Wavelet analysis of white beam x-ray fluorescence holograms: determination of lattice sites and imaging of local atomic structure

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Abstract. The prospects of atomic structure imaging with the continuous spherical wavelet transform (CSWT) as applied to white beam x-ray fluorescence holograms (XFH) are discussed. Recording of XFH with a white x-ray beam eliminates holographic twin images and minimizes extinction effects. However, the lack of these parasitic effects is accompanied by a limited radial resolution. In this work, by introducing an approximation of the white x-ray spectrum based on the Gumbel distribution, we propose an improvement both in generation of white beam XFH and in data analysis. Using approximate analytical models and realistic numerical simulations, we give a detailed description of the properties and resolution of local structure projections directly obtained from XFH by using wavelet analysis. It is demonstrated that the CSWT and, in particular, its windowed inversion can be effectively used to enhance and speed up reliability factor (R-factor) analysis of the data, which enables precise fully three-dimensional localization of multiple lattice sites of dopants. For this, an exact analytic formula for the inversion is given, enabling its fast calculation in a single step. As an example system, we consider magnetic ions in wurtzite GaN.

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1. Introduction

X-ray fluorescence holography (XFH) [1] is a structural probe capable of providing images of local atomic structure. In this work, we discuss a variant of XFH carried out in absorption geometry [2], in which fine structures of x-ray absorption anisotropy are interpreted in terms of holograms of local atomic structure around absorbing atoms. X-ray fluorescence is used to monitor the absorption and provides element selectivity. XFH is usually performed using monochromatic x-ray excitation and the maps of x-ray absorption anisotropy give information in reciprocal space. The conversion to real space is achieved by a holographic reconstruction [3]. For a recent review of XFH, see [4].

In [5], it was shown that the use of broad-band illumination enables one to interpret x-ray absorption anisotropy patterns as quasi-real space projections of atomic structure. This particular feature originates from the very short longitudinal coherence length of the white x-ray beam (of the order of 1 Å), which implies that the interference effects are only visible close to the forward scattering direction, i.e. around interatomic directions. This removes the problem of the holographic twin images [6] and makes the study of systems with lower symmetry possible. For monochromatic illumination, high symmetry is required as the XFH data need to be extended to a wide angular range for the holographic integral transform. Furthermore, white beam illumination minimizes the so-called extinction effects which make data analysis in holographic methods cumbersome [7].
Initially, white-beam x-ray absorption anisotropy could only be measured using the total electron yield as a secondary signal [8]. However, recently, the possibility of recording it with characteristic fluorescence radiation was demonstrated [9]. Consequently, the names white beam x-ray absorption anisotropy and white beam x-ray fluorescence holography will be used interchangeably.

The analysis of white beam XFH data is still an open issue. Among the proposed approaches are the direct comparison of angular maps with geometrical projections of the atomic structure around absorbing atoms [10] and a tomographic algorithm [8]. The first approach provides only qualitative information and the tomographic procedure is, in practice, limited to cubic samples. Quantitative analysis of white beam XFH can be performed by means of the most recently proposed and still developed approach: the continuous spherical wavelet transform (CSWT) [11]. The main drawback of this approach is related to the limited resolution in the radial direction or, in other words, in the accuracy in determination of inter-atomic bonds.

In this paper we present a detailed study of the wavelet analysis of white beam XFH. We focus on two aspects of such an analysis. Firstly, we investigate the potential of the wavelet transform as a tool for obtaining direct projections of local atomic structure. Secondly, we show that wavelets can be used as an efficient tool to enhance and speed up conventional methods of structural data analysis such as R-factor [12] procedures, which provide precise, fully three-dimensional (3D) information about structure.

The presented work is based on computer simulations and is constructed as follows. The first part is devoted to an improvement of the generation of white beam XFH patterns. A new approximation of a white beam synchrotron spectrum is proposed (based on the Gumbel distribution), which takes into account its heavily skewed nature. Next, analytical formulae for the resolution of the CSWT are derived and its sensitivity to the local structure is examined. For example, in monochromatic XFH, it was reported that signals from periodic lattice can severely influence the images of local structure [13–15]. For a white beam, these effects are studied using a model scatterer chain and wurtzite GaN atomic clusters. It is demonstrated that high-quality imaging, e.g. sensitive to light atoms, such as nitrogen in GaN, can only be achieved at the expense of losses in the radial resolution. In such a case the 3D wavelet analysis is replaced by a two-dimensional (2D) windowed inverse wavelet transform. A derivation of an analytic formula is presented for such a transformation, which allows for its fast and effective computation in a single computation step. It is shown that projections of the local atomic structure obtained with this approach are nearly free of artefacts and robust to noise. Finally, we propose a combined wavelet-assisted R-factor analysis for the imaging of the local atomic structure and determination of multiple-lattice sites from white beam holograms. As an example we discuss magnetic impurities in the GaN matrix.

