

Focusing characteristics of cylindrically bent Laue crystals

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Based on paraxial optics and the Takagi-Taupin theory, we establish an analytical framework for cylindrically bent Laue crystals that treats them as bulk diffraction devices and decomposes their behavior into geometric, kinematical, and higher-order scattering contributions. In this framework, we derive three fundamental results: a conservation relation accounting for aperture effects, a monochromatic focusing condition, and a polychromatic focusing condition. We further clarify the origin and limitations of common focusing conditions derived from geometric-optics arguments. These results deepen the fundamental understanding of bent Laue crystals and reshape their design logic, paving the way for practical applications.

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Introduction. High-performance x-ray sources have promoted the wide application of bent crystals as diffractive optical elements for x-ray beam manipulation [1–4]. Among them, cylindrically bent Laue crystals (CBLCs) are pivotal monochromatizing components (with focusing or collimating capabilities) in hard x-ray beamlines for their low absorption and high flux. Over recent decades, theoretical models, including ray-tracing, multilamellar, Penning-Polder, and wave-optics models [5], have been developed to describe CBLCs' optical properties, yet most only partially describe CBLCs' diffraction behavior, bearing inherent limitations. The advent of new-generation high-coherence sources has rendered these models inadequate, necessitating rigorous wave-optics approaches. The Takagi-Taupin (TT) dynamical theory of x-ray diffraction (XRD) is a widely used wave-optics technique for describing diffraction effects in such crystals [6,7].

The recognition that Laue crystals exhibit a dynamical focusing effect dates back to the 1970s [8,9]. Theoretical and experimental evidence shows dynamical effects cause CBLCs' focusing to deviate from geometrical optics predictions [10–17]. To account for the rich dynamical diffraction effects of CBLCs, it is necessary to solve the TT equations either numerically or analytically. Notably, an analytical integral solution to the TT equations exists for CBLCs [10], but it relies on the confluent hypergeometric function (CHF), complicating related research.

Subsequent studies based on this solution have addressed selected aspects of CBLCs' focusing behavior [10,14–16,18],

but they typically fall into two limited categories: analyses focused on isolated scattering mechanisms or global wave-front propagation treatments that obscure the internal structure of the diffracted field. Thus, developing a comprehensive and unified description of CBLCs' focusing characteristics based on the physical nature remains a critical challenge, particularly when disentangling their hierarchical influence mechanisms.

In this Letter, we combine paraxial optics with the Takagi-Taupin theory to establish a physically transparent, hierarchical description of wave-front transformation between the incident and diffracted waves in CBLCs. We show that the diffracted-wave envelope can be decomposed into three distinct contributions corresponding to geometric optics, kinematical scattering, and higher-order scattering (HOS) effects. This decomposition enables a unified and hierarchical analysis of CBLC diffraction. Based on this framework, we introduce several fundamental concepts, including an aperture-related conservation relation, a monochromatic (mono-) focusing condition, and a polychromatic (poly-) focusing condition. Moreover, the framework validates and clarifies many commonly used focusing conditions, in particular, resolving the geometric-optics-derived “magic condition” [2].

Theoretical method. We follow the formulation established in our previous work [17] in the TT framework. In CBLCs, the crystal wave is the coherent superposition of the transmitted wave $\mathcal{E}_0 \exp(i\mathbf{k}_0 \cdot \mathbf{r})$ and the diffracted wave $\mathcal{E}_h \exp(i\mathbf{k}_h \cdot \mathbf{r})$, where $\mathbf{k}_h = \mathbf{k}_0 + \mathbf{h}$, and $\mathbf{h}$ denotes the diffraction vector of the undeformed crystal. $\mathbf{k}_0$ is set equal to the incident wave vector $\mathbf{k}$ in vacuum ($|\mathbf{k}| = k = 2\pi/\lambda$, λ being the wavelength of x-rays), which simplifies the boundary condition [7]. Under polychromatic illumination, the actual incident wave vector may slightly deviate from the exact Bragg condition. For reference, the energy satisfying the Bragg condition is defined as the Bragg (or center) energy E_B , with the corresponding wave vector $\mathbf{k}_B$ ($|\mathbf{k}_B + \mathbf{h}| = |\mathbf{k}_B| = k_B$) and Bragg angle θ_B . The amplitudes $\mathcal{E}_0$ and $\mathcal{E}_h$ are governed by the well-known TT

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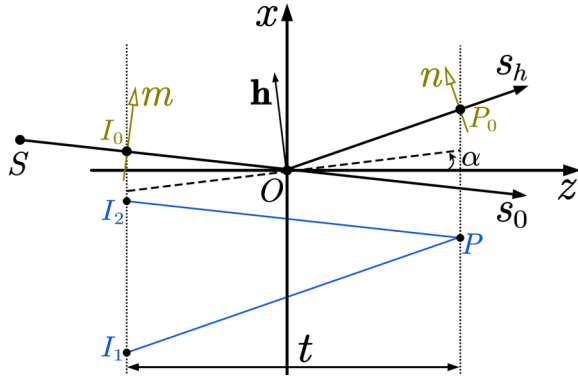


