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1993 J. Phys.: Condens. Matter 5 4903

(http://iopscience.iop.org/0953-8984/5/28/006)

J. Phys.: Condens. Matter 5 (1993) 4903–4908. Printed in the UK

X-ray dynamical diffraction in superlattices

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Received 21 December 1992, in final form 5 April 1993

Abstract. A new approach to calculating x-ray dynamical scattering in Bragg diffraction geometry in ideal superlattices has been proposed. The method is based on the Bloch theorem and effectively takes advantage of the periodic properties of superlattices.

1. Introduction

X-ray diffraction is widely used for structural characterization of semiconductor superlattices (SLs). By means of x-ray diffraction it is possible to determine such parameters of the SL as the period and the average lattice parameter [1–5].

A kinematical approximation which provides a simple and obvious description of diffraction scattering is widely used for analysis of the x-ray rocking curves from SLs [6]. It provides, however, overestimated low-order satellite intensities and is not applicable in the neighbourhood of the substrate Bragg peak. One could take into account dynamical effects within the framework of the conventional approach based on the solution of the non-linear first-order differential equation for the scattering amplitude [7]. This method, however, does not take into account such characteristic features of SLs as the periodic dependence on the structural and scattering parameters. Below we present a method of calculation of the dynamical x-ray scattering in SLs which effectively takes advantage of the above-mentioned property.

We shall start with the conventional Takagi–Taupin [7, 8] equations for the refracted wave amplitude D_0 and the diffracted wave amplitude D_h:

$$\frac{\mathrm{d}}{\mathrm{d}z}\begin{bmatrix} D_0 \\ D_h \end{bmatrix} = \frac{\mathrm{i}k}{2\gamma_0}\begin{bmatrix} \chi_0(z) & \chi_{\bar{h}}(z)\exp[\mathrm{i}\phi(z)] \\ -\beta\chi_h(z)\exp[-\mathrm{i}\phi(z)] & -[\chi_0(z)-\alpha]\beta \end{bmatrix}\begin{bmatrix} D_0 \\ D_h \end{bmatrix}. \qquad (1)$$

Here $k = 2\pi/\lambda$ is the wavevector; the asymmetry factor $\beta = \gamma_0/|\gamma_h|$ (γ_0 and γ_h are the directing cosines of the refracted and diffracted beams, respectively); χ_0, χ_h and $\chi_{\bar{h}}$ are the Fourier components of the crystal polarizability; the parameter $\alpha = -2\sin(2\vartheta_{\mathrm{Br}})((\vartheta - \vartheta_{\mathrm{Br}})$ specifies the angular deviation from the exact Bragg angle ϑ_{Br}); $\phi(z) = \boldsymbol{h}\cdot\boldsymbol{u}(z)$ ($\boldsymbol{h}$ is the reciprocal-lattice vector); the displacement of atomic planes is given by $u(z) = -\int_0^z \mathrm{d}s(\Delta d/d)(s)$ ($\Delta d/d$ is the lattice space modification with respect to crystal substrate).

After the substitution $D_h \to D_h\exp[\mathrm{i}\phi(z)]$ the set (1) transforms to

$$\frac{\mathrm{d}}{\mathrm{d}z}\begin{bmatrix} D_0 \\ D_h \end{bmatrix} = \frac{\mathrm{i}k}{2\gamma_0}\begin{bmatrix} \chi_0(z) & \chi_{\bar{h}}(z) \\ -\chi_h(z)\beta & -[\beta\chi_0(z)-\alpha-\Delta\alpha(z)] \end{bmatrix}\begin{bmatrix} D_0 \\ D_h \end{bmatrix} \qquad (2)$$

where

$$\Delta\alpha = (2\gamma_0/k\beta)(\mathrm{d}/\mathrm{d}z)\phi(z) = -(2\gamma_0/k\beta)(2\pi/d)(\Delta d/d)(z). \tag{3}$$

In an SL the coefficients of the matrix of the set (2) are periodic functions of the coordinate z. In accordance with the Bloch theorem [9], fundamental solutions of such a set for an arbitrary value of z must satisfy the following equality:

$$D_{0,h}(z+T) = \rho D_{0,h}(z) \tag{4}$$

where T is the period of the SL and ρ is called a multiplier [10].