2. White beam x-ray fluorescence holograms

2.1. Basic properties

Before diving into data analysis a few remarks on the origin and generation of XFH patterns have to be made. For monochromatic x-rays the absorption coefficient can be written as [16]

$$\mu(k) = \mu_0[1 + \chi_0(k)],$$  

(1)

where $\mu_0$ is the absorption coefficient of isolated atoms and $\chi_0(k)$ is the absorption anisotropy or the hologram. It originates from the interference of an incident plane wave with spherical
waves scattered inside the sample and in the first Born approximation is given as [17]

$$\chi_0(\mathbf{k}) = -2r_e \text{Re} \left[ \int_V \rho(\mathbf{r}) \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{r} e^{-i\mathbf{k} \cdot \mathbf{r}} dV \right],$$

(2)

where by convention [11] \( \mathbf{k} \) is a vector antiparallel to the wave vector of the incident radiation, \( r_e \) is the Thomson scattering length and \( \rho(\mathbf{r}) \) is the electron density at site \( \mathbf{r} \).

For polychromatic radiation the absorption anisotropy \( \chi(\hat{\mathbf{k}}) \) is defined as [11]

$$\chi(\hat{\mathbf{k}}) = \int_0^\infty N_0(k) \mu_0(k) \chi_0(\mathbf{k}) \, dk,$$

(3)

where \( N_0(k) \) is the incident beam spectrum. The quantity

$$N_0(k) \mu_0(k) \equiv N(k)$$

(4)

will be referred to as the effective spectrum. Expression (3) can be rewritten as

$$\chi(\hat{\mathbf{k}}) = -2r_e \int_V \rho(\mathbf{r}) h(\vartheta, r) \, dV$$

(5)

with \( h(\vartheta, r) \) given by the real part of the Fourier transform of the effective spectrum

$$h(\vartheta, r) = \text{Re} \left[ \int_{-\infty}^\infty N(k) e^{ikr} \, dk \right],$$

(6)

where \( t = 1 - \cos \vartheta \) and \( \vartheta = \arccos(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) \). For the subsequent analysis it is worth defining

$$\chi_\delta(\vartheta) = -\frac{2r_e}{r} h(\vartheta, r),$$

(7)

which corresponds to a hologram of a point \( \delta \)-like scatterer. From the basic properties of Fourier transforms it follows that for broadband radiation, \( h(\vartheta, r) \) becomes localized around \( t = 0 \) and the small angle approximation \( t \approx \vartheta^2/2 \) becomes valid and shall be used in the remainder of this paper. From (6) it is clear that the effective spectrum plays a crucial role in the description of white beam x-ray fluorescence holograms.

2.2. Approximating the effective spectrum \( N(k) \)

For energies far above the absorption edges, \( \mu_0(k) \sim Z^4/k^3 \) [18] implies that the shape of \( N(k) \) is approximately independent of the kind of absorbing atom. Thus, the spectrum is mainly determined by the x-ray source and by absorber filters, which are used to harden the spectrum.

Figure 1 shows an example effective spectrum calculated with the XOP package [19] for the Diamond I12 hard x-ray wiggler (www.diamond.ac.uk/home/beamlines/i12.html). This spectrum will be used in the remainder of this paper. This spectrum closely resembles the one at DORIS BW5 wiggler for which white beam experiments have been performed [9].

Until now, the Lorentzian distribution with the mean value \( k_0 \) and full-width at half-maximum \( \Delta k \)

$$N_L(k) = \frac{1}{2\pi} \frac{\Delta k}{(k - k_0)^2 + (\Delta k/2)^2}$$

(8)

was used for a rather crude approximation of such spectra. When inserted into (6), it gives the following expression for \( h(\vartheta, r) \):

$$h_L(\vartheta, r) = e^{-\beta_0 \vartheta^2} \cos(q \vartheta^2)$$

(9)
Figure 1. Simulated shape of the effective x-ray spectrum for the Diamond Light Source I12 beamline with a 2 mm Cu absorber. The effective spectrum is a product of the incident photon flux in units of (photons$^{-1}$ keV$^{-1}$) and absorption cross-section. Dots represent the simulation. Dashed and solid lines are the Lorentz and Gumbel fits, respectively. Fitted parameters: $k_0 = 36.1$ Å$^{-1}$, $\Delta k = 15.8$ Å$^{-1}$, $\mu = 34.7$ Å$^{-1}$, $\alpha = 7.8$ Å$^{-1}$.

with

$$\beta = \frac{\Delta k}{2k_0}, \quad q = \frac{k_0r}{2}.$$  \hspace{1cm} (10)

The $\beta$ parameter measures the bandwidth of the incident radiation and as shown in [11] is a key parameter in the transition from monochromatic to polychromatic holograms. However, from figure 1 it is evident that the Lorentzian does not take into account the heavily skewed nature of the spectrum.