FIG. 1. Laue diffraction geometry for a bent crystal. The s_0 and s_h axes parallel $\mathbf{k}_0$ and $\mathbf{k}_h$, respectively; Oz is along the inward normal to entrance surface (at $z = -t/2$). O : bending center; t : normal crystal thickness; α (asymmetry angle): directed angle from z axis to predeformation diffraction plane (dashed line); θ_1 : directed angle from z axis to s_0 axis; θ_2 : directed angle from z axis to s_h axis. All angles are positive counterclockwise. PI_1I_2 is the inverted BM triangle, with I an arbitrary point on I_1I_2 . S is a polychromatic source with the SO direction (or s_0 axis) fixed at Bragg energy for a given $\mathbf{h}$, making θ_2 energy dependent.

equations [6,7,17]:

$$\begin{aligned} \frac{\partial \mathcal{E}_0}{\partial s_0} &= \frac{ik}{2} [\chi_0 \mathcal{E}_0 + \chi_{-h} \exp(i\mathbf{h} \cdot \mathbf{U}) \mathcal{E}_h], \\ \frac{\partial \mathcal{E}_h}{\partial s_h} &= \frac{ikc_k}{2} [(\chi_0 + w) \mathcal{E}_h + \chi_h \exp(-i\mathbf{h} \cdot \mathbf{U}) \mathcal{E}_0], \end{aligned} \quad (1)$$

where $c_k = k/k_h$, $w = (k^2 - k_h^2)/k^2$, and $\chi_{0,\pm h}$ are the Fourier coefficients of the susceptibility. For the diffraction geometry in Fig. 1, the deformation phase $\mathbf{h} \cdot \mathbf{U}$ [Eq. (A1)] in the s_0Os_h system is quadratic in the coordinates, which permits an analytical solution of Eq. (1) via the Riemann method [10,17]. Then, the diffracted amplitude $\mathcal{E}_h$ at an arbitrary point $P(t/2, x')$ on the exit surface in Fig. 1 is given by [17]

$$\mathcal{E}_h(P) = \frac{\cos \theta_1}{\sin(\theta_2 - \theta_1)} \int_{I_1I_2} dx \psi_0(x) G_h(x; x', t). \quad (2)$$

The kernel in Eq. (2) takes the following form:

$$\begin{aligned} G_h(x; x', t) &= i \frac{kc_k \chi_h}{2} \exp[-i\mathbf{h} \cdot \mathbf{U}(s_{0P}, s_{hI})] \\ &\times \exp \left[i \frac{k\chi_0}{2} s'_0 + i \frac{kc_k}{2} (\chi_0 + w) s'_h \right] \\ &\times {}_1F_1 \left(-i \frac{\sigma}{b}, 1; -ib s'_0 s'_h \right), \end{aligned} \quad (3)$$

where b is the strain gradient defined in Eq. (A1), (s_{0P}, s_{hP}) and (s_{0I}, s_{hI}) are the coordinates of points P and I in s_0Os_h system, respectively, $s'_0 = s_{0P} - s_{0I}$, $s'_h = s_{hP} - s_{hI}$, and $\sigma = k^2 c_k \chi_h \chi_{-h}/4$. ${}_1F_1$ denotes the CHF of the first kind. This kernel delineates the wave field generated by a monochromatic point source on the entrance surface, confined to the Borrmann (BM) fan ($s'_0, s'_h \geq 0$). Crucially, the ${}_1F_1$ term in this kernel encodes the HOS effect, while the remaining terms correspond to the first-order (or kinematical) scattering. This distinction follows from the role of $\chi_{\pm h}$, which mediate energy

exchange between the $\mathcal{E}_0$ and $\mathcal{E}_h$ wave fields: Setting $\chi_{-h} = 0$ eliminates energy feedback from $\mathcal{E}_h$ to $\mathcal{E}_0$ (matching kinematical scattering behavior), yielding the ${}_1F_1$ function identically equal to 1.

$\psi_0(x)$ denotes the vacuum incident wave amplitude from a point source in a two-dimensional (2D) sense; under the paraxial approximation, it reads [14,17]

$$\psi_0(x) = \frac{1}{\sqrt{\lambda f_s}} \exp \left[ik \frac{(x - x_{I_0})^2 \cos^2 \theta_1^2}{2 f_s} \right],$$

where f_s is the incident distance (distance between S and O in Fig. 1). Motivated by the phase structure of $\psi_0(x)$, we introduce the following key transformations:

$$(x - x_{I_0}) \cos \theta_1 = m, \quad (x' - x_{P_0}) \cos \theta_2 = n, \quad (4)$$

which shifts our perspective to two rectangular coordinate systems, with origins at I_0 and P_0 , respectively (Fig. 1). With these transformations, Eq. (2) becomes

