The Ray Transfer Function for Diffracting Crystals

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(Dated: August 13, 2010)

As fourth generation synchrotron sources such as the Cornell ERL continue to be developed, brighter, higher quality x-ray beams will be available for experimenters. The ability to simulate these x-rays directly from knowing the charged particle optical properties would be a huge aid to beamline and experimental design. BMAD is a subroutine library that is currently able to simulate relativistic charged particle optics, and it is our goal to extend it to photon optics. In this regard, an algorithm for simulating Bragg diffraction through perfect crystals, such as those frequently used as monochromators, is described in this paper. This algorithm is able to handle the most general case of asymmetric Bragg reflection.

I. INTRODUCTION

In this paper, we will outline an algorithm to propagate x-rays in phase space through a diffracting crystal element with a tilted Bragg geometry, where the incoming beam, the crystal normal, and the crystal's lattice plane normals are not coplanar. The general algorithm will consist of two steps. The first step is to find the direction of the outgoing reference rays, which will correspond to the center of the reflection. Next, incoming rays that are off-axis will be transformed in phase space to the outgoing rays, and their orientations will be given in the basis defined by the outgoing reference ray.

However, unlike magnets or mirrors which produce an outgoing particle or ray for each incoming particle (ray), there is an additional restriction on the incident angles that the incoming rays must satisfy. This restriction is approximately given by Bragg's Law [1],

$$\theta_B = \sin^{-1} \frac{\lambda}{2d} \tag{1}$$

where λ is the wavelength of the radiation. The exact angles and corrections are given by the theory of dynamical diffraction, as described by Batterman and Cole [2].

The presence of this restriction implies that the user is not free to define arbitrary orientations for the crystal to produce a reflection. Instead, the graze angle and tilt correction are now outputs of the program. These are two angles that tell the user how to orient the crystal to obtain the center of the reflection. The full list of inputs and outputs is given in Table 1.

Input Parameters		Output Parameters	
variable name	symbol	variable name	symbol
`psi_angle`	ψ	`tilt_corr`	θ_{tiltcorr}
`tilt_angle`	θ_{tilt}	`graze_angle_in`	θ_{graze}
`d_spacing`	d		
`v_unitcell`	V		
`f0_re`	F_0'		
`f0_im`	F_0''		
`b_param`	b		
`e_tot`	E_{ref}		

Table I: Table of input and output parameters to the subroutine, together with the symbol which refers to them that will be used in this paper. These outputs tell the user how to orient the crystal, and are in addition to the output reference ray vector and the transfer function.

From these, we can calculate 3 other important parameters: λ, the wavelength of the plane wave corresponding to a photon in the reference trajectory; θ_B, the Bragg angle; and α, the asymmetry angle.

$$\lambda = \frac{hc}{E_{\text{ref}}}$$

$$\theta_B = \sin^{-1}\frac{\lambda}{2d}$$

$$\alpha = \tan^{-1}\left(\tan\theta_B \frac{b+1}{b-1}\right)$$

In the most general case, the tilt angle is given by the user, and it specifies the plane in which the outgoing reference ray lies. A tilt angle of 0 refers to a reflection occurring in the $x-z$ plane of the incoming local coordinate system (defined by the incoming reference ray), while a tilt angle of $\frac{\pi}{2}$ causes the reflection to be deflected downwards in the $y-z$ plane, towards the $-y$ direction. In effect, changing the tilt angle corresponds to a rotation of the system around the incoming reference ray (in accordance to the right hand rule). This definition is exactly the same as that for the mirror element in BMAD [3].

We shall first consider the coplanar case of asymmetric Bragg reflection (a case that is already well studied[2, 4, 5]), before moving on to the more general case where the crystal may be rotated about its surface normal by an angle ψ. In both of these cases, we assume that $\theta_{\text{tilt}} = 0$. A non-zero tilt angle is achieved by calling the subroutine `tilt_coords` in BMAD, which is in effect a rotation of the incoming local coordinates by an angle $-\theta_{\text{tilt}}$.