Hence, in this work a new approximation is proposed, based on the Gumbel distribution [20]

$$N_{G}(k) = \frac{1}{\alpha} \exp \left[ -\frac{k - \mu}{\alpha} - \exp \left( -\frac{k - \mu}{\alpha} \right) \right].$$ \hspace{1cm} (11)

with $\mu$ being its mode and $\alpha$ the scale parameter that determines its spread. The comparison of the fits of the two distributions to the effective spectrum is presented in figure 1. The Gumbel distribution much more accurately resembles the desired shape. Importantly, the approximation based on the Gumbel distribution accurately reproduces the effective spectra of various other existing sources and was tested for bending magnets, asymmetric multipole wiggler (ESRF ID15 [21]) and for an array of damping wigglers, which is planned to be used as an intense hard x-ray source at PETRA III [22].

Moreover, for the Gumbel distribution, we obtain a compact analytic expression for $h(\theta, r)$ which reads

$$h_{G}(\theta, r) = \text{Re} \left[ e^{i\alpha r \theta^2 / 2} \Gamma \left( 1 - i\alpha r \theta^2 / 2 \right) \right],$$ \hspace{1cm} (12)

where $\Gamma$ is the gamma function [23].

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Figure 2. White beam x-ray fluorescence hologram $\chi_\delta$ of a single point scatterer placed at position $r$ relative to the absorber. (a) The geometry of the absorber-point scatterer system with a 2D view of the hologram generated with the Gumbel approximation. (b) Profile along $\theta$ of the hologram from (a). The solid and dashed lines show profiles generated using the Gumbel and Lorentz spectrum approximations, respectively.

For a direct comparison of Lorentz and Gumbel approximations, a white beam x-ray fluorescence hologram was generated for a simple system consisting of an absorber and a point scatterer as shown in figure 2(a). The system is aligned along the $z$-axis and the distance between the absorber and the scatterer was set to 3.19 Å (Ga–Ga bond length in GaN). The comparison of the holographic profiles along $\theta$ is shown in figure 2(b). The main differences arise in the remnant diffraction fringes, which are of profound importance to the wavelet transform analysis.

The above improvement in the description of the effective spectrum should in principle allow for an abandonment of $h_L(\theta, r)$. However, due to its simplicity several useful analytic results can be derived. In the following sections, we will use both (9) and (12) to simultaneously generate white beam XFH for various systems, analyse and compare the results.

3. Wavelet analysis of white beam x-ray fluorescence holography: model systems

A peculiar feature that was explored in [11] is that white beam holograms have wavelet-like characteristics making the wavelet transform [24] a natural choice for their analysis. The CSWT is defined as a generalized correlation between the signal from (5) and specially prepared, scaled and rotated wavelets $\psi_{\hat{k}_0, s}$

$$\tilde{\chi}(\hat{k}_0, s) = \int_{\Omega} \psi_{\hat{k}_0, s}(\hat{k}) \chi(\hat{k}) d\Omega,$$

where $s$ is the scale parameter and $\hat{k}_0$ determines the wavelet position on the sphere [25]. Generally, the shape of wavelets can be adjusted to a given problem, the only requirement being that the admissibility (i.e. zero mean) condition is fulfilled. In our case the family of wavelets
in (13) is generated from a localized around the north pole mother wavelet \( \psi(\hat{k}) = \psi(\theta) \) given as [11]

\[
\psi(\theta) = -\frac{1}{s} \exp(-\beta q_0 \theta^2/s^2) \left[ \cos\left(\frac{q_0 \theta^2}{s^2}\right) - \beta \sin\left(\frac{q_0 \theta^2}{s^2}\right) \right],
\]

where the scale parameter \( s = (r/r_0)^{-1/2} \) is related to the real space distance and \( q_0 = k_0 r_0/2 \). The parameter \( r_0 \) is chosen in such a way that the small angle approximation holds for scales \( s \leq 1 \) (in the remainder of this paper it is set to \( r_0 = 1 \text{ Å} \)). The considered wavelet family almost perfectly matches the white beam holographic signal for the Lorentzian spectrum approximation. As will be shown, it can also be effectively used to analyse holographic patterns generated with the Gumbel spectrum, which give a much more realistic description of the experimental data.

