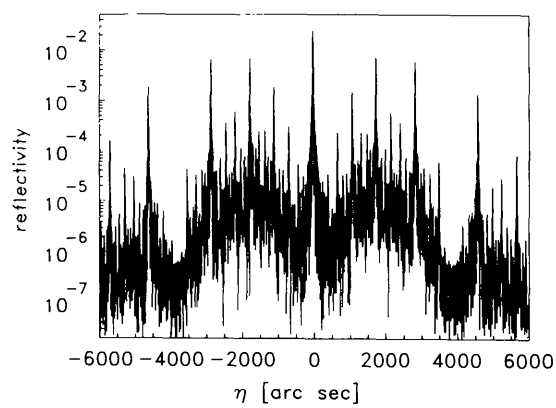

Fig. 2. Diffraction curve (reflectivity *vs* angular departure from the exact Bragg angle η) of the 12th generation of the FSL as well as of the generalized FSL with $r = 1, s = 10$. Symmetrical diffraction 002, substrate peak is not shown. Parameters of the FSL: GaAs substrate, building layer A is 15 mL GaAs, building layer B is 9 mL AlAs.

be re-expressed explicitly and the positions of the maxima cannot be found analytically. Therefore, we use an approximate approach based on the knowledge of the discrete Fourier transform of quasiperiodically arranged layers, which gives us an approximate formula for the reflectivity as well as for the positions of the maxima.

The two layers A, B have different scattering properties (structure factors). Therefore, we decompose the sum in (2) into two sums going through the layers of the same type and we suppose that the SL is infinite

$$\mathcal{F}^{\infty} = F_A \sum_{\substack{l=1 \\ \text{layer } A}}^{\infty} \exp(-i\varphi_l) + F_B \sum_{\substack{l=1 \\ \text{layer } B}}^{\infty} \exp(-i\varphi_l)$$
$$\equiv F_A S_A + F_B S_B. \tag{5}$$

To calculate the sums S_A, S_B we use the self-similarity of the FSL. In general, the Fibonacci lattice can be viewed as being built by two layers of type α and β. Their thicknesses, lattice parameters and phases are d_k, Δc_k and $\phi_k(d_k, \Delta c_k)$, where $k = \alpha, \beta$. The corresponding sum

$$S(\phi_\alpha, \phi_\beta) = \sum_{k=1}^{\infty} \exp(-i\varphi_k) \tag{6}$$

will be determined later. Firstly, we show how the sums S_A, S_B are expressed. If we group together the layers in the FSL to formal groups starting with layer A and containing just one A layer, then the FSL is represented as

$$F = \boxed{\text{AB}}\boxed{\text{A}}\boxed{\text{AB}}\boxed{\text{AB}}\boxed{\text{A}}\boxed{\text{AB}}\boxed{\text{A}}\boxed{\text{AB}}\boxed{\text{A}}\ldots$$

and the sequence of groups of layers $\alpha = \boxed{\text{AB}}$ and $\beta = \boxed{\text{A}}$ also forms the Fibonacci lattice. Thus, we have

$$S_A = S(\phi_A + \phi_B, \phi_A).$$

If the same is done with the B layers, the FSL alternative arrangement is

$$F = \boxed{\text{A}}\boxed{\text{BAA}}\boxed{\text{BA}}\boxed{\text{BAA}}\boxed{\text{BAA}}\boxed{\text{BA}}\ldots,$$

thus

$$S_B = \exp(-i\phi_A) S(\phi_B + 2\phi_A, \phi_B + \phi_A)$$

because the sequence of groups $\alpha = \boxed{\text{BAA}}$ and $\beta = \boxed{\text{BA}}$ following the first A layer forms the FSL.

By calculation of the sum $S(\phi_\alpha, \phi_\beta)$, it is possible to express the phases φ_k by means of positions of layers z_k according to Fig. 1. If we approximate the relative occurrences of layers α and β between the first and the kth layer $n_k(\beta)/n_k(\alpha) \simeq \tau$ for each layer k then $n_k(\alpha) \simeq z_k/d_{\alpha\beta}$, $n_k(\beta) \simeq \tau z_k/d_{\alpha\beta}$. We have introduced the averaged layer thickness $d_{\alpha\beta} = d_\alpha + d_\beta\tau$. The phases are then expressed as

$$\varphi_k = n_{k+1}(\alpha)\phi_\alpha + n_{k+1}(\beta)\phi_\beta$$
$$= z_{k+1}[u/\gamma_h + h_z(d_\alpha \Delta c_\alpha + d_\beta \tau \Delta c_\beta)/d_{\alpha\beta}]$$
$$\equiv z_{k+1}\kappa. \tag{7}$$