II. COPLANAR ASYMMETRIC BRAGG REFLECTION

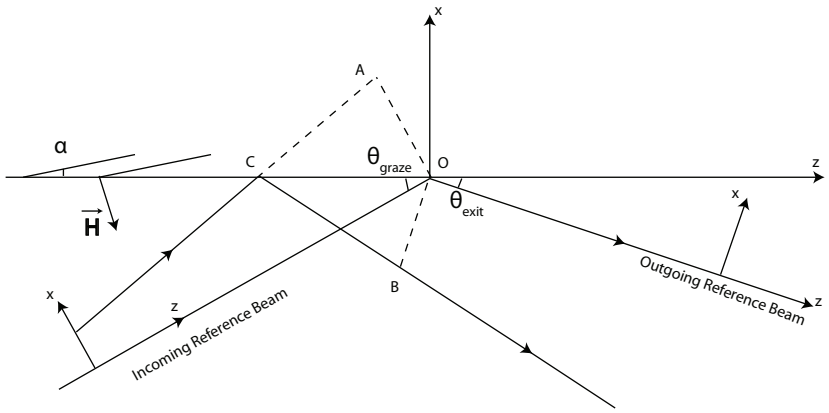

Figure 1: Ray diagram showing how the 3 sets of basis vectors are defined. The y-axis for all 3 of the bases are defined to point out of the paper. In this diagram, all lines and rays are in the plane of the paper, except for those defined by the off-axis photons which may have a y' component. This means that the points A, B, C do not necessarily lie in the $x-z$ plane.

A. Finding the Reference Trajectory

This corresponds to the case where $\psi = 0$, and is sometimes known as the simple asymmetric Bragg reflection. In this case, the Bragg plane normal, $\mathbf{H}$, is in the $x-z$ plane. Reflection occurs only over a very narrow angular range (on the order of arcseconds), and a sensible choice for reference trajectory would be the trajectory that occurs at the center of this angular range. Following Brauer et al. [6], we can obtain the angles of incidence and reflection at this center,

$$\triangle\,\theta_{i0} = \tan\theta_B |F_0| \frac{b-1}{b} \times \frac{r_e d^2}{\pi V}$$

$$\triangle\,\theta_{e0} = -b \triangle\,\theta_{i0}$$

$$\theta_{\text{graze}} = \theta_B + \alpha + \triangle\,\theta_{i0}$$

$$\theta_{\text{exit}} = \theta_B - \alpha + \triangle\,\theta_{e0}$$

Thus, in the crystal's basis, the outgoing reference beam is directed along the vector

$$\mathbf{k_{out}} = \frac{1}{\lambda}\begin{pmatrix} -\sin\theta_{\text{exit}} \\ 0 \\ \cos\theta_{\text{exit}} \end{pmatrix}. \tag{2}$$

B. Obtaining x'_e, y'_e

The critical relation between the incoming and outgoing rays is that the component of the wavevector parallel to the surface is conserved [2]. This condition is equivalent to requiring

$$\mathbf{k_e} - \mathbf{k_i} = N\hat{\mathbf{n}}_\mathbf{s} + \mathbf{H}, \tag{3}$$

where N is some real number, $\mathbf{k_{e,i}}$ are exit and entrance wavevectors, $\hat{\mathbf{n}}_\mathbf{s}$ is the surface crystal normal and $\mathbf{H}$ is the reciprocal lattice vector. We work in the crystal surface normal basis, so that $\hat{\mathbf{n}}_\mathbf{s} = \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix}$, $\mathbf{H} = \frac{1}{d}\begin{pmatrix} -\cos\alpha \\ 0 \\ \sin\alpha \end{pmatrix}$. The advantage of this is that N is automatically eliminated from the second and third components of Eq. (3). If the incoming reference vector is $\mathbf{k_{in}} = \frac{1}{\lambda}\begin{pmatrix} \sin\theta_{\text{graze}} \\ 0 \\ \cos\theta_{\text{graze}} \end{pmatrix}$, a ray which is represented by $[x, x', y, y']$ in 4-D phase space will have its wavevector given by

$$\mathbf{k_i} = \frac{1}{\lambda}\mathbf{M}_{in}\begin{pmatrix} x'_i \\ y'_i \\ \sqrt{1 - x_i'^2 - y_i'^2} \end{pmatrix} = \frac{1}{\lambda}\begin{bmatrix} \cos\theta_{\text{graze}} & 0 & \sin\theta_{\text{graze}} \\ 0 & 1 & 0 \\ -\sin\theta_{\text{graze}} & 0 & \cos\theta_{\text{graze}} \end{bmatrix} \cdot \begin{pmatrix} x'_i \\ y'_i \\ \sqrt{1 - x_i'^2 - y_i'^2} \end{pmatrix}.$$

The exit wavevector is given by a similar expression,

$$\mathbf{k_e} = \frac{1}{\lambda}\mathbf{M}_{out}\begin{pmatrix} x'_e \\ y'_e \\ \sqrt{1 - x_e'^2 - y_e'^2} \end{pmatrix} = \frac{1}{\lambda}\begin{bmatrix} \cos\theta_{\text{exit}} & 0 & -\sin\theta_{\text{exit}} \\ 0 & 1 & 0 \\ \sin\theta_{\text{exit}} & 0 & \cos\theta_{\text{exit}} \end{bmatrix} \cdot \begin{pmatrix} x'_e \\ y'_e \\ \sqrt{1 - x_e'^2 - y_e'^2} \end{pmatrix},$$

and we see immediately from the second component of Eq. (3) that $y'_e = y'_i$.