$$\begin{aligned} \mathcal{E}_h(n) &= C_h \times \exp[i\Phi_{\text{cle}}(n)] \\ &\times \int_{-a_0}^{a_0} dv \exp[i\Phi_{\text{kin}}(n, v)] \times F_{\text{hos}}(v), \end{aligned} \quad (5)$$

where

$$\begin{aligned} C_h &= ikc_k \chi_h / 2 / \sin(\theta_2 - \theta_1) / \sqrt{\lambda f_s}, \\ \Phi_{\text{cle}}(n) &= A\gamma^2 n^2 + B\gamma n + Cn^2 + Dn + E, \\ \Phi_{\text{kin}}(n, v) &= Av^2 + [(2A\gamma + B_0)n + B_1]v, \\ F_{\text{hos}}(v) &= {}_1F_1 \left[-i \frac{\sigma}{b}, 1; -ib\xi(v) \right], \\ \xi(v) &= (a_0^2 - v^2) / [\gamma \sin^2(\theta_2 - \theta_1)]. \end{aligned}$$

Here, $\gamma = \cos \theta_1 / \cos \theta_2$. $a_0 = t \sin(\theta_2 - \theta_1) / (2 \cos \theta_2)$ is half the projection of the inverted BM base I_1I_2 onto the m axis. The coefficients A, B, B_0, B_1, C, D , and E are given in Eq. (A3) and are, in general, functions of k (Fig. 1).

Equation (5) disentangles the hierarchical physical contributions to CBLCs' focusing behavior. The term $\Phi_{\text{cle}}(n)$ gives the crystal lens equation (CLE) for Bragg diffraction optics [Eq. (A6)], which is independent of bulk effects and can also be obtained via a simple geometric-optics model [16]. The term $\Phi_{\text{kin}}(n, v)$ describes the kinematical contribution and depends on the exit coordinate n , whereas $F_{\text{hos}}(v)$ represents the spatially invariant HOS effect.

Setting the n coefficient in Φ_{kin} to zero removes the spatial dependence of the scattering integral, leading to $2A\gamma + B_0 = 0$, which yields $f_s = R \cos \theta_1$. Inserting this value into Φ_{cle} gives the focal length $-R \cos \theta_2$, where both incident distance and focal length satisfy the Rowland geometry requirements. This analysis provides a wave-optics justification for the widespread applicability of the Rowland condition.

Generally, the n -dependent scattering integral in Eq. (5) perturbs the phase Φ_{cle} , causing deviations of the actual focal length from CLE predictions. As bulk diffraction elements, CBLCs exhibit thickness-induced effects, characterized by parameter a_0 in Eq. (5) via two ways: modifying the integration limits (reflecting the size variation of the triangle PI_1I_2 in Fig. 1) and affecting the HOS process. In the thin-crystal limit, Av^2 in Φ_{kin} is a second-order infinitesimal, and the ${}_1F_1$

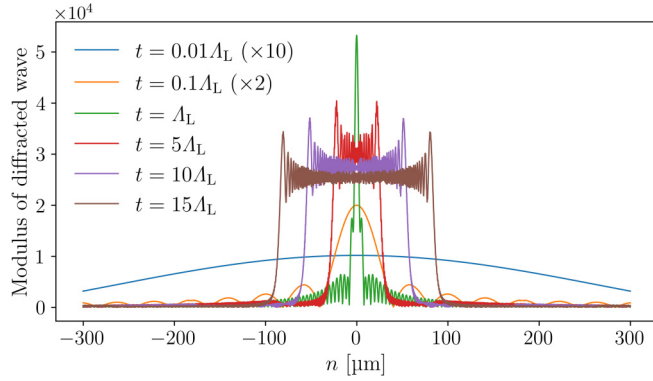


FIG. 2. Modulus of $\mathcal{E}_h(n)$ as a function of thickness at a Bragg energy of 28.814 keV. The blue and orange lines are magnified by a factor of 10 and 2, respectively. When $t > \Lambda_L$, the numerical aperture size is in good agreement with the theoretical value derived from Eq. (9). [$\Lambda_L = 89 \mu\text{m}$, Si(311) reflection, $\alpha = -3.102^\circ$, $R = 2 \text{ m}$, $f_s = 22 \text{ m}$, $v = 0.22$.]

function approximates to 1, reducing the scattering integral in Eq. (5) to

$$\int_{-a_0}^{a_0} dv \exp\{i[(2A\gamma + B_0)n + B_1]v\}.$$

Defining $n' = (2A\gamma + B_0)n + B_1$, the integral admits an analytical solution $2 \sin(n'a_0)/n'$. Notably, this sinc-type result matches the reflectivity formula under the thin-crystal approximation ($t \ll \Lambda_L$, Λ_L is the *Pendellösung* distance) in classical dynamical XRD theory [19]. As the thickness approaches zero, the central peak of $2 \sin(n'a_0)/n'$ broadens infinitely (despite very low diffraction efficiency) (Fig. 2). In this case, the scattering integral does not significantly modulate Φ_{cle} , such that the CBLC focal length is governed by CLE. With increasing thickness, Av^2 and F_{hos} become significant, driving a transition from the kinematical to the full-wave regime [20], as depicted in Fig. 2.

