

The role of absorption in 3D electron diffraction dynamical structure refinement

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The role of absorption in 3D electron diffraction is established through analytical theory, simulation and dynamical refinement. A two-beam expression for the absorbed integrated intensity in centrosymmetric crystals is derived, showing that for $t/\xi_g \ll 1$ reflections follow a uniform exponential decay set by the mean absorptive potential U_0' . Many-beam simulations of both centrosymmetric and non-centrosymmetric crystals reveal additional reflection-specific anomalous absorption beyond the uniform attenuation set by U_0' . Neglecting these effects in dynamical refinement of integrated intensities incurs an error that increases approximately linearly with thickness, with this error becoming more severe near zone axes. Dynamical refinements were performed on CsPbBr₃, quartz and borane, with the inclusion of absorption yielding an improvement in R_{obs} from 6.4 to 5.3% for CsPbBr₃, and negligible improvements for quartz and borane. Anomalous absorption may therefore be ignored for routine refinement of integrated intensities except in high- Z materials at thicknesses approaching ξ_g .

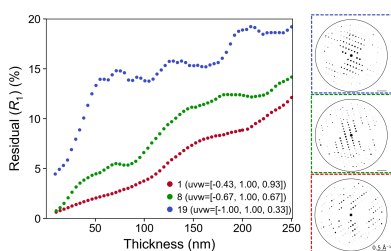
1. Introduction

Electron diffraction (ED) has become an established tool for determining the structures of nanocrystalline materials that are inaccessible to conventional X-ray crystallography. Developments such as precession electron diffraction (PED) (Vincent & Midgley, 1994) and continuous-rotation 3D ED have expanded its applicability, enabling routine structure determination across inorganic, hybrid and molecular crystals (Gemmi *et al.*, 2019).

Building on this foundation, dynamical refinement against 3D ED data (Palatinus *et al.*, 2015a; Palatinus *et al.*, 2015b), as implemented in *e.g.* JANA2020 (Petříček *et al.*, 2023), has enabled a continuing series of breakthroughs, including hydrogen localization (Palatinus *et al.*, 2017), multipolar refinements (Olech *et al.*, 2024) and ionization-state analysis via κ refinement (Suresh *et al.*, 2024). Alternative formulations of dynamical refinement continue to be developed (Malik *et al.*, 2026), extending the range and precision of these methods.

Refinement is the process by which a structural model is iteratively adjusted until convergence is achieved between simulated and observed diffraction intensities. Its accuracy is governed by the extent to which the scattering simulation reproduces the true physical interaction. The kinematical approach offers a simplified model, while dynamical simulation captures the full complexity of multiple scattering and can achieve far higher physical fidelity.

Despite these advances, inelastic scattering has generally been neglected in 3D ED refinement (Saha *et al.*, 2022; Pala-



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tinus *et al.*, 2013; Thomas *et al.*, 2024). Such processes are known to alter diffracted intensities in ways not captured by purely elastic models (Eggeman *et al.*, 2013). Their omission thus limits the completeness of current refinements, potentially introducing artefacts into solved structures.

In high-energy ED, where accelerating voltages typically exceed 50 keV, incident electrons can exchange energy with the material through three inelastic mechanisms: thermal diffuse scattering (TDS), plasmon excitations and core-loss ionization. Historically, the term *absorption* has been used to describe the effects arising from TDS. In reality, no true absorption occurs; rather, these processes lead to a loss of elastic intensity and a redistribution of diffracted intensity among beams (Humphreys & Hirsch, 1968), in contrast to the genuine absorption of photons in X-ray diffraction (Albrecht, 1939). Here, it is worth noting that although many kinematical 3D ED refinements make use of X-ray software and absorption corrections (van Genderen *et al.*, 2016; Simoncic *et al.*, 2023; Leung *et al.*, 2024), these corrections model a fundamentally different phenomenon.

While the electron-specific absorption formalism has previously been incorporated in convergent-beam electron diffraction (CBED) refinements (Bird & Saunders, 1992; Zuo & Spence, 1991; Midgley *et al.*, 1995; Zuo *et al.*, 1999; Nakashima *et al.*, 2025), its use in 3D ED remains limited. Beyond CBED, absorption has been addressed through simulations of precession data using a constant absorptive potential, where comparisons with elastic-only calculations revealed only minor differences, but no systematic investigation of the impact of absorption on refinement was undertaken (Palatinus *et al.*, 2013).

In CBED, a stationary crystal is illuminated by a convergent probe, producing Bragg discs that encode the full 2D region surrounding a reciprocal-lattice vector. In 3D ED and PED, crystal rotation or beam precession integrates intensities over linear or circular trajectories, effectively averaging orientation-specific dynamical contrast. The consequence is a set of integrated intensities that more closely match the kinematical approximation (Blackman, 1939), making them well suited for structure solution techniques originally devised for X-ray data.

These considerations raise the central question: under what conditions does absorption materially influence structure refinement, and when can it safely be neglected? To address this, Bloch-wave simulations were performed with and without absorption across multiple materials and orientations, revealing its effect on integrated intensities. Dynamical refinements including absorption were subsequently performed on experimental data, establishing the practical limits of the elastic-only approximation.

2. Methods

2.1. Thermal effects in quantitative electron diffraction

The present analysis builds upon the dynamical refinement method reported by Malik *et al.* (2026), which implements a

differentiable Bloch-wave framework. Unlike the kinematical approximation, which assumes single scattering, Bloch-wave methods explicitly account for coupling between diffracted beams.

Thermal vibrations in crystals give rise to diffuse scattering that removes electrons from the coherent diffracted beams, thereby producing an attenuation of diffracted intensities (Hashimoto *et al.*, 1962). These effects can be decomposed into TDS, arising from random atomic displacements, and phonon scattering (Wang, 1992; Eggeman *et al.*, 2013). Both processes produce sub-eV energy losses that fall within the ‘zero-loss’ peak, rendering most commercially available energy filters ineffective at removing absorption effects and requiring treatment through cooling or explicit modelling (Nakashima *et al.*, 2025). Beyond thermal effects, additional inelastic scattering processes, sometimes also grouped under the term absorption, such as plasmon scattering and core-loss ionization, can, in principle, be removed through energy filtering, although the extent to which this improves diffraction refinement remains unclear (Jansen *et al.*, 2004; Eggeman *et al.*, 2013; Yang *et al.*, 2022; Kim *et al.*, 2010; Gemmi & Oleynikov, 2013; Palatinus *et al.*, 2015a; Latychevskaia & Abrahams, 2019).

