

Simulation of XFEL pulse propagation through double crystal Laue monochromator

Summer student work report

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Motivation

In 2014 European X-ray free electron laser (XFEL) will start operating. It has some essential differences from the synchrotron source, thus it needs new optics. Monochromator for synchrotron radiation is a well known device, which should extract exact energy from the continual spectrum of synchrotron radiation. Usually Si perfect crystals in Bragg geometry are used for this purpose. The width of crystal reflection curve is typically in order of 10^{-4} - 10^{-5} rad, which is sufficiently lower than beam divergence.

For XFEL source the peak brilliance, and thus the peak heat loads, are much greater. To stand in this condition one should use diamond crystals in Laue geometry. Another change is that the divergence of XFEL pulses is very small, so incident beam angular width is substantially less than the reflection curve of the crystal. Also the beam is nearly fully coherent. For such source Gaussian beam seems to be a good model. But usually plane or spherical wave approximation is used in dynamical diffraction theory [2]. Recently a general approach that allows to consider crystal diffraction of a pulse limited in space and time was developed [1].

Originally it was planned that XFEL pulse will have average wavelength of 1 Å. However, for most applications it is necessary to operate with a range of energies. Thus it is interesting to know, how successfully the device designed for a particular photon energy will operate at various energies.

The main purpose of this project was to simulate propagation of the Gaussian beams of energies within range 8-20 keV from source to a Laue double crystal monochromator, between crystals and further to the detector.

Some facts from dynamical diffraction theory

In order to understand the principles of a double crystal monochromator one has to go into dynamical diffraction theory. Now we will consider the very basic equations of this theory, which were used in the program.

We shall consider diffraction reflection and transmission of a pulse of X-ray radiation

$$E_{in}(x, t) = A_{in}(x, t) \exp(iK_{0x}x - i\omega_0 t), \quad (1)$$

which is the field incident on a single-crystal plate of thickness d on the crystal surface $z = 0$. In this equation $A_{in}(x, t)$ is a slowly varying complex amplitude (the envelope of a wave packet), $K_{0x} = K_0 \sin \Theta_0$, $K_0 = \omega_0/c$ and c is the speed of light in vacuum; the axis x is directed along the crystal surface and the axis z is directed inside the crystal along the normal \mathbf{n} to the surface (Fig. 1). The angle of incidence of the radiation to the normal \mathbf{n} is $\Theta_0 = \psi - \Theta_B - \Delta\Theta$, where Θ_B is the Bragg angle for the central (average) frequency ω_0 , which is determined by the expression (2) $K_0 \sin \Theta_B = h$ (Laue condition), where h is the modulus of the

reciprocal lattice vector, $\Delta\Theta$ is the deviation from the exact Bragg angle, and ψ is the inclination angle of reflecting crystal planes to the normal \mathbf{n} .

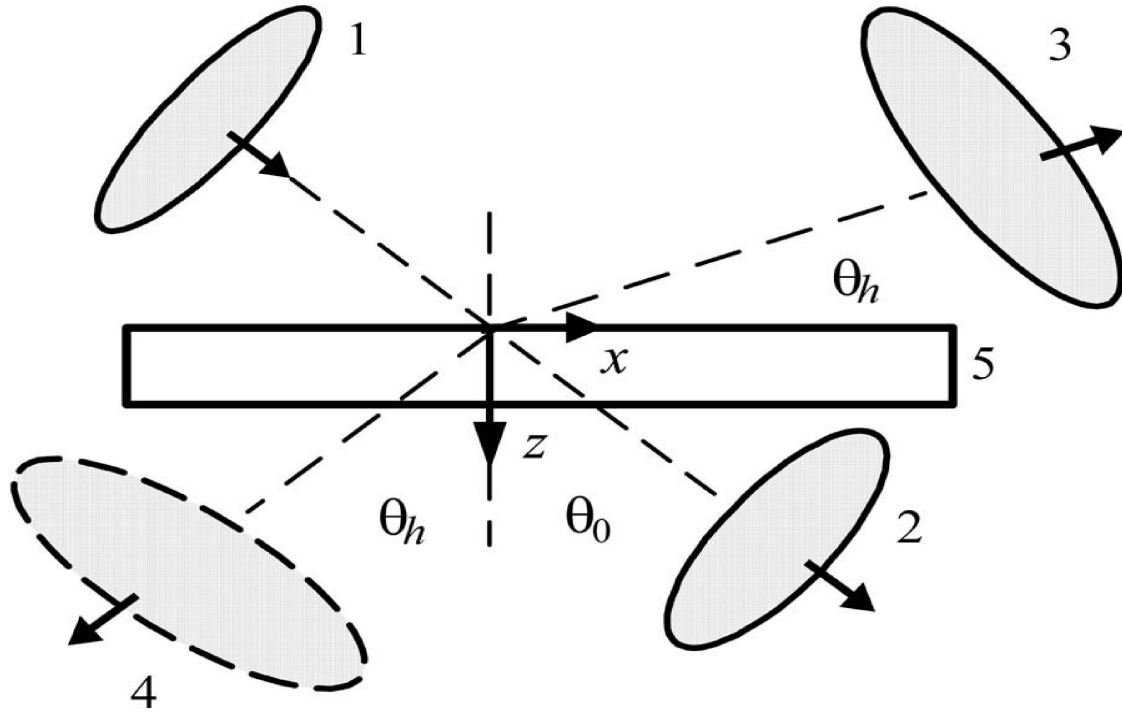


Fig. 1 Geometry in real space of X-ray pulse diffraction in the Bragg and Laue cases.

1: incident pulse $E_{in}(r, t)$;

2: transmitted pulse $E_0(r, t)$;

3: reflected pulse $E_h(r, t)$ in the Bragg case;

4, reflected pulse $E_h(r, t)$ in the Laue case;

5, the crystal;

Θ_0 and Θ_h are the angle of incidence of the initial pulse and the angle of reflection of the diffracted pulse, respectively, relative to the axis z .

