

MCM - program for calculating a multocrystal monochromator bandpass

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Abstract

The article contains an introduction for users-beginners to the program MCM. The program allows one to calculate and to see a two-dimensional distribution of monochromator transmissivity (bandpass) on the plane of parameters energy-angle as well as integral dependencies on energy and angle.

1. The theory of Bragg diffraction reflectivity of one single crystal plate

The dynamical theory of X-ray diffraction in single crystals is elaborated for a plane wave scattering. Let a plane monochromatic wave with a wave vector \mathbf{k}_0 and frequency ω be incident on the crystal plate. When the Bragg condition for the reciprocal lattice vector \mathbf{h} is fulfilled, namely, $\mathbf{k}_h^2 \approx \mathbf{k}_0^2$ where $\mathbf{k}_h = \mathbf{k}_0 + \mathbf{h}$, the second plane wave is generated inside the crystal. Therefore the wave field inside the crystal may be considered as a superposition of shortened Bloch wave $E(\mathbf{r}, t) = E(\mathbf{r}, \omega) \exp(-i\omega t)$ where

$$E(\mathbf{r}, \omega) = \sum_{j=1,2} [E_0^{(j)} \exp(i\mathbf{k}_0 \mathbf{r}) + E_h^{(j)} \exp(i\mathbf{k}_h \mathbf{r})] \exp(iK\varepsilon_j \mathbf{n}) \quad (1)$$

where $K = \omega/c = 2\pi/\lambda$, c is a speed of light, λ is a wavelength, \mathbf{n} is a unit vector normal to the crystal plate surface. Note that the condition $\mathbf{k}_0^2 = K^2$ follows from the Maxwell's equation in air. Here a possible refraction of plane waves is taken into account by introducing the parameter ε_j called dispersion error. We assume that all waves are sigma-polarized so that the unit vector of polarization is normal to the scattering plane of vectors \mathbf{k}_0 and \mathbf{k}_h .

It is enough for our purpose to use Maxwell's equation for the amplitude $E(\mathbf{r}, \omega)$ as follows

$$[-\nabla^2 - K^2]E(\mathbf{r}, \omega) = K^2 \chi(\mathbf{r})E(\mathbf{r}, \omega) \quad (2)$$

where $\chi(\mathbf{r})$ is a susceptibility of the crystal lattice that has the same translation symmetry. A substitution of Eq.(1) to Eq.(2) and averaging the equation over unit cell leads to the same set of equation for any value of index j as follows

$$\begin{aligned} [(\mathbf{k}_0 + K\varepsilon\mathbf{n})^2 - K^2(1 + \chi_0)] E_0 &= K^2\chi_{\bar{h}}E_h \\ [(\mathbf{k}_h + K\varepsilon\mathbf{n})^2 - K^2(1 + \chi_0)] E_h &= K^2\chi_hE_0 \end{aligned} \quad (3)$$

where χ_0 , χ_h and $\chi_{\bar{h}}$ are coefficients of Fourier series expansion of $\chi(\mathbf{r})$ over the reciprocal lattice vectors: zero, \mathbf{h} and $-\mathbf{h}$. These are complex values. Under usual approximation these values may be calculated by means of formula

$$\chi_h = -\frac{\lambda^2 r_0}{\pi V_0} \sum_{j=1}^N \exp(-i\mathbf{h}\mathbf{r}_j) \exp[-W_j(\mathbf{h})][f_j(\mathbf{h}) + f'_j + if''_j] \quad (4)$$

where $r_0 = e^2/mc^2$ is a classical electron radius, e and m are charge and mass of electron, V_0 is a volume of unit cell, therefore $1/V_0$ is a number of unit cells in the unit volume of the crystal. The sum is over all atoms inside the unit cell, \mathbf{r}_j is a relative coordinate of the atom inside the unit cell, $W_j(\mathbf{h}) = \langle (\mathbf{h}\mathbf{u}_T)^2 \rangle / 2$ is an exponent of the Debye-Waller factor due to thermal vibrations of atoms with a displacement \mathbf{u}_T , $f_j(\mathbf{h})$ is a Fourier image of electron density of atom with an index j . The values $f'_j + if''_j$ are known as resonant addition to the formfactor due to a photoelectric interaction. These depend on \mathbf{h} very slowly, therefore for small enough reciprocal lattice vectors one may neglect this dependence. The dimensionless value f''_j describes an absorption of X-ray beam. It may be expressed through physical values $f''_j = \sigma_j / (2\lambda r_0)$ where σ_j is a cross section of the photoelectric absorption. Today these parameters may be obtained directly from different Internet sites. One of them is a program X0H made by Sergey Stepanov "http://sergey.bio.aps.anl.gov".