Further, noting that $\Phi_{\text{kin}}(n, v)$ is quadratic in v , we rewrite Eq. (5) via completing the square as

$$\begin{aligned} \mathcal{E}_h(n) &= C_h \times \exp[i\Phi_{\text{km}}(n)] \\ &\times \int_{-a_0}^{a_0} dv \exp[i\Phi_{\text{ape}}(n, v)] \times F_{\text{hos}}(v), \end{aligned} \quad (6)$$

where

$$\begin{aligned} \Phi_{\text{km}}(n) &= K_2 n^2 + K_1 n + K_0, \\ \Phi_{\text{ape}}(n, v) &= A \left[v + \left(\gamma + \frac{B_0}{2A} \right) n + \frac{B_1}{2A} \right]^2. \end{aligned}$$

K_2, K_1, K_0 are defined in Eq. (B1). Compared with Eq. (5), Eq. (6) separates the kinematical contribution into two parts: One directly affects the propagation process and is absorbed into Φ_{cle} to form Φ_{km} , while the other, $\Phi_{\text{ape}}(n, v)$, explicitly represents the aperture effect, as shown below. For the HOS term $F_{\text{hos}}(v)$, our previous work [17] numerically identified b and t as the dominant control parameters in typical configurations. At large b or t , as shown in Fig. 9 of Ref. [17], HOS process reduces to a static scattering factor describing energy dissipation without phase modulation [10], as

experimentally validated [11]. Accordingly, $F_{\text{hos}}(v)$ may be approximated as an energy-dissipation constant (Appendix D: Analysis of higher-order scattering effects), with diffracted-wave propagation governed primarily by kinematical effects (the quasiclassical approximation [10]). Even in geometries with strong HOS effects, as demonstrated below, the kinematical process remains the foundation of CBLC focusing, with HOS acting as a higher-order modulation.

Aperture effect. The factor $\exp[i\Phi_{\text{ape}}(n, v)]$ constitutes the Gaussian integral kernel. Setting

$$F_1(n) = \int_{-a_0}^{a_0} dv \exp \left[iA \left(v + N_c n + \frac{B_1}{2A} \right)^2 \right] \quad (7)$$

with $N_c = \gamma + B_0/(2A)$, and noting that A is of order k , standard properties of Gaussian integrals imply that $F_1(n)$ rapidly decays as n moves away from the center (Fig. 2). Accordingly, $F_1(n)$ acts as an aperture function [in a one-dimensional (1D) sense], restricting the effective spatial extent of the diffracted wave on the exit surface. The aperture size can be obtained analytically by differentiating $F_1(n)$ with respect to n , yielding

$$\frac{dF_1(n)}{dn} = N_c [\exp(iAu_2^2) - \exp(iAu_1^2)], \quad (8)$$

with $u_1 = -a_0 + N_c n + B_1/(2A)$ and $u_2 = a_0 + N_c n + B_1/(2A)$. This derivative is the difference of two Gaussian phase terms with identical form but shifted stationary points along the n axis. Upon integration, only the neighborhoods of these stationary points (i.e., $u_1 = 0$ and $u_2 = 0$) contribute, implying that $F_1(n)$ is appreciable only between them. This directly leads to the conservation relation for the effective aperture size,

$$\Delta n = 2a_0/N_c, \quad (9)$$

where Δn denotes the aperture width in the n direction. This relation is further confirmed in Fig. 2, which shows that Δn scales linearly with the crystal thickness for $t > \Lambda_L$. Since N_c depends on multiple system parameters, the aperture size Δn is highly sensitive to the diffraction geometry. Consequently, aperture effects must be taken into account when propagating the outgoing diffracted wave using the free-space diffraction formalism. Approximate approaches, such as the stationary-phase method, may therefore lead to reduced accuracy and observable deviations in practical applications.

Monochromatic focusing. Kinematically, $\Phi_{\text{km}}(n)$ in Eq. (6) characterizes the primary propagation behavior of CBLCs' diffracted waves. Its quadratic coefficient K_2 represents the focusing property in accordance with paraxial optics principles [21]. Defining the kinematical focal length as

$$f_{\text{km}} = -k/(2K_2), \quad (10)$$

$K_2 > 0$ corresponds to a virtual focus and $K_2 < 0$ to a real focus. In Bragg incidence, a closed-form expression for K_2 is provided in Eq. (B2). Substituting $f_s = R \cos \theta_1$ into Eq. (B2) immediately yields $f_{\text{km}} = -R \cos \theta_2$, thereby recovering the Rowland geometry once again. In particular, for symmetric diffraction, where $B_0 = 0$, the kinematical focal length reduces to $f_{\text{km}} = -R \cos \theta_2$, which is independent of the incident distance. In this case, the actual focusing behavior of CBLCs is governed by the full scattering integral in Eq. (6).