Let us now write the field $E_{in}(x, t)$ in the form of a two-dimensional Fourier integral,

$$E_{in}(x, t) = \iint E_{in}(k_{0x}, \omega) \exp(ik_{0x}x - i\omega t) dk_{0x} d\omega \quad (2)$$

where

$$E_{in}(k_{0x}, \omega) = (2\pi)^{-2} \iint E_{in}(x, t) \exp(ik_{0x}x - i\omega t) dx dt, \quad (3)$$

Here and further on, all integrations are carried out over the infinite limits from $-\infty$ to $+\infty$. Substituting the field $E_{in}(x, t)$ (1) into (3) and introducing new variables

$$q = k_{0x} - K_{0x}, \quad \Omega = \omega - \omega_0, \quad (4)$$

one obtains a set of Fourier amplitudes of the field, $E_{in}(k_{0x}, \omega) = A_{in}(q, \Omega)$, with

$$A_{in}(q, \Omega) = (2\pi)^{-2} \iint A_{in}(x, t) \exp(-iqx + i\Omega t) dx dt, \quad (5)$$

Expression (2) describes a set of plane monochromatic waves with amplitudes $A_{in}(q, \Omega)$, wave-vectors $k_0 = (k_{0x}, k_{0z})$ and frequencies ω .

For each single component wave in (2) transmitted (T) and reflected (R) coefficients can be calculated using the plane-wave dynamical diffraction theory. Not going into details, let us take the solution well known from the dynamical diffraction theory (so called pendulum solution):

$$R(y) = \frac{\chi_h}{\chi_{\bar{h}}} \frac{\sin^2(A\sqrt{1+y^2})}{1+y^2}, \quad (6)$$

where

$$A = \pi \frac{d}{L_{ext}}, \quad (7)$$

In these equations y is convenient angular variable, χ_h - Fourier transformation of polarisation, d - thickness of the crystal, L_{ext} - extinction length.

Even if a crystal is infinitely thick, only the crystal volume within the extinction length contributes considerably to the diffraction in Bragg geometry. In Laue geometry extinction length is not so demonstrative, but determines the shape of the reflectivity curve (see (6) and (7)). It could be calculated as

$$L_{ext} = \lambda \frac{\sqrt{|\gamma_0 \gamma_h|}}{\pi |\operatorname{Re}(\chi_h)|}, \quad \gamma_h = \cos(\Theta_h), \quad (8)$$

where $g=0, h$.

As one can see at fig. 2, this solution represents a series of interchanging maxima and minima, which can be understood as interchanging of dominant beam (reflected or transmitted).

It is clear from equations (6) and (7), that the shape of the reflectivity curve determined by the ratio d/L_{ext} . In Laue case the reflection coefficient is maximal if the crystal thickness satisfies the condition

$$d = \frac{\pi}{2} L_{ext} (2n), \quad (9)$$

where $n=0, 1, 2, \dots$ is an integer.