The values $\chi_{0,h}$ are of order 10^{-5} or smaller. Therefore the parameters ε is of approximately the same order of value. The normal case of diffraction occurs when both parameters $\gamma_0 = (\mathbf{k}_0\mathbf{n})/K = \cos\psi_0$ and $\gamma_h = (\mathbf{k}_h\mathbf{n})/K = \cos\psi_h$ have no small values (see Fig.1). Then one can use an approximation where ε^2 terms are negligible compared to the first degree terms. In this case the set of equations (3) can be approximated by

$$\begin{aligned} [2\varepsilon\gamma_0 - \chi_0]E_0 - \chi_{\bar{h}}E_h &= 0 \\ -\chi_hE_0 + [2\varepsilon\gamma_h + \alpha_h - \chi_0]E_h &= 0 \end{aligned} \quad (5)$$

where $\alpha_h = (\mathbf{k}_h^2 - \mathbf{k}_0^2)/K^2$ is a parameter of deviation from the Bragg condition. This is a set of two homogeneous equations which can have a solution only if the determinant of the matrix is equal zero. The condition is, in fact, an equation for calculating the unknown parameter ε .

$$\left(\varepsilon - \frac{\chi_0}{2\gamma_0}\right) \left(\varepsilon - \frac{\chi_0}{2\gamma_h} + \frac{\alpha_h}{2\gamma_h}\right) - \frac{\chi_h\chi_{\bar{h}}}{4\gamma_0\gamma_h} = 0 \quad (6)$$

We shall consider only the Bragg case of diffraction when the diffracted wave go out the crystal through the same surface that the incident wave come in. In this case the parameter γ_h is negative. Below we shall use this property in an explicit form. On the

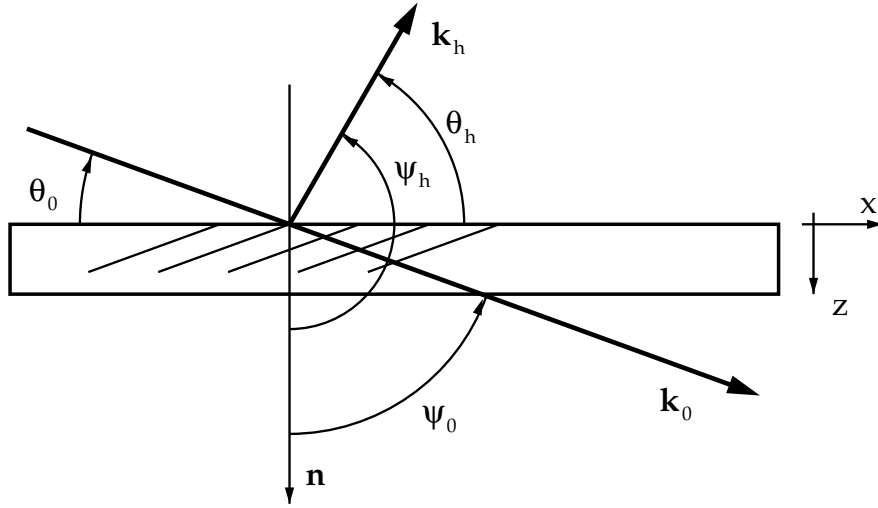


Figure 1: The geometrical parameters of the Bragg diffraction.

other hand, the parameter α_h depends on both the angular deviation $\Delta\theta$ of incident wave from the Bragg angle and angle of crystal rotation $\Delta\varphi$ as well as on relative energy shift $\Delta E/E$ of the photon energy $E = \hbar\omega$ from the Bragg energy for given angle of incidence. Since we are interested only in small values we may accept a reference values of angle and energy and consider a linear approximation

$$\alpha_h = -2 \sin 2\theta_B \left[\Delta\theta + \tan \theta_B \frac{\Delta E}{E} - \Delta\varphi \right] \quad (7)$$

The equation (6) is solved analytically and we have two solutions which may be written as

$$\varepsilon_{1,2} = \frac{1}{2\gamma_0} \left(\chi_0 + p \pm \sqrt{p^2 - q^2} \right) \quad (8)$$

with

$$p = \frac{1}{2}[\alpha_h b - \chi_0(1+b)], \quad q^2 = \chi_h \chi_h^* b, \quad b = \frac{\gamma_0}{|\gamma_h|} \quad (9)$$

where the square root is assumed to have positive imaginary part. We note that one solution ε_1 has positive imaginary part while another solution ε_2 has negative imaginary part. It is easy to verify at least for nonabsorbing crystal when $p^2 < q^2$. However it is general property for all values of α_h .