While the original Bloch-wave formalism developed by Bethe (1928) treats only elastic scattering, the effects of TDS absorption can be included through the complex Fourier coefficient of the potential (Yoshioka, 1957). For a reciprocal-lattice vector $\mathbf{g}$, this coefficient can be approximated as (Bird & King, 1990)

$$\begin{aligned} U_{\mathbf{g}}^{\text{tot}} &= U_{\mathbf{g}} + iU'_{\mathbf{g}} \\ &= -\frac{h^2}{2m_0\Omega} \sum_{\kappa} \exp[-2i\pi(\mathbf{g} \cdot \mathbf{r}_{\kappa})] \\ &\quad \times [f_{\kappa}(s) + if'_{\kappa}(s, B_{\kappa})] \exp(-B_{\kappa}s^2), \end{aligned} \quad (1)$$

where $s = |\mathbf{g}|/2$, $\mathbf{r}_{\kappa}$ is the position of atom κ in the unit cell, m_0 , h and Ω denote the electron rest mass, Planck’s constant and the unit-cell volume, respectively. Here $f_{\kappa}(s)$ is the elastic scattering factor and $f'_{\kappa}(s, B_{\kappa})$ its absorptive counterpart, calculated within the Einstein-model approximation using the isotropic Debye–Waller factor $B_{\kappa} = 8\pi^2\langle u_{\kappa}^2 \rangle$, where $\langle u_{\kappa}^2 \rangle$ is the mean-squared vibrational displacement.

This displacement depends on the stiffness of the inter-atomic potential. Materials with high Debye temperatures (Θ_D) maintain relatively small $\langle u^2 \rangle$ when compared with materials with low Θ_D under the same conditions. Cooling reduces $\langle u^2 \rangle$ and correspondingly diminishes the magnitude of the absorptive effects (Humphreys & Hirsch, 1968).

Despite its quantitative improvements over the elastic-only model, this formulation remains approximate. A principal limitation is the assumption that absorbed electrons are removed rather than redistributed into diffuse background intensity (Humphreys & Hirsch, 1968). Although background subtraction mitigates the effect, it cannot fully separate diffuse inelastic contributions from the elastic signal. Analytical treatments of TDS suggest that thermally scattered electrons, while centred on Bragg discs, are distributed over far larger

scattering angles than elastically scattered electrons (Wang, 1995). As an example, for InP at 250 keV and 300 K, only 4.2% of TDS electrons are expected to fall within a 10 mrad semi-angle (Jordan *et al.*, 1991); for a conservatively large Bragg-disc radius of 2.5 mrad, the resulting influence on the measured Bragg intensities is therefore expected to be small.

Another important approximation concerns the use of isotropic atomic vibrations, represented by a single parameter U_{iso} , or calculated as $U_{\text{iso}} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$ when anisotropic displacement parameters are available. While anisotropic forms of f'_k exist, they are considerably more demanding computationally, and the errors introduced in f'_k by using isotropic Debye–Waller factors are typically on the order of 1–5% for low- and medium-order reflections (Peng, 1997).

A further limitation arises from the use of the Einstein model, which assumes independent oscillators and fails to describe systems with strong phonon correlations. A more complete description is provided by the frozen phonon method (Wang, 1995; Allen *et al.*, 2015), which conserves total scattering intensity and recovers the diffuse background by averaging over many thermal configurations. While the frozen phonon method can be incorporated into the Bloch-wave framework (Yamazaki *et al.*, 2013; Mendis, 2025), it typically requires averaging over dozens of thermal configurations, imposing a computational burden that restricts its practical use in refinement.

2.2. Two-beam absorption formalism

The two-beam approximation represents the simplest extension beyond the kinematical model, coupling the incident and a single diffracted beam while neglecting higher-order interactions. Although it fails to describe the complex coupling present in strongly diffracting systems or near high-symmetry zone axes, it is often valuable for analytical derivations and in theoretical interpretation.

The two-beam approximation gives analytical expressions for the diffracted-beam intensity under absorption in centrosymmetric crystals (Hashimoto *et al.*, 1962):

$$|\Psi_{\mathbf{g}}|_{\text{abs}}^2 = \exp(-2\kappa_0 t) \frac{[\cosh(2\Delta\kappa t) - \cos(2\pi\Delta\kappa t)]}{2(1+x^2)} \quad (2)$$

with the following definitions:

$$\kappa_0 = \frac{\pi}{\xi'_0}, \quad \Delta\kappa = \frac{\sqrt{1+x^2}}{\xi_{\mathbf{g}}}, \quad \Delta\kappa = \frac{\pi}{\xi'_{\mathbf{g}}\sqrt{1+x^2}},$$

$$\xi'_0 = \frac{K}{U'_0}, \quad \xi'_{\mathbf{g}} = \frac{K}{U'_{\mathbf{g}}}, \quad \xi_{\mathbf{g}} = \frac{K}{|U_{\mathbf{g}}|}, \quad x = \xi_{\mathbf{g}} S_{\mathbf{g}}.$$

Here, $K = |\mathbf{K}| = 1/\lambda$ is the magnitude of the incident electron wavevector $\mathbf{K}$, corresponding to the radius of the Ewald sphere. The excitation error $S_{\mathbf{g}}$ is defined as (Spence & Zuo, 1992)

$$S_{\mathbf{g}} = \frac{K^2 - |\mathbf{K} + \mathbf{g}|^2}{2K},$$

which may be interpreted as the distance of a reciprocal-lattice point from the Ewald-sphere surface.

The quantity ξ'_0 determines the mean absorption, while $\xi'_{\mathbf{g}}$ governs the strength of anomalous absorption; Hashimoto *et al.* (1962) describe $\xi'_{\mathbf{g}}$ as the absorption distance.

