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The optics of focusing bent-crystal monochromators on X-ray powder diffractometers with application to lattice parameter determination and microstructure analysis

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Abstract

The use of an Incident Beam Monochromator (IBM) in an X-ray powder diffractometer modifies both the shape of the spectrum from the X-ray source, and the relation between the apparent diffracted angle and the actual wavelength of the X-ray. For high-accuracy work, the traditional assumption of a narrow line of typically Gaussian shape does not suffice. Both the shape of the tails of peaks, and their width, can be described by a new model which couples the dispersion from the optic to the dispersion from the powder sample, and to its transport to a detector. This work presents such a model, and demonstrates that it produces excellent fits via the Fundamental Parameter Approach, and requires few free parameters to achieve this. Further, the parameters used are directly relatable to physical characteristics of the diffractometer optics. This agreement is critical for the evaluation of high-precision lattice parameters and crystal microstructural parameters by powder diffraction.

I. INTRODUCTION

The use of monochromators on powder diffractometers greatly simplifies the shape of a powder diffraction pattern by removing extraneous emission lines, such as the Ka_2 line in the copper emission spectrum that lies quite close to Ka_1 and creates doubled peaks. It also simplifies microstructural analysis of powders by trimming the very long intrinsic Lorentzian tails of an atomic emission line. The use of bent-crystal monochromators for X-ray diffraction work dates at least to Johann's work with singly-bent crystals in 1931 [1]. It was quickly followed by the spherical-aberration-free crystals of Johansson in 1933 [2]. Over the years, numerous papers have been published on the properties of the spectrum passed by such a crystal ([3-5], *e.g.*).

By considering the system of monochromator and powder sample together as a special case of a two-crystal monochromator, one arrives at a new, more complete description of its behavior. In a diffractometer of Bragg-Brentano geometry, there are two effects which are not completely accounted for in the earlier literature. First, the spectrum passed by any crystal is dispersed; the direction of the center of the x-ray beam is correlated with the x-ray wavelength, and this dispersion will be shown to modify the line profile of powder

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diffraction peaks. Second, the effects of the finite size of the x-ray source is not taken into account, and it will be shown to be the primary factor setting the bandwidth of the transmitted spectrum.

We present, then, a detailed model of the behavior of a Johansson optic in a Bragg-Brentano diffractometer. The model will be compared to ray-tracing Monte Carlo calculations and to data from the NIST Divergent Beam Diffractometer (DBD) [6]. This model yields improved fits of the line shape across the 2θ diffraction angle range, and thus will result in improved consistency of the apparent lattice parameter when measured from each of the reflections in the pattern, as compared to the global optimum from a least-squares Pawley [7] fit. The model is suitable for computing the shape of powder diffraction lines using the Fundamental Parameters Approach (FPA) to powder diffraction [8-12] to model the Instrument Profile Function (IPF). It introduces a correction for the crystal dispersion and a semi-empirical passband which scales the well-known atomic emission spectrum by a shape which can be estimated from the Monte Carlo results and refined on the pattern of a material with very sharp lines, such as SRM 660 [13].

Because of the dependence of the models provided on dynamical diffraction theory and computation, we provide as supplementary data code that implements the dynamical diffraction methods of Batterman and Cole [14] in an efficient way, in the form of components which work with the McX-Trace Monte-Carlo code [15]. We also provide a macro for the Topas 5¹ code for analysis of diffraction patterns [16] which implements this model.

II. THEORY

A. Dispersion

A typical Bragg-Brentano instrument with a Johansson [2] IBM acts as a 2-crystal “+—” monochromator, per figure 15.8 of Authier [17] (*e.g.*). A sketch of a system representative of what we are describing is in figure 1. A Johansson monochromator crystal, or other focusing or collimating optic, is bent so that the lattice curvature results in the Bragg condition being satisfied across the entire face of the crystal for rays emanating from any point near the Rowland circle. Therefore, the outgoing angle θ_m of a beam of wavelength λ from the crystal is just the Bragg diffraction angle from the optic lattice with spacing d_m which satisfies $\lambda = 2d_m \sin \theta_m$. If θ_s is the Bragg angle of the specimen, and $2\theta(\lambda)$ is the traditional outgoing angle $2\theta_s(\lambda) - \theta_m(\lambda) + \theta_m(\lambda_0)$ of the beam from the specimen surface (where λ_0 is the central wavelength of the system), the purely angular dispersion of this system derived by differentiating Bragg’s law with respect to λ , is

$$\frac{d(2\theta)}{d\lambda} = \frac{1}{\lambda}(2 \tan \theta_s - \tan \theta_m). \quad (1)$$