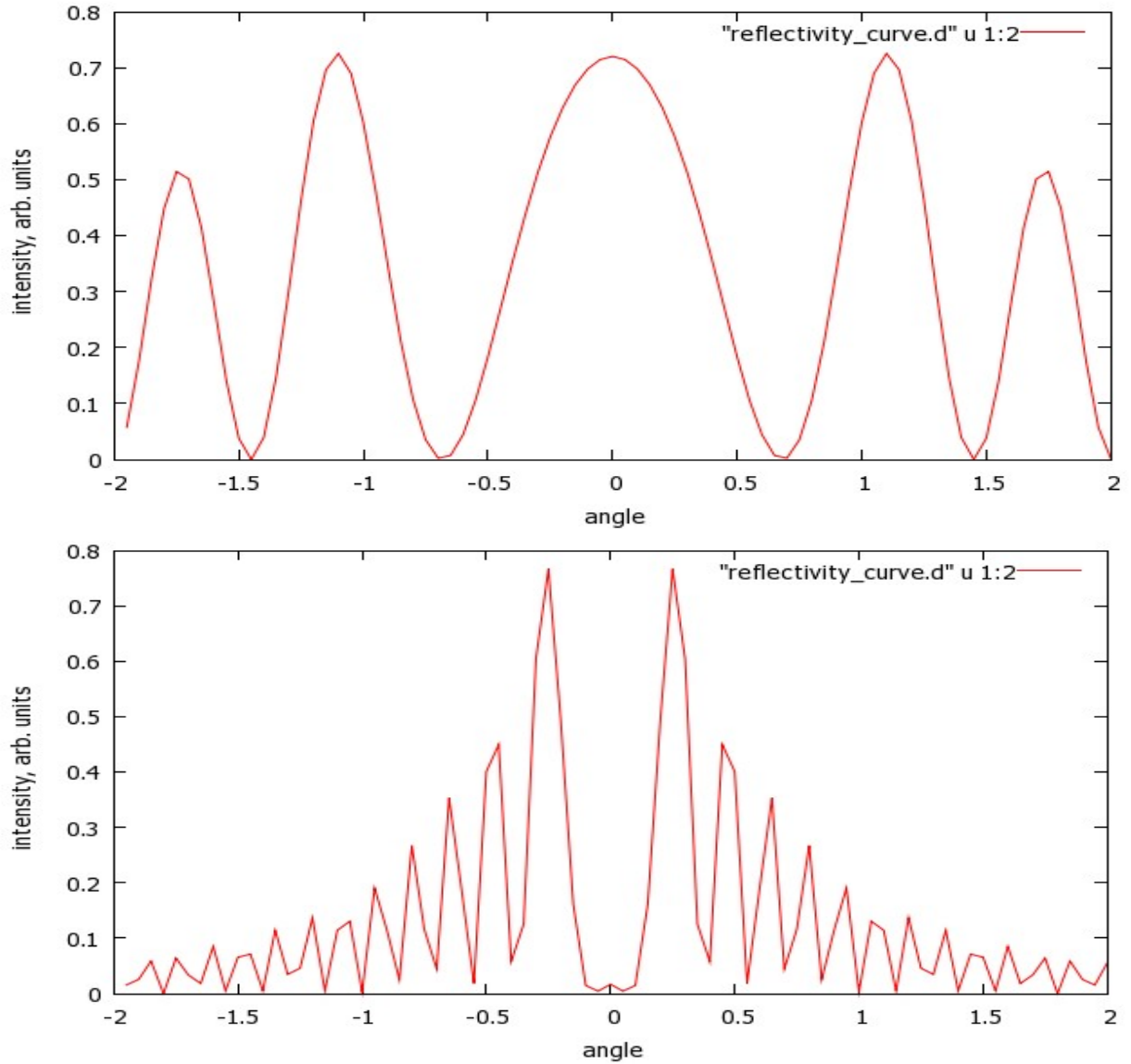


Fig. 2 Reflected intensity for the case of fulfilled (a) and not fulfilled (b) condition (9).

If condition (9) is satisfied, one will see the picture like fig. 2a with broad central maximum, otherwise it will take form of fig. 2b. In practice one can use side maxima to find reflection in the last case, but the intensities will be significantly smaller.

Transmitted coefficient can be determined as $T=1-R$. Now we can obtain the distribution of field $E_g(x, z, t)$ for transmitted ($g=0$) and reflected ($g=h$) pulses at any point of space (x, z) outside the crystal and at any moment of time t ,

$$E_g(r, t) = \iint B_g(q, \Omega) A_{in}(q, \Omega) \exp(ik_g r - i\omega t) dq d\Omega \quad (10)$$

where $B_0=T$, $B_h=R$.

Gaussian beam

As it was already mentioned, we consider that our beam is Gaussian. In this chapter the main properties of it are discussed.

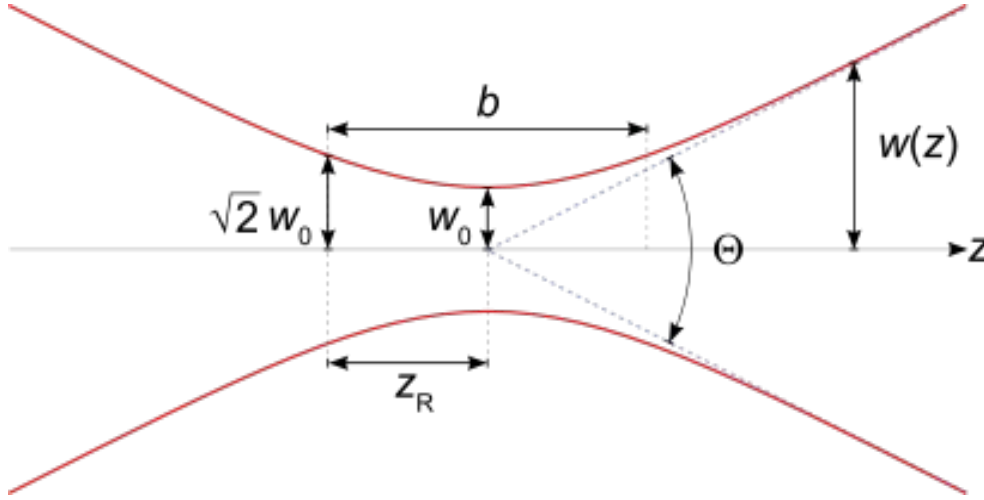


Fig. 3 Gaussian beam geometry

The geometry and behaviour of a Gaussian beam are governed by a set of beam parameters, the most important are the radius at which the field amplitude drops to $1/e$ of its axial value $w(z)$, angular divergence Θ and wavelength λ (see fig. 3). The parameter $w_0 = w(0)$, named waist size, and also is frequently used for the description of Gaussian beam. The parameter $w(z)$ approaches a straight line for big distances. The angle between this straight line and the central axis of the beam is called the divergence of the beam Θ . It can be calculated as

$$\theta \equiv \frac{\lambda}{\pi w_0}, \quad (11)$$

where θ is given in radians.

In our case energy (or wavelength) was shifted at each iteration and source size was kept constant during the operation, but could be changed in the input file Laue_2x.d (variable r0W). Angular divergence was recalculated automatically.

Results and discussion

Using the programs, which were described in chapter ‘program manuals’, following results were obtained. Firstly, let’s take a look at Fig.4 where the reflection from one crystal is shown.