The mean absorptive potential U'_0 is defined as (Rez *et al.*, 1994)

$$U'_0 = \frac{\gamma}{\pi} \frac{\sum_i n_i f'_i(0)}{\Omega}, \quad (3)$$

where γ is the relativistic correction factor, n_i are the site occupancies, $f'_i(0)$ are the absorptive scattering factors at $\mathbf{g} = 0$ and the sum is over all atoms in the unit cell. In the absence of absorption, the two-beam diffracted intensity simplifies to (Hirsch *et al.*, 1965):

$$|\Psi_{\mathbf{g}}|_{\text{no abs}}^2 = \frac{\sin^2(\pi t \Delta\kappa)}{(1+x^2)}, \quad (4)$$

which can be rewritten as

$$|\Psi_{\mathbf{g}}|_{\text{no abs}}^2 = \frac{1 - \cos(2\pi t \Delta\kappa)}{2(1+x^2)}. \quad (5)$$

In equation (2), absorption enters through a global damping term $\exp(-2\kappa_0 t)$ and a reflection-specific term $\cosh(2\Delta\kappa t)$. When $U'_0 = U'_{\mathbf{g}} = 0$, both reduce to unity, and equation (2) reverts to the elastic form of equation (5). While equations (2) and (5) are given for diffraction at a specific orientation $S_{\mathbf{g}}$, in 3D ED the quantity of interest is the integrated rocking-curve intensity. Starting from the non-absorbed two-beam expression [equation (5)], the relevant quantity is

$$I_{\text{no abs}}^{\text{int}}(t) = \int_{-\infty}^{\infty} |\Psi_{\mathbf{g}}|_{\text{no abs}}^2 dx, \quad x = \xi_{\mathbf{g}} S_{\mathbf{g}}. \quad (6)$$

Following Blackman's treatment of two-beam integrated intensities (Blackman, 1939), we introduce $A = \pi t/\xi_{\mathbf{g}}$, giving (Own, 2005)

$$I_{\text{no abs}}^{\text{int}}(t) = \int_{-\infty}^{\infty} \frac{\sin^2(A\sqrt{1+x^2})}{1+x^2} dx = \pi \int_0^A J_0(2u) du, \quad (7)$$

where J_0 is the zeroth-order Bessel function of the first kind.

As derived in Section S1 (in the supporting information), carrying out the corresponding integral for the absorbed case in the weak-absorption limit ($t/\xi_{\mathbf{g}} \ll 1$) yields

$$\frac{I_{\text{abs}}^{\text{int}}(t)}{I_{\text{no abs}}^{\text{int}}(t)} \approx \exp(-2\kappa_0 t) \left[1 + \frac{\pi t \xi_{\mathbf{g}}}{2\xi_{\mathbf{g}}^2} \left(1 - \frac{\pi^2 t^2}{3\xi_{\mathbf{g}}^2} + \frac{\pi^4 t^4}{20\xi_{\mathbf{g}}^4} \right)^{-1} \right]. \quad (8)$$

For centrosymmetric crystals, absorption therefore modifies the integrated two-beam intensity in two distinct ways. The global factor $\exp(-2\kappa_0 t)$ applies a uniform thickness-dependent attenuation, given by U'_0 . The second factor represents the anomalous contribution arising from the reflection-specific $U'_{\mathbf{g}}$. At large thickness, this anomalous term causes reflections to diverge from the uniform decay. Reflections with large $U'_{\mathbf{g}}$

Table 1
Crystallographic parameters for the three materials used in this study.
For full experimental acquisition and data reduction details, see the original references.

Parameters	CsPbBr ₃	α-Quartz (SiO ₂)	Borane (B ₁₈ H ₂₂)
Source dataset	Suresh <i>et al.</i> (2024)	Klar <i>et al.</i> (2023)	Suresh <i>et al.</i> (2024)
Space group	<i>Pbnm</i>	<i>P3₂21</i>	<i>Pccn</i>
Unit cell (<i>a</i> , <i>b</i> , <i>c</i>) (Å)	8.119, 8.359, 11.759	4.923, 4.923, 5.400	10.770, 11.990, 10.736
Angles (α, β, γ) (°)	90, 90, 90	90, 90, 120	90, 90, 90
Volume (Å ³)	798.1	113.3	1386.9

(small ξ_g') show the largest departures, since the anomalous term scales approximately as $\xi_g/\xi_g'^2$.
For non-centrosymmetric crystals, additional first-order absorptive contributions may also arise from phase differences between the elastic and absorptive structure factors (Bird, 1990). These effects are discussed in Section S2, where additional simulations indicate that the resulting additional non-centrosymmetric contributions remain comparatively small.
To obtain experimentally meaningful quantities, the two-beam integrated expressions in equations (6)–(8) must include an additional Lorentz correction of the form $I_{2\text{-beam}}^{\text{int}} \times L$, where L accounts for the angular dwell time of a reflection near its Bragg condition, which is inversely proportional to the velocity of Bragg-crossing during rotation (McIntyre & Stansfield, 1988; Zhang *et al.*, 2010).
In a continuous-rotation experiment, this velocity is set by the component of the reciprocal-lattice vector perpendicular to the rotation axis (Holmes, 2014). If ϕ denotes the angle between $\mathbf{g}$ and the rotation axis, the intersection speed is proportional to $|\mathbf{g}|\sin\phi$. The correction therefore takes the form $L = 1/|\mathbf{g}|\sin\phi$, which expresses the fact that reflections near the rotation axis remain near their Bragg condition for

longer and contribute more strongly to the observed experimental intensity.

3. Results

3.1. Comparison of two- and many-beam models of absorption

The material caesium lead bromide (CsPbBr₃) was examined using the structure reported by Suresh *et al.* (2024), with the corresponding structural parameters listed in Table 1. This compound was selected because it contains atoms of large atomic number and correspondingly strong elastic and absorptive scattering factors f and f' , making absorption especially significant.
Two-beam and many-beam integrated intensities were simulated for CsPbBr₃ at 200 keV using the first experimentally observed orientation, $[uvw] = [-0.43, 1.00, 0.93]$, taken from the 3D ED dataset reported by Suresh *et al.* (2024) and determined during data reduction using *PETS2* (Palatinus, 2011). This orientation defines the centre of a virtual frame, as described by Klar *et al.* (2023), with each virtual frame corresponding to a small angular range in α around the central orientation, where α is the rotation axis of the goniometer. In this study, all orientations correspond to experimentally observed ones, while specific angular positions within a virtual frame are referred to as tilts.
The two-beam integrated intensities for this orientation were computed by numerically integrating equations (2) and (4) with an additional Lorentz correction. In the many-beam case, calculations were performed using the full Bloch-wave code described by Malik *et al.* (2026), with the parametrized form of the absorptive scattering factors f' adapted from Thomas *et al.* (2024). Here, no Lorentz correction is required

