Table 1. 25 *Values of* $\mathscr{P}_+$ *and* $\mathscr{Q}_+$ *for a derivative of* β*-lactam*

Signs in parentheses are the true signs of the main reflections.

Number	Indices of main terms: h			Indices of main terms: k			Observed magnitudes, $\lvert E \rvert$: h	k	$\frac{1}{2}$(h+k)	$\frac{1}{2}$(h−k)	Heavy-atom contribution E^P: h	k	$\mathscr{P}_+$	$\mathscr{Q}_+$
1	4	8	9	2	0	11	2·46(−)	2·81(−)	3·49	2·34	−1·91	−1·04	0·99	0·95
2	2	13	3	0	1	3	2·35(−)	2·06(−)	2·79	2·60	−0·58	−1·86	0·98	0·91
3	9	4	4	5	4	12	2·61(+)	2·05(+)	2·04	1·89	1·86	1·99	0·97	0·73
4	9	4	4	3	12	6	2·61(+)	2·12(+)	2·11	2·06	1·86	1·65	0·97	0·78
5	2	11	7	2	9	1	2·50(+)	2·54(+)	2·36	2·06	1·06	1·87	0·97	0·83
6	8	9	2	2	11	0	2·21(+)	2·63(+)	2·36	0·84	1·59	1·86	0·97	0·75
7	4	17	0	2	7	0	2·56(+)	2·10(+)	2·33	2·04	1·98	1·20	0·97	0·80
8	7	13	1	3	13	9	2·70(+)	2·50(+)	2·38	1·56	1·96	1·57	0·96	0·74
9	4	10	3	4	8	9	2·03(−)	2·46(−)	1·88	2·06	−1·60	−1·91	0·95	0·73
10	6	2	10	2	2	6	2·06(+)	2·05(+)	2·23	1·95	1·46	0·92	0·89	0·75
11	3	14	2	1	6	0	2·31(+)	2·60(+)	1·88	2·34	1·34	0·56	0·88	0·79
12	4	11	3	0	1	3	2·01(+)	2·06(−)	1·92	3·14	0·01	−1·86	0·86	0·86
13	5	7	5	5	3	1	2·20(+)	3·00(+)	2·26	2·59	−0·09	1·37	0·83	0·89
14	2	10	4	0	2	2	2·36(−)	2·59(−)	1·43	2·34	−1·59	−0·67	0·82	0·69
15	3	5	8	3	11	2	2·85(+)	2·00(+)	3·05	2·59	1·89	−0·48	0·76	0·93
16	6	14	2	2	4	12	2·57(−)	2·38(−)	1·85	2·08	−0·42	0·11	0·74	0·75
17	8	8	4	2	2	6	2·25(−)	2·05(+)	0·88	2·61	0·93	0·92	0·63	0·53
18	5	5	7	3	13	9	2·14(−)	2·50(+)	1·50	2·34	−0·69	1·57	0·53	0·69
19	9	5	3	1	7	11	2·06(−)	2·12(+)	1·99	0·53	−0·35	−0·77	0·50	0·49
20	3	5	8	3	3	10	2·85(+)	3·05(−)	1·78	1·11	1·89	−0·66	0·50	0·59
21	6	14	2	2	2	6	2·57(−)	2·05(+)	1·80	0·16	−0·42	0·92	0·48	0·49
22	4	11	3	2	1	11	2·01(+)	2·69(−)	1·99	0·54	0·01	−1·58	0·48	0·48
23	4	16	2	2	2	6	2·00(−)	2·05(+)	2·89	2·26	−1·66	0·92	0·46	0·87
24	3	14	2	3	6	0	2·30(+)	2·16(−)	2·06	2·07	1·34	−1·39	0·43	0·76
25	5	5	3	1	7	11	2·26(−)	2·12(+)	1·99	0·74	1·85	−0·81	0·41	0·51

to employ the higher neighborhoods for the better estimation of structure invariants and seminvariants.