Accordingly to Eq.(1) this means that one Bloch wave decreases itself with increasing a depth while another Bloch wave increases itself. It is evident from the boundary condition that increasing wave have no large weight. In thin crystal plate it contributes after a reflection from the bottom boundary of the crystal plate. The interference of two solutions leads to interference fringes on the angular or energy dependencies of

intensity. In thick crystal plate the increasing solution does not contribute completely in the intensity of diffracted beam. Therefore we must take only the solution ε_1 with a positive imaginary part. In this case a relative intensity may be obtained from any of the Eq.(5). The reflectivity P_R is determined as a ratio of outgoing and incoming energy flows. For example, from the first equation we have

$$P_R(\Delta\theta, \Delta E) = \frac{1}{b} \left| \frac{E_h^{(1)}}{E_0^{(1)}} \right| = \frac{1}{b} \left| \frac{2\gamma_0\varepsilon_1 - \chi_0}{\chi_{\bar{h}}} \right|^2 = \frac{1}{b} \left| \frac{p + \sqrt{p^2 - q^2}}{\chi_h} \right|^2 \quad (10)$$

In crystals with an inversion centre we have $\chi_{\bar{h}} = \chi_h$ and only two parameters are essential. Accordingly to optical definition we may write $\chi_0/2 = n = -\delta + i\beta$ where δ is a decrement of refractive index, β is an index of absorption. We introduce a similar definition for $\chi_h/2 = -\delta_h + i\beta_h$. In a case of transparent crystal when $\beta = \beta_h = 0$ the region of maximal reflectivity has a width which is determined from the condition $p^2 < q^2$. The centre of this region in an angular axis is shifted from the kinematical Bragg angle on the value

$$\Delta\theta_c = \frac{\delta}{\sin 2\theta_B} \left(1 + \frac{1}{b} \right), \quad (11)$$

the width of the region equals

$$\Delta\theta_w = \frac{1}{b^{1/2}} \frac{4\delta_h}{\sin 2\theta_B}. \quad (12)$$

The maximal value of reflectivity is $P_{R,\max} = 1$.

Fig.2 shows a result of accurate calculation of P_R using the Eq.(10) for the case of (12 2 2) diffraction of 14.41 keV X-rays in silicon. One can see that the properties shown in the Fig.2 can be estimated analytically. With decreasing the angle between the incident beam and the surface $\theta_0 = \pi/2 - \psi_0$ the shift of reflectivity region from the kinematical value grows drastically, the width of this region grows also but not so quickly while the reflectivity drops slightly. The integral reflectivity can be estimated analytically as

$$P_{R,\text{int}} = P_{R,\max} \Delta\theta_w = \frac{4\delta_h}{\sin 2\theta_B} \frac{1}{b^{1/2}} \quad (13)$$

For example, in the case shown in Fig.2 we have $\sin 2\theta_B = 0.420$, $\delta = 2.34 \mu\text{rad}$, $\beta = 0.0174 \mu\text{rad}$, $\delta_h = 0.1908 \mu\text{rad}$, $\beta_h = 0.00847 \mu\text{rad}$. For the case of 1° glancing incidence angle we have $b = 0.041$. This leads to a shift $\Delta\theta_c = 144 \mu\text{rad}$, to a width $\Delta\theta_w = 9 \mu\text{rad}$ and $P_{R,\max} = 1$. These values coincide with the accurate calculation shown in figure except the fact that the real reflectivity becomes smaller $P_{R,\max} = 0.61$ due to an absorption inside the extinction domain of crystal (see Fig.2). The detailed comparison of two curves obtained in the present approach and in an extended approach, taking into account the ε^2 terms, shows a slight additional shift of the accurate curve for $\theta_0 = 1^\circ$. Nevertheless one may conclude that approximate analytical theory is valid up to 1° angle of incidence θ_0 .