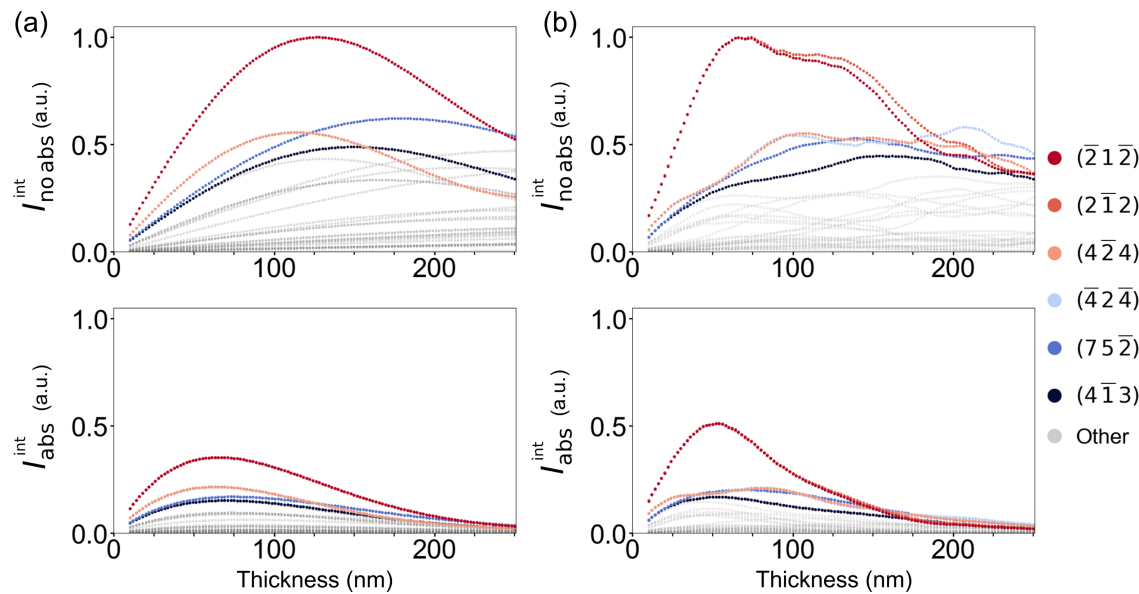


Figure 1
Integrated intensity versus thickness for CsPbBr₃, 200 keV, $[uvw] = [-0.43, 1.00, 0.93]$, without (top) and with absorption (bottom), for the (a) two-beam, (b) many-beam model. The six most intense reflections are highlighted in colour, with all others shown in grey for clarity.

because the rotation geometry is already encoded through explicit tilt sampling.

A $\pm 1.5^\circ$ sweep around the experimental orientation was simulated with 60 uniformly spaced tilt samples, and the corresponding rocking curves were summed to obtain the integrated intensities. Unless otherwise stated, 60 tilt samples per orientation were used throughout.

Simulations were performed for thicknesses between 10 and 250 nm. This lower limit was chosen as the width of rocking curves scales inversely with thickness in the kinematic limit (Hirsch *et al.*, 1965), and therefore at very small thicknesses (where the kinematic approximation is valid), the curves may exceed the angular range defined by the virtual frame. As a result, part of the diffracted intensity may fall outside the sampling window, making these reflections not fully integrated.

The resulting two-beam and many-beam integrated intensities, with and without absorption, are shown in Fig. 1.

While the two-beam curves show smooth Pendellösung-type oscillations, the many-beam case develops the expected irregularities from multiple strongly coupled reflections. In the two-beam model, pairs such as $(\bar{2}1\bar{2})/(\bar{2}\bar{1}2)$ and $(4\bar{2}4)/(\bar{4}2\bar{4})$ maintain identical intensities over the full thickness range. In the many-beam calculation, however, these pairs begin to diverge at thicknesses approaching 100 nm, reflecting the redistribution of intensity through additional dynamical pathways.

In both models, absorption clearly attenuates intensities, but this plot alone does not reveal the reflection-specific decay rates or how the models compare. To address this comparison, Fig. 2 shows the ratio of absorbed to non-absorbed integrated intensities ($I_{\text{abs}}^{\text{int}}/I_{\text{no abs}}^{\text{int}}$) as a function of thickness for the two- and many-beam models.

In the two-beam case [Fig. 2(a)], fitting an exponential decay to each individual hkl yields a mean absorption length of $\bar{\lambda} = 89.9$ nm with a standard deviation of $\sigma_{\lambda} = 2.0$ nm. From the two-beam absorption formalism, the decay constant is

determined by the global damping term, with $\lambda_{2\text{-beam}} = K/(2\pi U_0')$. Using $K = 39.87 \text{ \AA}^{-1}$ at 200 keV and $U_0' = 0.0072 \text{ \AA}^{-2}$ for CsPbBr₃, the predicted absorption length is $\lambda_{2\text{-beam}} = 88.4$ nm, in excellent agreement with the fitted value.

As expected, the two-beam model shows little reflection-dependent variation in the absorption ratios. $(4\bar{2}4)$ and $(\bar{4}2\bar{4})$ begin to depart from the otherwise nearly uniform attenuation trend for $t > 150$ nm [$(4\bar{2}4)$ is not visible because it lies directly beneath $(\bar{4}2\bar{4})$]. These reflections have the largest values of U_{g} and U_{g}' among the observed set, with $U_{\text{g}} = 0.013 \text{ \AA}^{-2}$, $U_{\text{g}}' = 0.003 \text{ \AA}^{-2}$, giving $\xi_{\text{g}} \approx 300$ nm and $\xi_{\text{g}}' \approx 1400$ nm. Equation (8) predicts that the anomalous contribution increases when t approaches ξ_{g} , in agreement with the observed behaviour. To further illustrate the deviation from uniform attenuation in the two-beam model as t approaches ξ_{g} , an extended version of Fig. 2(a) covering 0–350 nm is shown in Fig. S1(a) (in the supporting information).