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The Dynamic Theory of X-ray Diffraction by the One-dimensional Ideal Superlattice. I. Diffraction by the Arbitrary Superlattice

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Abstract

The theory of X-ray two-beam dynamic diffraction by the one-dimensional ideal superlattice (SL) in the Laue and Bragg cases is developed. The reflection and transmission amplitudes of the SL are expressed by those for one period of the SL. General expressions revealing the behavior of the diffraction pattern, irrespective of the particular model, are obtained. A detailed analysis is carried out for the most important case: $z_0 \ll \bar{\Lambda}$ (z_0 and $\bar{\Lambda}$ being the SL period and the mean extinction length of the crystal, respectively).

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1. Introduction

Superlattices (SL) are crystalline structures, in which electrons are affected by, besides the periodic lattice potential, an additional periodic potential with period considerably exceeding the lattice parameter. Owing to a number of unique properties, the SL has good prospects of being widely applicable to microelectronics and computer engineering (Shick, 1974). Being important in applications, the SL perfection has been investigated by various methods of X-ray and electron microscopy analysis (Matthews & Blakeslee, 1974, 1975, 1976; Petroff, Gossard, Savage & Wiegmann, 1979). The theoretical investigations of X-ray diffraction on various types of natural (superstructures, layered semiconductor compounds, polytype structures, charge density wave structures) and artificial SLs (the use of ultrasonics, multilayer thin-film structures based on heterojunctions) were confined to the kinematic approximation treatment (de Fontaine, 1966; Korekawa, 1967; Segmüller & Blakeslee, 1973; Böhm, 1975), which holds if $z_0 \ll \bar{\Lambda}$ (z_0 is the SL period and $\bar{\Lambda}$ the mean crystal extinction length) and $D \ll \Lambda_m$ (D is the thickness and Λ_m the extinction length of SL, respectively). While the first condition is usually satisfied for most SL types, this is not the case for the second.

The dynamic theory, which takes into account the interaction between the incident and reflected waves, was employed in the problem of X-ray diffraction on the harmonic model SL. The solution of Takagi's equations for small amplitudes of the additional potential is given by Khapachev, Kolpakov, Kouznetzov & Kouz'min (1979). At $z_0 \ll \bar{\Lambda}$ the problem is reduced to well known two-wave dynamic theory (Köhler, Möhling & Peibst, 1974). At $z_0 \simeq \bar{\Lambda}$ an interesting resonance, which is very sensitive to weak ultrasonic strains, has been theoretically studied and then experimentally found (Entin, 1978).

The characteristic matrix method employed in the theory of X-ray diffraction in multilayer crystalline films was developed by Kolpakov & Belyaev (1982). However, the authors restricted themselves to the detailed analysis of a two-layer system only.

X-ray dynamic reflection from the SL, consisting of the ideal layers of crystalline lattices equally shifted with respect to each other, is considered by Vardanyan & Manoukyan (1982).

In the present paper the two-beam dynamic theory of X-ray diffraction on the one-dimensional ideal SL is developed.

2. The SL reflection and transmission amplitudes

(a) *Laue case*

Let a plane monochromatic X-ray wave of unit amplitude be incident on the SL consisting of N identical crystalline layers, which we call the SL cells (see Fig. 1). We introduce the following designations: Φ_{hN} and Φ_{0N} are, respectively, the reflection and transmission amplitudes of the SL consisting of N cells; r_h, $r_{\bar{h}}$ and t_0, $t_{\bar{0}}$ are, respectively, the reflection and transmission amplitudes of one cell; **h** is the reciprocal-lattice vector and the dash corresponds to incidence from the back of the reflecting planes.