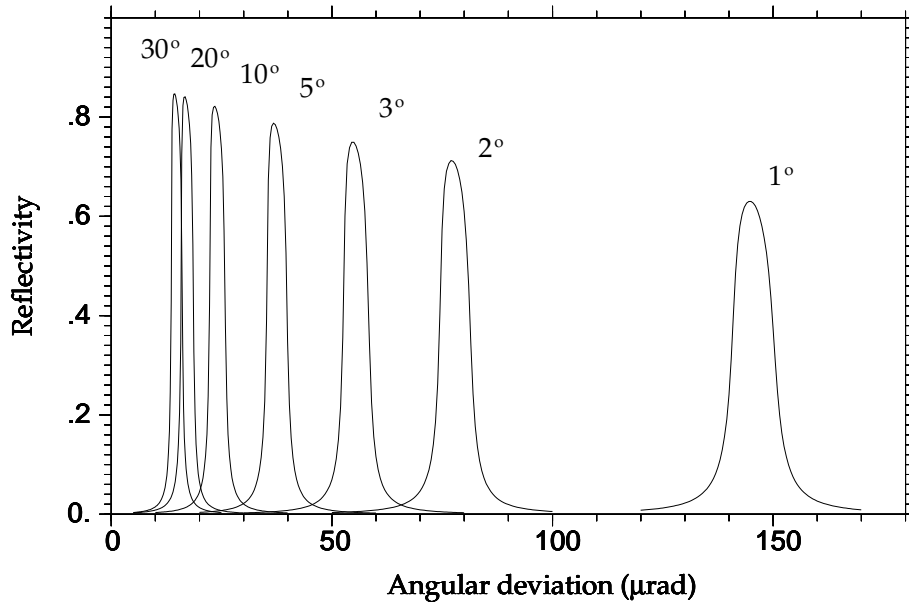


Figure 2: The reflectivity of X-rays for (12 2 2) diffraction in silicon and different values of glancing angle θ_0 of incident beam. The values of θ_0 are shown near the curves. The energy $E = 14.41$ keV. One may see that an angular dynamical shift of the maximum increases while a height of maximum decreases with decreasing θ_0 . The latter occurs due to absorption.

2. Transmissivity of multicrystal monochromator

Let us consider the properties of multicrystal monochromator consisting of few perfect crystal plates which reflect the beam successively to transmit the beam inside some range on the plane of parameters energy-angle. The theory for thick crystals presented in the preceding section will be used. The expression for the reflectivity of one crystal P_R is given by Eq.(10). It depends on the angular shift $\Delta\theta$, angular position of the crystal plate $\Delta\varphi$ and energy shift ΔE from the reference value. However, we need in the relation between these values for different crystal plates.

The Bragg diffraction in crystals cannot change the energy of X-rays therefore ΔE is the same after the reflection by n -th crystal, $\Delta\varphi$ is constant but may be different for different crystals while the angular shift $\Delta\theta$ may be changed in process of reflection by each crystal when asymmetrical diffraction takes place. When crystals are cut out of blocks of different matters then θ_B , χ_0 , χ_h , b and $\Delta\varphi$ may be different in different crystals.

Let us consider now the angular deviation of diffracted wave $\Delta\theta'$. We have the coordinates of wave vector of incident wave in crystal (see Fig.1 for x and y axes)

$$\begin{aligned} k_{0x} &= K \cos(\theta_0 + \Delta\theta) \approx K \cos \theta_0 - K \sin \theta_0 \cdot \Delta\theta, \\ k_{0z} &= K \sin(\theta_0 + \Delta\theta) \approx K \sin \theta_0 + K \cos \theta_0 \cdot \Delta\theta + K\varepsilon \end{aligned} \quad (14)$$

The coordinates of diffracted wave in air will differs from these by reciprocal lattice

vector and additional z-component $K\sigma$ to satisfy the dispersion law in air, namely

$$\begin{aligned} k_{hx} &\approx K \cos \theta_h - K \sin \theta_0 \cdot \Delta\theta, \\ k_{hz} &\approx -K \sin \theta_h + K \cos \theta_0 \cdot \Delta\theta + K\varepsilon + K\sigma \end{aligned} \quad (15)$$

Here we take into account that the coordinates of reciprocal lattice vector are $h_x = K(\cos \theta_h - \cos \theta_0)$, $h_z = -K(\sin \theta_h + \sin \theta_0)$. The angles θ_0 and θ_h are shown in Fig.1. One must find the new value σ from the condition $k_{hx}^2 + k_{hz}^2 = K^2$ at least in linear in $\Delta\theta$ approximation. A simple calculation gives

$$\sigma = -\varepsilon - \frac{\sin(\theta_h + \theta_0)}{\sin \theta_h} \Delta\theta \quad (16)$$

We may write

$$\begin{aligned} k_{hx} &= K \cos \theta_h - K \sin \theta_h \cdot \Delta\theta' \approx K \cos(\theta_h + \Delta\theta'), \\ k_{hz} &= -K \sin \theta_h - K \cos \theta_h \cdot \Delta\theta' \approx -K \sin(\theta_h + \Delta\theta') \end{aligned} \quad (17)$$

with the relation

$$\Delta\theta' = \Delta\theta \frac{\sin \theta_0}{\sin \theta_h} = b\Delta\theta \quad (18)$$

This is well known general relation which does not depend on the conditions of diffraction. As it follows from Eq.(18) for $b < 1$ the asymmetric diffraction increases the width of the beam and decreases the angular divergence of the beam.