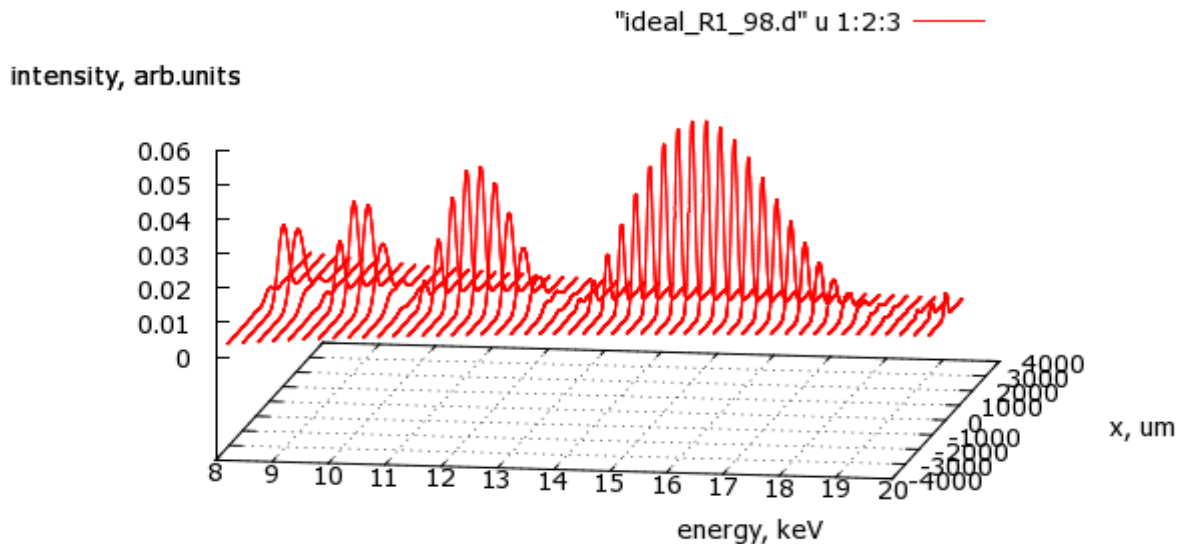


Fig. 4 Distribution of intensity of the beam reflected from the single crystal.

This picture is typical for our simulations and was calculated for a 98 μm thick diamond crystal. It represents a wiggling curve with maxima and minima corresponding to condition (9). The purpose of this work was to find nice construction of a double crystal monochromator. By looking at fig. 4 one can say, that there are energies at which crystal doesn't reflect at all, thus it can't be used. If crystal thickness will be changed, maxima and minima of reflectivity changes, so it is possible to find optimal crystal thickness for the given energy range. But in real cases one cannot change the monochromator for each energy during the experiment, so those minima about 1 keV range can become a problem.

For better understanding of these results one should look at the angular distributions of the incident beam in comparison with reflection curve of the crystal. Fig. 5 shows it for energies 13,25 and 16 keV (these energies have minimum and maximum peak intensities at fig. 4). The green line shows the spectrum of the beam. As one can see at 16 keV the green line lies in the middle of the main peak of the crystal reflection curve, thus most of the intensity goes into the reflected beam. Unlike the 13,5 keV case the beam is located between two side maxima, thus nearly all the intensity goes into the transition wave.

Following this approach one can find a simple way to get intensity even in the case of Fig.5.b. The crystal reflectivity curve can be displaced by rotating the crystal as it is shown at Fig. 6. In this case the intensity will not be as high as, for example, at 16 keV, but will be significantly increased.

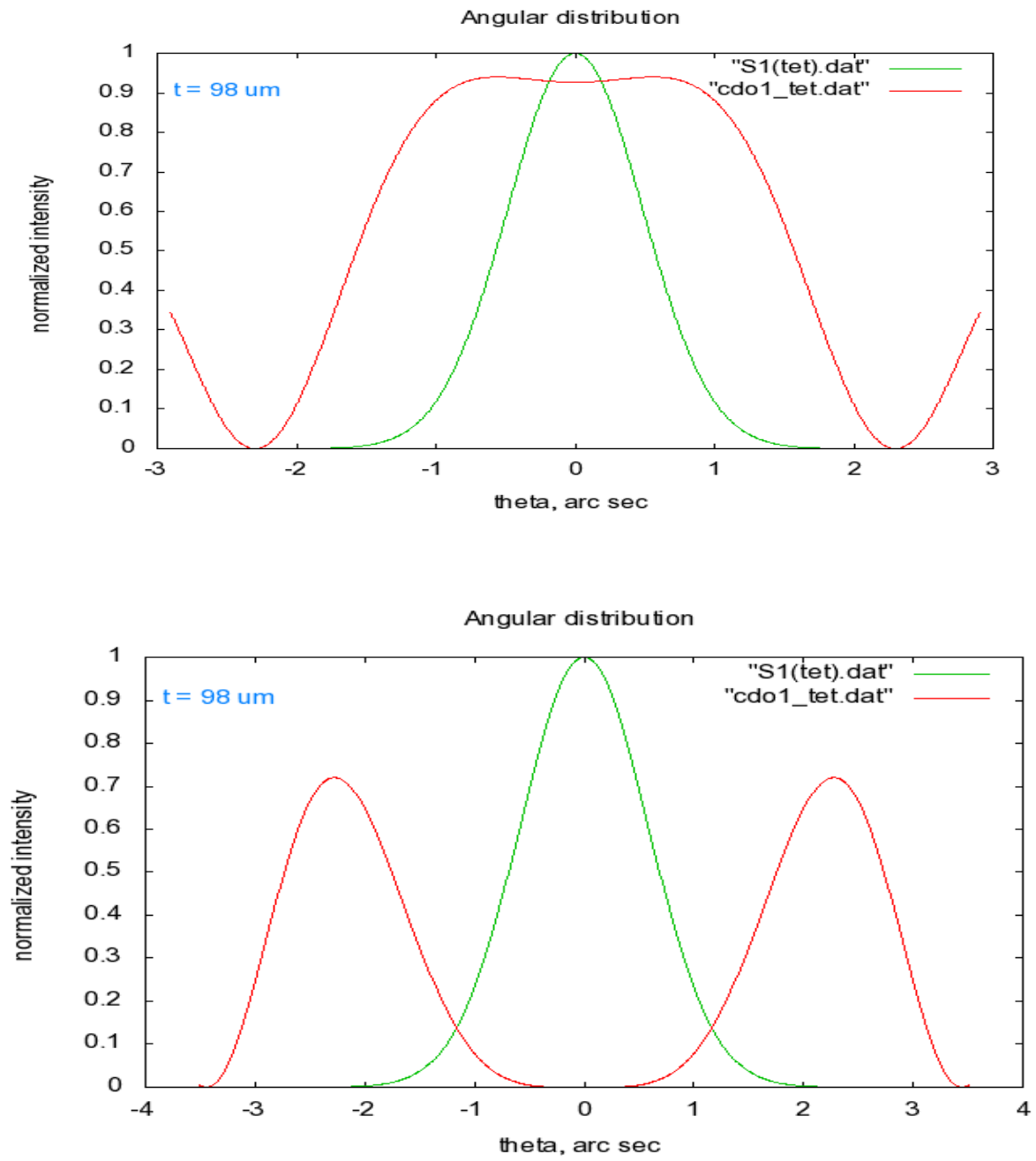


Fig. 5 Reflection curves (red lines) and angular distribution of the beam intensity (green lines) in case of different energies:
a. E=16 keV b. E= 13.25 keV