The waves $\Phi_{0(N-1)}$ and $\Phi_{h(N-1)}$ emerging from the set of $(N-1)$ layers are incident on the Nth layer, and for Φ_{hN} and Φ_{0N} we obtain the following recursion equations:

$$\Phi_{hN} = t_{\bar{0}}\Phi_{h(N-1)} + r_h\Phi_{0(N-1)} \tag{1}$$

$$\Phi_{0N} = r_{\bar{h}}\Phi_{h(N-1)} + t_0\Phi_{0(N-1)}. \tag{2}$$

For $N=0$ and $N=1$ we have

$$\Phi_{h0} = 0, \qquad \Phi_{h1} = r_h \tag{3}$$

and

$$\Phi_{00} = 1, \qquad \Phi_{01} = t_0. \tag{4}$$

The solutions of (1) and (2) are given in Appendix *A*, and are of the form

$$\Phi_{hN} = i\left(\frac{r_h}{r_{\bar{h}}}\right)^{1/2} \frac{\sin(N\varphi)}{(1+\xi^2)^{1/2}} \tag{5}$$

$$\Phi_{0N} = \cos(N\varphi) - \frac{i\xi}{(1+\xi^2)^{1/2}}\sin(N\varphi), \tag{6}$$

where

$$\xi = (t_{\bar{0}} - t_0)/2(r_h r_{\bar{h}})^{1/2} \tag{7}$$

$$\sin\varphi = -i(r_h r_{\bar{h}})^{1/2}(1+\xi^2)^{1/2}. \tag{8}$$

Expressions (5) and (6) are similar to the formulae for the reflection and transmission amplitudes of an ideal crystal (Pinsker, 1978), with the only difference

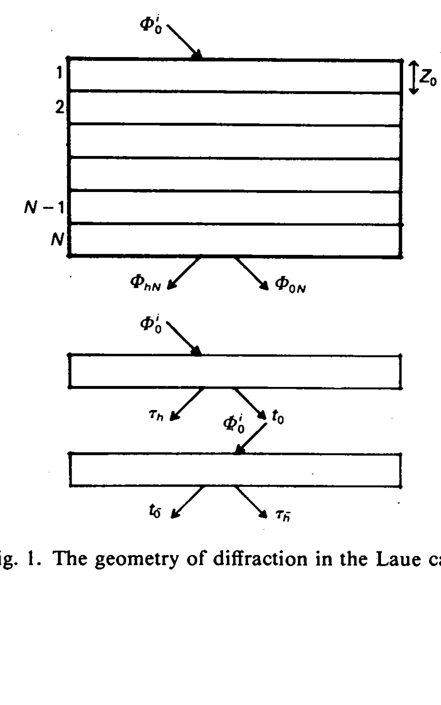

Fig. 1. The geometry of diffraction in the Laue case.

being that instead of the deviation parameter from the Bragg angle θ_B,

$$s = 2k \sin \theta_B(\theta - \theta_B), \tag{9}$$

here we have the parameter $\xi(s)$, dependent on the SL model. If the crystal is ideal (*i.e.* the superperiodicity is absent) one may suppose it to be composed of N equal layers each of thickness z_0, and substituting the corresponding formulae for reflection and transmission amplitudes of the ideal layer in (7) and (8), we obtain

$$\xi(s) = s/\beta \tag{10a}$$

$$N\varphi = \pi D(s^2 + \beta^2)^{1/2}, \tag{10b}$$

where D is the crystal thickness and

$$\beta = \frac{kC(\chi_h\chi_{\bar{h}})^{1/2}}{\cos \theta_B} = \frac{\pi}{\Lambda} \tag{11}$$

is the inverse extinction length; $k = 1/\lambda$ is the wave number in vacuum; C is the polarization factor; χ_h and $\chi_{\bar{h}}$ are the Fourier components of crystal susceptibility. The directions of the diffraction maxima (satellites) correspond to the roots of the equation

$$\xi(s) = 0. \tag{12}$$

(*b*) *Bragg case*

The reflection geometry is given in Fig. 2. Taking into account the multifold reflections from the boundaries of the SL cells, we obtain the following recursion equations:

$$\Phi_{hN} = r_h + t_0t_{\bar{0}}\Phi_{h(N-1)} + t_0t_{\bar{0}}r_{\bar{h}}\Phi^2_{h(N-1)} + \dots$$
$$= \frac{r_h + \Phi_{h(N-1)}(t_0t_{\bar{0}} - r_hr_{\bar{h}})}{1 - r_{\bar{h}}\Phi_{h(N-1)}} \tag{13}$$

$$\Phi_{0N} = t_0\Phi_{0(N-1)}/[1 - r_{\bar{h}}\Phi_{h(N-1)}] \tag{14}$$

under conditions (3) and (4).