The one-dimensional wave vector $\kappa = \kappa(\phi_\alpha, \phi_\beta)$ depends only on the structural composition of the whole lattice (and on an incidence angle of course). The expression of z_k for the Fibonacci lattice is well known and the discrete Fourier transform $S(\phi_\alpha, \phi_\beta) = S(\kappa) = \sum_n \exp(-i\kappa z_n)$ can be calculated according to the modulated phase method, resulting in (Levine & Steinhardt, 1986)

$$S(\kappa) = (1/d_\beta) \sum_{pq} \operatorname{sinc}(\Phi_{pq}/2) \exp(-i\Phi_{pq}/2)\, \delta(\kappa - \kappa_{pq}), \tag{8}$$

where the phase $\Phi_{pq} = 2\pi q - (d_\alpha - d_\beta)\kappa_{pq}$ and the wave vector of the maxima $\kappa_{pq} = 2\pi(p/\tau + q)/d_{\alpha\beta}$, where p and q are integers.

2.3.1. *Formula for the diffraction amplitude of FSL.* Rearranging (5) in the presented way, we find the final expression for the SGF of the infinitely long FSL:

$$\mathcal{F}^{\infty}(\eta) = \sum_{pq} \{[F_A(\kappa_{pq})/d_A] \exp(-i\Phi_{pq}/2) \operatorname{sinc}(\Phi_{pq}/2)$$
$$+ [\exp(-id_A\kappa_{p+q,p}) F_B(\kappa_{p+q,p})/(d_A + d_B)]$$
$$\times \exp(i\tau\Phi_{pq}/2) \operatorname{sinc}(\tau\Phi_{pq}/2)\} \delta[\kappa(\eta) - \kappa_{pq}], \tag{9}$$

where the phase $\Phi_{pq} = 2\pi q - (d_A - d_B)\kappa_{pq}$, the wave vector of the maxima $\kappa_{pq} = 2\pi(p + q\tau)/d$ and $d = d_A + d_B\tau$ the average layer thickness. The wave-vector angular dependence is $\kappa(\eta) = u(\eta)/\gamma_h + h_z(d_A\Delta c_A + d_B\tau\Delta c_B)/d$. Expressing the angular departure from the previous expressions as η, we see that the angular positions of the maxima of $\mathcal{F}^{\infty}(\eta)$ are labelled by two integers p and q,

$$\eta_{pq} = [-\chi_0(1 - \gamma_h/\gamma_0)/2 \sin 2\theta_B]$$
$$- (h_z\gamma_h/K \sin 2\theta_B)[(d_A\Delta c_A + d_B\tau\Delta c_B)/d]$$
$$+ (\lambda/d)(\gamma_h/\sin 2\theta_B)(p + q\tau). \tag{10}$$

Hence, the angular position of the main (zeroth, $p = q = 0$) satellite is

$$\eta_{00} = -\chi_0(1 - \gamma_h/\gamma_0)/2 \sin 2\theta_B$$
$$- (h_z\gamma_h/K \sin 2\theta_B)(d_A\Delta c_A + d_B\tau\Delta c_B/d) \tag{11}$$

and it depends on the thicknesses d_A, d_B and on the compositions Δc_A, Δc_B. Further, it follows from (10) that the angular departure of the pqth satellite from the main one is

$$\Delta\eta_{pq} = \eta_{00} - \eta_{pq} = (\lambda/d)(|\gamma_h|/\sin 2\theta_B)(p + q\tau) \tag{12}$$

and it depends only on the averaged layer thickness d. This formula was previously reported by Tapfer & Horikoshi (1987).