By contrast, the many-beam case [Fig. 2(b)] exhibits a broader distribution of decay constants, with $\bar{\lambda} = 93.2$ nm and $\sigma_{\lambda} = 10.1$ nm, indicative of the effects of anomalous, reflection-specific absorption.

Beyond integrated intensities, rocking-curve analysis provides further insight into how absorption modifies scattering pathways. Many-beam rocking curves for all reflections considered in the above calculation at $t = 200$ nm are shown in Fig. S5. While not representative of the original sample thickness observed by Suresh *et al.* (2024), 200 nm serves as an illustrative high-thickness example, where absorption is especially pronounced.

Fig. S5 shows that absorption can modify the tilt-dependent intensity profile (*i.e.* rocking curve) in ways that vary markedly across reflections: for some, the effect is nearly uniform across all tilts, while for others it is strongly tilt dependent. Despite these local tilt variations, the corresponding integrated intensities exhibit far smaller differences between absorptive and elastic simulations. This contrast helps explain why absorption plays a significant role in CBED analysis, where

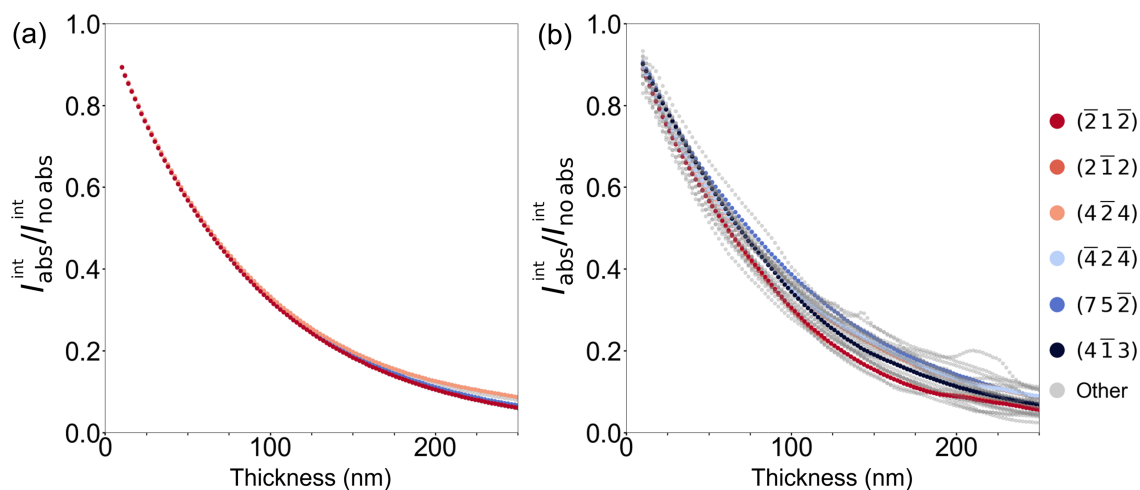


Figure 2

Ratio of integrated intensity ($I_{\text{abs}}^{\text{int}}/I_{\text{no abs}}^{\text{int}}$) as a function of thickness for CsPbBr₃ with $[uvw] = [-0.43, 1.00, 0.93]$. (a) Two-beam model; (b) many-beam model. A decaying exponential was fitted to each hkl curve, yielding absorption parameters $\bar{\lambda} = 89.9$ nm, $\sigma_{\lambda} = 2.0$ nm (two-beam) and $\bar{\lambda} = 93.2$ nm, $\sigma_{\lambda} = 10.1$ nm (many-beam).

rocking-curve shapes are fitted directly (Zuo & Spence, 1991), but a reduced one in 3D ED, where integration suppresses tilt-specific behaviour.

3.2. Implications of neglecting absorption in dynamical refinement

The discrepancy between elastic and absorptive simulations can be further quantified using a residual. A standard choice is R_1 , defined as

$$R_1 = \frac{\sum_i |\sqrt{I_i^{\text{exp}}} - \sqrt{I_i^{\text{calc}}}|}{\sum_i \sqrt{I_i^{\text{exp}}}},$$

where I_i^{exp} denotes the experimentally observed intensity of reflection i , and I_i^{calc} the corresponding simulated intensity. Because R_1 does not weight reflections by their experimental uncertainties, it is particularly sensitive to noisy, low-intensity reflections. Consequently, practical refinements typically report R_{obs} , defined as R_1 evaluated only over reflections satisfying $I_i^{\text{exp}}/\sigma_i > 3$, where σ_i is the estimated measurement error (Palatinus *et al.*, 2019). Another alternative is the weighted form wR_{all} , which considers all intensities and weights the contribution of each I_i according to its uncertainty σ_i and its magnitude. To estimate the influence of absorption, R_1 can be adapted to measure the deviation between absorptive and purely elastic simulations:

$$R_1(t) = \frac{\sum_i |\sqrt{I_i^{\text{int,abs}}(t)} - \sqrt{I_i^{\text{int,no abs}}}|}{\sum_i \sqrt{I_i^{\text{int,no abs}}}}. \quad (9)$$

Here, a global scale factor corresponding to the mean absorptive attenuation has been omitted for simplicity, such that only reflection-dependent deviations contribute to the residual; the full derivation is given in Section S3. If the ratio of integrated intensities $I_i^{\text{int,abs}}/I_i^{\text{int,no abs}}$ is approximated as an exponential decay with mean decay constant $\bar{\lambda}$ and a Gaussian spread of λ_i , the resulting thickness dependence of the residual can be estimated in closed form,

$$R_1(t) \approx \sqrt{\frac{2}{\pi}} \frac{t \sigma_{\lambda}}{2 \bar{\lambda}^2}, \quad R_1(t) \propto t, \quad (10)$$

so that the slope of the residual is

$$\frac{dR_1}{dt} = \sqrt{\frac{2}{\pi}} \frac{\sigma_{\lambda}}{2 \bar{\lambda}^2}. \quad (11)$$

R_1 is therefore expected to increase linearly with thickness, governed by both the mean absorption length $\bar{\lambda}$ and its relative spread σ_{λ} . A uniform absorptive attenuation, such as that predicted by the two-beam model, is therefore expected to have no impact on residuals, in contrast to the anomalous absorption observed in many-beam simulations.