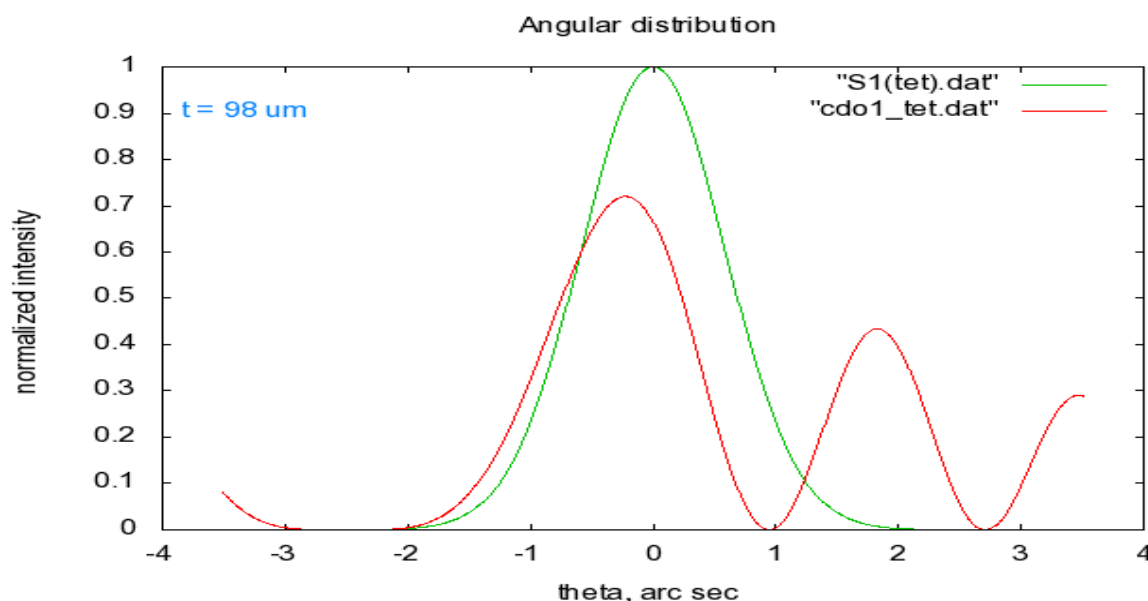


Fig. 6 Reflection curve (red line) and angular distribution of the beam intensity (green line) in case of energy $E=13.25 \text{ keV}$ and inclination angle of the crystal $\alpha=2.5 \text{ arc. sec.}$

Now let's look at the picture for two crystals (Fig. 7). Both crystals have the same thickness of 107 um .

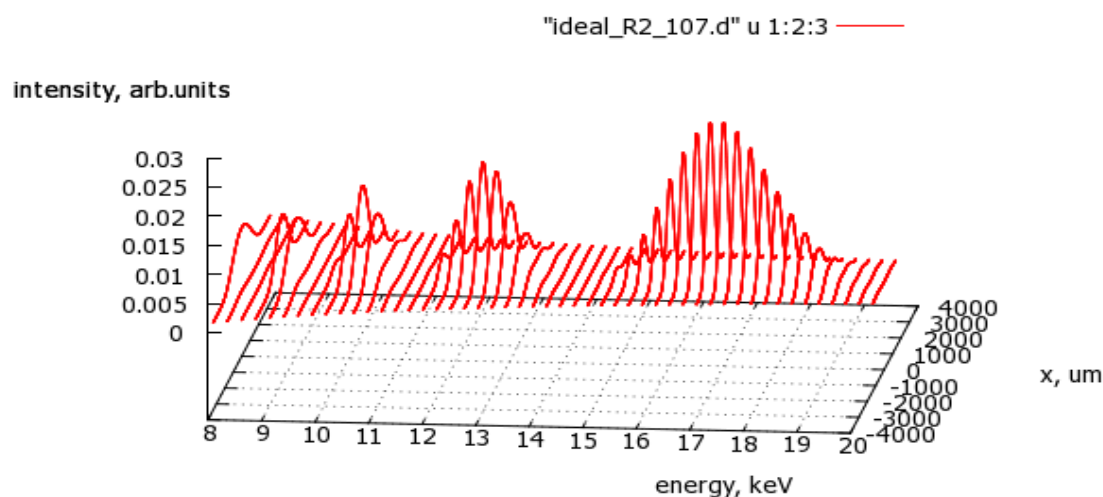


Fig. 7 Distribution of intensity of the beam reflected from two crystal monochromator. Crystal thicknesses 107 um .

This picture is quite similar to the one from the single crystal, but has lower intensities. It's more demonstrative to look at a 2D graph with integral intensities. The red line at Fig. 8 shows integral intensities for non-rotated crystal and the green one corresponds to the case of rotating by 2 arc. sec. (in order to have maximum intensity at 14 keV).

