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A Bayesian Approach to Rocking-Curve Analysis in Dark-Field X-ray Microscopy

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Abstract. Dark-field X-ray microscopy (DFXM) maps crystal lattice distortions and defects in millimeter-sized samples by recording rocking curves with sub-micrometer spatial resolution. Quantitative analysis is complicated by overlapping diffraction contributions within single voxels, which limits the reliability of standard peak-fitting approaches. Here, we formulate rocking-curve decomposition as a Bayesian inverse problem, jointly inferring the shapes and spatial distributions of distinct diffraction components with uncertainty quantification. The method separates weak-beam and strong-beam contributions, distinguishing regions where defect contrast is enhanced from the central region dominated by dynamical diffraction. The resulting decomposition reduces data complexity and facilitates dislocation identification.

1 Introduction

Dislocations govern the mechanical and functional properties of crystalline materials, carrying plastic deformation and controlling processes such as yielding, hardening, and failure [1], while also influencing electrical conductivity, magnetic response, and diffusion [2]. Most experimental techniques used to study them exploit diffraction contrast: dislocations introduce long-range strain fields that locally tilt lattice planes by small angles, typically milliradians, modifying the diffraction condition relative to that of the ideal crystal and producing measurable contrast.

Transmission electron microscopy (TEM) provides direct observation of dislocation cores at high spatial resolution [3, 4], but its requirement for thin samples limits its applicability to bulk materials. Dark-field X-ray microscopy (DFXM) offers a complementary approach, using Bragg diffraction of high-energy synchrotron radiation to map lattice distortions in bulk samples with sub-micrometer resolution and an angular sensitivity the order of 10^{-4} rad [5] (figure 1). Weak-beam contrast, adapted from TEM [6], further enhances dislocation visibility by probing the tails of the rocking curve [7].

Despite these capabilities, rocking-curve analysis remains challenging when multiple diffraction contributions overlap in angular space. Parametric peak fitting can capture dominant features but struggles with asymmetry and overlapping signals. Mathematical decompositions



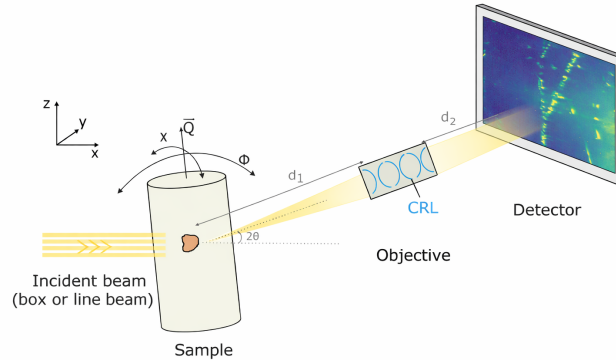


Figure 1: Schematic of a dark-field X-ray microscopy setup. An incident X-ray beam illuminates the sample, and only scattered (diffracted) rays corresponding to a selected Bragg reflection are collected by an objective lens system.

such as principal component analysis [8] or orthogonal basis methods [9] yield compact representations without guaranteed physical meaning, while data-driven approaches including machine learning [10] extract latent structure but are not constrained to correspond to specific diffraction conditions.

In this work, we adopt a different strategy and introduce a Bayesian framework for the decomposition of local rocking curves into physically motivated components associated with strong-beam (SB) and weak-beam (WB) conditions. Within diffraction theory, SB contrast is more strongly influenced by dynamical diffraction, where multiple (non-local) scattering redistributes intensity and complicates interpretation, whereas WB conditions suppress these effects and are better approximated by the kinematic regime. In this limit, lattice tilts shift the Bragg condition toward higher or lower angles, rendering the tails of the rocking curve particularly sensitive to deviations from the ideal lattice while reducing non-local contributions. Rather than enforcing orthogonality or relying on fully agnostic latent representations, the model incorporates prior physical knowledge to guide the decomposition, while explicitly accounting for uncertainty. This approach provides an interpretable alternative to existing methods, enabling the separation of overlapping diffraction contributions and the quantification of their reliability within a unified probabilistic framework.