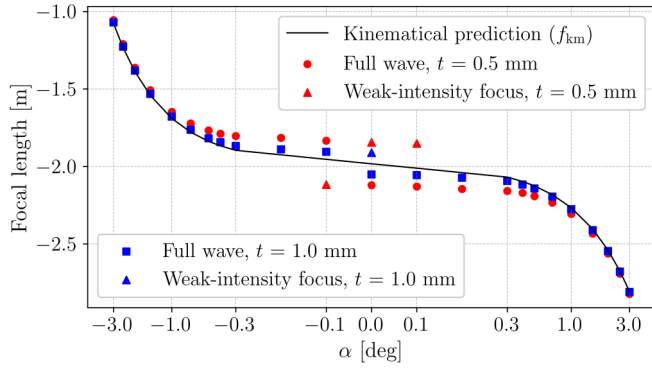


FIG. 3. Monochromatic virtual focal length as a function of α at a Bragg energy of 28.814 keV. Full-wave numerical results by Eq. (5) closely surround the analytical results from f_{km} . HOS effects suppression by b and t is also evident. Triangle markers denote the weaker of the two focal points. For red triangles, intensity ratios (weak/strong focus) are $\alpha = -0.1^\circ$, 44%; $\alpha = 0.0^\circ$, 82%; $\alpha = 0.1^\circ$, 29%. For blue triangles, $\alpha = 0.0^\circ$, 77%. Ratios <20% are omitted, and they decay rapidly. [Si(311) reflection, $R = 2$ m, $f_s = 22$ m, $\nu = 0.22$.]

As noted in Appendix D: Analysis of higher-order scattering effects, HOS effects under symmetric diffraction give rise to two focal points around $-R \cos \theta_2$ (Fig. 3), with deviations in opposite directions. When an asymmetry angle is introduced, the strain gradient b becomes effective [Eq. (A2)]. This asymmetry suppresses HOS effects, with the suppression strength increasing with $|b|$. Consequently, the kinematical focal length f_{km} provides an increasingly accurate description of the true focusing behavior, as illustrated in Fig. 3.

Polychromatic focusing. In Ref. [17], we numerically demonstrated that the poly-focusing behavior of CBLCs is governed by wave optics; the validity of the geometric-optics-based magic condition, which defines an achromatic state through the coincidence of the geometric and single-ray foci [Eqs. (A7) and (A8)], is restricted to limited regimes. Here, we use the analytical model developed herein to elucidate CBLCs' poly-focusing behavior. Retaining the carrier $\exp(i\mathbf{k}_h \cdot \mathbf{r})$, which is essential for free-space propagation, and temporarily neglecting the scattering integral in Eq. (6), the general propagation term for diffracted waves assumes the form

$$\psi_e(n) = \exp[i\Phi_{\text{km}}(n)] \exp[i(\mathbf{k} + \mathbf{h}) \cdot \mathbf{r}]. \quad (11)$$

Under paraxial optics, $\exp[i\Phi_{\text{km}}(n)]$ serves as the envelope (defining wave-front modulation center), while $\exp[i(\mathbf{k} + \mathbf{h}) \cdot \mathbf{r}]$ describes the tilt of the diffraction optical axis. Expressing $\psi_e(n)$ in a rectangular frame whose q axis serves as the reference optical axis [Fig. 4(a)], we obtain

$$\begin{aligned} \psi_e(n) = & \exp\{iK_2[n - \Delta_n(k)]^2\} \\ & \times \exp[ik\Delta\theta(k)n + i\mathbf{k}\mathbf{e}_q \cdot \mathbf{r} + \phi_0], \end{aligned} \quad (12)$$

where ϕ_0 denotes a constant phase. $\Delta_n(k)$ and $\Delta\theta(k)$ are defined in Eq. (C1). Geometrically, $\Delta_n(k)$ denotes the lateral offset of P_F from the reference axis, approximated as $\mathbf{e}_n \cdot \vec{P_C P_F}$, while $\Delta\theta(k)$ is the corresponding angular offset of the diffraction optical axis (FP_F). Kinematically, the poly-

