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A Criterion for the Dynamical to Kinematical Transition of X-Ray Diffraction on a Bent Crystal

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A criterion is given in answer to the question: "To what extent is it possible to bend a crystal without loss of X-ray peak reflectivity?" An expression based on the work of Chukhovskii, Gabrielyan and Petrashen [1], is formulated that applies to anisotropic cubic crystal and that can be used not only for conventional asymmetric Bragg diffraction, but also for inclined crystal diffraction. The following special cases are treated as examples: isotropic crystal, standard symmetrical Bragg diffraction, extremely asymmetric diffraction, and backscattering with Bragg angles near 90° . In addition, an asymptotic behavior for high energies is detailed.

Introduction

It is well known that the peak reflectivity of a bent crystal, generally speaking, is smaller than that of a plane crystal, and it goes to zero when the crystal curvature goes to infinity. The reason for this is the transition between dynamical and kinematical diffraction that takes place as the crystal curvature increases. The physical explanation is as follows: the deviation from exact Bragg position along the beam changes so fast that the thickness over which the beam is within a Darwin width becomes too small to reflect the beam. Bent crystals are widely used as focusing elements in X-ray optics, and estimation of whether or not a bent crystal is still perfect enough to provide good reflectivity is of great importance.

Currently the Advanced Photon Source (APS) is considering a number of bent crystals as focusing elements for future APS beamlines, including a sagittally focusing monochromator [2] and bent backscattering analyzer for inelastic X-ray scattering experiments.

The quantitative criterion for the transition between dynamical and kinematical diffraction has been formulated by F. Chukhovskii and others [1]. These authors have obtained the exact solution of the Takagi-Taupin equations. These equations are given by,

$$\begin{aligned} i \frac{dE_0}{ds_0} + \frac{k \chi_0}{2 \gamma_0} E_0 + \sigma_1 \exp(i \mathbf{h} \cdot \mathbf{u}(\mathbf{r})) E_1 &= 0 \\ i \frac{dE_1}{ds_1} + \frac{k \chi_0}{2 \gamma_1} E_0 + \sigma_{-1} \exp(-i \mathbf{h} \cdot \mathbf{u}(\mathbf{r})) E_0 &= 0. \end{aligned} \quad (1)$$

Here $\mathbf{u}(\mathbf{r})$ is a displacement field in a crystal. In a case of a homogeneously bent crystal or a crystal with a constant thermal gradient a displacement field is described by a general quadratic form:

$$\mathbf{h} \cdot \mathbf{u}(\mathbf{r}) = 4 \sigma_{-1} \sigma_1 (A s_0^2 + 2 B s_0 s_1 + C s_1^2). \quad (2)$$

Here E_0 and E_1 - are the amplitudes of the incident and diffracted waves,
(s_0, s_1) - are the coordinates in the diffraction plane, defined by the relations:

$$\mathbf{r} = \frac{\mathbf{k}_0}{k \gamma_0} s_0 + \frac{\mathbf{k}_1}{k \gamma_1} s_1, \quad (3)$$

where $\mathbf{k}_0$ and $\mathbf{k}_1$ are the wave vectors of the incident and diffracted beam, $2\pi/\lambda = |\mathbf{k}_0| = |\mathbf{k}_1|$. Here and below, an index 0 denotes the incident beam and 1 the diffracted beam; γ_i are absolute values of cosines of the angles between wave the vector of the beam and the normal to the crystal surface:

$$\gamma_0 = \sin(\theta - \alpha) \cos(\phi), \quad \gamma_1 = \sin(\theta + \alpha) \cos(\phi).$$

Variables in the above expressions are defined as follows:

- α is the asymmetry (positive for the grazing incidence);
- ϕ is the inclination angle, i.e., the angle between the diffraction plane and the normal to the crystal surface;
- θ is the Bragg's angle;
- $\mathbf{u}(\mathbf{r})$ is the displacement field;
- $\mathbf{h}$ the diffraction vector, $|\mathbf{h}| = 2\pi/d_{hkl}$;
- d_{hkl} is the interplanar distance.