2 Methodology

In a typical DFXM experiment, the sample is illuminated by either a quasi-parallel box beam or a one-dimensionally focused sheet beam. A diffracting grain or subgrain is brought into Bragg condition, and the diffracted signal passes through an objective lens, typically a compound refractive lens (CRL), forming a magnified real-space image on a far-field detector (figure 1). Only rays corresponding to the selected Bragg reflection contribute to the image. By tilting the diffraction vector relative to the sample, the local crystallographic orientation is scanned through the Bragg condition pixel by pixel, producing a spatially resolved rocking curve. The data used here consist of image series acquired at successive rocking angles for fixed χ and 2θ (figure 1); further experimental setup details can be found in Ref. [11].

The aim is to decompose each local rocking curve into three contributions associated with SB, WB-left, and WB-right. This is formulated within a Bayesian framework, which enables estimation of both the basis functions along the rocking-angle axis and the corresponding spatial coefficient maps, together with their uncertainty estimates. The dataset is written as $I(\phi_k, x, y)$, x and y are real space coordinates (detector pixels) with $x = 1, \dots, H$, $y =$

$1, \dots, W$ and $k = 1, \dots, K$, where ϕ_k denotes the k -th rocking angle. The full rocking-angle range is retained, since the separation of SB, WB-left, and WB-right depends not only on peak positions but also on the overall curve shape and asymmetry.

The data are arranged as a $K \times H \times W$ array. A logarithmic compression is applied, $\tilde{I} = \log(1 + I)$, followed by normalization to the interval $[0, 1]$. The rocking-angle axis is shifted so that the SB condition is approximately centered at $\phi = 0^\circ$, corresponding to the nominal Bragg angle.

A central region of interest (ROI) is used to estimate representative rocking curves with improved signal-to-noise ratio. If the ROI contains N pixels, the data matrix is $\mathbf{I}_{\text{ROI}} \in \mathbb{R}^{K \times N}$. To preserve a positive, intensity-like representation, each curve is transformed by subtracting a pixel-wise baseline and normalizing by its local amplitude:

$$I_{\text{fit}}(\phi_k, i) = \frac{\tilde{I}(\phi_k, i) - \tilde{I}_{\min}(i)}{\tilde{I}_{\max}(i) - \tilde{I}_{\min}(i)}. \quad (1)$$

2.1 Bayesian decomposition

For each pixel i in the ROI, the normalized rocking curve is modeled as a linear combination of three components:

$$I_{\text{fit}}(\phi_k, i) \approx c_{\text{SB}}(i) v_{\text{SB}}(\phi_k) + c_{\text{WB,left}}(i) v_{\text{WB,left}}(\phi_k) + c_{\text{WB,right}}(i) v_{\text{WB,right}}(\phi_k). \quad (2)$$

Here, v_{SB} , $v_{\text{WB,left}}$, and $v_{\text{WB,right}}$ are latent basis functions defined along the rocking-angle axis, and $c_{\text{SB}}(i)$, $c_{\text{WB,left}}(i)$, and $c_{\text{WB,right}}(i)$ are the corresponding pixel-wise coefficients.

The model is implemented in PyMC Python [12]. The basis functions are constrained to be non-negative using truncated normal priors, while the coefficients are assigned half-normal priors, ensuring an additive decomposition.

The prior for SB is chosen as a symmetric Gaussian centered near $\phi = 0^\circ$. For WB-left and WB-right, skewed Gaussian priors are used to better represent asymmetric profiles, with different widths on either side of the mean. The observation model is Gaussian:

$$p(I_{\text{obs}} | \Theta) = \prod_{k,i} \mathcal{N}(I_{\text{obs}}(\phi_k, i) | I_{\text{model}}(\phi_k, i), \sigma^2), \quad (3)$$

where Θ denotes the full set of model parameters, including the basis functions, pixel-wise coefficients, and noise parameter. Given the prior specification and the likelihood, the posterior distribution is given by Bayes' rule:

$$p(\Theta | I_{\text{obs}}) \propto p(I_{\text{obs}} | \Theta) p(\Theta), \quad (4)$$

Posterior sampling is performed using the No-U-Turn Sampler (NUTS) [13]. After sampling, the basis functions are normalized for comparison. Since WB-left and WB-right may exchange labels during sampling, a relabeling step is applied by comparing each sample with the prior templates.