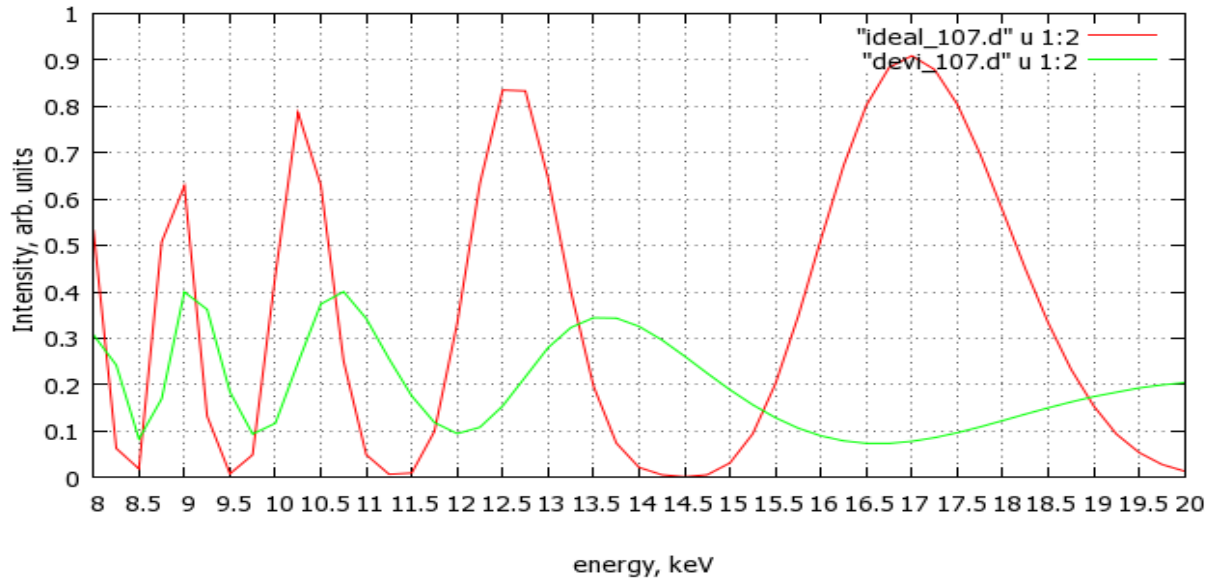


Fig. 8 Integral intensities of the beam reflected from inclined (green line) and not inclined (red line) crystals.

One can do such realignment for every energy of incoming beam to investigate what intensity can be achieved by alignment crystals with given thicknesses and energy of incident beam. Results of simulations for 107 μm thick crystals (optimal thickness for 1 A) are shown at Fig. 9.

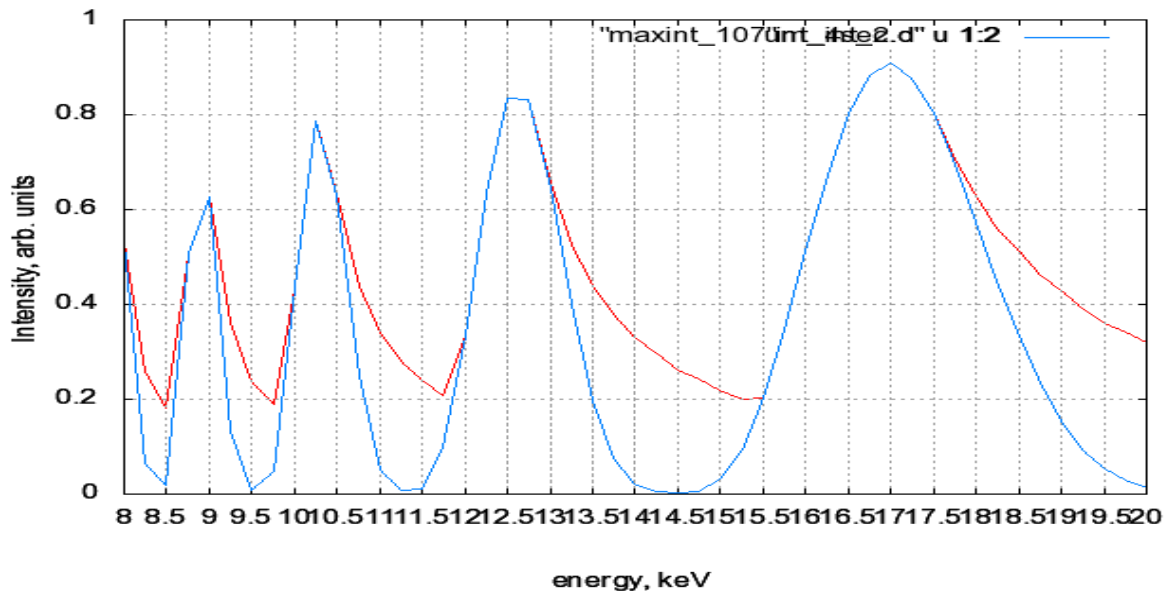


Fig. 9 Integral intensity of the beam reflected from not inclined (blue line) and optimally inclined (red line) crystals.

One more thing in which we were interested in was comparison of different thicknesses: in order of 100 μm and 400 μm . Simulations shows, that oscillation of diffraction reflection curves become more frequent with increasing of thickness. Fig.6 shows reflectivity from two 400 μm thick crystals in the same

scale as at Fig. 7. According to this one can say, that 100 μm crystal looks more suitable for our purposes. However, for thicker crystal the main peak of diffraction reflection curve becomes narrower, compatible with angular divergence of incoming beam. 2D model should be used for crystals with thicknesses 400 μm and bigger.