However, the relation (18) was obtained under an assumption of monochromatic wave of energy E . It is necessary for us to consider the finite energy bandwidth and to analyse a direction of reflected beam in the same coordinate system for all energies inside the bandwidth. In addition we want to take into account the rotation of crystal in the same coordinate system. In this case we need to write the Eq.(18) in a more complete form

$$\theta' - \theta_h = b(\theta - \theta_0) \quad (19)$$

Then we have to bear in mind that the Bragg angle becomes different for different energies. Therefore we choose the middle value of energy E as a reference value and consider small deviations ΔE from the reference value. From the Bragg condition $2d \sin \theta_B = \lambda$ we may find

$$\begin{aligned} \Delta\theta_B &= \frac{\Delta\lambda}{\lambda} \tan \theta_B = -\frac{\Delta E}{E} \tan \theta_B, \\ \theta_0 &= \theta_{0m} - \frac{\Delta E}{E} \tan \theta_B + \Delta\varphi, \\ \theta_h &= \theta_{hm} - \frac{\Delta E}{E} \tan \theta_B - \Delta\varphi. \end{aligned} \quad (20)$$

Here the angle $\Delta\varphi$ is introduced in addition for taking into account a rotation of the crystal. Now the Eq.(18) may be written in more general form where the angular deviation are used in a reference coordinate system independent on the energy

$$\Delta\theta' = b\Delta\theta + \frac{\Delta E}{E} (b-1) \tan \theta_B - \Delta\varphi(b+1) \quad (21)$$

The angular deviation $\Delta\theta'$ may be used as an angular deviation of incoming wave for the next crystal plate. Each crystal changes an angular divergence in accord with it's asymmetry, therefore

$$\Delta\theta_{\text{out}} = b\Delta\theta_{\text{in}} + (\Delta E/E)(b-1) \tan \theta_B - \Delta\varphi(b+1).$$

However, this angular deviation is equal to the angular deviation of incoming wave for next crystal $\Delta\theta_{\text{in}}^{\text{next}} = \Delta\theta_{\text{out}}$ only in the case of $(n, -m)$ setting when the reciprocal lattice vectors of diffraction in two crystals make an angle more than $\pi/2$. In the case of (n, m) setting we need to change a sign $\Delta\theta_{\text{in}}^{\text{next}} = -\Delta\theta_{\text{out}}$. It is because the direction of counting the angles for incident and diffracted beams are opposite to each other. In the case of $(n, -m)$ setting an additional change of the reciprocal lattice vector direction compensates this difference.

The same takes place for the angle of rotation. However, now just for $(n, -m)$ settings we need to change the direction of the angle of rotation by the opposite one. It is convenient to introduce the multiplier z_n which is equal to 1 for $(n, -m)$ and -1 for (n, m) . Then we have a recurrent relations

$$\begin{aligned} \Delta\theta_1 &= \Delta\theta, & \Delta\theta_{n+1} &= z_n[\Delta\theta_n b_n + (\Delta E/E)(b_n - 1) \tan \theta_{B,n} - \Delta\varphi_n(b_n + 1)] \\ s_1 &= 1, & s_{n+1} &= z_n s_n, & \Delta\varphi_n &= s_n (\Delta\varphi_n)_{\text{in}} \end{aligned}$$

The total reflectivity $P_R^{(n)}(\Delta\theta, \Delta E)$ of multicrystal monochromator is obtained by the recurrent relation

$$P_R^{(n)}(\Delta\theta, \Delta E) = P_R^{(n-1)}(\Delta\theta, \Delta E) P_{R,n}(\Delta\theta_n, \Delta E), \quad n = 1, 2, \dots \quad (22)$$

where $P_{R,n}(\Delta\theta_n, \Delta E)$ is a reflectivity of n -th crystal plate determined by Eq.(10), $P_R^{(0)} = 1$ This value is, in fact, a transmissivity of the beam because oftenly the beam direction stays the same.