The coordinates (s_0, s_1) can be expressed as follows:

$$\begin{aligned} x &= a_0 s_0 + a_1 s_1 \\ y &= (s_0 - s_1) \tan(\phi) \\ z &= s_0 - s_1, \end{aligned} \quad (4)$$

where (x, y, z) are the Cartesian coordinates with x directed along the crystal surface in the diffraction plane and z normal to the surface and directed inward.

The coefficients in Eq. (4) can be written as:

$$a_0 = \cos(\theta - \alpha) / \gamma_0, \quad a_1 = \cos(\theta + \alpha) / \gamma_1.$$

The values of the coefficients σ_{-1} and σ_1 in the Takagi-Taupin equations (1) are equal to:

$$\begin{aligned} \sigma_{-1} &= \pi \chi_{-1} / (\gamma_0 \lambda), \\ \sigma_1 &= \pi \chi_1 / (\gamma_1 \lambda). \end{aligned} \quad (5)$$

Here χ are the Fourier coefficients of the crystal polarizability:

$$\chi_{hkl} = \frac{r_e \lambda^2}{\pi a^3} F_{hkl}, \quad (6)$$

here r_e is the classical electron radius, F_{hkl} is the usual X-ray structure factor, and a is a lattice parameter.

Equation (2) is an implicit definition of the dimensionless parameter B which is proportional to the parameter B_c introduced by Chukhovskii and others [1]:

$$B = \frac{B_c}{2 \sigma_{-h} \sigma_h}. \quad (7)$$

X-ray diffraction from a crystal with a displacement field depending only on the z coordinate is considered in the kinematical approximation in Appendix I. It is shown that the maximum reflectivity of the crystal in this case is the reciprocal of parameter B defined as in Eq. (7).

It has been theoretically shown [1] that the coefficients A and C in Takagi-Taupin equations (1) affect only the phase multipliers of the solutions, while the value of parameter B affects the intensity distribution and, therefore, the crystal reflectivity. Parameter B represents the projection of the strain gradient to the diffraction plane. In accordance with Chukhovskii and others [1], the criterion of the transition between dynamical to kinematical diffraction is:

$$B = 1. \quad (8)$$

More specifically, when $B=1$, the maximum reflectivity is approximately equal to 50% (see Fig. 1c). In order to get crystal reflectivity close to that of a perfect (plane) crystal, it is necessary to satisfy the condition:

$$B \ll 1. \quad (9)$$

It automatically means that when one satisfies this condition, not only the peak reflectivity, but the whole shape of the crystal's reflecting curve will be close to that of the perfect (plane) crystal.

In order to use this criterion it is necessary to know the value of the parameter B, which is implicitly defined by equation (2). However, no explicit expression for this parameter was given by Chukhovskii et al [1], and this task has been left to a reader. We provide here ready-to-use formulas for different cases allowing one to ascertain to what extent it is possible to bend a crystal without loss of X-ray reflectivity.

The Explicit Expression for the Criterion

The most general expression for the displacement field in an elastically bent thin crystal of the constant thickness is as follows [4]:

$$\begin{aligned} u_x &= \frac{xz}{R_x} + \beta yz + \alpha_x \frac{z^2}{2} \\ u_y &= \frac{yz}{R_y} + \beta xz + \alpha_y \frac{z^2}{2} \\ u_z &= - \left(\frac{x^2}{R_x} + \frac{y^2}{R_y} + \beta xy + \alpha_z \frac{z^2}{2} \right). \end{aligned} \quad (10)$$

Again, x and y are the Cartesian coordinates in the plane of the thin crystal plate. Z is normal to the crystal, and R_x , R_y , and β are the parameters of the crystal surface shape $u_z(x,y)$ described by a general quadratic form given by:

$$u_z = - \left(\frac{x^2}{R_x} + \frac{y^2}{R_y} + \beta xy \right). \quad (11)$$

Let us suppose, that the parameters R_x , R_y and β are known. It has been shown [4] that all other parameters in Eq. (10) can then be expressed through these parameters as follows:

$$\begin{vmatrix} \alpha_x/2 \\ \alpha_y/2 \\ -\alpha_z \end{vmatrix} = D \begin{vmatrix} 1/R_x \\ \beta \\ 1/R_y \end{vmatrix}. \quad (12)$$

The matrix D depends on the crystal elastic constants and crystal axis orientation. (The algorithm of the computation of this matrix is given in the Appendix of ref. [4], elastic constants for Si and Ge are taken from the article [3]).