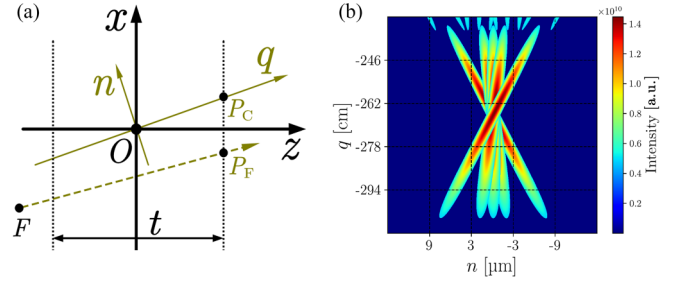


FIG. 4. (a) The rectangular coordinate system for free-space propagation with unit axis vectors $\mathbf{e}_q$, $\mathbf{e}_n$, and $\mathbf{e}_q \parallel \mathbf{k}_B + \mathbf{h}$. F denotes the virtual image point. P_F denotes the wave-front modulation center. (b) Focus profiles for energy offsets of -2 , -0.5 , 0 , 0.5 , and 2 eV relative to E_B with $t = 0.5$ mm. The variation in energy offset from small to large aligns with the clockwise rotation of the focus. [Si(311) reflection, $E_B = 28.814$ keV, $\alpha = -2.641^\circ$, $R = 5$ m, $f_s = 38$ m, $\nu = 0.22$.] This diffraction geometry is taken from Ref. [17], and the magic condition requires $f_s = 22$ m.

focal length (Appendix C: Derivation of the polychromatic focusing condition) f_{kp} is given by

$$f_{\text{kp}} = -f_{\text{km}} \frac{\left(\frac{B_0}{2A\gamma} + 1\right)\gamma \tan \theta_B}{\gamma \tan \theta_1 - \tan \theta_2}. \quad (13)$$

The magic condition seeks to eliminate the mismatch between poly- and mono-foci, yielding the minimum achievable focus size. In our model, this condition corresponds to $f_{\text{kp}} = f_{\text{km}}$, which leads to $B_0 = 2A$. Substituting this result into f_{km} recovers the geometric-optics focusing condition [Eq. (A7)], demonstrating that the magic condition is valid at the kinematical level, equating to stringent constraints on diffraction geometry via Eqs. (A7) and (A8). This clarifies our earlier numerical observation [17]: The magic condition aligns the optical axes of diffracted waves with different energies, whereas HOS effects misalign their mono-foci.

As shown in Fig. 8 of Ref. [17] and Eq. (5), HOS effects exhibit spatial invariance and a weak energy dependence. It therefore merely leads to an axial stretching or compression of the mono-focal length along the propagation axis. This implies that the poly-focal positions are predominantly governed by the kinematical process; i.e., Eq. (13) remains valid in the full-wave sense.

For HOS-dominated diffraction configurations, where the magic condition breaks down, the more rigorous poly-focusing condition [Eq. (13)] provides a quantitative multiparameter compensation strategy. Namely, one can adjust the diffraction geometry according to Eq. (13) to enforce the matching between f_{kp} and the actual mono-focal length. For instance, one practical approach is to vary the incident distance. Figure 4(b) confirms that such tuning restores the achromatic state even in strongly HOS-dominated configurations reported in Ref. [17].

Conclusions. We have presented a unified theoretical framework for cylindrically bent Laue crystals that enables a systematic understanding of their optical behavior beyond surface- or geometric-optics-based descriptions. By separating geometric, kinematical, and higher-order scattering contributions, the framework provides a hierarchical view of

how bulk diffraction effects govern focusing properties in these optical systems.

Within this picture, several long-standing focusing conditions used in practice are placed on a firm theoretical footing, and the poly-focusing effect is shown to arise naturally within a full wave-optical treatment. The analysis further reveals previously unrecognized constraints and focusing regimes associated with finite aperture and bulk scattering, highlighting limitations inherent to purely geometric interpretations.

Beyond clarifying existing models, the results establish fundamental principles that reshape the design logic of bent Laue crystal optics, enabling more predictive control of their performance. A recommended design procedure may proceed as follows. First, a candidate design is generated by applying the kinematical focusing equations, specifying the design energy E_B , crystal-related parameters such as $\chi_{0,\pm h}$, α , and R , the source distance, and the target focal properties. A crystal thickness exceeding Λ_L is typically chosen to ensure sufficient diffraction efficiency. Second, the design is validated using full-wave simulations. The focal intensity distribution is calculated via numerical Fresnel propagation, enabling direct evaluation of the focal position and chromatic overlap. Third, the design is iteratively optimized. Deviations from the target performance are analyzed with particular attention to aperture and HOS effects, and the design parameters are refined until the required specifications are satisfied.

The concepts and methods developed here are not restricted to cylindrically bent Laue crystals and can be readily extended to bent Bragg crystals commonly used in x-ray spectrometry.

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Data availability. Data may be available upon request.

Appendix A: Derivation of the crystal lens equation. The deformation phase for a cylindrically bent isotropic crystal in the system $s_0O s_h$ shown in Fig. 1 has the form [17]

$$\mathbf{h} \cdot \mathbf{U} = \frac{a}{2}s_0^2 + bs_0s_h + \frac{c}{2}s_h^2, \quad (\text{A1})$$

with

$$a = \frac{h}{R} [\cos \alpha \sin 2\theta_1 + \sin \alpha (\sin^2 \theta_1 + \nu \cos^2 \theta_1)],$$

$$b = \frac{h}{R} [\cos \alpha \sin(\theta_1 + \theta_2) + \sin \alpha (\sin \theta_1 \sin \theta_2 + \nu \cos \theta_1 \cos \theta_2)],$$

$$c = \frac{h}{R} [\cos \alpha \sin 2\theta_2 + \sin \alpha (\sin^2 \theta_2 + \nu \cos^2 \theta_2)],$$

where ν is the Poisson ratio and R (bending radius) is positive for concave-side incidence and negative for convex-side inci-

dence. In Bragg incidence, b is simplified to

$$\frac{h \sin \alpha}{R} \left[1 + \frac{1 + \nu}{2} (\cos 2\alpha + \cos 2\theta_B) \right], \quad (\text{A2})$$

which means that b is primarily influenced by the bending radius and the asymmetry angle.