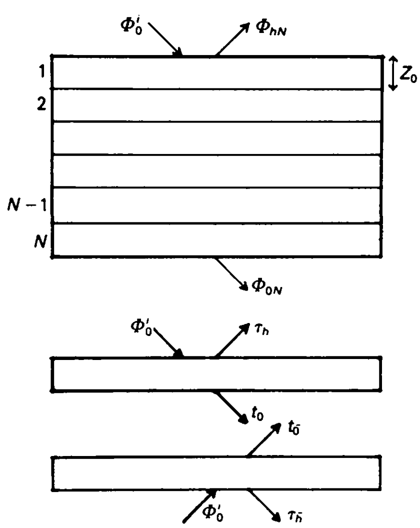

Fig. 2. The geometry of diffraction in the Bragg case.

The solutions (13) and (14), given in Appendix *B*, are of the form

$$\Phi_{hN} = \left(\frac{r_h}{r_{\bar{h}}}\right)^{1/2} \frac{\sin(N\varphi)}{\sin(N\varphi + \arccos \xi)} \tag{15}$$

$$\Phi_{0N} = \left(\frac{t_0}{t_{\bar{0}}}\right)^{N/2} \frac{\sin(\arccos \xi)}{\sin(N\varphi + \arccos \xi)}, \tag{16}$$

where

$$\xi = [1 - t_0t_{\bar{0}} + r_hr_{\bar{h}}]/2(r_hr_{\bar{h}})^{1/2} \tag{17}$$

and

$$\sin \varphi = [(r_hr_{\bar{h}}/t_0t_{\bar{0}})(1 - \xi^2)]^{1/2}. \tag{18}$$

In the Bragg case the deviation parameter from the Bragg angle is

$$s = 2k \cos \theta_B(\theta - \theta_B - \chi_0/\sin 2\theta_B), \tag{19}$$

where χ_0 is the zeroth Fourier component of crystal susceptibility.

In the case of an ideal crystal $\xi(s) = s/\beta$, where

$$\beta = \pi kC(\chi_h\chi_{\bar{h}})^{1/2}/\sin \theta_B. \tag{20}$$

For the thick SL ($N \to \infty$) from (15) we obtain

(*a*) at $|\xi| > 1$

$$\Phi_{h\infty} = \left(\frac{r_h}{r_{\bar{h}}}\right)^{1/2} [\xi \mp (\xi^2 - 1)^{1/2}], \tag{21}$$

where the upper sign corresponds to $\xi > 1$ (type III ranges) and the lower one corresponds to $\xi < -1$ (type I ranges).

The reflectivity

$$R^{\mathrm{I,III}}_{h\infty} = [|\xi| - (\xi^2 - 1)^{1/2}]^2 \tag{22}$$

decreases rapidly with increasing $|\xi|$;

(*b*) at $|\xi| \le 1$ (type II ranges)

$$\Phi_{h\infty} = \left(\frac{r_h}{r_{\bar{h}}}\right)^{1/2} [\xi - i(1 - \xi^2)^{1/2}] \tag{23}$$

and the reflectivity is

$$R^{\mathrm{II}}_{h\infty} = 1. \tag{24}$$

Thus, a total reflection of an incident X-ray wave occurs from a thick nonabsorbing SL within certain ranges of incidence.

Directions of the diffraction maxima (satellites) are found from (12).