The values of this matrix for some crystal orientations are given in the Table II. In isotropic approximation this matrix is given by:

$$D = \begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\nu/(1-\nu) & 0 & -\nu/(1-\nu) \end{vmatrix}, \quad (13)$$

where ν is Poisson's ratio.

Now by substituting Eqs. (10), (12), and (4-5) into Eq. (2) and comparing left and right parts, we obtain an expression for B (see expression 1 in Table I).

Formulas 2-5 in Table I are derived in the *isotropic* crystal approximation, and are also valid for the following orientation of *anisotropic* Si or Ge: $z=\langle 001 \rangle$ and x and y in the (001) plane. The effective values of the ratio $\nu/(1-\nu)$ are equal to 0.386 for Si and 0.369 for Ge. Expression 5 for backscattering is also valid for Si and Ge plates with the surface orientation (111) . Values of $\nu/(1-\nu)$ for Si and Ge in this case are equal to 0.221 and 0.184 correspondingly.

Numerical Examples

All expressions for the parameter B given in the Table I have the same generic format given by:

$$B = \frac{R_{Cx}}{R_x} + \frac{R_{Cy}}{R_y} \quad (14)$$

where R_x and R_y are actual crystal curvature radii and R_{Cx} and R_{Cy} are constants depending on the diffraction geometry, reflections, crystal orientation, and elastic properties. They are equal to the values of the "critical radii" where the transition between the dynamical and kinematical diffraction takes place ($B=1$). In this section the values of the critical radii will be provided for the different cases. In all examples below, R_{Cx} and R_{Cy} are in meters.

The structure of equation 1 in the Table I clearly shows that there are several ways to satisfy the condition $B \ll 1$.

1) Soft radiation and low order reflections giving small values of λ/χ^2

In order to illustrate the influence of the crystal material, reflection order, and wavelength on the character of the X-ray diffraction in a bent crystal, we compare the Si(777) and Ge(444) reflections.

Orientation in both cases is: $x=\langle 1 -1 0 \rangle$ and $y=\langle 1 1 -2 \rangle$, Backscattering ($\lambda = 2 d_{hkl}$), symmetric diffraction $\alpha = 0$, and spherical bending ($R_x = R_y$) are assumed:

a) Si (7 7 7) critical radii are $R_{Cx} = R_{Cy} = 28$ m. This means that a crystal with $R_x=R_y=3$ m will be reflecting kinematically ($B=18.7$), with a very small reflectivity.

b) Ge (4 4 4) critical radii $R_{Cx} = R_{Cy} = 0.036$ m. Crystal with $R_x=R_y=1$ m will be reflecting dynamically ($B=0.072$). This case is shown in Fig. 1a. Results for bending to the critical radius corresponding to $B=1$ are shown in Fig. 1c, intermediate case of $B=0.5$ is shown in Fig. 1b, and the case of further bending up to $B=2$ is shown on the Fig. 1d. The results in Fig. 1 were obtained using a 2x2 matrix formulation of dynamical diffraction [5].

2) Special orientations and/or Bragg angles providing $R_{cx}=0$

Search for conditions when $R_{cx}=0$ can be clearly illustrated with the use of the equation 4 in Table I for the isotropic approximation, that is when $\cot^2(\theta) = v/(1-v)$.

Let us substitute the effective value $v/(1-v) = 0.221$ (see Table II) and we obtain: $\theta=64.82^\circ$. At this Bragg angle Si crystal with (111) surface will reflect X-rays dynamically *at any curvature*.