Let $S_\theta = 1/\sin(\theta_2 - \theta_1)$; the coefficients in Eq. (5) are given by

$$\begin{aligned} A &= \frac{k}{2f_s} - S_\theta^2 \frac{c}{2}, \quad B_0 = S_\theta^2 b, \quad B_1 = -\frac{k\eta}{2\gamma}, \quad C = -S_\theta^2 \frac{a}{2}, \\ D &= \frac{k\eta}{2}, \quad \eta = [-\chi_0 + c_k(\chi_0 + w)\gamma] S_\theta, \\ E &= \frac{kt[\chi_0 + c_k(\chi_0 + w)\gamma]}{4 \cos \theta_1}, \quad B = B_0 n + B_1. \end{aligned} \quad (\text{A3})$$

Substituting them into $\Phi_{\text{cle}}(n)$ gives

$$\Phi_{\text{cle}}(n) = Qn^2 + E, \quad Q = \frac{k}{2f_s} \gamma^2 + S_\theta^2 \left(-\frac{c}{2} \gamma^2 + b\gamma - \frac{a}{2} \right). \quad (\text{A4})$$

In Bragg incidence, with the relations $\theta_1 = \alpha - \theta_B$, $\theta_2 = \alpha + \theta_B$, $h = 2k \sin \theta_B$, the key relations

$$b\gamma - a = c\gamma - b = \frac{k \sin^2 2\theta_B}{R \cos \theta_2} \quad (\text{A5})$$

are derived. Substituting them into Q gives

$$Q = \frac{k}{2} \frac{1}{\cos^2 \theta_2} \left(\frac{\cos^2 \theta_1}{f_s} + \frac{-\cos \theta_1 + \cos \theta_2}{R} \right), \quad (\text{A6})$$

which leads to the CLE in geometric optics [16].

Two common geometric optics focusing conditions are noted here [3]: The geometric focus f_g (essentially a poly-focusing condition from the neutral plane) is given by

$$\frac{\cos \theta_1}{f_s} - \frac{\cos \theta_2}{f_g} = \frac{2}{R} \quad (\text{A7})$$

and the single-ray focus f_p (another poly-focusing condition from the incident ray path) is given by

$$f_p = \frac{R \sin 2\theta_B}{2 \sin \theta_1 + (1 + \nu) \sin 2\alpha \cos \theta_1}. \quad (\text{A8})$$

Appendix B: Derivation of the monochromatic focusing condition. The coefficients in $\Phi_{\text{km}}(n)$ have the forms

$$K_2 = \frac{B_0^2}{-4A} + C, \quad K_1 = \left(\frac{B_0}{2A\gamma} + 1 \right) \frac{k}{2} \eta, \quad K_0 = \frac{B_1^2}{-4A} + E. \quad (\text{B1})$$

In Bragg incidence, with Eq. (A5) applied again, K_2 is simplified to

$$K_2 = \frac{k \left(\frac{1}{R \cos \theta_1} - \frac{1}{f_s} \right) \left(\frac{k}{R \cos \theta_2} - B_0 \gamma \right) + \frac{B_0 k}{\gamma R \cos \theta_2}}{2 \left[k \left(\frac{1}{R \cos \theta_1} - \frac{1}{f_s} \right) + \frac{B_0}{\gamma} \right]}. \quad (\text{B2})$$

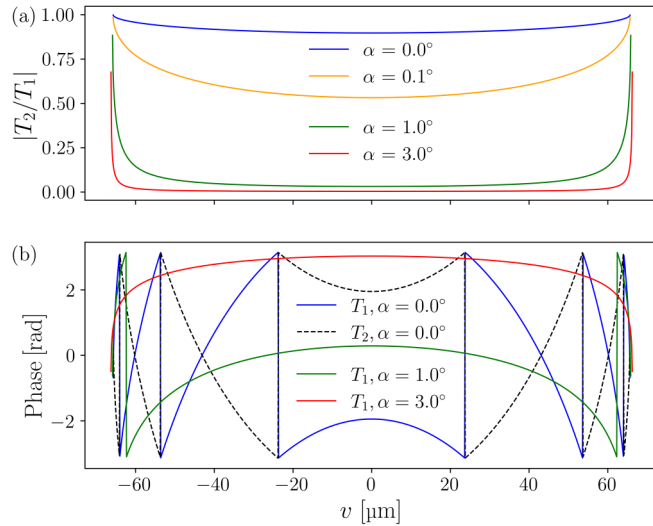


FIG. 5. (a) Amplitude ratio $|T_2/T_1|$ and (b) phase evolution of T_1 and T_2 vs spatial variable v for different asymmetry angles α . At $\alpha = 0^\circ$, T_1 and T_2 have comparable magnitude and are in opposite phase. As α increases, T_2 becomes much weaker than T_1 , and the phase of T_1 is approximately constant. [Si(311) reflection, $E_B = 28.814$ keV, $t = 0.5$ mm, $R = 2$ m, $f_s = 22$ m, $v = 0.22$.]