¹Certain commercial equipment, instruments, or materials are identified in this paper in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the U.S. government, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

However, this is not the complete description of the relation between the wavelength and the diffraction angle which is inferred from where such a ray intersects either a receiving slit or a pixel on a position-sensitive detector. The apparent outgoing angle $2\theta_{\text{apparent}}$, which is the angle usually recorded by diffractometer software, is the angle relative to the diffractometer axis at which an outgoing diffracted ray crosses the Rowland circle; many well-known aberrations such as sample transparency, sample height, and flat-specimen corrections affect this. Examining figure 1, one can see the transverse offset x of the beam from the monochromator onto the sample due to the dispersion of the monochromator as the difference between where the solid green line and the dashed green line cross the sample surface. The range of allowed x values is limited by a combination of the rocking curve width of the monochromator crystal and the source size; this is discussed in more detail in section II B. This produces a displacement in $2\theta_{\text{apparent}}$ of x/R where R is the distance from the sample center to the detector. The distance x can be computed from the dispersion of the monochromator and the distance D between the monochromator crystal and the sample center:

$$\frac{d\Delta x}{d\lambda} = \frac{1}{\lambda} D \tan \theta_m \quad (2)$$

and, converting this to an apparent angle offset and combining with eq. 1 result in:

$$\frac{d(2\theta_{\text{apparent}})}{d\lambda} = \frac{1}{\lambda} \left(2 \tan \theta_s + \left(\frac{D}{R} - 1 \right) \tan \theta_m \right). \quad (3)$$

For the specific case of a Johansson optic, which is set up with a focus at a distance b_m from the crystal, and a distance R from this focus to the sample (so the system is parafofocussing), the distance D from the crystal to the sample is $D = b_m + R$ and eq. 3 becomes

$$\frac{d(2\theta_{\text{apparent}})}{d\lambda} = \frac{1}{\lambda} \left(2 \tan \theta_s + \frac{b_m}{R} \tan \theta_m \right). \quad (4)$$

This, then, allows one to compute the shape of the diffracted spectrum (ignoring other instrumental and sample convolutions) as a function of diffraction angle $2\theta_{\text{apparent}}$ in the region of the reflection from a lattice plane. If the spectrum, as will be computed in the next section, has an intensity distribution $I(\lambda)$, then the diffracted intensity $I'(2\theta_{\text{apparent}})$ from a lattice plane with spacing d_{hkl} in a region centered at $2\theta_{hkl}$, will be:

$$I'(2\theta_{\text{apparent}}) \propto I \left(2d_{hkl} \sin \theta_{hkl} \left(1 + \frac{(2\theta_{\text{apparent}} - 2\theta_{hkl})}{2 \tan \theta_{hkl} + \frac{b_m}{R} \tan \theta_m} \right) \right). \quad (5)$$

B. Passband

If a single crystal (bent or not) is illuminated with a source of x-rays, the characteristics of the Bragg-diffracted radiation is described in full generality by dynamical x-ray diffraction theory, as presented in the modern treatment in Batterman and Cole [14]. In the simple case

of a perfectly collimated, broadband beam on a crystal with low x-ray absorption, the theory of Darwin [18] gives a shape of the reflected spectrum. For a real source, the effects of finite source size and angular spread of the beam at different positions on the crystal surface result in a wider range of transmitted wavelength (passband) than predicted by simple Darwin theory. This has been recognized and modeled in the past in less detail, for example, in [19]. To determine the passband, we split this problem into two parts: an analytic estimate of the passband width, from a purely geometrical view, and a parametric model of its actual shape, supported by comparison to a Monte Carlo ray-tracing model of a diffractometer.