3) Sagittal focusing

Consider the dependence of the critical radius for sagittal focusing R_{cy} on wavelength for the given reflection. For cylindrical bending, the term proportional to $1/R_x$ can be omitted. Because the polarizability χ is proportional to λ^2 (see Eq. 6), and $\sin(\theta)$ is proportional to λ for any given reflection, it is easy to see that the critical radius for the given reflection does not depend on wavelength:

$$B = \frac{v}{2\pi (\chi/\lambda^2)^2 (2 d_{hkl})^3 (1-v)} \frac{1}{R_y} \quad (15)$$

As an example, consider the expression for B for different energies is as follows:

orientation: $x=<1 \ -1 \ 0>$ and $y=<1 \ 1 \ -2>$, Si(1 1 1), asymmetry $\alpha = 0^\circ$. This geometry has been discussed [2] for a sagittally focusing monochromator. We obtain:

$$\theta = 14.23^\circ \text{ (Cu } K_\alpha \text{ radiation):} \quad B = -0.0883/R_x + 0.00128/R_y$$

$$\theta = 6.51^\circ \text{ (Mo } K_\alpha \text{ radiation):} \quad B = -0.442/R_x + 0.00128/R_y$$

$$\theta = 5.13^\circ \text{ (Ag } K_\alpha \text{ radiation):} \quad B = -0.714/R_x + 0.00128/R_y$$

The critical radius in the sagittal direction in all three cases is: $R_{cy} = 1.28$ mm.

This result means that the Si or Ge plate with the (111) surface will reflect X-rays without loss of X-ray reflectivity at any practically achievable curvature in a sagittal direction.

4) Asymmetric diffraction giving $\sin(\theta+\alpha) \sin(\theta-\alpha) \ll 1$

Orientation: $x=<1 \ 1 \ 1>$ and $y=<1 \ -1 \ 0>$, reflection Si(9 9 9), $\theta=89.94^\circ$, asymmetry $\alpha=89^\circ$,
 $B = 93/R_x + 2.08/R_y$.

An asymmetric backscattering monochromator for the APS with the focusing distance $L = 15$ m must have a curvature:

$$R_x = 1 / \sin(\theta-\alpha) = 859 \text{ m}, \quad B = 0.108,$$

which satisfies the condition of dynamical scattering.

5) High energy asymptotic behavior

For small Bragg angles in formula 4 in Table I it is possible to neglect the terms containing $v/(1-v)$ in comparison with $\cot^2(\theta)$. This means that the crystal elastic properties do not affect the result, i.e. it does not matter whether we use the anisotropic or isotropic approximation or what orientation the crystal has. For example, for the two brightest reflections in the Si and Ge crystals we obtain the following expressions for the critical radii (for symmetric diffraction and a non inclined geometry):

$$\begin{array}{llll} \text{reflection (111):} & R_{CX} = 0.00147 E^2 & \text{for Si} & \text{and} & R_{CX} = 2.76 \cdot 10^{-4} E^2 & \text{for Ge,} \\ \text{reflection (220):} & R_{CX} = 0.00184 E^2 & \text{for Si} & \text{and} & R_{CX} = 3.11 \cdot 10^{-4} E^2 & \text{for Ge.} \end{array}$$

where R_{CX} is in meters and energy E is in KeV. This means that for high energies (like $E=100$ KeV) critical radii are very large, especially for Si, and it is difficult to achieve the dynamical diffraction in this region.

6) Extremely inclined diffraction plane

The case in which the diffraction plane is not perpendicular to the crystal surface (i.e. $\phi \neq 0$) is known as "inclined geometry". Recently, it was proposed [6] as an approach for solving the high heat load problem in the monochromators for the new generation synchrotrons.