To test this, equation (9) was evaluated across thickness for CsPbBr₃ at $[uvw] = [-0.43, 1.00, 0.93]$, with the results shown in Fig. 3(a).

Although the comparison involves only simulated intensities, the calculation was restricted to reflections classified as experimentally observed in the original dataset of Suresh *et al.* (2024), with $I_i^{\text{exp}}/\sigma_i > 3$, such that the predicted residuals correspond to those expected for a real experimental refinement. The corresponding dataset and crystallographic parameters are summarized in Table 1.

In Fig. 3(a), the dark-blue curve is calculated from integrated intensities, obtained by summing 60 tilts across the full $\pm 1.5^\circ$ tilt series, while residuals at individual tilts (non-integrated intensities) are shown in light blue. The comparison demonstrates reduced anomalous absorption achieved by integration: although individual tilts can show strong deviations, these largely cancel when averaged.

At low thicknesses the predicted effect of absorption is minimal, with R_1 remaining below 5% for thicknesses under 100 nm. Using the parameters $\bar{\lambda} = 93.2$ nm and $\sigma_{\lambda} = 10.1$ nm, the predicted slope from equation (11) is $dR_1/dt = 0.046\% \text{ nm}^{-1}$, in close agreement with the best-fit slope of $0.048\% \text{ nm}^{-1}$ shown in Fig. 3(a).

This residual can be interpreted as a nominal attainable lower bound on an elastic-only dynamical refinement. To

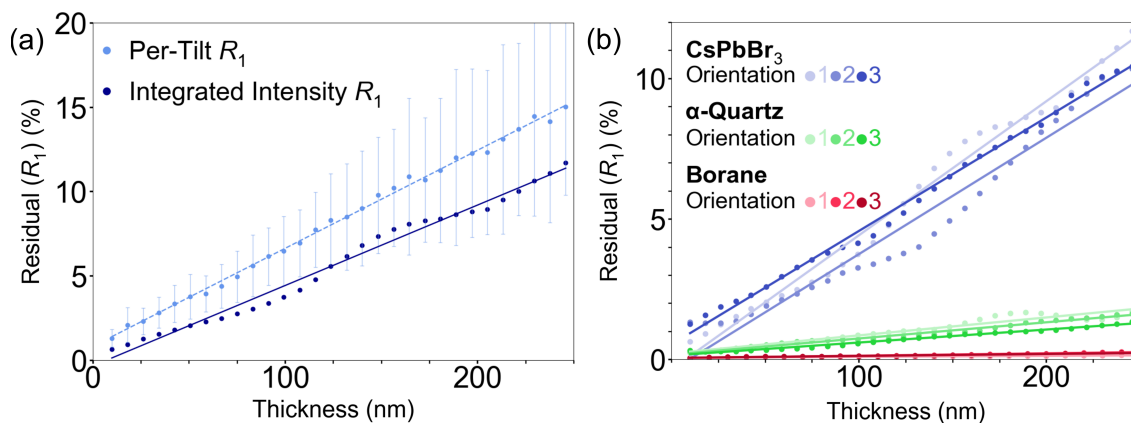


Figure 3 Thickness dependence of residual error R_1 (%) between simulated I_{abs} and $I_{\text{no abs}}$. (a) Integrated intensities (dark blue) compared with per-tilt intensities (light blue) for CsPbBr₃ at $[uvw] = [-0.43, 1.00, 0.93]$; light-blue points are R_1 averages across $\pm 1.5^\circ$ tilt series with error bars showing standard deviation around the mean. Best-fit slopes were determined, yielding 0.048 and $0.058\% \text{ nm}^{-1}$ for the integrated intensities and per-tilt values, respectively. (b) Integrated intensity R_1 curves for CsPbBr₃, α -quartz and borane, each shown with three representative orientations (best-fit slopes and $[uvw]$ indices given in Table S3).

compare this predicted lower bound with real refinements, we consider the elastic-only refinements of the same CsPbBr₃ dataset reported by Suresh *et al.* and re-analysed by Malik *et al.* (2026). Suresh *et al.* reported an overall $R_{\text{obs}} = 5.3\%$, while Malik *et al.* yielded a value of $R_{\text{obs}} = 6.5\%$. Because the present study employs the refinement framework and simulation pipeline of Malik *et al.*, all comparisons refer specifically to their results, ensuring that parameters are defined and controlled consistently.

While the true specimen thickness is not known, the hybrid physics machine learning framework used in this study and introduced by Malik *et al.* (2026) extracts an orientation-dependent thickness distribution directly from the diffraction data through joint refinement of structural and experimental parameters. For the orientation shown in Fig. 3(a), this corresponds to a thickness of $t \approx 50$ nm, for which the predicted effect of neglecting absorption is around 2%. This comparison shows that the low refinement residuals reported are consistent with the predicted effect of absorption at this thickness, indicating that only a minor improvement would be expected from incorporating absorption in the refinement.

While the preceding comparison concerns only a single orientation, absorption and resulting residuals are expected to vary with orientation. To quantify this effect, $R_1(t)$ between absorptive and purely elastic simulations was computed for a range of orientations and materials typical of 3D ED experiments. Fig. 3(b) compares these results for three materials taken from recently reported continuous-rotation 3D ED datasets: CsPbBr₃ (Suresh *et al.*, 2024), α -quartz (Klar *et al.*, 2023) and octadecaborane (hereafter referred to as borane) (Suresh *et al.*, 2024).

In each case, the first three experimentally observed orientations were simulated, with equation (9) evaluated only for reflections with $I_i^{\text{exp}}/\sigma_i > 3$. These materials were selected to capture a wide range of structural and physical characteristics: CsPbBr₃ is a halide perovskite with high atomic number, quartz is an inorganic oxide with moderate atomic number, and borane is an inorganic molecular crystal composed of light

elements. Additionally, CsPbBr₃ (*Pbnm*) and borane (*Pccn*) are centrosymmetric, whereas α -quartz (*P3₂21*) is non-centrosymmetric. Their crystallographic parameters are listed in Table 1.

From Fig. 3(b), clear material-dependent trends emerge. For all three materials, the first three orientations lie within a narrow mean-thickness range, giving values of approximately 50 nm for CsPbBr₃, 85 nm for α -quartz and 170 nm for borane, as determined from the orientation-dependent thickness profile obtained in the elastic-only refinements (see Fig. S8). At these thicknesses, absorption contributes *ca.* 2% for CsPbBr₃, 0.6% for α -quartz and 0.2% for borane.