2. SL with abrupt interfaces

Let us consider x-ray diffraction in an SL with abrupt interfaces between constituent layers. For simplicity first we restrict ourselves to the case of an SL each period of which consists of two layers. The thickness of the first layer is denoted by t, and the thickness of the second layer by $T-t$. Within each layer, Fourier components $\chi_0^{(i)}$, $\chi_h^{(i)}$ and $\chi_{\bar{h}}^{(i)}$ of polarizability and Fourier components $(\Delta d/d)^{(i)} (i = 1, 2)$ of lattice mismatch are assumed to be constant.

The general solution of (2) in the first layer ($0 \leqslant z \leqslant t$) may be written in the following form:

$$\boldsymbol{D}(z) \equiv \begin{bmatrix} D_0(z) \\ D_h(z) \end{bmatrix} = \omega \boldsymbol{D}_1^{(1)} \exp(\mathrm{i}k\epsilon_1^{(1)} \tfrac{1}{2} z\gamma_0) + \delta \boldsymbol{D}_2^{(1)} \exp(\mathrm{i}k\epsilon_2^{(1)} \tfrac{1}{2} z\gamma_0) \tag{5}$$

where

$$\epsilon_{1,2}^{(1)} = \tfrac{1}{2}[\![(\alpha + \Delta\alpha^{(1)})\beta + (1-\beta)\chi_0^{(1)} \pm \{[(\alpha + \Delta\alpha^{(1)})\beta - (1+\beta)\chi_0^{(1)}]^2 - 4\beta\chi_{\bar{h}}^{(1)}\chi_h^{(1)}\}^{1/2}]\!] \tag{6}$$

are the eigenvalues of the matrix of (2) in the interval $0 \leqslant z \leqslant t$ and

$$\boldsymbol{D}_{1,2}^{(1)} = \begin{bmatrix} 1 \\ -(\chi_0^{(1)} - \epsilon_{1,2}^{(1)})/\chi_{\bar{h}}^{(1)} \end{bmatrix} \tag{7}$$

are the relevant column eigenvectors, and ω and δ are constants.

It is convenient to represent solution (5) in the matrix form

$$\boldsymbol{D}(z) = \mathbf{Q}_1(z) \begin{bmatrix} \omega \\ \delta \end{bmatrix}. \tag{8}$$

The columns of the matrix $\mathbf{Q}_1(z)$ are formed by the eigenvectors $\boldsymbol{D}_{1,2}^{(1)}$ with appropriate multipliers:

$$\mathbf{Q}_1(z) = [\boldsymbol{D}_1^{(1)} \exp(\mathrm{i}k\epsilon_1^{(1)} \tfrac{1}{2} z\gamma_0), \boldsymbol{D}_2^{(1)} \exp(\mathrm{i}k\epsilon_2^{(1)} \tfrac{1}{2} z\gamma_0)]. \tag{9}$$

In the second layer ($t \leqslant z \leqslant T$),

$$\boldsymbol{D}(z) = \eta \boldsymbol{D}_1^{(2)} \exp(\mathrm{i}k\epsilon_1^{(2)} \tfrac{1}{2} z\gamma_0) + \nu \boldsymbol{D}_2^{(2)} \exp(\mathrm{i}k\epsilon_2^{(2)} \tfrac{1}{2} z\gamma_0) \tag{10}$$

or, in the equivalent matrix form,

$$D(z) = \mathbf{Q}_2(z) \begin{bmatrix} \eta \\ \nu \end{bmatrix} \tag{11}$$

where

$$\mathbf{Q}_2(z) = [D_1^{(2)} \exp(ik\epsilon_1^{(2)} \tfrac{1}{2} z\gamma_0), D_2^{(2)} \exp(ik\epsilon_2^{(2)} \tfrac{1}{2} z\gamma_0)]. \tag{12}$$

At the interface between layers ($z = t$) the amplitudes of the refracted and diffracted waves must match:

$$\mathbf{Q}_1(t) \begin{bmatrix} \omega \\ \delta \end{bmatrix} = \mathbf{Q}_2(t) \begin{bmatrix} \eta \\ \nu \end{bmatrix}. \tag{13}$$