For the extremely inclined diffraction plane with an inclination angle ϕ approaching 90° coefficients C_X and C_Y in the expression 1 from Table I approach the limits:

$$C_X = \cos(\alpha) \cot(\theta - \alpha) \cot(\theta + \alpha) + \sin(\alpha) [\cot(\theta - \alpha) - \cot(\theta + \alpha)] \quad (16)$$

$$C_Y = \cos(\alpha).$$

These expressions do not depend on the elastic constants of the crystal. It is easy to see from the structure of expression 1 in the Table I that for ϕ close to 90° parameter B is proportional to the $\cos(\phi)$. This means that inclined geometry provides us a method with which to achieve dynamical diffraction on a bent crystal. For example, for the Si(111) reflection, radiation 8 KeV, symmetrical diffraction $\alpha = 0$, and inclination angle $\phi = 85^\circ$, we obtain:

$$B = \frac{7.82 \text{ mm}}{R_X} + \frac{0.49 \text{ mm}}{R_Y}.$$

This implies that an inclined crystal will be reflecting dynamically at any practically achievable curvature. This allows one to use a bent inclined crystal for the sagittal focusing as proposed by Ice and Sparks [7].

Conclusion

Analytical expressions for the criterion that must be met in order to obtain dynamical diffraction of X-rays in bent crystals are provided in different approximations in Table I. Those formulas include the matrix D , which depends on the crystal elastic constants and orientation. The values of this matrix are provided in Table II for some special orientations and in isotropic approximation. The results of this work allow one to determine to what extent is it possible to bend a crystal without loss of X-ray reflectivity.

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Table I. Expressions for the parameter B derived in several approximations

Asym met ry	Incli nati on	Bragg angle	Iso tro pic *	Expression for B	
α	ϕ	θ			
1. General case				λ	$C_X \quad C_Y$
			No	$B = \frac{\lambda}{2 \pi \chi^2} \sin(\theta) \sin(\theta+\alpha) \sin(\theta-\alpha) \cos(\phi)$	$(\frac{C_X}{R_X} + \frac{C_Y}{R_Y})$
				$C_X = \cos(\alpha) [D_{31} \cos^2(\phi) + \cot(\theta-\alpha) \cot(\theta+\alpha) + D_{21} \sin(2\phi)]$	
				$+ \sin(\alpha) [2D_{11} \cos(\phi) + \cot(\theta-\alpha) - \cot(\theta+\alpha)]$	
				$C_Y = \sin(\alpha) 2 D_{13} \cos(\phi)$	
				$+ \cos(\alpha) [D_{33} \cos^2(\phi) + D_{23} \sin(2\phi) + \sin^2(\phi)]$	
				For the values of matrix D see Table II.	
2. Isotropic approximation*				λ	$C_X \quad C_Y$
			Yes	$B = \frac{\lambda}{2 \pi \chi^2} \sin(\theta) \sin(\theta+\alpha) \sin(\theta-\alpha) \cos(\phi)$	$(\frac{C_X}{R_X} + \frac{C_Y}{R_Y})$
				$C_X = \cos(\alpha) [(-\nu/(1-\nu)) \cos^2(\phi) + \cot(\theta-\alpha) \cot(\theta+\alpha)]$	
				$+ \sin(\alpha) [\cot(\theta-\alpha) - \cot(\theta+\alpha)]$	
				$C_Y = -\nu/(1-\nu) [2 \sin(\alpha) \cos(\phi) + \cos(\alpha) \cos^2(\phi)]$	
3. Above approximation + non inclined geometry				λ	$C_X \quad C_Y$
	$\phi=0$		Yes	$B = \frac{\lambda}{2 \pi \chi^2} \sin(\theta) \sin(\theta+\alpha) \sin(\theta-\alpha) \cos(\phi)$	$(\frac{C_X}{R_X} + \frac{C_Y}{R_Y})$
				$C_X = \cos(\alpha) [-\nu/(1-\nu) + \cot(\theta-\alpha) \cot(\theta+\alpha)]$	
				$+ \sin(\alpha) [\cot(\theta-\alpha) - \cot(\theta+\alpha)]$	
				$C_Y = -\nu/(1-\nu) [2 \sin(\alpha) + \cos(\alpha)]$	
4. Above approximations + symmetric diffraction				λ	$\nu \quad 1 \quad \nu \quad 1$
$\alpha=0$	$\phi=0$		Yes	$B = \frac{\lambda}{2 \pi \chi^2} \sin(\theta)^3 [(\cot^2(\theta) - \frac{\nu}{1-\nu}) \frac{1}{R_X} - \frac{\nu}{1-\nu} \frac{1}{R_Y}]$	
5. Above approximations + backscattering**				$\lambda \quad \nu \quad 1 \quad 1$	
$\alpha=0$	$\phi=0$	$\theta \rightarrow \pi/2$	Yes	$B = - \frac{\lambda}{2 \pi \chi^2} \frac{\nu}{1-\nu} (\frac{1}{R_X} + \frac{1}{R_Y})$	
6. High-energy limit, symmetric non inclined geometry				λ^2	
$\alpha=0$	$\phi=0$	$\theta > 0$	No	$B = - \frac{\lambda^2}{4 \pi d_{hkl} \chi_{hkl}^2 R_X}$	