The rough estimation of the area inside which the monochromator transmits a radiation may be obtained by means of DuMond diagram. Each crystal reflects the X-ray beam inside the strip with the central line determined by the equation $\alpha_n = 0$, namely,

$$\frac{\Delta E}{E} = -\cot \theta_{B,n} \cdot (\Delta\theta_n - \Delta\varphi_n) + \frac{\delta_n}{2 \sin^2 \theta_{B,n}} \left(1 + \frac{1}{b_n} \right) \quad (23)$$

where n is a number of the crystal. At the plane $(\Delta\theta, \Delta E)$ this line has the inclination angle $-(\pi/2 - \theta_{B,n})$ which is determined by only the Bragg angle of n -th crystal. The asymmetry of diffraction as well as the scattering amplitude (decrement of refractive index) leads to a shift of this line which can be compensated by an additional small rotation of the crystal. However, the initial angular deviation $\Delta\theta = \Delta\theta_1$ is changed in the process of asymmetrical reflection therefore after n reflections it is found from the recurrent relation

$$\Delta\theta_{n+1} = B_n \left(\Delta\theta_n + \frac{\Delta E}{E} C_n - \Delta\varphi_n D_n \right) \quad (24)$$

where

$$B_n = z_n b_n, \quad C_n = (1 - 1/b_n) \tan \theta_{B,n}, \quad D_n = (1 + 1/b_n)$$

Therefore the Eq.(23) must be written as

$$\begin{aligned} \frac{\Delta E}{E} &= -\cot \theta_{B,n} B_{n-1} \cdots B_1 \Delta \theta + \frac{\delta_n}{2 \sin^2 \theta_{B,n}} \left(1 + \frac{1}{b_n}\right) \\ &\quad - \frac{\Delta E}{E} \cot \theta_{B,n} (C_{n-1} B_{n-1} + C_{n-2} B_{n-1} B_{n-2} + \cdots + C_1 B_{n-1} \cdots B_1) \quad (25) \\ &\quad + \cot \theta_{B,n} (\Delta \varphi_n + \Delta \varphi_{n-1} D_{n-1} B_{n-1} + \cdots + \Delta \varphi_1 D_1 B_{n-1} \cdots B_1) \end{aligned}$$

The solution in common of these equations already exists in case of two crystals in the region close to the point of intersection of two lines. For a number of crystals more than 2 the additional symmetry is necessary for existing the solution without an additional rotating the crystals ($\Delta \varphi_n = 0$).

In general case when each crystal has an independent rotation axis one can find the solution by means of fine adjustment. *The solution exists for arbitrary number of crystals when all crystals have different Bragg angle and asymmetry and settings only when*

$$\begin{aligned} \Delta \varphi_n &= B_{n-1} \cdots B_1 (\Delta \theta)_{ip} + \tan \theta_{B,n} \left(\left(\frac{\Delta E}{E} \right)_{ip} A_n - \frac{\delta_n}{2 \sin^2 \theta_{B,n}} \left(1 + \frac{1}{b_n}\right) \right) \\ &\quad - \Delta \varphi_{n-1} D_{n-1} B_{n-1} - \cdots - \Delta \varphi_1 D_1 B_{n-1} \cdots B_1 \quad (26) \end{aligned}$$

where

$$A_n = 1 + \cot \theta_{B,n} (C_{n-1} B_{n-1} + C_{n-2} B_{n-1} B_{n-2} + \cdots + C_1 B_{n-1} \cdots B_1)$$

where $(\Delta \theta)_{ip}$ and $(\Delta E/E)_{ip}$ are the coordinate of the intersection point. One may choose the origin as the point of intersection then $(\Delta \theta)_{ip} = 0$ and $(\Delta E/E)_{ip} = 0$ and the formula has more simple form

$$\begin{aligned} \Delta \varphi_n &= -\frac{\delta_n}{2} \left(1 + \frac{1}{b_n}\right) \left(\tan \theta_{B,n} + \frac{1}{\tan \theta_{B,n}} \right) \\ &\quad - \Delta \varphi_{n-1} D_{n-1} B_{n-1} - \cdots - \Delta \varphi_1 D_1 B_{n-1} \cdots B_1 \quad (27) \end{aligned}$$

To calculate this expression we define

$$f_n = -\frac{\delta_n}{2} \left(1 + \frac{1}{b_n}\right) \left(\tan \theta_{B,n} + \frac{1}{\tan \theta_{B,n}} \right)$$

and then the algorithm looks as follows

$$\Delta \varphi_n = f_n - \sigma_n, \quad \sigma_{n+1} = B_n (\sigma_n + \Delta \varphi_n D_n), \quad \sigma_1 = 0$$

Let us consider first terms from the general equation

$$\begin{aligned} \Delta \varphi_n &= f_n + \Delta \theta_n, \\ \Delta \varphi_1 &= f_1, \quad \sigma_1 = 0 \\ \Delta \theta_2 &= -\Delta \varphi_1 D_1 B_1, \quad \sigma_2 = \Delta \varphi_1 D_1 B_1, \quad \Delta \varphi_2 = f_2 - \Delta \varphi_1 D_1 B_1 \end{aligned}$$

and so on.