To eliminate δ functions in (9), we have to take into account the finite thickness of a real FSL. According to the standard approach in the kinematical theory of diffraction, we multiply the electron susceptibility by the shape function, which is 1 inside and 0 outside the superlattice. In the Fourier transform, this causes the convolution of the diffraction curve of the infinitely long lattice with the Fourier transform of the shape function. Formula (9), rewritten for the SGF of the FSL with thickness L, is then

$$\begin{aligned}\mathcal{F}_L^{\infty}(\eta) = \sum_{pq}\{&[F_A(u_{pq})/d_A]\,\mathrm{sinc}(\Phi_{pq}/2)\exp(-i\Phi_{pq}/2)\\ &+ [\exp(-id_A\kappa_{p+q,p})F_B(u_{p+q,p})/(d_A+d_B)]\\ &\times \mathrm{sinc}(\tau\Phi_{pq}/2)\exp(i\tau\Phi_{pq}/2)\}\\ &\times L\,\mathrm{sinc}[(u-u_{pq})L/2\gamma_h]\\ &\times \exp[-i(u-u_{pq})L/2\gamma_h], \qquad (13)\end{aligned}$$

where $u_{pq} = u(\eta_{pq})$. The factor in the sum cannot be factorized into the product of the structure and geometric factors like in the case of periodic SL (Holý, Kuběna & Ploog, 1990) rather it has a form like the diffraction amplitude of a system of two interpenetrating incommensurate sublattices.

The zeroth-order maximum (the main satellite) fulfils the condition $\Phi_{pq} = 0$, which requires $p = q = 0$. Moreover, we can define the approximates of the main maxima requiring $\Phi_{pq} \simeq 0$, from which $q - p\tau \simeq 0$, so the indices p and q can be the subsequent Fibonacci numbers (Steinhardt & Levine, 1987) or these multiplied by the same arbitrary integer.

For greater angular departures η, the reflectivity decreases because $F_{A,B}$ diminishes.

3. Numerical simulations

We have performed numerical calculations of diffraction curves of FSLs using both exact and quasicrystalline approximate methods. Within the exact method, the SGF of one finite generation of the FSL is directly calculated by means of the exact recurrent formula (3). Within the approximate method, the SGF of a finite FSL is given by (13). We have found that the approximated curve fits the exactly calculated one very well. This is shown in Figs. 3 and 4 for two arbitrarily chosen angular regions of the diffraction curve. The approximated curve has the same profile as the exact one but the absolute intensities differ slightly.

The summation over an infinite number of indices p and q in (13) was replaced by a summation over a small number of them where a good convergence was obtained. If the SL thickness is increased, new low-intensity maxima occur and the p, q region must be increased to calculate this profile.

The self-similarity of the curve is expressed by the self-similarity of $\Delta\eta_{pq}$ as represented by (12) by the invariance with respect to any multiplication by $r + s\tau$, r, s integers. This property is valid for both cases $d_B/d_A \neq \tau$ and $d_B/d_A = \tau$, as was found recently (Merlin *et al.*, 1985), and depends only on the averaged layer thickness d and not on the chemical composition.

The agreement of both diffraction curves allows us to use (10) to label the peak positions.

4. Experiment

The generalized FSL with $r = 1$ and $s = 10$, as described at the end of §2.2 and shown in Fig. 1, was used as the sample. The multilayer was grown on a GaAs (001) substrate. The nominal thickness of the GaAs layer A is

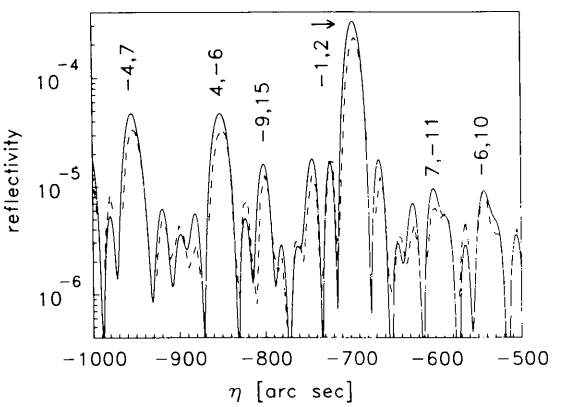

Fig. 3. Comparison of the diffraction curves of the 12th generation of FSL calculated using the exact formula (3) (full line) and the approximate formula (13) (dashed line). The peaks are labelled by two integers p, q according to formula (10). Diffraction and SL parameters are the same as in Fig. 2.