1. Passband width—First, we estimate the width of the passband. If the x-ray source has a full width w in the diffracting plane of the monochromator, and lies a distance a_m from the monochromator, one can apply the dispersion relation $\theta = \lambda \tan \theta_m / \lambda$ to get the full width δ_0 of the transmitted spectrum, ignoring the dynamical width and any aberrations (such as axial divergence on the IBM crystal) which influence it:

$$\delta_0 \equiv \frac{\Delta\lambda}{\lambda} = \frac{w}{a_m \tan \theta_m}. \quad (6)$$

2. Passband profile—Next, we need the shape for the passband. This is, in general, very difficult to compute, since it involves all of the optics of the system, both before and after the IBM crystal. To first order, it should be the convolution of the shape of the dynamical rocking curve for the IBM crystal with the shape of the x-ray source in the diffraction plane of the IBM. However, the axial divergence and behavior of the beam across slits modifies this, to the point that an analytical model is not practical.

Therefore, we will carry out a full ray tracing of a typical system, and seek a parametric model for the spectrum shape which can be applied in FPA codes for the analysis of data. We do this using McXTrace [15, 20] extended with some locally-developed models described in the Appendix. The system on which we base the ray tracing is the NIST DBD [6], which has a focal distance $R = 217.5\text{mm}$, a Ge 111 IBM operating at $\theta_m = 13.635^\circ$, an object distance for the IBM of $a_m = 119\text{mm}$ and an image distance $b_m = 217.5\text{mm}$. It is coincidental that the image distance is the same as the focal length of the machine. The source we model is a copper fine-focus line of length 8mm and a nominal width $w = 40\text{ }\mu\text{m}$. This instrument is likely to be fairly typical in these parameters, such that the parametric model we provide may be directly useful on other instruments, with only adjustment of the instrument-specific parameters.

Figure 1 shows the basic layout of the machine we simulate. For a Johansson optic [2], given the object distance a_m and the image distance b_m , and the Bragg angle θ_m , one can calculate the lattice radius of curvature R_1 by solving the appropriate angles of rays from a cylindrical surface; if θ_a is the angle on the incoming side from the surface, and θ_b is the angle on the outgoing side, and $\theta_a + \theta_b = 2\theta_m$ and $\theta_a - \theta_b = \alpha$ which is the asymmetry angle, we define $x = a_m/b_m$.

$$\begin{aligned}
\cos \theta_a &= \frac{1 + x \cos 2\theta_m}{\sqrt{1 + x^2 + 2x \cos 2\theta_m}} \\
\sin \theta_a &= \frac{x \sin 2\theta_m}{\sqrt{1 + x^2 + 2x \cos 2\theta_m}} \\
\sin \theta_b &= \frac{\sin \theta_a}{x} \\
R_1 &= \frac{a_m}{\sin \theta_a}.
\end{aligned} \tag{7}$$

The surface radius of curvature $R_m = R_1/2$ for a Johansson optic. The lattice planes are rotated counterclockwise around the center of the surface of the crystal by an angle α_m relative to the surface. These equations are explicitly included in the sample code provided.

For the passband simulations, we use a source with a constant spectral distribution instead of the copper atomic emission spectrum, since this maps the output intensity directly to the passband. The sample is removed in this simulation, and the detector arm is moved to place the detector in the direct beam. The detector is an ideal energy detector in the place of what normally would be a silicon position-sensitive detector (SiPSD). Figure 2 shows the result of these simulations for various sizes w of the x-ray source, plotted against energy instead of wavelength as would be used in equation 5. The curve labeled “no divergence” uses a completely collimated beam from the source, and is essentially the rocking curve of the IBM. The curve with $w = 0$ shows the small broadening due to axial divergence. The $w = 40 \mu\text{m}$ curve is appropriate for the nominal source size of our x-ray tube. The $w = 80 \mu\text{m}$ curve shows the shape with further broadening.

The parametric model presented here is based on noting that the tails of the rocking curve look much like the Lorentzian (*i.e.* $1/(x^2 + a^2)$) tails of a Darwin rocking curve. Convolution of a Lorentzian with a rectangular function of width δ_0 representing the x-ray source size results in a function which involves arctan. If we define

$$\zeta(u) = \arctan\left(\frac{u - u_0\delta_0 + \delta_0/2}{\delta_3\delta_0}\right) - \arctan\left(\frac{u - u_0\delta_0 - \delta_0/2}{\delta_3\delta_0}\right), \tag{8}$$

with adjustable parameters of δ_0 (which sets the width of the flat top and should be close to the physically predicted value from eq. 6), δ_3 , which sets the width of the Lorentzian model of the Darwin curve, and u_0 , which is the tuning error of the crystal from the center of the peak (in units of the passband). δ_3 , with the formula written as above, is also in units of the passband width, and should be roughly $\delta_3 \approx (\delta_D/2)/\delta_0$, where δ_D is the Darwin full-width at half maximum; δ_3 is about 0.1 for the NIST DBD.