Also, since the reference ray (where $x' = y' = 0$ for both incident and exit rays) has to satisfy Eq. (3),

$$\cos\theta_{\text{exit}} - \cos\theta_{\text{graze}} = \frac{\lambda}{d}\sin\alpha. \tag{4}$$

If we make the approximation that the $\sqrt{1 - x'^2 - y'^2} \approx 1$, we obtain from Eq. (3)

$$x'_e\sin\theta_{\text{exit}} + x'_i\sin\theta_{\text{graze}} + \cos\theta_{\text{exit}} - \cos\theta_{\text{graze}} = \frac{\lambda}{d}\sin\alpha. \tag{5}$$

Simplifying,

$$x'_e = -\frac{\sin\theta_{\text{graze}}}{\sin\theta_{\text{exit}}}x'_i.$$

Recall that $\theta_{\text{graze}} = \theta_B + \alpha + \triangle\,\theta_i$, $\theta_{\text{exit}} = \theta_B - \alpha + \triangle\,\theta_e$, so if we can make the approximation that the deviation from Bragg's Law is small,

$$x'_e = -\frac{\sin(\theta_B + \alpha)}{\sin(\theta_B - \alpha)}x'_i = bx'_i,$$

our results will be in agreement with Brauer et al. [6] and Matsushita and Kaminaga [4].

C. Obtaining x_e,y_e

To find the change in position in phase space, we consider the geometry shown in Fig. 1. The displacement of the ray off the nominal ray is described by 2 variables, x_i and y_i. These are obtained by projecting the rays to the point so that **OA** is perpendicular to the reference ray. In the incoming local coordinate system, $\mathbf{OA} = \begin{pmatrix} x_i \\ y_i \\ 0 \end{pmatrix}$. In other words, the problem is to find **OB** in the outgoing reference basis as a function of **OA** in the incoming reference basis and the angles found previously.

We rewrite $\mathbf{OC} = \mathbf{OA} + \mathbf{AC} = \mathbf{OA} + n\lambda\mathbf{k_i}$, where n has units of length, and $\mathbf{OA} = x_i \begin{pmatrix} \cos\theta_{\text{graze}} \\ 0 \\ -\sin\theta_{\text{graze}} \end{pmatrix} + y_i \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$. Using the condition that $\mathbf{OC} \cdot \hat{\mathbf{n_s}} = 0$, one can solve for n and find **OC**,

$$n = -\frac{x_i \cos\theta_{\text{graze}}}{\sin\theta_{\text{graze}} + x_i' \cos\theta_{\text{graze}}},$$

$$\mathbf{OC} = \begin{pmatrix} 0 \\ y_i - \frac{x_i y_i' \cos\theta_{\text{graze}}}{\sin\theta_{\text{graze}} + x_i' \cos\theta_{\text{graze}}} \\ -\frac{x_i}{\sin\theta_{\text{graze}} + x_i' \cos\theta_{\text{graze}}} \end{pmatrix} \approx \begin{pmatrix} 0 \\ y_i \\ -\frac{x_i}{\sin\theta_{\text{graze}}} \end{pmatrix}.$$

Note that this approximation is only valid for large graze angles, $\theta_{\text{graze}} \gg x_i'$. We use the same technique to find $\mathbf{OB} = \mathbf{OC} + \mathbf{CB} = \mathbf{OC} + m\mathbf{k_e}$, except that the condition is now

$$\mathbf{OB} \cdot \mathbf{k_{exit}} = \mathbf{OB} \cdot \begin{pmatrix} -\sin\theta_{\text{exit}} \\ 0 \\ \cos\theta_{\text{exit}} \end{pmatrix} = 0,$$

which gives

$$m = \frac{x_i \cos\theta_{\text{exit}}}{\sin\theta_{\text{graze}} + x_i' \cos\theta_{\text{graze}}},$$

$$\mathbf{OB} = \begin{pmatrix} x_i \frac{\cos\theta_{\text{exit}}(x_i' \cos\theta_{\text{exit}} - \sin\theta_{\text{exit}})}{\sin\theta_{\text{graze}} + x_i' \cos\theta_{\text{graze}}} \\ y_i + x_i \frac{(y_e' \cos\theta_{\text{exit}} - y_i' \cos\theta_{\text{graze}})}{\sin\theta_{\text{graze}} + x_i' \cos\theta_{\text{graze}}} \\ x_i \frac{\sin\theta_{\text{exit}}(x_e' \cos\theta_{\text{exit}} - \sin\theta_{\text{exit}})}{\sin\theta_{\text{graze}} + x_i' \cos\theta_{\text{graze}}} \end{pmatrix} \approx \begin{pmatrix} -x_i \frac{\sin\theta_{\text{exit}} \cos\theta_{\text{exit}}}{\sin\theta_{\text{graze}}} \\ y_i \\ -x_i \frac{\sin^2\theta_{\text{exit}}}{\sin\theta_{\text{graze}}} \end{pmatrix}.$$