3. Diffraction by the SL of a short period

To find the expression $\xi(s)$, it is necessary to obtain the reflection and transmission amplitudes of a single SL cell, which at $z_0 \gtrsim \Lambda$ can be done by solving the Takagi (1969) equations. The analytical solution of these equations can be found for particular cases only, and generally they are solved numerically. The formulae obtained in this paper make it possible to reduce the numerical solution of the Takagi equations for an arbitrary ideal SL to the one for a single SL cell, which greatly reduces the operation time. The problem is much simplified for the case $z_0 \ll \bar{\Lambda}$. This approximation is valid for superstructures, multilayer thin-film heterostructures, and a crystal placed in a short-wave ultrasonic field, *etc.* In this case the dispersion surfaces of different diffraction maxima do not intersect and the two-wave approximation is valid (Köhler, Möhling & Peibst, 1974). When $z_0 \ll \bar{\Lambda}$ one can write for t_0, $t_{\bar{0}}$ and r_h, $r_{\bar{h}}$ their kinematic formulae (James, 1948):

$$\begin{aligned} t_0 &= \exp[-i\pi\bar{s}z_0] \\ t_{\bar{0}} &= \exp[i\pi\bar{s}z_0] \end{aligned} \tag{25}$$

and

$$\begin{aligned} r_h &= \frac{i\pi k C\bar{\chi}_h}{\cos\bar{\theta}_B}\exp(i\pi\bar{s}z_0)\int_0^{z_0}\exp[-i2\pi\bar{s}(z)z\,\mathrm{d}z \\ r_{\bar{h}} &= \frac{i\pi k C\bar{\chi}_{\bar{h}}}{\cos\bar{\theta}_B}\exp(-i\pi\bar{s}z_0)\int_0^{z_0}\exp[i2\pi\bar{s}(z)z]\,\mathrm{d}z, \end{aligned} \tag{26}$$

where $s(z)$ is defined by (9) and indicates the local deviation from the Bragg angle and $\bar{s}$, $\bar{\chi}_h$, $\bar{\chi}_{\bar{h}}$ and $\bar{\theta}_B$ are mean values of the corresponding quantities averaged over the SL period:

$$\bar{s} = \bar{s}(z_0) = \frac{1}{z_0}\int_0^{z_0} s(z)\,\mathrm{d}z = 2k\cos\bar{\theta}_B(\theta - \bar{\theta}_B) \tag{27}$$

$$\bar{\chi}_{h,\bar{h}} = (1/z_0)\int_0^{z_0}\chi_{h,\bar{h}}(z)\,\mathrm{d}z \tag{28}$$

$$\bar{\theta}_B = (1/z_0)\int_0^{z_0}\theta_B(z)\,\mathrm{d}z. \tag{29}$$

Substituting (25) and (26) in (7), we find

$$\xi(\bar{s}) = \frac{\sin(\pi\bar{s}z_0)}{\pi\bar{\beta}z_0|M(\bar{s})|}, \tag{30}$$

where

$$M(\bar{s}) = \frac{1}{z_0}\int_0^{z_0}\exp[-i2\pi\bar{s}(z)z]\,\mathrm{d}z \tag{31}$$

and $\bar{\beta}$ is the average value of β.

Solving (12), we obtain

$$\bar{s}_m = m/z_0 \quad (m = 0; \pm 1; \pm 2; \ldots). \tag{32}$$

The distance between the satellites

$$\Delta = 1/z_0 \tag{33}$$

is independent of the satellite order.

Let us expand $\xi(\bar{s})$ in a Taylor series in the vicinity of $\bar{s}_m$ points and restrict ourselves to the first term:

$$\xi(\bar{s}) = \frac{(-1)^m}{\bar{\beta}M_m}(\bar{s} - \bar{s}_m), \tag{34}$$

where

$$M_m = |M(\bar{s}_m)| < 1. \tag{35}$$

Substituting (26) into (8) we obtain

$$\varphi(\bar{s}) = \pi\bar{\beta}M_m z_0(1 + \xi^2)^{1/2}. \tag{36}$$

The comparison of (34) and (36) with (10) shows that within the mth satellite one may consider the SL as an ideal crystal with the modified Fourier components of crystal susceptibility

$$|\chi_{hm}| = |\bar{\chi}_h|M_m. \tag{37}$$

The parameter M_m depends on the SL model and satisfies the following condition (see Appendix C):

$$\sum_{m=-\infty}^{\infty} M_m^2 = 1. \tag{38}$$

The same conclusion is valid in the Bragg case. Since $M_m \leq 1$ holds for any model, then the widths of the SL diffraction maxima are less than those for an ideal crystal, and the Bormann effect is weaker.