Stable and physically reasonable values for δ_0 and δ_3 can be easily determined by refining a powder pattern of a material with sharp lines and no microstrain broadening, such as SRM 660c or SRM 640e [13, 21], using the FPA [9-12]. Materials with significant microstrain are not good candidates for this refinement, since the width of a line due to microstrain scales with $\tan \theta_s$, which is not linearly independent of the $\tan \theta_s$ in eq. 4.

The effect of this passband model on the X-ray spectrum incident on a sample is shown in figure 3. Because the passband for our system is significantly wider than the $\text{CuK}\alpha_1$ emission complex, the resulting spectrum has that peak transmitted nearly unmodified, but more remote peaks mostly cut off. This has the useful property that the position of that peak is not strongly influenced by modest mistuning of the crystal (such that the transmitted intensity is within a few percent of its peak). If the passband were narrower than the peak being filtered, the centroid of the peak would follow the mistuning of the crystal, and potentially be less stable if the crystal or source move. For the purposes of metrological traceability, this is important since the invariant characteristics of the emission line dominate the shape of the spectrum, rather than the details of the tuning of the crystal.

III. COMPARISON TO POWDER DIFFRACTION DATA

In this section, we will carry out comparisons between our models and data. We will use the FPA to model the IPF of the instrument and the sample characteristics. We will compare FPA peak models computed in Bruker Topas 5 to measured line shapes, using both the dispersion and passband described above, for LaB_6 SRM 660b [22]. SRM 660b (and later revisions) has sharp lines due to its large crystallite size and lack of strain, and very high linear attenuation, so that its line shapes are not perturbed by microstructural aberrations or sample packing. A “good” model is one which provides both low residuals (good χ^2) for the fit, and for which the resulting fitting parameters are physically meaningful.

In figure 4, we show details of three regions of 2θ space, which highlight different characteristics of the fit and spectral model. The extracted parameters from the fits are compared in table I. In the low-angle range (figure 4a), the peak is highly asymmetric due to axial divergence and flat-specimen effects; more critically, the $\tan \theta_m$ term in equation 4, which is independent of the diffraction angle, adds to the expected width of the peak, even though the $\tan \theta_B$ term is quite small. In the mid-angle region (figure 4b), the axial divergence term approaches zero, and the flat specimen correction is quite small. The peaks are almost symmetrical, and most of the width results from the spectral broadening combined with real material parameters such as transparency and crystallite size. At high angles (figure 4c), the powder contribution to the spectral broadening dominates, along with some axial divergence.

Another test for the quality of the fits is a d plot, which shows “pulling” of peak positions from the values calculated from the lattice parameters when the peaks are allowed to move independently. This is implemented by computing a Pawley [7] fit to determine the lattice parameter d_0 of the material and any other material and machine parameters, and then freezing all the parameters while allowing the peaks to move independently. If the resulting fit yields a position $2\theta_{hkl}$ (in radians) for the peak indexed by hkl which is associated with a d -spacing d_{hkl} and $\theta_B(d_0, hkl)$ is the Bragg angle from the Pawley fit, the quantity

$$\Delta d_0 \equiv d_0 \frac{\Delta d_{hkl}}{d_{hkl}} = -d_0 \frac{(\theta_{hkl} - \theta_B(d_0, hkl))}{\tan \theta_{hkl}} \quad (9)$$

is the apparent shift in the lattice parameter d_0 that would be calculated based on the $hk\ell$ peak by itself. Figure 5 shows the results of this, with the results scaled to femtometers. The error bars displayed are pure 1σ statistical errors from the fitting procedure. The systematic oscillations in this result are of unknown origin, but are much smaller than the uncertainties on the lattice parameter of this material quoted in its certificate.