Finally, to obtain x_e and y_e we have to transform into the outgoing ray's basis,

$$\begin{pmatrix} x_e \\ y_e \\ 0 \end{pmatrix} = \mathbf{M}_{out}^{-1}\mathbf{OB} = \begin{pmatrix} -\frac{\sin\theta_{\text{exit}}}{\sin\theta_{\text{graze}}} x_i \\ y_i \\ 0 \end{pmatrix}. \tag{6}$$

Putting all the results together, the transformation in 4-dimensional phase space is

$$\begin{pmatrix} x_e \\ x_e' \\ y_e \\ y_e' \end{pmatrix} = \begin{bmatrix} \frac{1}{b'} & 0 & 0 & 0 \\ 0 & b' & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{pmatrix} x_i \\ x_i' \\ y_i \\ y_i' \end{pmatrix}, \qquad b' = -\frac{\sin\theta_{\text{graze}}}{\sin\theta_{\text{exit}}}.$$

D. Wavelength dependence of x'

Consider Eq. (5). If we introduce a difference in wavelength, we can rewrite Eq. (5) as

$$x_e' \sin\theta_{\text{exit}} + x_i' \sin\theta_{\text{graze}} + \cos\theta_{\text{exit}} - \cos\theta_{\text{graze}} = \frac{\lambda + \triangle\lambda}{d} \sin\alpha.$$

Eq. (4) can be substracted from this equation to obtain

$$x'_e \sin\theta_{\rm exit} + x'_i \sin\theta_{\rm graze} = \frac{\triangle\,\lambda}{\lambda}\frac{\lambda}{d}\sin\alpha. \tag{7}$$

Using Bragg's Law,

$$x'_e = -x'_i \frac{\sin\theta_{\rm graze}}{\sin\theta_{\rm exit}} + \frac{\triangle\,\lambda}{\lambda}\frac{2\sin\alpha\cos\theta_B}{\sin\theta_{\rm exit}}\tan\theta_B.$$

If we make the same approximation as above that the deviation from the Bragg angle is small,

$$\begin{aligned} x'_e &= -x'_i \frac{\sin\theta_{\rm graze}}{\sin\theta_{\rm exit}} + \frac{\triangle\,\lambda}{\lambda}\frac{\sin\theta_{\rm graze}-\sin\theta_{\rm exit}}{\sin\theta_{\rm exit}}\tan\theta_B \\ &= bx'_i - \frac{\triangle\,\lambda}{\lambda}(1+b)\tan\theta_B. \end{aligned}$$

This reproduces the result in Matsushita and Kaminaga [5].

III. GENERAL ASYMMETRIC BRAGG REFLECTION

A. Finding the Reference Trajectory

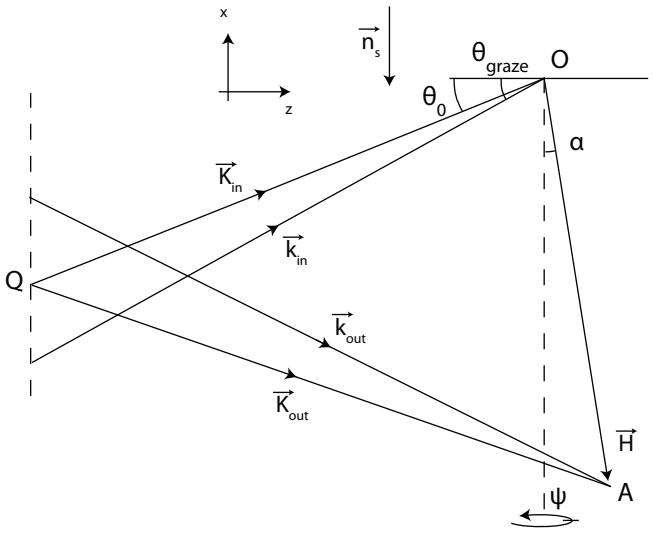

Figure 2: Diagram showing the construction in reciprocal space to find the directions of the center of reflection. All points shown in the diagram are in the plane of the paper, except for the point A. The y-axis points out of the plane of the paper.