The SL extinction length

$$\Lambda_m = \bar{\Lambda}/M_m \tag{39}$$

is larger than that of an ideal crystal, therefore the X-ray wave penetrates into the SL deeper than into an ideal crystal.

The kinematic approximation for the SL holds, if $D \ll \Lambda_m$, D being the SL thickness.

Formulae (32) and (37) may also be obtained by the following considerations. The SL is characterized by an average over the SL period value $\bar{\theta}_B$. From the Laue condition

$$2\pi k z_0(\sin\theta_m - \sin\bar{\theta}_B) = \pi m$$

and assuming $\theta - \bar{\theta}_B \ll 1$, we find

$$\bar{s}_m = m/z_0.$$

When the SL period is small, one may neglect multifold reflections inside the SL cell. Then

$$\begin{aligned} |\chi_{hm}| &= \left|\frac{1}{z_0}\int_0^{z_0}\chi_h(z)\exp[-i2\pi\bar{s}(z)z]\,\mathrm{d}z\right| \\ &= |\bar{\chi}_h|M_m. \end{aligned}$$

The calculation of the superstructure factors M_m for various SL models is carried out in paper II (Vardanyan, Manoukyan & Petrosyan, 1985).

4. The absorption effect

The formula for the amplitude reflected from the SL X-ray wave is obtained using the corresponding formula for an ideal crystal when replacing the parameter s/β by ξ. Therefore, to take into account X-ray absorption in the SL, it is sufficient to replace $\mathrm{Re}\,(s/\beta)$ and $\mathrm{Im}\,(s/\beta)$ by $\mathrm{Re}\,\xi=\xi_r$ and $\mathrm{Im}\,\xi=\xi_i$, respectively, in the corresponding formulae for an ideal absorbing crystal given by Pinsker (1978).

The reflectivity for the SL with an infinite number of elements is of the form

$$R_m=E_m-(E_m^2-1)^{1/2}, \tag{40}$$

where

$$E_m=[1+(\xi_r^2+\xi_i^2)^2-2(\xi_r^2-\xi_i^2)]^{1/2}+\xi_r^2+\xi_i^2. \tag{41}$$

At X-ray incidence in the $\bar{s}_m$ direction, *i.e.* when $\xi_r=0$, we have

$$R_m(\bar{s}_m)=[R(0)]^{1/M_m}, \tag{42}$$

$R(0)$ being the reflectivity of an ideal absorbing bulk crystal with averaged parameters.

Since $R(0)<1$, then at relatively small values of M_m the mth-order reflection intensity will be too low.

APPENDIX *A*

Let us show that in the Laue case

$$t_0t_{\bar{0}}-r_hr_{\bar{h}}=1. \tag{A-1}$$

The coefficients t_0, r_h and $t_{\bar{0}}$, $r_{\bar{h}}$ are defined by the Howie–Whelan equations (Amelinckx, 1964):

$$\begin{aligned}\frac{\mathrm{d}t_0}{\mathrm{d}z}+i\pi s(z)t_0&=i\beta\left(\frac{\chi_h}{\chi_{\bar{h}}}\right)^{1/2}r_h\\ \frac{\mathrm{d}r_h}{\mathrm{d}z}-i\pi s(z)r_h&=i\beta\left(\frac{\chi_{\bar{h}}}{\chi_h}\right)^{1/2}t_0\end{aligned} \tag{A-2}$$

and

$$\begin{aligned}\frac{\mathrm{d}t_{\bar{0}}}{\mathrm{d}z}-i\pi s(z)t_{\bar{0}}&=i\beta\left(\frac{\chi_{\bar{h}}}{\chi_h}\right)^{1/2}r_{\bar{h}}\\ \frac{\mathrm{d}r_{\bar{h}}}{\mathrm{d}z}+i\pi s(z)r_{\bar{h}}&=i\beta\left(\frac{\chi_h}{\chi_{\bar{h}}}\right)^{1/2}t_0,\end{aligned} \tag{A-3}$$