Finally, we compare computed microstructural parameters, using the FPA, from SRM 1979 [23], a set of ZnO powders with two different nanometer-scale crystallite size distributions. This material was analyzed on the DBD and on a synchrotron at APS 11BM Wang et al. [24]; because of the optical properties (very low axial divergence and energy spread $E/E \approx 10^{-4}$) of the synchrotron beam, the microstructure derived from it can be considered definitive. The NIST DBD has been assumed to have marginal resolution to correctly measure the size distribution of the large ('75 nm') crystallites from SRM 1979; see figure 5 of [25], which was computed using the *ad hoc* multi-Gaussian model of [6]. However, using this model, the situation for the large crystallites, which are most sensitive to peak shape errors, since they have the narrowest peaks, is significantly improved. In table II, we show the comparison. Note that the volume-weighted mean crystallite size $\langle L \rangle_{\text{vol}}$ is most sensitive to the overall peak shape, since it depends on high-frequency components in Fourier-transform space. The fact that the DBD result for $\langle L \rangle_{\text{vol}}$ now approaches the high-resolution result from the synchrotron implies the line shape is very well represented by the models presented in this work, combined with the FPA parameters describing the rest of the DBD.

IV. SUMMARY AND CONCLUSIONS

A new optical model for the behavior of a powder diffractometer with an IBM has been developed. This model incorporates two characteristics of the IBM: the angular dispersion of the beam resulting from the Bragg diffraction from its crystal planes, and the bandwidth limiting of the transmitted radiation due to the interaction of the dynamical diffraction intensity from the crystal and the finite size of the X-ray source. Combining these into an FPA model of the IPF results in high-quality fits to data from samples with even very sharp diffraction peaks. This model will be useful both for high-precision lattice constant measurements of powders, where it reduces the "pulling" of peaks away from their true position, and for microstructure determination, where the agreement of the line shape across the entire angular range on a specimen with very sharp lines implies that the IPF is very well modeled.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

Appendix A:: Description of supplementary data

1. Topas macro

The file "dbd_ibm_setup_atan_20181116.inc" is an example of a Topas [16] macro which implements the model described above for the specific case of the NIST DBD, with the copper $K\alpha_{11}$, $K\alpha_{12}$, $K\alpha_{21}$, and $K\alpha_{22}$ lines included in the spectrum. It should be easily

adaptable to other similar instruments, and also provides a specific example of how to apply this in general.

2. McXTrace sample code

The files in the zip archive “nist-crystals.zip” contain all the components necessary to represent a fairly complete model of the NIST DBD, and are provided to show how the dynamical diffraction calculations in the appendix are implemented. The non-DBD-specific components of these will appear in an upcoming release of McXTrace [15, 20] as part of the official distribution, and in the future should be obtained from there, where they will be maintained.

Appendix B:: Approach to dynamical diffraction

To implement the ray-tracing model, we have developed new dynamical crystal reflection models for the McXTrace [15] code, based on the work of Batterman and Cole [14]; code implementing these are attached as supplementary data. The discussion below is very brief, and assumes that the reader is using it in conjunction with [14]. We provide 3 new models, all based on the discussion below. The first two are for Bragg reflection from a thick crystal, the first for flat crystals and the second which allows bending of the crystal on a single axis, with independent bending of the lattice and the surface (as needed for a Johansson optic) and are nearly identical except for the geometry calculation. The third model computes Laue diffraction (transmission) through a flat crystal; it is based on the same solution to the dispersion relations discussed below, but carries out the interference calculation (which creates Pendellösung fringes) between the two propagated rays.

In a previous work [26], we described a smaller improvement to the McXTrace crystal models, which involved improving already extant algorithms; the method described here is a complete rewrite from the start.