As before, we require the reference trajectory to occur at the center of reflection. To find the center of reflection, we follow the construction in reciprocral space shown in Fig. 2. The point Q is sometimes known as the Lorentz point, which is the centre of the hyperboloid describing the dispersion surface. We shall work in the basis where the crystal normal is given by $\begin{pmatrix}-1\\0\\0\end{pmatrix}$ and the incoming reference ray is in the x-z plane. This is the element coordinate system. In reciprocral space, the lengths of the vectors are known,

$$|\mathbf{k_{out}}| = |\mathbf{k_{in}}| = \frac{1}{\lambda},$$

$$|\mathbf{K_{out}}| = |\mathbf{K_{in}}| = \frac{1}{\lambda(1+\delta)}.$$

where $\delta = \frac{\lambda^2}{2}\frac{r_e}{\pi V}|F_0|$ gives the average refractive index's deviation from unity in terms of r_e, the classical electron radius. The angle ψ defines the direction of $\mathbf{H}$: ψ in $(0, \pi)$ causes $\mathbf{H}$ to have a positive y-component in the crystal basis.

$$\mathbf{H} = \frac{1}{d}\begin{pmatrix} -\cos\alpha \\ \sin\alpha\sin\psi \\ \sin\alpha\cos\psi \end{pmatrix} \tag{8}$$

Now, we can form a vector equation with triangle OQA,

$$\begin{aligned} \mathbf{QA} &= \mathbf{QO} + \mathbf{H} \\ \begin{pmatrix} b_1 \\ b_2 \\ \sqrt{1-b_1^2-b_2^2} \end{pmatrix} &= \begin{pmatrix} \sin\theta_0 \\ 0 \\ \cos\theta_0 \end{pmatrix} + \frac{\lambda(1+\delta)}{d}\begin{pmatrix} -\cos\alpha \\ \sin\alpha\sin\psi \\ \sin\alpha\cos\psi \end{pmatrix}. \end{aligned}$$

b_1 and b_2 can be eliminated, allowing us to find the angle of the wavevector in the crystal, θ_0, by solving the equation

$$\frac{\lambda(1+\delta)}{2d} = \cos\alpha\sin\theta_0 - \sin\alpha\cos\psi\cos\theta_0, \tag{9}$$

which gives

$$\theta_0 = \sin^{-1}\frac{\lambda(1+\delta)}{2d\sqrt{1-\sin^2\alpha\sin^2\psi}} + \tan^{-1}(\tan\alpha\cos\psi).$$

Note that θ_0 must lie in the first quadrant. The required graze angle is therefore

$$\theta_{\text{graze}} = \cos^{-1}\frac{\cos\theta_0}{1+\delta}. \tag{10}$$

We also need to determine the outgoing reference ray vector, $\mathbf{k_{out}} = \begin{pmatrix} k_{out_1} \\ k_{out_2} \\ k_{out_3} \end{pmatrix}$. Two of the components should equal to the corresponding components in $\mathbf{QA}$,

$$\begin{aligned} k_{out_2} &= \frac{1}{d}\sin\alpha\sin\psi, \\ k_{out_3} &= \frac{1}{d}\sin\alpha\cos\psi + \frac{1}{\lambda(1+\delta)}\cos\theta_0. \end{aligned}$$

so k_{out_3} is simply the value which causes the vector have a magnitude of $\frac{1}{\lambda}$,

$$\mathbf{k_{out}} = \begin{pmatrix} -\sqrt{\frac{1}{\lambda^2} - k_{out_2}^2 - k_{out_3}^2} \\ k_{out_2} \\ k_{out_3} \end{pmatrix}. \tag{11}$$

The negative square root is taken as the reflection is expected to travel out of the crystal.

B. Local Coordinate Systems

The incoming coordinate basis matrix can be specified by writing down a matrix $\mathbf{M}_{in}$ in the crystal coordinate system,

$$\begin{aligned} \mathbf{M}_{in} &= \begin{bmatrix} \mathbf{x_{in}} & \mathbf{y_{in}} & \hat{\mathbf{k}_{\mathbf{in}}} \end{bmatrix} \\ &= \begin{bmatrix} \cos\theta_{\text{graze}} & 0 & \sin\theta_{\text{graze}} \\ 0 & 1 & 0 \\ -\sin\theta_{\text{graze}} & 0 & \cos\theta_{\text{graze}} \end{bmatrix}. \end{aligned}$$

Due to the asymmetric cut of the crystal, the outgoing reference ray may have an out of plane component. We will account for the out of plane component by making a correction to the tilt, which is a rotation about $\mathbf{k_{in}}$. A rotation

by the angle θ about this axis is represented by the matrix $\mathbf{M}_{in} \cdot \left[\begin{smallmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{smallmatrix}\right] \cdot \mathbf{M}_{in}^{-1}$, so in order to find θ_{tiltcorr}, we solve

$$\left(\mathbf{M}_{in} \cdot \left[\begin{smallmatrix} \cos\theta_{\text{tiltcorr}} & \sin\theta_{\text{tiltcorr}} & 0 \\ -\sin\theta_{\text{tiltcorr}} & \cos\theta_{\text{tiltcorr}} & 0 \\ 0 & 0 & 1 \end{smallmatrix}\right] \cdot \mathbf{M}_{in}^{-1} \cdot \mathbf{k_{out}}\right) \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

to obtain

$$\theta_{\text{tiltcorr}} = \tan^{-1} \frac{k_{out_2}}{k_{out_3} \sin\theta_{\text{graze}} - k_{out_1} \cos\theta_{\text{graze}}}. \tag{12}$$