In matrix notation the Bloch condition (4) has the following form:

$$\rho \mathbf{Q}_1(0) \begin{bmatrix} \omega \\ \delta \end{bmatrix} = \mathbf{Q}_2(T) \begin{bmatrix} \eta \\ \nu \end{bmatrix}. \tag{14}$$

By expressing the vector $\begin{bmatrix} \eta \\ \nu \end{bmatrix}$ from equation (13) as

$$\begin{bmatrix} \eta \\ \nu \end{bmatrix} = \mathbf{Q}_2^{-1}(t)\mathbf{Q}_1(t) \begin{bmatrix} \omega \\ \delta \end{bmatrix} \tag{15}$$

and substituting (15) in (14), we obtain the following relation:

$$\rho \begin{bmatrix} \omega \\ \delta \end{bmatrix} = \mathbf{Q}_1^{-1}(0)\mathbf{Q}_2(T)\mathbf{Q}_2^{-1}(t)\mathbf{Q}_1(t) \begin{bmatrix} \omega \\ \delta \end{bmatrix}. \tag{16}$$

In equations (15) and (16) and hereafter, $\mathbf{Q}^{-1}$ denotes the inverse of the matrix $\mathbf{Q}$.

From (16) it follows that ρ is the eigenvalue of the 2×2 matrix $\mathbf{Q}_1^{-1}(0)\mathbf{Q}_2(T)\mathbf{Q}_2^{-1}(t)\mathbf{Q}_1(t)$. We denote by $\rho_{1,2}$ and $\begin{bmatrix} \omega \\ \delta \end{bmatrix}_{1,2}$ the eigenvalues and the relevant eigenvectors of the above-mentioned matrix. Then the general solution of (2) at $(n-1)T \leqslant z \leqslant (n-1)T+t$ ($n = 1, 2, 3, \ldots$) may be represented in the following form:

$$D(z) = A\rho_1^{n-1}\mathbf{Q}_1[z-(n-1)T] \begin{bmatrix} \omega \\ \delta \end{bmatrix}_1 + B\rho_2^{n-1}\mathbf{Q}_1[z-(n-1)T] \begin{bmatrix} \omega \\ \delta \end{bmatrix}_2 \tag{17}$$

where A and B are constants.

At $(n-1)T + t \leqslant z \leqslant nT$ ($n = 1, 2, 3, \ldots$),

$$D(z) = A\rho_1^{n-1}\mathbf{Q}_2[z-(n-1)T \begin{bmatrix} \eta \\ \nu \end{bmatrix}_1 + B\rho_2^{n-1}\mathbf{Q}_2[z-(n-1)T] \begin{bmatrix} \eta \\ \nu \end{bmatrix}_2 \tag{18}$$

where

$$\begin{bmatrix} \eta \\ \nu \end{bmatrix}_{1,2} = \mathbf{Q}_2^{-1}(t)\mathbf{Q}_1(t) \begin{bmatrix} \omega \\ \delta \end{bmatrix}_{1,2}. \tag{19}$$

Equations (17) and (18) seem to be convenient for the analysis of the diffraction wave fields in the SL. The constants A and B in them could be determined from the amplitude continuity equations at the SL–substrate and SL–vacuum boundaries. At the entrance surface of the substrate the wave field may be represented as

$$D_s = D_{0s}\begin{bmatrix} 1 \\ R \end{bmatrix} \tag{20}$$

where D_{0s} is the amplitude of the wave transmitted through the SL wave, and R is the reflection amplitude of the substrate which can be easily calculated within the framework of the conventional dynamical theory [11].

If the SL is composed of N periods, then by taking into account (17) the continuity condition at the boundary with the substrate may be written as follows:

$$A\rho_1^N \mathbf{Q}_1(0)\begin{bmatrix} \omega \\ \delta \end{bmatrix}_1 + B\rho_2^N \mathbf{Q}_1(0)\begin{bmatrix} \omega \\ \delta \end{bmatrix}_2 = D_{0s}\begin{bmatrix} 1 \\ R \end{bmatrix}. \tag{21}$$

At the boundary with the vacuum the continuity condition is

$$A\mathbf{Q}_1(0)\begin{bmatrix} \omega \\ \delta \end{bmatrix}_1 + B\mathbf{Q}_1(0)\begin{bmatrix} \omega \\ \delta \end{bmatrix}_2 = \begin{bmatrix} E_0 \\ E_h \end{bmatrix} \tag{22}$$

where $E_0 = 1$ is the amplitude of the wave incident on the SL and E_h is the amplitude of the diffracted wave under study. Equations (21) and (22) form the set of linear equations of fourth order with respect to the quantities A, B, D_{0s} and E_h and allow one to obtain a complete solution of the problem of diffraction scattering of x-rays in an SL.