3. How to use a computer program MCM

The formula (27) as well as all others obtained above was used in elaborating the computer program which calculates the transmission properties of the multicrystal monochromator consisting of up to ten different crystals. As a result of calculation, the reflectivity distribution $P_R^{(n)}(\Delta\theta, \Delta E)$ as a map of levels is shown as well as the integral over angle and over energy curves. The UNIX version of the program is elaborated as a command batch-file MCM which contains 4 lines (command)

```
dtpad mcm.par
mcm.exe < mcm.par
vkps
ghostview -a4 -magstep -1 mcm.ps
```

First line runs the text editor `dtpad` for preparing the text file `mcm.par` of input data for the calculating program `mcm.exe`. The structure of input data may be found in the bottom part of the same file. Below the structure of data is also described:

- First line contains an arbitrary text in apostrophes. For example:

'Case 1: 3-crystal monochromator'.

The text may contain up to 128 symbols. This text is a title of the variant as well as the title of figure which is shown at the bottom line of the page. The file may contain many variants with different titles. However, only first variant at the top of the file is currently used.

- Second line contains three numbers which defines the energy axis. One has to specify the first (`den1`) and last (`den2`) values of ΔE and a number of points (`nden`) that is a dimension of array of energy dependence. Energies are measured in meV.

- Third line contains three numbers which defines the angular axis. One has to specify the first (`dt1`) and last (`dt2`) values of $\Delta\theta$ and a number of points (`ndt`) that is a dimension of array of angular dependence.

- Fourth line contains three numbers which defines number of crystals of multicrystal monochromator (`ncr`), the energy of X-rays in keV (`energy`) and the parameter (`mod`). The last parameter allows user to reject the adjustment of all crystals is `mod = 0` or use it if `mod = 1`. Since the adjustment is calculated automatically the user does not know the real angles of rotations. Sometimes it is inconvenient.

- The rest lines specify the parameters of each crystal. The parameters are: the Bragg angle θ_B (`teta_B`), the parameters of scattering δ (`del`), β (`bet`), δ_h (`delh`), and β_h (`beth`), the asymmetry factor b (`b`) and the angular position $\Delta\varphi$ (`phi`) of the crystal relative to the accurate position of the maximum transmission defined by formula (27). Thus for a maximum transmission all `phi`-parameters must be equal zero. The asymmetry factor has a sign which specifies the setting of the next crystal. So (`b`) is positive if the next crystal is in $(n, -m)$ setting and it is negative for (n, m) setting. The parameter of scattering may be taken from the internet site "<http://sergey.bio.aps.anl.gov>". The number of lines equals to the number of crystals.

After saving data and closing the window with an editor the second command runs the calculating program `mcm.exe` which takes the data from the file `mcm.par`. The program calculates the results and saves them in the files `mcm.map`, `mcm.iem`, `mcm.ian`.

The file `mcm.map` is a direct access file that contains two-dimensional array of reflectivity in a computer format of numbers. The files `mcm.iem` and `mcm.ian` contains the integral over angle (energy dependence) and integral over energy (angular dependence) which are written as usual two-columns text files.

After calculating the results in the numeric form the program writes the file `vkps.par` that is used by the program `vkps` for preparing the PostScript file of the figure showing the results in graphical form.

The third command of the batch-file just runs the program `vkps`. The PostScript file has the name `mcm.ps`. It may be used for printing the figure of results by the command `lp` as well as for looking the results on the terminal's monitor by means of the program `ghostview`.

The fourth command just runs `ghostview` with some options which is useful to see the full page on a screen simultaneously.

The example of input data and figure of the results are enclosed.

Appendix 1. How to convert direct access data to text format data

The file `mcm.map` contains the numbers in a direct access (computer) format. Therefore it is impossible to see them by means of text editor. To use other graphics program (not `vkps`) one may need to have the data as a multicolumn text format. Such an operation of converting the format of data may be performed by means of universal program `vkdc.exe`. One may run the program by means of the command batch-file

```
vkdc
```

This file has two lines:

```
dtpad vkdc.par
vkdc.exe < vkdc.par
```

In the text file `vkdc.par` one has to prepare previously the input data for the work of conversion. The file has 4 lines. In first two lines the names of incoming and outgoing data files must be specified in first 12 positions from the first position and without apostrophes. The next line contains the parameters of first argument; first (`x1`) and last (`xn`) values and number of dots (`nx`). The last line contains three numbers: number of functions (`nf`), number of first function (`nff`) and number of operation (`CO`). If `CO = 0` then the conversion: direct access to text is performed. If `CO = 1` then the reverse conversion: text to direct access is made. In the last case the parameters of argument values are not used, however, if `x1 = 1` then the transformation of the function $f(x)$ to the function $\log_{10}[f(x)]$ is made, if `x1 = -1` then the transformation of the function $f(x)$ to the function $10^{f(x)}$ is made. For other values of `x1` the format change goes without a function transformation. An example of input data file is:

```
mcm.map
mcm.mtt
1. 101. 101
101 1 0
```