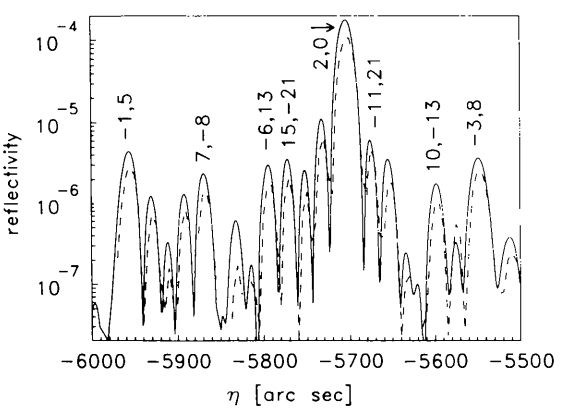

Fig. 4. As Fig. 3 for a different angular region.

15 monolayers (mL, half of the lattice parameter) and 143 layers in total, that of AlAs layer B is 9 mL (88 layers in total), total thickness of the superlattice is 831 nm. Owing to the pseudomorphic structure of the SL, the lattice parameter c_A has been supposed to equal that of the substrate $c = 5.65325$ Å. Therefore, the three free structural parameters (thicknesses d_A, d_B and lattice parameter c_B) had to be determined by a fit of the measured diffraction curve. The measurement of the diffraction curve was made using a double-crystal X-ray diffractometer with Cu $K\alpha$ symmetrical 111 diffraction on a perfect silicon crystal and symmetrical 002 diffraction on the sample.

The fit of the relative peak distances according to (12) gives the averaged layer thickness $d = d_A + d_B\tau = 56.7(2)$ Å. Use of (11) for the position of the zeroth-order satellite with respect to the position of the substrate peak gave the parameter c_B as a function of the ratio d_B/d_A keeping d fixed. To estimate the third free parameter c_B, the third condition is necessary. Usually the fit of the whole experimental diffraction curve is employed in such cases. Low primary intensity involved in the measurement made it impossible because the low-intensity peaks, which are more sensitive to the d_B/d_A ratio, were not distinguished. To have another condition to estimate the remaining parameter, we have supposed that the ratio d_B/d_A equals the ratio of the nominal thicknesses (9 mL AlAs/15 mL GaAs), which was assumed by the producer of the sample. The calculation of all three parameters under this assumption gave the values $d_A = 14.6(1)$ mL, $d_B = 8.8(1)$ mL, $c_B = 5.668(1)$ Å. The lattice parameter c_B was found to be the same as the value usually found in the periodic GaAs/AlAs superlattices measured with high precision (Holý, Kuběna & Ploog, 1990). This confirms the validity of our assumption. The measured and the best-fitted curves are shown in Fig. 5.

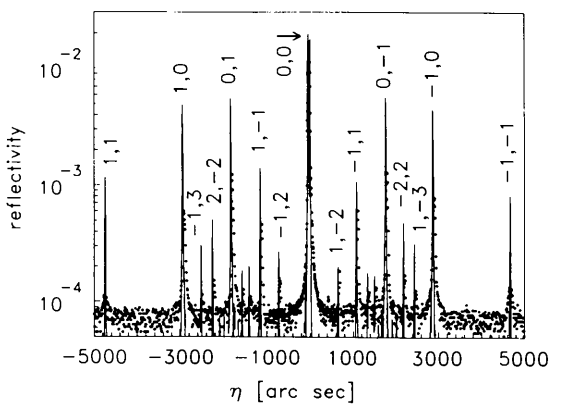

Fig. 5. Experimental diffraction curve (points) and the best-fitted curve (full line) of the generalized Fibonacci superlattice described in the text. The experimental arrangement enabled the measurement of intensity over four orders of magnitude.

5. Concluding remarks

Full calculation of the diffraction curve of the Fibonacci superlattice in the semi-kinematical approximation with two approaches has been reported. We have compared the results of the exact formula (3) calculated recurrently with those of the approximate formula (13) derived by means of the discrete Fourier transform of quasiperiodically arranged layers in the infinite lattice and successively restricted to a finite thickness. Good agreement of the peak positions and of the intensities of the diffraction curves was found. The agreement between exact and approximate diffraction curves increases with the number of layers, hence increasing the SL thickness. The exact approach can be used for the diffraction-curve numerical calculation, while the approximate approach provides clearer information on the diffraction-curve profile, mostly from equation (10), which describes the diffraction-curve peak positions. The derived approximate formulae were found to be useful to fit the layer thicknesses and lattice parameters of the generalized Fibonacci superlattice. We have shown that it is possible to fit the structural parameters of this quasiperiodic superlattice even if low experimental resolution did not allow the fitting of the whole diffraction curve.

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