We use an approach based on the exact dispersion relation in equation 17 of [14], and a purely vector computation of the results. The notation we will use follows closely that of [14], with $\vec{k}_0, \vec{k}_H$ being the free-space incoming and diffracted wave vectors, $\vec{k}_0, \vec{k}_H$ being the incoming and diffracted wave vectors in the crystal, $\vec{H}$ being the wave vector perpendicular to the diffraction plane, and $\hat{n}$ being the surface outer normal of the crystal. The dispersion relation is:

$$\begin{vmatrix} k^2(1 - \Gamma F_0) - \vec{K}_0 \cdot \vec{K}_0 & -k^2 P \Gamma F_H \\ -k^2 P \Gamma F_H & k^2(1 - \Gamma F_0) - \vec{K}_H \cdot \vec{K}_H \end{vmatrix} = 0 \quad (\text{B1})$$

This approach deviates from traditional approaches in a number of ways. The primary difference is keeping all the equations in the form of vector dot product relations, so that the results remain explicitly valid for arbitrary off-axis geometries, which is very difficult to achieve in methods which convert the equations into angular space. The second difference is that we use the exact quartic solution to eq. B1, instead of the quadratic approximation

almost universally used. This results in a small correction at very high asymmetries, and is mostly included for formal correctness. Third, no approximate expansion of the solutions are carried out in terms of a rocking curve width around a central Bragg diffraction angle. We present the equations used, which can be seen directly in the code.

The first step of solving for the dynamical diffraction is to find the relationship between all of the wave vectors, including the refraction of the waves at the crystal surface. Using the tangential continuity of electric fields at surfaces, and defining q_0 and q_H to be the discontinuity in the normal component of the incoming and outgoing wave vector, the following must hold:

$$\vec{k}_H = \vec{k}_0 + kq_0\hat{n} + \vec{H} + kq_H\hat{n} = \vec{k}_0 + \vec{H} + k(q_0 + q_H)\hat{n} \quad (\text{B2})$$

and if we define $q = q_0 + q_H$, and solve $\vec{k}_0 \cdot \vec{k}_0 = \vec{k}_H \cdot \vec{k}_H$ (since the incoming and outgoing photons have the same wavelength):

$$k^2q^2 + 2kq(\vec{k}_0 + \vec{H}) \cdot \hat{n} + (2\vec{k}_0 \cdot \vec{H} + H^2) = 0 \quad (\text{B3})$$

for its two real roots kq_1 and kq_2 . We will define kq_2 to be the smaller of these in absolute value, which is the physically real one which represents the small refraction. The code uses a macro which computes both roots of a quadratic equation, in a manner which is always accurate for both roots, to achieve this. kq_2 can then be substituted for $k(q_0 + q_H)$ in eq. B2 to compute $\vec{k}_H$.

Next, given $\vec{k}_0$, $\hat{n}$, P , χ_0 , χ_H , and $\chi_{\bar{H}}$, with $\chi_0 \equiv -\Gamma F_0$, $\chi_H = -\Gamma F_H$, and $\chi_{\bar{H}} = -\Gamma F_{\bar{H}}$, (still in the notation of [14]), and noting that $k(1 - \chi_0) = k_0$ which for $\chi_0 \ll 1$ yields $k^2(1 - \chi_0) \approx k_0^2(1 + \chi_0)$, one defines the on-diagonal terms of eq. B1:

$$\begin{aligned} p_1 &= \left| \vec{k}_0 + kq_0\hat{n} \right|^2 - k_0^2(1 + \chi_0) \\ &= k^2q_0^2 + 2kq_0\vec{k}_0 \cdot \hat{n} - k_0^2\chi_0 \\ p_2 &= \left| \vec{k}_0 + kq_0\hat{n} + \vec{H} \right|^2 - k_0^2(1 + \chi_0) \\ &= p_1 + 2kq_0\vec{H} \cdot \hat{n} + 2\vec{k}_0 \cdot \vec{H} + H^2. \end{aligned} \quad (\text{B4})$$

We then solve eq. B1, rewritten as

$$p_1p_2 = k_0^4P^2\chi_H\chi_{\bar{H}} \equiv \varepsilon, \quad (\text{B5})$$

for its complex roots $(kq_0)_n$ (noting that we never need to explicitly calculate k independently of q). In our code implementation, we first solve approximate quadratics which give roots which are refined with Newton's method to get the exact quartic roots; this could also be achieved by calling a library function which returns quartic solutions directly. This approach allows one to only solve for as many of the quartic roots as needed; in the Bragg case, this is only one root, and for Laue, it is two roots. Also, in the code, the