Appendix C: Derivation of the polychromatic focusing condition. In Eq. (12),

$$\begin{aligned} \Delta_n(k) &= -K_1/(2K_2), \quad \Delta k = k - k_B, \\ \Delta\theta(k) &= \Delta k(\gamma \tan \theta_1 - \tan \theta_2)/k. \end{aligned} \quad (C1)$$

Then, the kinematical poly-focal length f_{kp} is given by

$$f_{kp} = \frac{-[\Delta_n(k) - \Delta_n(k_B)]}{\Delta\theta(k) - \Delta\theta(k_B)} = \frac{\frac{k}{2K_2}[K_1(k) - K_1(k_B)]}{\Delta k(\gamma \tan \theta_1 - \tan \theta_2)}, \quad (C2)$$

where we use that K_2/k exhibits weak energy dependence near the Bragg energy. Since $B_0/(2A\gamma)$ also shows weak energy dependence, the variation in K_1 primarily arises from $k\eta$. In fact, η corresponds to the deviation parameter in classical dynamical XRD theory [19]. Its variation near the Bragg energy is dominated by w , which has the form [19] $w \simeq 4 \sin^2 \theta_B \Delta k/k$. Then, we have

$$\eta(k) \simeq \eta(k_B) + 2\gamma \tan \theta_B \Delta k/k. \quad (C3)$$

Substituting it into Eq. (C2) leads to

$$f_{kp} \simeq -f_{km} \frac{(\frac{B_0}{2A\gamma} + 1)[\gamma \tan \theta_B \Delta k + \frac{\Delta k}{2} \eta(k_B)]}{\Delta k(\gamma \tan \theta_1 - \tan \theta_2)}. \quad (C4)$$

Neglecting $\Delta k \eta(k_B)$ due to the small magnitude of χ_0 in the hard x-ray regime, we obtain Eq. (13). In general, however, $k\eta$ remains nonzero for negligible χ_0 , leading to a nonzero wave-front center offset even at Bragg energy [$\Delta_n(k_B) \neq 0$]. This physically accounts for mono-foci's minor offset from the q axis at Bragg energy [17].

Appendix D: Analysis of higher-order scattering effects. Mathematically, $F_{hos}(v)$ can be expanded as [10]

$$F_{hos}(v) = T_1(v) + T_2(v), \quad (D1)$$

with

$$\begin{aligned} T_1(v) &= \frac{\exp(\epsilon \pi \frac{\sigma}{b})}{\Gamma(1 + i \frac{\sigma}{b})} \Psi\left[-i \frac{\sigma}{b}, 1; -ib\xi(v)\right], \\ T_2(v) &= -\frac{\exp[\epsilon \pi \frac{\sigma}{b} - ib\xi(v)]}{\Gamma(-i \frac{\sigma}{b})} \Psi\left[1 + i \frac{\sigma}{b}, 1; ib\xi(v)\right], \end{aligned}$$

where Γ is the gamma function; if $\arg[-ib\xi(v)] > 0$, then $\epsilon = 1$, else $\epsilon = -1$. Ψ is the CHF of the second kind. T_1 and T_2 have historically been referred to as generalized wave fields, which correspond to the weakly absorbing wave mode and the strongly absorbing wave mode, respectively [18]. When $\alpha = 0$, $T_1(v)$ and $T_2(v)$ reduce to

$$T_1(v) = \frac{1}{2} H_0^{(1)}[2\sqrt{\sigma\xi(v)}], \quad T_2(v) = \frac{1}{2} H_0^{(2)}[2\sqrt{\sigma\xi(v)}].$$

$H_0^{(1)}$ and $H_0^{(2)}$ are Hankel functions of the first and the second kind, respectively. In typical applications, $H_0^{(1)}$ and $H_0^{(2)}$ exhibit comparable intensities and opposite phases (Fig. 5), yielding a bifocal pattern located around the kinematical focus. As $|\alpha|$ increases, T_2 weakens progressively and T_1 becomes dominant, leading to a single focal point. For sufficiently large $|b|$, $F_{hos}(v)$ [or $T_1(v)$] acts as a static scattering factor, where the focusing condition is governed by f_{km} . These physical processes are clearly illustrated in Figs. 3 and 5. Further discussions can be found in Ref. [10].

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