It is possible to show that the modulus of one of the eigenvalues ρ is always less than unity while the modulus of the other always exceeds unity. Thus, if x-ray diffraction takes place in a semi-infinite SL ($N = \infty$), then it is necessary to keep, in equations (17) and (18), only one term for which

$$|\rho| < 1. \tag{23}$$

Condition (23) provides damping of the wave fields in the bulk of the SL. In this case the continuity condition (22) at the boundary with the vacuum has the following form:

$$A\mathbf{Q}_1(0)\begin{bmatrix} \omega \\ \delta \end{bmatrix} = \begin{bmatrix} E_0 \\ E_h \end{bmatrix}. \tag{24}$$

The x-ray rocking curve calculated from a semi-infinite absorbing SL is depicted in figure 1(a). Figure 1(b) demonstrates the differences between the dynamical and kinematical approximations when calculating the 'zero' peak of the above-mentioned SL.

The formulae obtained allow generalization of the case when each period of the SL contains not two but m layers with thicknesses t_i ($\sum_{i=1}^{m} t_i = T$). Then instead of (16) we have the following relation for determination of ρ and eigenvectors of the first period of the SL:

$$\rho\begin{bmatrix} \omega \\ \delta \end{bmatrix} = \mathbf{Q}_1^{-1}(0)\mathbf{Q}_m(T)\left[\prod_{k=m}^{2}\mathbf{Q}_k^{-1}\left(\sum_{j=1}^{k-1} t_j\right)\mathbf{Q}_{k-1}\left(\sum_{j=1}^{k-1} t_j\right)\right]\begin{bmatrix} \omega \\ \delta \end{bmatrix}. \tag{25}$$

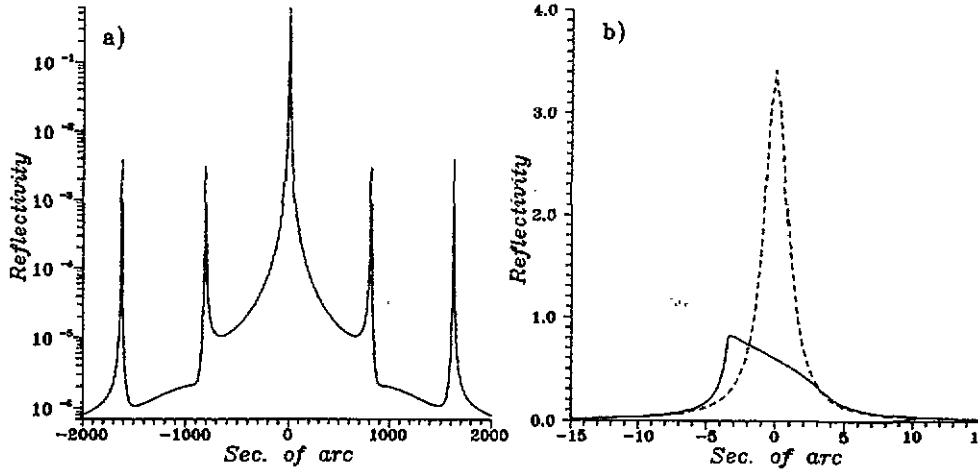

Figure 1. (*a*) X-ray rocking curve calculated from a semi-infinite SL with the period $T = 230$ Å. (*b*) 'Zero' peak of a semi-infinite SL in a linear scale: ——, dynamical approximation; - - - -, kinematical approximation.