* Expressions 2-5, derived in isotropic approximation, are also valid for anisotropic Si and Ge plates with (001) surface.

** Expression 5 for backscattering is also valid for Si and Ge plates with the surface (111). For effective values of the ratio $\nu/(1-\nu)$ see Table II.

Table II. The matrix D from expression (12) for different crystal orientations

Orientation	Si	Ge
$z=\langle 001 \rangle$ $x \text{ \& } y \text{ in } (001) \text{ plane}$ or Isotropic crystal	$\begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -0.386^* & 0 & -0.386 \end{vmatrix}$	$\begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -0.369^* & 0 & -0.369 \end{vmatrix}$
$x = \langle 1 \ -1 \ 0 \rangle, y = \langle 1 \ 1 \ -2 \rangle$	$\begin{vmatrix} 0 & 0.222 & 0 \\ 0.111 & 0 & -0.111 \\ -0.221^{**} & 0 & -0.221 \end{vmatrix}$	$\begin{vmatrix} 0 & 0.250 & 0 \\ 0.125 & 0 & -0.125 \\ -0.184^* & 0 & -0.184 \end{vmatrix}$
$x = \langle 1 \ 1 \ -2 \rangle, y = \langle 1 \ -1 \ 0 \rangle$	$\begin{vmatrix} 0.111 & 0 & -0.111 \\ 0 & 0.222 & 0 \\ -0.221^{**} & 0 & -0.221 \end{vmatrix}$	$\begin{vmatrix} 0.125 & 0 & -0.125 \\ 0 & 0.250 & 0 \\ -0.184 & 0 & -0.184 \end{vmatrix}$
$x = \langle 111 \rangle, y = \langle 1 \ -1 \ 0 \rangle$	$\begin{vmatrix} 0.026 & 0 & 0.144 \\ 0 & 0.192 & 0 \\ -0.236 & 0 & -0.301 \end{vmatrix}$	$\begin{vmatrix} 0.025 & 0 & 0.159 \\ 0 & 0.212 & 0 \\ -0.199 & 0 & -0.276 \end{vmatrix}$
$x = \langle 111 \rangle, y = \langle 1 \ 1 \ -2 \rangle$	$\begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -0.232 & 0.138 & -0.281 \end{vmatrix}$	$\begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -0.195 & 0.159 & -0.251 \end{vmatrix}$
$x = \langle 1 \ -1 \ 0 \rangle, y = \langle 1 \ 1 \ 1 \rangle$	$\begin{vmatrix} 0 & -0.192 & 0 \\ -0.144 & 0 & -0.026 \\ -0.301 & 0 & -0.236 \end{vmatrix}$	$\begin{vmatrix} 0 & -0.212 & 0 \\ -0.159 & 0 & -0.025 \\ -0.276 & 0 & -0.199 \end{vmatrix}$
$x = \langle 1 \ 1 \ -2 \rangle, y = \langle 1 \ 1 \ 1 \rangle$	$\begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -0.281 & 0.138 & -0.232 \end{vmatrix}$	$\begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -0.251 & 0.159 & -0.195 \end{vmatrix}$

* The effective value of the ratio $-v/(1-v)$ for the correspondent crystal orientations in the formulas 2-5 in the Table I.

** The effective value of the ratio $-v/(1-v)$ for the correspondent crystal orientations in the formula 5 in the Table I.