In this example a direct access file `mcm.map` is copied as a text file `mcm.mtt`. The file `mcm.map` has 101*101 matrix therefore the file `mcm.mtt` has 102 columns (first is argument) with 101 values in each column. The argument is simply a number of line. The information about an argument is absent in the file `mcm.map`. One needs to know

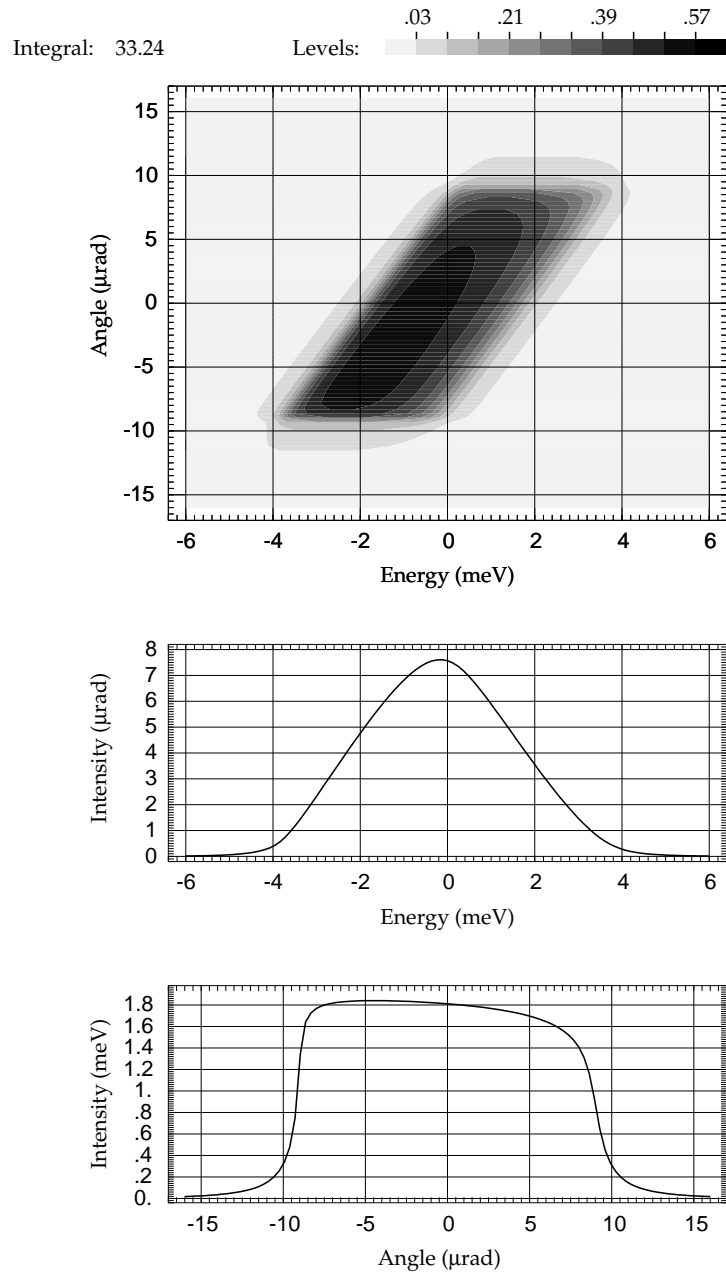
it independently.

Appendix 2. An example of input and output data

Here one example is considered to give an understanding of input and output data. If the file `mcm.par` has the following content

```
'6.4 meV monochromator of four reflections (4 2 2, 12 2 2, 12 2 2, 4 2 2)'  
-6.  6.  101  
-16. 16.  101  
4 14.41 1  
22.83 2.34 0.0174 1.0101 0.0154 -0.097 0.  
80.47 2.34 0.0174 0.1313 0.00591 1.  0.  
80.47 2.34 0.0174 0.1313 0.00591 -1.  0.  
22.83 2.34 0.0174 1.0101 0.0154 10.3 0.
```

then the program creates and shows a PostScript file shown in Fig.3. The integral values are obtained by summing the two-dimensional array over one coordinate and multiplying by the step value. Therefore the two-dimensional region must be large enough to include the whole maximum of transmissivity. The total integral is a sum over all points multiplied by both steps.



6.4 meV monochromator of four reflections (4 2 2, 12 2 2, 12 2 2, 4 2 2)

1

Figure 3: Example of output figure.