As shown earlier, in the two-beam limit, inclusion of absorption produces almost no per-reflection variation, with intensities attenuated uniformly. Under many-beam conditions, however, absorption alters the inter-beam coupling, changing how intensity is redistributed with thickness. The resulting deviation from the elastic-only solution therefore reflects the degree of many-beam interaction. In CsPbBr₃, the heavy constituent atoms lead to the simultaneous excitation of many strong beams. In contrast, α -quartz and borane exhibit much weaker many-beam character at these thicknesses. Their lower atomic numbers result in fewer simultaneously excited strong reflections, so scattering is dominated by quasi-two-beam interactions. In such regimes, the inclusion of absorption does not result in significant redistribution of diffracted intensity. The behaviour observed for quartz further suggests that the additional absorptive effects associated with non-centrosymmetric crystals remain comparatively weak under the present conditions.

3.3. Orientation dependence of absorption effects

In addition to the strong material dependence, little systematic variation is observed across orientations in Fig. 3(b). This may be explained by the geometry of the orientations examined, with each lying away from strongly diffracting zone axes. This behaviour is characteristic of 3D ED datasets, where randomly orientated crystals are rotated through large angular ranges that remain predominantly off-zone, typically intersecting perhaps only a single major zone axis over the course of the tilt series. At such zone-axis conditions, however, where many-beam effects are strongest, a correspondingly greater influence of absorption is expected.

To examine this behaviour explicitly, three representative orientations from the CsPbBr₃ dataset were selected to span off-zone, intermediate and near-zone regimes. While several orientations in the dataset fall into each category, orientations 1, 8 and 19 were chosen for illustration, with the corresponding simulated diffraction patterns shown in Fig. 4(b). Orientation 1 ($[uvw] = [-0.43, 1.00, 0.93]$) serves as the representative off-zone reference, orientation 8 ($[uvw] = [-0.67, 1.00, 0.67]$) corresponds to a direction near $[232]$ and orientation 19 ($[uvw] = [-1.00, 1.00, 0.33]$) lies close to $[331]$.

In Fig. 4(a), the variation of $R_1(t)$ with crystal orientation is shown, highlighting the strengthening of many-beam coupling and the associated enhancement of anomalous absorption

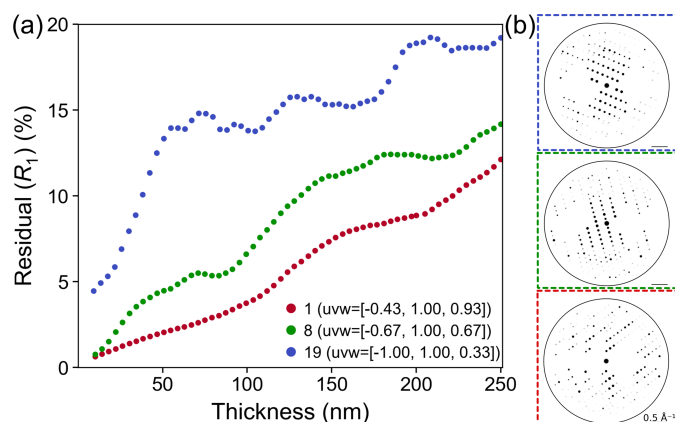


Figure 4
Orientation dependence of absorption effects in CsPbBr₃. (a) Thickness dependence of R_1 between simulated $I_{\text{abs}}^{\text{int}}$ and $I_{\text{no abs}}^{\text{int}}$ for orientations 1, 8 and 19. (b) Corresponding simulated diffraction patterns, each enclosed by a dashed box in the colour of its respective curve in (a).

effects as the crystal is tilted towards a strongly diffracting zone axis. Orientation 1 [seen previously in Figs. 3(a), 3(b)] is representative of most orientations in the dataset, with an approximately linear thickness dependence in R_1 . Orientation 8 displays a markedly steeper trend, indicating stronger many-beam coupling, while orientation 19 shows the strongest and most nonlinear response, rising to nearly 13% by 50 nm. Such a large residual indicates that an elastic-only refinement would perform poorly for this orientation, with a correspondingly large improvement expected if absorption is included.

Further insight into this behaviour is provided in Fig. S6, in which $I_{\text{abs}}^{\text{int}}/I_{\text{no abs}}^{\text{int}}$ is plotted as a function of thickness for the corresponding curves. These simulations show that the decaying-exponential attenuation underlying the linear $R_1(t)$ trend no longer holds as the crystal approaches a zone axis.

Comparable behaviour has been reported in recent dynamical refinements, where orientations near zone axes exhibit anomalously high residuals, previously ascribed to crystal imperfections and excessive dynamical effects (Olech *et al.*, 2024). In that study, 15 frames corresponding to these orientations were omitted from the refinement, representing a significant loss of usable data. The present results indicate that exclusion of such frames may be unwarranted, as the elevated residuals are largely attributable to previously unmodelled absorption effects.

3.4. Elastic and absorptive refinements of experimental 3D ED data

Although the preceding simulations indicate that the inclusion of absorption will significantly alter simulated intensities, it remains unclear whether these differences will yield measurable benefits in refinement accuracy or in the recovered structure. To answer this question, full dynamical refinements were carried out for CsPbBr₃, α -quartz and borane, with and without absorption.

For each material, refinements followed the complete workflow described by Malik *et al.* (2026). This included orientation-dependent thickness refinements. The corresponding refined thickness-tilt curves for all three materials are shown in Fig. S8; overall the absorptive and elastic models give similar trends, but notable deviations occur for specific orientations (e.g. CsPbBr₃ ~55 versus 48 nm; borane ~200 versus 170 nm).

The resulting refinement statistics are summarized in Table 2, with refinement parameters provided in Table S4.

Across all three materials, the inclusion of absorption produces only modest changes in the refinement residuals. CsPbBr₃ shows a clear improvement when absorption is included, while the refinement residuals of α -quartz and borane remain effectively unchanged.