The inferred basis functions are then propagated from the ROI to the full field of view. The full dataset is processed in the same way as the ROI, so that each pixel is represented by a rocking curve sampled over the same set of rocking angles. For a given pixel i , the measured rocking curve is written as a vector in $\mathbb{R}^K$ and is approximated as a linear combination of the three inferred basis functions collected in the matrix $\mathbf{V} \in \mathbb{R}^{K \times 3}$. The corresponding coefficient vector is obtained by solving the regularized least-squares problem

$$\mathbf{c}(i) = \arg \min_{\mathbf{c}} \|I(\phi_k, i) - \mathbf{V}\mathbf{c}\|_2^2 + \lambda \|\mathbf{c}\|_2^2, \quad (5)$$

where λ is a small regularization parameter introduced to stabilize the inversion and to reduce sensitivity to noise or near-collinearity between components. In practice, this step assigns to each pixel the combination of SB, WB-left, and WB-right weights that best reproduces its local rocking curve in the least-squares sense. Repeating the reconstruction over all pixels yields the spatial coefficient maps

$$c_{\text{SB}}(x, y), \quad c_{\text{WB, left}}(x, y), \quad c_{\text{WB, right}}(x, y), \quad (6)$$

which describe how the three contributions are distributed across the image.

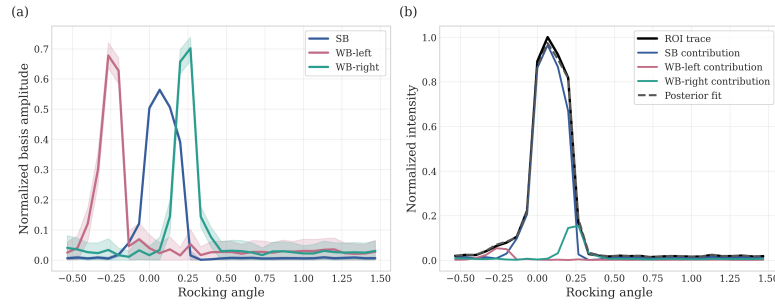


Figure 2: Posterior basis functions and ROI fit from the Bayesian decomposition. Panel (a) shows the posterior mean basis functions for SB, WB-left, and WB-right, with shaded credible intervals. Panel (b) shows the mean ROI rocking curve together with the corresponding SB, WB-left, and WB-right contributions and the posterior fit.

3 Results and Discussion

We applied our Bayesian method to DFXM data acquired from pure single-crystal aluminum samples at Beamline ID06-HXM (now ID03) of the European Synchrotron Radiation Facility (ESRF) [11]. The sample is single crystal of industrially pure aluminum (99.99%), with dimensions $0.7 \times 0.7 \times 10 \text{ mm}^3$, oriented with the long $[1\bar{1}0]$ axis perpendicular to the scattering plane. Prior to the experiments, the samples were annealed for 10 h at 590°C in atmospheric air and slowly cooled in the furnace to minimize residual strain. More information about the experimental setup can be found in [14].

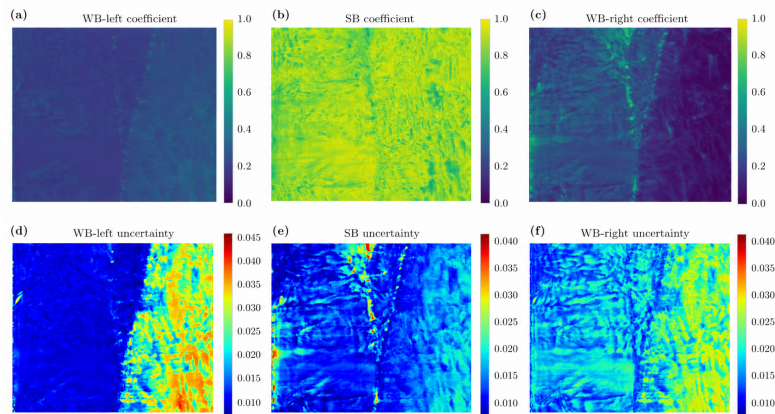


Figure 3: Bayesian decomposition of the rocking-curve dataset. Panels (a)–(c) show the posterior mean coefficient maps for SB, WB-left, and WB-right. Panels (d)–(f) show the corresponding uncertainty maps obtained from posterior sampling estimated from the spread of the reconstructed coefficient maps over the posterior samples.