3. SL with continuously varying characteristics

Let us consider now the x-ray diffraction in an SL whose structural characteristics χ_0, χ_h and $\chi_{\bar{h}}$ and lattice mismatch $\Delta d/d$ are continuously varying periodic functions of the coordinate z. This occurs for example for SLs whose interface between constituent layers is not atomically abrupt. In this case it is impossible to construct exact analytical expressions for the wave fields in the SL.

Let us denote the amplitudes of the wave fields at the entrance surface of the SL as $\begin{bmatrix} D_0(0) \\ D_h(0) \end{bmatrix}$. From the linearity of the initial set of differential equations (2), it follows that

$$\begin{bmatrix} D_0(T) \\ D_h(T) \end{bmatrix} = \mathbf{M} \begin{bmatrix} D_0(0) \\ D_h(0) \end{bmatrix} \tag{26}$$

where $\mathbf{M}$ is the 2×2 matrix depending only on the scattering angle, structural characteristics and value of T. For determination of the elements of the matrix $\mathbf{M}$ it is necessary to solve equations (2) twice by numerical methods or perturbation techniques in the interval $0 \leqslant z \leqslant T$.

In fact, if we set

$$\begin{bmatrix} D_0(0) \\ D_h(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{27}$$

then it is easy to see that

$$M_{11} = D_0(T) \qquad M_{21} = D_h(T). \tag{28}$$

If

$$\begin{bmatrix} D_0(0) \\ D_h(0) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{29}$$

then

$$M_{12} = D_0(T) \qquad M_{22} = D_h(T). \tag{30}$$

The Bloch condition (4) has the following form:

$$\rho \begin{bmatrix} D_0(0) \\ D_h(0) \end{bmatrix} = \mathbf{M} \begin{bmatrix} D_0(0) \\ D_h(0) \end{bmatrix} \tag{31}$$

i.e. ρ is the eigenvalue and $\begin{bmatrix} D_0(0) \\ D_h(0) \end{bmatrix}$ is the eigenvector of the matrix $\mathbf{M}$. Further operations are obvious; they coincide with those described in the previous section.

4. Conclusion

A new method based on the periodic properties of an SL to calculate x-ray dynamical diffraction has been proposed. In comparison with the existing methods the new approach has some advantages as well as deficiencies. Probably the most interesting feature of the new approach is that computing time is independent of the number of periods in the SL. The proposed method is also applicable to x-ray grazing incidence diffraction on the SL [12]. As for deficiencies, it is less simple and illustrative than the kinematical approximation. It is also not clear at the present stage whether this method could be modified to take into account the random variations in the SL period, concentration profiles, etc. Random variations, however, reveal themselves mainly in high-order satellites where dynamical effects are negligible and it is easier to use the kinematical approximation for analysis [13].

References

[1] Chang L L, Segmuller A and Esaki L 1976 *J. Appl. Phys. Lett.* **28** 39
[2] Segmuller A, Krishna P and Esaki L 1977 *J. Appl. Crystallogr.* **10** 1
[3] Fleming R M, Mewhan D B, Gossard A C *et al* 1980 *J. Appl. Phys.* **51** 357
[4] Kashihara Y, Kase T and Harada J 1986 *Japan. J. Appl. Phys.* **25** 1834
[5] Afanas'ev A M, Imamov R M, Mockerov V G, Maslov A V, Mukhamedzhanov E Kh, Pashaev E M and Zaitsev A A 1992 *Proc. Phys. Tech. Inst. Russ. Acad. Sci.* at press
[6] Speriosu V S and Vreeland T Jr 1984 *J. Appl. Phys.* **56** 1591
[7] Taupin D 1964 *Bull. Soc. Fr. Minéral Cristallogr.* **87** 469
[8] Takagi S 1969 *J. Phys. Soc. Japan* **26** 1239
[9] Ziman J M 1964 *Principles of the Theory of Solids* (Cambridge: Cambridge University Press) p 15
[10] Fedoryuk M V 1985 *Ordinary Differential Equations* (Moscow: Nauka) p 227
[11] Pinsker Z G 1978 *Dynamical Scattering of X-rays in Crystals* (Berlin: Springer) p 262
[12] Melikyan O G, Imamov R M and Novikov D V 1992 *Fiz. Tverd. Tela* **34** 1572
[13] Chrzan D and Dutta P 1986 *J. Appl. Phys.* **59** 1504