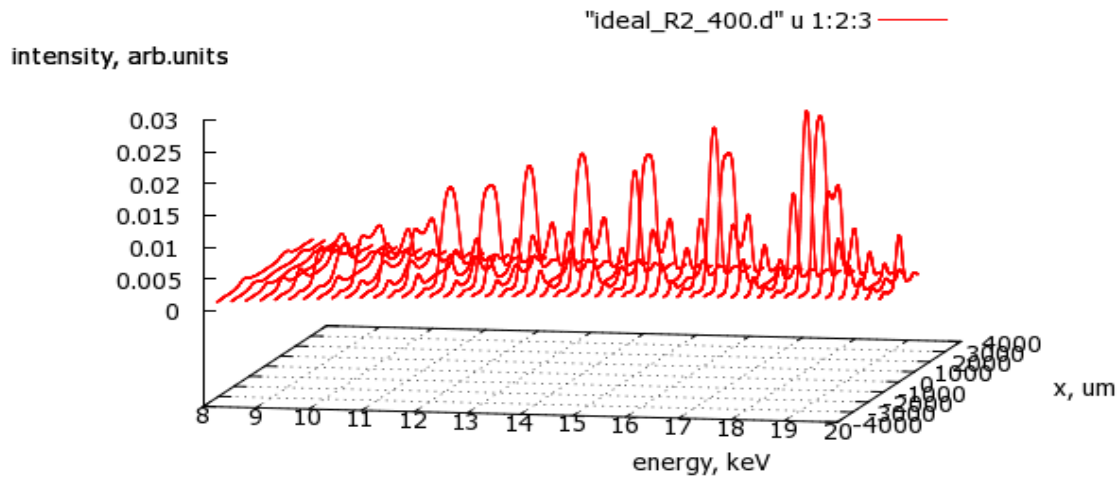


Fig. 9 Distribution of intensity of the beam reflected from two crystal monochromator. Crystal thicknesses 400 μm .

Natural spectral bandwidth of XFEL beam $\Delta E \sim 10$ eV is much less than period of oscillations at Fig. 8 and 9, and does not affect the results.

Conclusions

One of the important conclusions answers the question how strong slight deviations of parameters from the ideal case will effects to the resulting intensities. Simulations shows that deviations of inclination angles within few degrees, deviations from Bragg angle within fractions of urad, deviations in thicknesses within few microns does not lead to critical changes in relation to ideal case.

Small thickness crystals (about 100 μm) seems to be more suitable.

Crystal thickness cannot be optimized for entire energy range (8-20 keV).

Environment for Laue DCM optimization was developed and can be used for further simulations.

Acknowledgements

I would like to thank my supervisors Liubov Samoylova and Harald Sinn for useful advices and great support. Thanks to them I learn new skills and was introduced into new for me field of physics. I would also like to thank all peoples, who made this Summer Student Program 2010 available. It was a great experience and interesting summer.

References

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- [2] A. Authier, “Dynamical theory of X-ray diffraction”, 2001
- [3] http://sergey.gmca.aps.anl.gov/x0h_search.html S. Stepanov’s web server.
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Appendix

A1 Manual for the program Laue_2x.for *

* Original core of the program (calculations of reflection curve) was written by V.A. Bushuev

The program Laue_2x.for was written for a line source, infinite in y direction and Gaussian in x direction, i.e. 1D case is assumed. The amplitude of the electric field can be written as

$$A_s(x, z=0) = \exp[-(x/r_0)^2 + i\alpha_0(x/r_0)^2], \quad (12)$$

where r_0 is a parameter, which describes source size in transverse direction. It can be connected with FWHM (full width at half maximum) by simple equation $r_w = 1.1774 * r_0$; α_0 – phase parameter, which describes parabolic curvature of wave front and additional angle divergence:

$$\Delta\theta \equiv \frac{\lambda}{\pi r_0} \sqrt{1 + \alpha_0^2}, \quad (13)$$

Intensity of the beam (11) in the maximum decreases as $1/z$ while distance z increases, which differs from the $1/z^2$ law usually used for 2D beam

$$A_s(x, y, z=0) = \exp[-(x/r_0)^2 - (y/r_0)^2 + i\alpha_0(x/r_0)^2 + i\alpha_0(y/r_0)^2]. \quad (14)$$

Such a beam should be registered by 2D detector. However, all calculations in the program can be considered as ones for propagation of the beam with detection of its intensity integrated along y direction. While free space propagation is under consideration it will be correct to multiply intensity profile in x direction (which is calculated by the program) by the same profile in the y direction (like in eq. 2). But in crystals it becomes much more complicated. Still one can use the same multiplying procedure for reflected beam, if the beam angular divergence in both directions is much less than the width of the main peak of the diffraction reflection curve. Such assumption is fulfilled in XFEL in case that crystal thickness is in order of 100 um, and spoils while the thickness increases.

The program Laue_2x.for can be used to calculate propagation of Gaussian beam in the route source – 1st Laue crystal – 2nd Laue crystal – detector. All reasonable distances and parameters can be set up in the input file Laue_2x.d. There are short descriptions and coded names of corresponding variables for each parameter in this file in order to make communication with the program comfortable. Only the first paragraph should be filled with reasonable data before running the program, the others are calculated and filled

in automatically by the program. The example of input file can be found in appendix A.

Let's briefly clarify some points. Psi_1 and Psi_2 are inclination angles, i.e. angles between surface and reflection planes for the first and the second crystals. They are positive then rotated counterclockwise (in this case asymmetry coefficient $b = \gamma_0/\gamma_h$ is less than one, where $\gamma_0 = \cos(\theta_B + \psi)$, $\gamma_h = \cos(\theta_B - \psi)$). Angular deviations from Bragg angle are positive than rotated counterclockwise (i.e. when the angle increases from normal to surface). Value CXmax shows maximum of coordinate of the incident beam in transverse direction in units of beam size. Boundaries for the angle Cq should be set in such way, that the entire angular spectrum could be described (Cq=3 is enough in most cases).

Below the list of parameters for program Laue_2x.for is printed. All number from the first paragraph done as example and can be shifted in reasonable ranges.