Figure 2(a) shows the posterior basis functions inferred for SB, WB-left, and WB-right. The three components remain distinct after inference, with SB centered around the main rocking

condition and the two WB components shifted on either side. The WB contributions appear as weaker side features on the flanks of the ROI rocking curve. This is physically consistent with the expected diffraction contrast: regions that remain closest to the Bragg condition contribute primarily to SB, whereas local lattice distortions, in particular around dislocations, shift part of the diffracted intensity away from the central Bragg condition and give rise to weaker side contributions associated with WB-left and WB-right.

The posterior credible intervals remain relatively narrow around the main peaks, indicating that the characteristic shapes of the three basis functions are reasonably well constrained within the fitted ROI. Away from the peak region, the intervals broaden, as expected, because the lower intensity provides weaker constraints on the decomposition. The quality of the decomposition can be assessed from the ROI-average fit shown in figure. 2(b). The posterior reconstruction follows the measured ROI trace closely: the dominant part of the signal is captured by the SB contribution, while WB-left and WB-right provide weaker corrections on the flanks of the rocking curve.

The spatial coefficient maps are shown in figure. 3(a)–(c). The SB map displays the dominant contribution across most of the field of view, while the WB-left and WB-right maps reveal weaker spatially varying features superimposed on the main structure. The two WB maps are not identical, indicating that the model separates left- and right-side weak-beam contributions. In this way, the decomposition distinguishes the dominant Bragg-related signal from weaker defect-sensitive features associated with local departures from the central rocking condition.

The uncertainty is estimated directly from the posterior samples and propagated through the spatial decomposition. For the basis functions, it is reflected by the credible intervals in figure. 2(a). For the coefficient maps, posterior samples of the basis functions are propagated through the reconstruction, producing ensembles of maps for SB, WB-left, and WB-right. The posterior mean and spread are then computed pixel-wise. The resulting uncertainty maps, shown in figure. 3(d)–(f), complement the mean coefficient maps by indicating where the decomposition is more or less constrained by the data. The uncertainty varies spatially and generally increases in regions where the separation between components is less stable. In particular, localized regions of elevated posterior uncertainty in the SB coefficient map are consistent with crystal defects, especially dislocations, for which the local rocking-curve shape departs from the average behavior encoded by the dominant basis functions. Defect regions are therefore characterized not only by modified mean coefficients, but also by increased posterior variability. The WB-left and WB-right uncertainty maps likewise indicate that the weak-beam separation is less consistent in some areas, which is consistent with their lower signal amplitude and partial overlap.

Compared with PCA or GSO, the present method does not impose orthogonality between components, but instead keeps the decomposition tied to physically defined SB, WB-left, and WB-right contributions [9]. Classical single-peak fitting yields local orientation and mosaicity, but does not explicitly separate SB and WB contributions [15]. More agnostic machine-learning approaches can recover latent structure, although without the same degree of direct physical interpretability [10]. In this sense, the present framework is best viewed as a complementary approach, providing a compact decomposition of the rocking-curve stack while preserving a physically meaningful interpretation and allowing the posterior variability of the decomposition to be assessed.

4 Conclusion

We have presented a Bayesian approach for the decomposition of rocking-curve data into physically interpretable components with associated uncertainty. The method provides a complementary analysis tool to existing rocking-curve techniques, combining physical insight with

statistical inference. Given its general formulation, the approach can in principle be extended to other diffraction-based imaging modalities, including transmission electron microscopy and X-ray topography, where similar challenges arise.

5 Acknowledgement

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6 Data Availability

The code associated with this work is available at GitHub repository.

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