This angle should be subtracted from the total tilt angle to determine how the crystal is oriented, and in effect, is a correction to the tilt to remove the out of plane component. This means that an additional tilt correction rotation should be applied to the incoming vectors, so that

$$\begin{pmatrix} x_i \\ y_i \end{pmatrix} = \begin{bmatrix} \cos\theta_{\text{tiltcorr}} & \sin\theta_{\text{tiltcorr}} \\ -\sin\theta_{\text{tiltcorr}} & \cos\theta_{\text{tiltcorr}} \end{bmatrix} \cdot \begin{bmatrix} \cos\theta_{\text{tilt}} & \sin\theta_{\text{tilt}} \\ -\sin\theta_{\text{tilt}} & \cos\theta_{\text{tilt}} \end{bmatrix} \cdot \mathbf{x}.$$

Similar rotations should be performed for $\mathbf{x}'$.

Furthermore, the correct definition of $\mathbf{M}_{out} = \left[\begin{smallmatrix} \mathbf{x_{out}} & \mathbf{y_{out}} & \hat{\mathbf{k}}_{\mathbf{out}} \end{smallmatrix}\right]$ in the crystal coordinate basis should have the second basis vector rotated by θ_{tiltcorr} around the axis defined by $\mathbf{k_{in}}$, as compared to $\mathbf{y_{in}}$. Note that if $\theta_{\text{tiltcorr}} = 0$, $\mathbf{y_{in}} = \mathbf{y_{out}}$.

$$\begin{aligned} \mathbf{y_{out}} &= \mathbf{M}_{in}^{-1} \cdot \begin{bmatrix} \cos\theta_{\text{tiltcorr}} & -\sin\theta_{\text{tiltcorr}} & 0 \\ \sin\theta_{\text{tiltcorr}} & \cos\theta_{\text{tiltcorr}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \mathbf{M}_{in} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\ \mathbf{x_{out}} &= \mathbf{y_{out}} \times \hat{\mathbf{k}}_{\mathbf{out}} \end{aligned}$$

C. Rays that are off-axis

Rays that travel off the optical axis are defined in phase space using the local coordinate system of the beam. The relationship between the incoming and outgoing rays are still governed by the boundary condition that the component of the wavevectors parallel to the surface should be the same. This is equivalent to requiring

$$\mathbf{k}_e - \mathbf{k}_i = N\hat{\mathbf{n}}_s + \mathbf{H}. \tag{13}$$

$\mathbf{k_i}, \mathbf{k_e}$ are not necessarily in the direction of the reference beam, for which different subscripts (in, out) are used in our notation. We would like to work in the crystal normal basis as in Section 2, so the phase space vectors have to be transformed into this coordinate system,

$$\mathbf{M}_{out} \cdot \begin{pmatrix} x_e' \\ y_e' \\ 1 \end{pmatrix} - \mathbf{M}_{in} \cdot \begin{pmatrix} x_i' \\ y_i' \\ 1 \end{pmatrix} = \lambda \begin{pmatrix} N \\ 0 \\ 0 \end{pmatrix} + \lambda \mathbf{H},$$

where we make the assumption that the angular deviation from the reference direction is small ($x', y' \ll 1$). This can be solved with

$$N = \frac{1}{\lambda \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \mathbf{M}_{out}^{-1} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}} \left[1 - \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \cdot \mathbf{M}_{out}^{-1} \cdot \left(\lambda \mathbf{H} + \mathbf{M}_{in} \cdot \begin{pmatrix} x_i \\ y_i \\ 1 \end{pmatrix}\right)\right], \tag{14}$$

$$\begin{pmatrix} x_e' \\ y_e' \\ 1 \end{pmatrix} = \mathbf{M}_{out}^{-1} \left(\lambda \begin{pmatrix} N \\ 0 \\ 0 \end{pmatrix} + \lambda \mathbf{H} + \mathbf{M}_{in} \cdot \begin{pmatrix} x_i \\ y_i \\ 1 \end{pmatrix}\right). \tag{15}$$