where

$$s(z)=s+\mathrm{d}(\mathbf{hu})/\mathrm{d}z$$

is the local deviation from the Bragg condition. From (*A*-2) and (*A*-3) it is readily seen that

$$\mathrm{d}(t_0t_{\bar{0}}-r_hr_{\bar{h}})/\mathrm{d}z=0 \tag{A-4}$$

and

$$t_0t_{\bar{0}}-r_hr_{\bar{h}}=\text{constant}. \tag{A-5}$$

At $z=0$ the boundary conditions are $t_0=t_{\bar{0}}=1$ and $r_h=r_{\bar{h}}=0$. Hence the ratio (*A*-1) is valid.

Taking into account (*A*-1) from (1) and (2) we obtain

$$\Phi_{j,N}=(t_0+t_{\bar{0}})\Phi_{j(N-1)}-\Phi_{j(N-2)}\quad(j=0,h). \tag{A-6}$$

The general solution of (*A*-6) is in the form of a linear combination of Chebyshev polynomials:

$$\Phi_{jN}=\alpha_jT_N(\eta)+\beta_jU_N(\eta), \tag{A-7}$$

where

$$T_N=\cos(N\varphi)$$
$$U_N=\sin[(N+1)\varphi]/\sin\varphi$$

are Chebyshev polynomials of first and second order, respectively (Gradstein & Rizjik, 1971) and

$$\eta=\cos\varphi=(t_0+t_{\bar{0}})/2. \tag{A-8}$$

The coefficients α_j and β_j are defined from conditions (3) and (4):

$$\beta_h=-\alpha_h=2r_h/(t_0+t_{\bar{0}}) \tag{A-9}$$

$$\beta_0=1-\alpha_0=(t_0-t_{\bar{0}})/(t_0+t_{\bar{0}}). \tag{A-10}$$

Substituting (*A*-9) and (*A*-10) into (*A*-7), we obtain

$$\Phi_{hN}=r_h\sin(N\varphi)/\sin\varphi \tag{A-11}$$

$$\Phi_{0N}=\cos(N\varphi)+\frac{t_0-t_{\bar{0}}}{2}\frac{\sin(N\varphi)}{\sin\varphi}. \tag{A-12}$$

Let us introduce the following designation:

$$\xi=\left(\frac{\eta^2-1}{r_hr_{\bar{h}}}-1\right)^{1/2}=\frac{t_{\bar{0}}-t_0}{2(r_hr_{\bar{h}})^{1/2}}. \tag{A-13}$$

Then (*A*-11) and (*A*-12) can be transformed to the form

$$\Phi_{hN}=i\left(\frac{r_h}{r_{\bar{h}}}\right)^{1/2}\frac{\sin(N\varphi)}{(1+\xi^2)^{1/2}} \tag{A-14}$$

$$\Phi_{0N}=\cos(N\varphi)-\frac{i\xi}{(1+\xi^2)^{1/2}}\sin(N\varphi), \tag{A-15}$$

where φ is connected with ξ by the following relation:

$$\sin\varphi=-i(r_hr_{\bar{h}})^{1/2}(1+\xi^2)^{1/2}. \tag{A-16}$$

APPENDIX *B*

We try the solution of (13) in the form

$$\Phi_{hN}=A_N/B_N. \tag{B-1}$$

Substituting (*B*-1) into (13), and comparing the obtained expression with (*B*-1), we obtain the set of recursion equations

$$\begin{cases}A_N=r_hB_{N-1}+(t_0t_{\bar{0}}-r_hr_{\bar{h}})A_{N-1}\\ B_N=B_{N-1}-r_{\bar{h}}A_{N-1}.\end{cases} \tag{B-2}$$

Eliminating B_N, we obtain

$$A_N = (1 + t_0 t_{\bar{0}} - r_h r_{\bar{h}}) A_{N-1} - t_0 t_{\bar{0}} A_{N-2}. \quad (B\text{-}3)$$