polarization factor P is called C . Only one of the two small roots of this equation, which we will call $(kq_0)_1$, will have attenuated waves going into the crystal; for Bragg reflection from a thick crystal, this is the correct root. This then permits the calculation of the internal wave vectors $\vec{K}_0 = \vec{k}_0 + (kq_0)_1 \hat{n}$ and $\vec{K}_H = \vec{K}_0 + \vec{H}$. Our current code ignores the second small root, which is necessary to describe leakage through a crystal in Bragg geometry, since the extinction in most typical systems is high compared to the crystal thickness; this may be addressed in future work. We evaluate the polynomials p_1 and p_2 at $kq = (kq_0)_1$. Now, to avoid cancellation and roundoff errors in computing ξ_0 and ξ_H , we define the larger in magnitude of p_1, p_2 as p_l and the smaller as p_s and recompute $p_s = \epsilon/p_l$ since the larger of the two polynomials does not involve delicate cancellation of terms. We then compute $\xi_0 = p_l/(2k_0)$ and $\xi_H = p_s/(2k_0)$. These then are applied as in eq. 24 of [14]:

$$E_H / E_0 = \frac{2\xi_0}{k_0 P \chi_H} \quad (\text{B6})$$

to compute the diffracted field strength. To correct this for the reflection geometry, as needed for the Monte Carlo, this is scaled by the asymmetry parameter b :

$$b = \frac{\vec{K}_0 \cdot \hat{n} / K_0}{\vec{K}_H \cdot \hat{n} / K_H}. \quad (\text{B7})$$

The actual reflection probability (or statistical weight) is then

$$R = \frac{|E_H / E_0|^2}{|b|}. \quad (\text{B8})$$

We then apply the polarization projection technique described in equations 19-21 of [26] to take an arbitrarily polarized incoming beam and produce the correctly polarized outgoing result.

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Figure 1:
Schematic of typical Bragg-Brentano DBD, with parameters labeled for theory section, and as modeled in Monte Carlo model. Black lines are optics; blue are measurements, and green are sample traces of the beam. Drawing is not to scale.

Figure 2:

Computed passbands and parametric models. Note that these are computed with the IBM set to an angle which is not corrected for the dynamical offset, so it is mistuned from the center of $\text{CuK}\alpha_1$. The symbols and the “no divergence” line are Monte-Carlo results with the source size as indicated. The solid lines are the model from equation 8, with best-fit parameters.

Figure 3:

Comparison of transmitted spectrum from a spatially broad source, which approximates the atomic emission spectrum, and the transmitted spectrum from a fairly realistic $w = 40 \mu\text{m}$ wide source. The passband is tuned slightly to the high-energy side of $\text{Cu}K\alpha_1$ to improve rejection of $\text{Cu}K\alpha_2$.

Figure 4:
Comparison FPA fits of LaB₆ diffraction patterns to data.

Figure 5:
Lattice constant bias d_0 from fits to SRM 660 data. See eq. 9 for definition.

Table I:

Comparison of fit parameters between multi-Gaussian model from [6] and the model in this work. Uncertainties quoted are pure 1σ statistical.

parameter ↓	model → theory	multi-Gaussian	this work
adjustable parameters in emission model		8	3
goodness of fit (χ^2/N)		1.13	1.002
attenuation length	$12\ \mu\text{m}$	$68 \pm 1.2\ \mu\text{m}$	$16 \pm 2\ \mu\text{m}$
equatorial beam divergence	0.79°	1.05°	0.86°
Lorentzian crystallite size broadening		$1.6 \pm 0.03\ \mu\text{m}$	$1.8 \pm 0.03\ \mu\text{m}$

Table II:

Comparison of computed microstructural parameters from DBD data to 11BM data. The “11BM” and “DBD cert” columns are from table 5 of the SRM 1979 certificate [23]. The high resolution of the 11BM beamline makes its results definitive for this measurement.

Parameter	11-BM	DBD cert	DBD (this work)
$\langle L \rangle_{\text{area}}$ (nm)	95.4(4)	75.3(9)	80.7(13)
$\langle L \rangle_{\text{vol}}$ (nm)	138.9(6)	97.2(14)	128.3(25)
deformation α	0.000 28(1)	0.000 18(3)	0.000 35(2)
stacking fault β	0.001 57(1)	0.001 64(5)	0.001 47(3)
Strain	0.033 71(11)	0.005 68(40)	0.020 46(23)