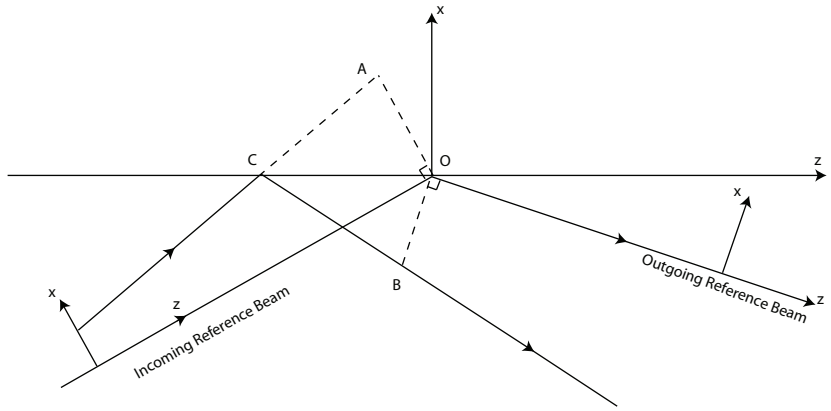

Figure 3: Diagram showing reference and off-axis rays in real space. In this diagram, only the incoming reference beam has to be in the plane of the paper; points A,B,C are not necessarily in the x-z plane.

To find the change in position in phase space, we consider the geometry shown in Fig. 3. The problem is to find OB in the outgoing reference basis as a function of OA in the incoming reference basis.

$$\begin{aligned}\mathbf{OC} &= \mathbf{OA} + \mathbf{AC} \\ &= \mathbf{M}_{in} \cdot \begin{pmatrix} x_i \\ y_i \\ 0 \end{pmatrix} + n\hat{\mathbf{k}_\mathbf{i}} \\ &= \mathbf{M}_{in} \cdot \begin{pmatrix} x_i \\ y_i \\ 0 \end{pmatrix} + n\mathbf{M}_{in} \cdot \begin{pmatrix} x_i' \\ y_i' \\ 1 \end{pmatrix}\end{aligned}$$

where n is an unknown with units of length. One can solve for $\mathbf{OC}$ using the condition that $\mathbf{OC} \cdot \hat{\mathbf{n}_\mathbf{s}} = 0$, so that

$$n = -\frac{\hat{\mathbf{n}_\mathbf{s}} \cdot \mathbf{M}_{in} \cdot \begin{pmatrix} x_i \\ y_i \\ 0 \end{pmatrix}}{\hat{\mathbf{n}_\mathbf{s}} \cdot \mathbf{M}_{in} \cdot \begin{pmatrix} x_i' \\ y_i' \\ 1 \end{pmatrix}}. \tag{16}$$

One can use the same method to find $\mathbf{OB} = \mathbf{OC} + m\hat{\mathbf{k}_\mathbf{e}}$, where m has units of length. The corresponding condition is that

$$\mathbf{OB} \cdot \hat{\mathbf{k}_\mathbf{out}} = 0$$

which gives

$$m = -\frac{\hat{\mathbf{k}_\mathbf{out}} \cdot \mathbf{OC}}{\hat{\mathbf{k}_\mathbf{out}} \cdot \mathbf{M}_{out} \cdot \begin{pmatrix} x_e' \\ y_e' \\ 1 \end{pmatrix}}. \tag{17}$$

Lastly, to obtain x_e, y_e, we do a coordinate transformation to the outgoing ray's basis,

$$\begin{pmatrix} x_e \\ y_e \\ 0 \end{pmatrix} = \mathbf{M}_{out}^{-1}\mathbf{OB}. \tag{18}$$

D. Reflectivity

While the usual methods of ray tracing do not consider effects due to the amplitude of the electric fields (or equivalently, the intensity of radiation), we may calculate the reflectivity of the crystal using dynamical diffraction theory and include the amplitude of the electric fields as another dimension in the phase space of the photons. Here,

we summarize results from Batterman and Cole [2]. One needs to find the parameters ξ_0 and ξ_H,

$$\xi_0 = \frac{\mathbf{K_0}.\mathbf{K_0} - k^2(1-\Gamma F_0)}{2k} \tag{19}$$

$$\xi_H = \frac{\mathbf{K_H}.\mathbf{K_H} - k^2(1-\Gamma F_0)}{2k}, \tag{20}$$

where $\mathbf{K_{0,H}}$ are the wavevectors inside the crystal, $\Gamma = \frac{r_e\lambda^2}{\pi V}$ and $k = \frac{1}{\lambda}$, so that the ratio of the complex amplitudes of the incoming and outgoing waves (from which intensities can be calculated) are

$$\frac{E_H}{E_0} = -\frac{kP\Gamma F_H}{2\xi_H}. \tag{21}$$

P is the factor used to account for differing polarization states. The σ polarization state refers to the case where the electric field vector is perpendicular to the plane of reflection, while the π state refers to the case there the electric field vector is parallel to the plane. With this understanding,

$$P = \begin{cases} 1 & \sigma \text{ polarization state} \\ \cos 2\theta_0 & \pi \text{ polarization state} \end{cases}. \tag{22}$$