Appendix I. The solution of the Taupin's problem in the kinematical approximation.

In the case of the backscattering (θ is close to 90°) the only term in the displacement field which affects the X-ray diffraction is the term, proportional to z^2 . In this case the general expression (2) reduces to (expression (5.1) from [1]):

$$\mathbf{h} \cdot \mathbf{u}(\mathbf{r}) = 4 \sigma_{-h} \sigma_h B z^2. \quad (17)$$

Such a displacement field describes the crystal with the deformation linear on z . The problem of the X-ray diffraction on the crystal with the displacement field like (17) is known as a Taupin's problem [8].

In kinematical approximation it is possible to write down the amplitude of the scattered wave as:

$$A = A_0 \int_{z=0}^{\infty} \exp(-i a z - i b z^2) dz \quad (18)$$

$$\text{where } a = - \frac{2 i \mu}{\sin(\theta)} + 4 \pi \sin(\theta) dE/hc, \quad (19)$$

μ is the absorption coefficient, h is a Plank's constant, and c is the speed of light. dE is the deviation of the photon energy from the wave which is in exact Bragg position at the top surface $z=0$ of the crystal. Also the following definitions apply:

$$b = \frac{2 \pi}{\lambda} \sin(\theta) \frac{v}{1-v} \left(\frac{1}{R_x} + \frac{1}{R_y} \right), \text{ and} \quad (20)$$

$$A_0 = \chi \pi / \lambda. \quad (21)$$

We suppose that the amplitude of the incident wave is equal to unity. Introducing new dimensionless variables $p = a / \sqrt{b}$ and $Z = z \sqrt{b}$ one can obtain:

$$A = A_0 \frac{1}{\sqrt{b}} \int \exp(-i p Z + i Z^2) dZ = A_0 \frac{1}{\sqrt{b}} F(p) \quad (22)$$

For a crystal with small absorption, p is proportional to the energy deviation dE . It is possible to show that the integral $F(p)$ in the equation (22) is given by:

$$F(p) = (1-i) (\pi/8)^{(1/2)} \cos(p^2/4) - p \cdot {}_1F_2(1, 3/4, 5/4, -p^4/64) + (1+i) (\pi/8)^{(1/2)} \sin(p^2/4) - p^3 \cdot {}_1F_2(1, 5/4, 7/4, -p^4/64). \quad (23)$$

Here ${}_1F_2$ is a hypergeometric function.

The diffracted intensity is proportional to the $|F(p)|^2$ and plotted on Fig. 2. With the accuracy of the multipliers listed below the Fig. 2 represents the reflecting curve of the crystal in the kinematical approximation. This graph has a maximum of $|F(3.05)| = 4.305$. Therefore, the absolute value of the maximum reflectivity of the crystal is equal to:

$$R_{\max} = A_0^2 \cdot 4.305 / b \quad (24)$$

Substituting (20-21) into (24) and comparing with the expression 5 in the Table I for the B for the backscattering, one can obtain:

$$R_{\max} = \frac{4.305}{4 B}$$

This provides us a very simple estimation of the asymptotic behavior of the reflectivity at the large curvatures (i.e. $B \gg 1$) as

$$R_{\max} \approx 1/B \quad (25)$$

This expression also gives us the limit of the applicability of the kinematical approximation:

$$B = 1. \quad (26)$$

Fig.1 Reflectivity of the spherically bent Ge (444) crystal in backscattering ($\theta \rightarrow 90^\circ$) as a function of photon energy for different values of parameter B (these results were obtained numerically using a 2x2 matrix formulation of dynamical diffraction [5]):

a) $R = 1 \text{ m}, B = 0.072;$	b) $R = 144 \text{ mm}, B = 0.5;$
c) $R = 72 \text{ mm}, B = 1;$	d) $R = 36 \text{ mm}, B = 2.$

Fig. 2 The reflectivity of the bent crystal in the kinematic approximation (arbitrary units); p - is the normalized deviation from the exact Bragg position; reflectivity is proportional to $|F(p)|^2$; $F(p)$ is the function given by expression (23).

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