Input file Laue_2x.d

```

30.000000  -r0W FWHM source size at z=0 (um)
0.000000   - alfa_0 in phase(x)=alfa_0*(x/r0)**2
2.000000   - dtetta_1 angle deviation of 1st crystal (urad)
0.000000   - Psi_1 inclination angle for 1st crystal (deg)
107.000000 - tc_1 1st crystal thickness (um)
2.000000   - dtetta_2 angle deviation of 2nd crystal (urad)
0.000000   - Psi_2 inclination angle for 2nd crystal (deg)
107.000000 - tc_2 2nd crystal thickness (um)
3.500000   - CXmax in Xmax=CXmax*r1W/2
2.000000   - regim_Cq: 1 - qMax=1/dx, 2 - qMax=Cq*(2/r1W)
3.000000   - Cq in qMax=Cq*(2/r1x)*sqrt(1+alfa1**2)(regim_Cq=2.)
900.000000 - number of points n over x and q (<901)
1.549800   - lam0 wavelenght (A)
1.258300   - d interplanar spacing for (220) Diamond (A)
500.000000 - Z0m distance between source and 1st crystal (m)
0.210000   - Z1 distance between two crystals (m)
500.000000 - Z2 distanse between 2nd crystal and detector(m)
-23.001999 - hi0r, real part of hi0 (in E-06)
0.050120   - hi0i,imaginary part of hi0 (in E-06)
7.335800   - hih, real part of hih (in E-06)
0.048562   - hihi,imaginary part of hi0 (in E-06)

```

=====calculated parameters=====

```

2.2795925  - dt_0 FWHM incident beam divergence (urad)
5.9633203  - dt_main1 1/2 width of main peak (urad)
1140.1909180 - r1W FWHM beam size at z=Z0 1st crystal (um)

```

37.9936104	- alfa_1 phase parameter at $z=Z0$
95.7155914	- max source intensity Beam0(x,z=0) (%)
2.6310306	- max incident intensity Beam(x,Z0) (%)
1.7001945	- Max reflected intensity BeamR1(x,Z1) 1st (%)
0.5996205	- Max reflected intensity BeamR2(x,Z2) 2nd (%)
1.0000000	- incident integral intensity at the source (a.u.)
0.4901979	- integral intensity 1st refl. BeamR1(x,Z1) (a.u.)
0.3075291	- integral intensity 2nd refl. BeamR2(x,Z2) (a.u.)
0.5786799	- cdo_1 for 1st crystal (plane wave)
0.5786799	- cdo_2 for 2nd crystal (plane wave)
8.3225679	- Lex1 extinction length for 1st crystal (um)
38.0123177	- tet01 incident angle on 1st crystal (deg)
-38.0123177	- teth1 reflected angle after 1st crystal (deg)
1.0000000	- b1 asymmetry factor for 1st crystal
8.3225679	- Lex2 extinction length for 2nd crystal (um)
38.0123177	- tet02 incident angle on 2nd crystal (deg)
-38.0123177	- teth2 reflected angle after 2nd crystal (deg)
1.0000000	- b2 asymmetry factor for 2nd crystal
38.0123177	- tB Bragg angle for Diamond(220) (deg)
7.5597310	- dtB1 1/2 BRAGG width for 1st crystal (urad)
7.5597310	- dtB2 1/2 BRAGG width for 2nd crystal (urad)
13.1601076	- Z0_Fr Fresnel distance from the source (m)
9534.9990234	- Z1_Fr= $2 \cdot r1^2 \cdot gh / (\lambda m0 \cdot b^2)$ (m)
-0.1641427	- sdvig_1 beam shift along x after 1st crystal (m)
390.8159485	- sdvig_2 beam shift after 2nd crystal (m)
20.3196049	- mu absorption factor (1/cm)
0.2759560	- mutl= $\mu \cdot tc_1 / g01$

A2 Macros description

Before starting to work with the program, one should set the new environmental system variable “gplot” in order to make the graphical representation of results available. It should contain the absolute path to the executive file “gnuplot.exe”. It is assumed, that *gnuplot* / *Octave* program is installed at your computer. You can download available version of this software package for MS Windows following the link http://sourceforge.net/projects/octave/files/Octave_Windows%20-%20MinGW/.

After setting up the input parameters run the program. You will see the sign “everything is working fine” and the wavelength on the screen. Now file Laue_2x.d contains a set of parameters which were calculated during operating, they are listed in the second and third paragraphs (the first one contains input data). Also a set of data files and pictures will be created by the program in the

current directory. Namely, spatial intensity distribution of the beam before the first crystal, incident and reflected beams after the first and second crystals, and diffraction reflection curves for both crystals.

In many cases it is important to see, how results will be changed if wavelength (or energy) is shifted. To obtain this information one should continuously call `Laue_2x.for`, shifting energies in every step. Octave script `Laue_scr.m` can be used for this purpose. Some of the input parameters are energy dependent, so it is essential to prepare one more input file `energy_par.dat`, containing tables with such parameters for each energy. All necessary formulas to calculate them were given in chapter Theory. In our case this parameters were taken from special web server X0h [3]. To set up alother input parameters edit file `Laue_shab.d` (it should be filled in the same way as `Laue_2x.d`).

As a result of running `Laue_scr.m` a new directory “\Laue” will be added (or replaced, if it already exists) to the current path. It will contain all information that `Laue_2x.for` gives placed in a separate directory for each energy (including `Laue_2x.d` with current wavelength and all recalculated parameters).

To visualize the results one can run the octave script `3dparam.m`. It will collect data from directories created by `Laue_scr.m` and form files `refl1.d` and `refl2.d` with three columns: energy, coordinate and intensity of reflected beam after first or second crystals. To extract any other parameter (such as integral intensities, extinction depth etc.) as a function of energy one can use octave script `2dparam.m`.

Also one can use octave script `ang_align.m` to calculate the maximum intensity which can be achieved by shifting angle deviations of both crystals (`dtetta_1` and `dtetta_2`).