The essential result from the theory of dynamical diffraction is that $\mathbf{K_0}$ and $\mathbf{K_H}$ are constrained to lie on the dispersion surface, which is described by

$$\xi_0\xi_H = \frac{1}{4}k^2P^2\Gamma^2F_HF_{\bar{H}}. \tag{23}$$

Keeping in mind the boundary conditions for the incoming wave vector and outgoing wavevector, we can write

$$\mathbf{K_0} = \mathbf{k_i} + qk\hat{\mathbf{n}_s}$$
$$\mathbf{K_H} = \mathbf{k_i} + \mathbf{H} + qk\hat{\mathbf{n}_s}$$

where $\mathbf{k_i} = k\mathbf{M}_{out} \cdot \begin{pmatrix} x_i' \\ y_i' \\ 1 \end{pmatrix}$ and q is, in general, a complex number in order to account for absorption. Under the assumption that $|q| \ll 1$ (which is the assumption that refraction effects are small), one can expand Eqs. (19) and (20) to first order in q, which yields

$$\xi_0 = q\mathbf{k_i}\cdot\hat{\mathbf{n}_s} + \frac{k\Gamma F_0}{2} \tag{24}$$

$$\xi_H = q(\mathbf{k_i}+\mathbf{H})\cdot\hat{\mathbf{n}_s} + \frac{k\Gamma F_0}{2} + \frac{H^2 + 2\mathbf{k_i}\cdot\mathbf{H}}{2k}. \tag{25}$$

Substitution into Eq. (23), neglecting terms in q^2 and solving for q, we obtain

$$q = \frac{k^2\Gamma^2(F_HF_{\bar{H}}P^2 - F_0^2) + \Gamma F_0(H^2 + 2\mathbf{k_i}\cdot\mathbf{H})}{2k\Gamma F_0(2\mathbf{k_i}+\mathbf{H})\cdot\hat{\mathbf{n}_s} + \frac{2}{k}\mathbf{k_i}\cdot\hat{\mathbf{n}_s}(H^2 + 2\mathbf{k_i}\cdot\mathbf{H})}. \tag{26}$$

This should be substituted back into Eqs. (25) and (21) to obtain the ratio of the outgoing to incoming electric fields. The reflectivity should be the absolute value squared of this ratio,

$$R = \left|\frac{E_H}{E_0}\right|^2. \tag{27}$$

E. Change in phase

The relative change in path length for an off-axis ray, compared to the reference ray, is $n + m$. In addition, there will be a phase change due to refraction effects, and this difference should be added to the total relative path, which

gives

$$\triangle\ z = n + m + \lambda \left(\arg \frac{E_H}{E_0} \right). \tag{28}$$

IV. DISCUSSION

The above results have been incorporated into BMAD under several subroutines. Typically, a user would specify the crystal type and reflection in terms of Miller indices (h,k,l), and so the subroutine `crystal_type_to_crystal_params` calculates the relevant input parameters as given in Table 1. The subroutine `crystal_attribute_bookkeeper` then calculates the orientation of the outgoing reference ray and associated coordinate systems. Finally, off-axis rays are propagated by the subroutine `track1_bmad`.

V. ACKNOWLEDGEMENTS

I would like to acknowledge Kenneth Finkelstein and David Sagan for their guidance throughout this project. Thanks also goes to Georg H. Hoffstaetter for initiating this work and putting us in touch, as well as all others who made the REU program possible, including Ivan Bazarov, Lora Hine, Monica Wesley. This work was supported in part by the Rawlings Cornell Presidential Research Scholarship, and in part by the National Science Foundation REU grant PHY-0849885.

Appendix A: NOMENCLATURE

λ	Wavelength of reference photon in vacuum
E_{ref}	Energy of the reference photon
α	Asymmetry angle; angle between the lattice normal and crystal surface normal
b	Asymmetry parameter
ψ	Angle with which the crystal is rotated about the crystal surface normal
d	interplanar spacing of the hkl reflection
$\mathbf{H}$	lattice vector $\begin{pmatrix} h \\ k \\ l \end{pmatrix}$ in reciprocal space, $\lvert\mathbf{H}\rvert = \frac{1}{d}$
F_0, F_0', F_0''	Structure factor for H=0, real part, imaginary part
F_H	Structure factor of the hkl reflection (can be complex)
V	Volume of a unit cell
δ	Average deviation of index of refraction from unity
Γ	$\frac{r_e \lambda^2}{\pi V}$
θ_B	Bragg Angle
θ_0	Angle between incoming wavevector inside the crystal and crystal surface
$\mathbf{M}_{in}, \mathbf{M}_{out}$	Basis matrices for incoming and outgoing coordinate systems
$\mathbf{k_{in}}, \mathbf{k_{out}}$	Incoming and outgoing reference wavevectors outside crystal
$\mathbf{k_i}, \mathbf{k_e}$	Off-axis wavevectors
$\mathbf{K_{in}}, \mathbf{K_{out}}$	Wavevectors inside crystal
P	Factor accounting for polarization states of the incoming radiation

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