While the earlier analysis predicted a reduction of R_{obs} for CsPbBr₃ from approximately 6.4% to 4.5%, the refinement only reaches 5.3%. This outcome likely reflects both the simplifying assumptions of the absorptive model, including its isotropic treatment of thermal motion and unmodelled phonon correlations, and the broader set of factors that

Table 2

Refinement residuals for CsPbBr₃, α -quartz and borane.

Residual (%)	CsPbBr ₃	α -Quartz	Borane
Elastic $R_{\text{obs}}/wR_{\text{all}}$	6.40/6.73	4.14/3.84	9.54/8.56
Absorptive $R_{\text{obs}}/wR_{\text{all}}$	5.26/5.31	4.00/3.66	9.48/8.51

contribute to the observed residual, such as plasmon and core-loss ionization, beam damage and crystal imperfections. These factors obscure the specific contribution of absorption, and the observed decrease in R_{obs} is therefore consistent with the expected behaviour under experimental conditions.

For quartz and borane, the predicted absorption effects were modest, and the refinements exhibit correspondingly small improvements. For both materials, absorption therefore plays no significant role in the refinement, and the remaining analysis focuses on CsPbBr₃, with the full quartz and borane results reported in the supporting information.

Beyond the overall improvement in residuals observed for CsPbBr₃, the orientation-dependent residuals (Fig. 5) show several pronounced outliers (orientations 19, 29, 46, 53). As discussed in Section 3.3, these orientations lie near strongly diffracting zone axes, where many-beam coupling is stronger and absorption has a larger influence.

Although the residuals of orientations 19, 29, 53 decrease markedly following the inclusion of absorption, they remain high outliers. This behaviour indicates that the present absorptive model corrects only part of the deviation and that additional zone-axis effects, possibly including plasmon and core-loss ionization contributions or more complex dynamical interactions, remain unaccounted for. While such orientations might warrant exclusion in an elastic-only refinement, the absorptive model provides a sufficient basis for their retention.

Additionally, several orientations exhibit worse residuals under the absorptive model. While it is not clear why this occurs, this may be attributable to experimental uncertainty together with the approximate treatment of absorption employed here.

To further assess the consequences of including absorption on the refined structure, Table S5 compares the atomic para-

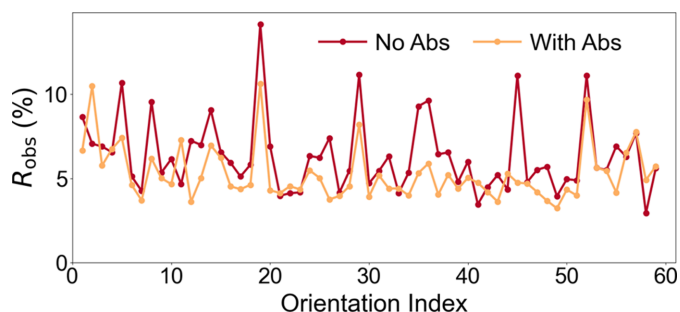


Figure 5

Results of dynamical refinements performed with and without the inclusion of absorption for CsPbBr₃. Residuals R_{obs} (%) are compared across rotation indices for refinements carried out on identical datasets and parameters. Fig. S7 shows the corresponding wR_{all} results for CsPbBr₃ and the full orientation-dependent residuals for α -quartz and borane.

meters obtained with and without the absorptive potential for CsPbBr₃. The inclusion of absorption produces only minor shifts in both fractional coordinates and anisotropic displacement parameters. The largest observed positional difference is approximately 0.001 in fractional coordinates, with corresponding changes in anisotropic displacement parameters below 0.003 Å², both within normal refinement precision (Brázda *et al.*, 2019), confirming that the refined structure remains stable under the modified scattering model. This indicates that even for a material with a large mean atomic number $\langle Z \rangle$ of 48.4, for thicknesses below 50 nm, absorption has little practical impact on the recovered structure. Consequently, omitting absorption from dynamical refinement simulations is expected to bias thermal and structural parameters only in high- Z materials at thicknesses approaching ξ_g .

4. Conclusion

This work presents what is, to our knowledge, the first implementation of absorption in 3D ED dynamical refinement, establishing its influence on experimental residuals and refined structures. Though central to CBED contrast, absorption has a much weaker influence on the relative intensities measured in 3D ED. This discrepancy arises from integration, which averages orientation-specific anomalous absorption.

The underlying theory is examined, beginning from the two-beam approximation, yielding a closed form expression for integrated intensities in the presence of absorption for centrosymmetric crystals. This shows that for $t \ll \xi_g$ reflections experience a uniform exponential decay with thickness, with a decay rate set by the mean absorptive potential U'_0 . In the many-beam limit, dynamical refinements that neglect absorption incur a systematic, thickness-dependent residual. The residual $R_1(t)$ grows approximately linearly with thickness, determined by the mean absorption length $\bar{\lambda}$ and its spread σ_λ , and with this effect becoming more severe near zone axes. This behaviour explains a longstanding observation that orientations near zone axes exhibit anomalously high residuals in elastic-only dynamical refinements and provides a framework for incorporating these data rather than discarding them.

Comparative refinements of CsPbBr₃ performed with and without absorption show a clear improvement in fit when absorption is included, reducing the refinement residual R_{obs} from 6.4% to 5.3%. In contrast, refinements of α -quartz and borane under identical conditions show little improvement in R_{obs} , consistent with expectations for lower- Z materials.

Absorption can therefore safely be neglected for routine refinements except in high- Z materials for thicknesses approaching ξ_g . Although not addressed in the present analysis, temperature is also expected to play a significant role, with materials observed at $T \geq \Theta_D$ likely to exhibit strong absorptive effects.

Additionally, the influence of omitting absorption in the determination of finer structural information such as bonding charge density remains unclear. It is worth noting that

deviations away from neutral-atom scattering factors will affect low-order reflections disproportionately. These have, in general, the largest U_g , U'_g and the effects of absorption will likely be appreciable.

Similarly, although the additional absorptive effects associated with non-centrosymmetric crystals were shown here to be comparatively small, these may still provide useful sensitivity to chirality and absolute structure determination through the breaking of Friedel equivalence.

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Conflict of interest

The authors disclose no conflicts of interest.

Data availability

All data, analyses and code used to produce the results are available in the GitHub repository <https://github.com/bcolmey/role-of-absorption-in-3DED-dynamical-refinement>.

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