We try the solution of (B-3) in the form

$$A_N = (t_0 t_{\bar{0}})^{N/2} F_N. \quad (B\text{-}4)$$

Substituting (B-4) into (B-3), we obtain

$$F_N = 2\eta F_{N-1} - F_{N-2}, \quad (B\text{-}5)$$

where

$$\eta = [1 + t_0 t_{\bar{0}} - r_h r_{\bar{h}}]/2(t_0 t_{\bar{0}})^{1/2}. \quad (B\text{-}6)$$

The solution of (B-5) is a linear combination of the Chebyshev polynomials:

$$F_N = \alpha T_N(\eta) + \beta U_N(\eta). \quad (B\text{-}7)$$

Substituting (B-7) into (B-4), we get

$$A_N = (t_0 t_{\bar{0}})^{N/2} [\alpha T_N(\eta) + \beta U_N(\eta)]. \quad (B\text{-}8)$$

From condition (3), we find $\alpha = -\beta$ and

$$A_N = (t_0 t_{\bar{0}})^{N/2} \beta \sin(N\varphi) \operatorname{cotan} \varphi, \quad (B\text{-}9)$$

where

$$\eta = \cos \varphi.$$

Determining B_N from (B-2) and substituting it into (B-1), we find

$$\Phi_{hN} = \left(\frac{r_h}{r_{\bar{h}}}\right)^{1/2} \frac{\sin(N\varphi)}{\sin(N\varphi + \arccos \xi)}, \quad (B\text{-}10)$$

where

$$\xi = (1 - t_0 t_{\bar{0}} + r_h r_{\bar{h}})/2(r_h r_{\bar{h}})^{1/2} \quad (B\text{-}11)$$

$$\sin \varphi = [(r_h r_{\bar{h}}/t_0 t_{\bar{0}})/(1 - \xi^2)]^{1/2}. \quad (B\text{-}12)$$

The solution of (14) is

$$\Phi_{0N} = \Phi_{00} \prod_{j=1}^{N} a_j, \quad (B\text{-}13)$$

where

$$a_j = t_0/[1 - r_{\bar{h}} \Phi_{h(j-1)}]. \quad (B\text{-}14)$$

Taking into account condition (14) and formula (B-10), from (B-13) we obtain

$$\Phi_{0N} = \left(\frac{t_0}{t_{\bar{0}}}\right)^{N/2} \frac{\sin(\arccos \xi)}{\sin(N\varphi + \arccos \xi)}. \quad (B\text{-}15)$$

APPENDIX C

The SL cell structure factor is defined by

$$M_m = \left|(1/z_0) \int_0^{z_0} \mathrm{d}z \exp\left[-i2\pi \int_0^z s(z)\, \mathrm{d}z\right]\right|. \quad (C\text{-}1)$$

The local deviation $s(z)$ may be represented by

$$s(z) = \bar{s}_m + q(z), \quad (C\text{-}2)$$

where

$$\bar{s}_m = m/z_0 \quad (C\text{-}3)$$

$$\int_0^{z_0} q(z)\, \mathrm{d}z = 0. \quad (C\text{-}4)$$

Substituting (C-2) and (C-3) in (C-1), we obtain

$$M_m = \left|(1/2\pi) \int_0^{2\pi} \mathrm{d}x \exp\left[-imx - i2\pi \int_0^{xz_0/(2\pi)} q(z)\, \mathrm{d}z\right]\right|.$$

Hence,

$$\sum_{m=-\infty}^{\infty} M_m^2 = [1/(2\pi)^2] \iint_0^{2\pi} \mathrm{d}x\, \mathrm{d}x' \times \exp\left[-i2\pi \int_{x'z_0/(2\pi)}^{xz_0/(2\pi)} q(z)\, \mathrm{d}z\right] \times \sum_{m=-\infty}^{\infty} \exp[-im(x - x')].$$

Since

$$\sum_{m=-\infty}^{\infty} \exp[-im(x - x')] = 2\pi\delta(x - x'),$$

where $\delta(x)$ is the Dirac function, so

$$\sum_{m=-\infty}^{\infty} M_m^2 = 1.$$

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