3.1. Spatial resolution

Several properties giving insight into the advantages and limitations of the CSWT can be shown by applying it to a simple point scatterer hologram \( \chi_\delta \) from the previous subsection. The resulting wavelet transform coefficients \( \tilde{\chi}_\delta \) are analogous to the holographic point spread function [26], which is, in this case, space dependent.

A 3D view of the CSWT computed for \( \chi_\delta \) from figure 2(a) is shown in figure 3(a). The numerical computations have been performed with the YAWTB toolbox [27]. Detailed 2D slices of the CSWT which depict the differences between the two approximations of the spectrum are given in figures 3(b) and (c). In both images, values to the left of the white line correspond to the Lorentzian while values to the right correspond to the Gumbel approximation. The reconstructed position of the scatterer is given by the visible distinct maximum. While \( \tilde{\chi}_\delta \) calculated for Lorentz and Gumbel approximations differ in details they have similar general character.

To show the dependence of \( \tilde{\chi}_\delta \) on the spectrum parameters and the scatterer’s position, it is worth giving a closed-form expression for it. Although this is only possible for the Lorentzian approximation, the general conclusions can be extended to the Gumbel approximation. The profile of the CSWT along the \( z \)-axis (along the central, vertical white line in figure 3(b)) is shown in figure 3(d). This profile is calculated to be

\[
\tilde{\chi}_\delta (r, r') = \int_0^{2\pi} \int_0^\pi \chi_\delta (\theta, r') \psi (\theta, r) \sin \theta \, d\theta \, d\phi
\]

\[
\approx \frac{4\pi r c \beta (r/r_0)^{1/2}}{k \left[ (r - r')^2 + \beta^2 (r + r')^2 \right]},
\]

where \( r' \) denotes the distance between the absorber and the scatterer. In the evaluation of (15) it was assumed that \( e^{-\Delta k (r + r')} \to 0 \) holds. In figure 3(d) this approximated analytic result is compared with the exact numerical calculations and the agreement is almost perfect. The FWHM \( \Delta r \) of \( \tilde{\chi}_\delta \) from (15) reads

\[
\Delta r \approx 4\beta r',
\]

and defines the radial resolution of reconstruction as predicted in [11]. Note that it gets worse with increasing distance from the absorber. For our spectrum and for the model absorber–scatterer system \( \Delta r \approx 2.79 \text{ Å} \).
Figure 3. Wavelet transform $\tilde{\chi}_\delta$ of a white-beam hologram generated for an absorber–point scatterer system from figure 2. (a) 3D view computed for the Gumbel approximation. (b) A magnified $r$–$\theta$ slice of the wavelet space near the scatterer’s position. (c) Spherical shell for $r = 3.19$ Å, i.e. for the exact scatterer’s position. The left parts of plots (b) and (c) have been computed with the Lorentzian while the right ones with the Gumbel approximations. (d) Radial profile along the $z$-axis. The vertical dashed line marks the position of the scatterer. (e) Angular profile at $r = 3.19$ Å. The vertical dashed line marks the position of $\theta_0$. In line plots, dots and dashed lines represent exact numerical calculation for the Lorentzian and Gumbel spectra, respectively. Solid lines are approximate analytical $\tilde{\chi}_\delta$ profiles given by (15) and (17).

A similar calculation is performed to evaluate the angular resolution. The angular profile $\tilde{\chi}_\delta$ for $r = r'$ (white dashed half circle in figure 3(b)) is given by

$$
\tilde{\chi}_\delta(\theta) \approx \frac{\pi r e^{r'r_0} e^{-(\beta^2+1)q^2/2\beta}}{2q' \beta (r'r_0)^{3/2}} \left[ 1 - \beta e^{q'^2/(2\beta)} \sin\left( \frac{q'\theta^2}{2} \right) \right].
$$

(17)

where $q' = \frac{kr'}{r}$. A comparison with an exact numerical calculation is presented in figure 3(e). The angular resolution can be estimated by evaluating the value of the first zero $\theta_0$ of (17) for which $\tilde{\chi}_\delta(\theta_0) = 0$. This value reads

$$
\theta_0 = \sqrt{2 \frac{\beta}{q'} \sqrt{W(\beta^{-2})}},
$$

(18)

where $W$ is the Lambert $W$ function [28]. For our example spectrum $\beta = 0.22$ and $W(\beta^{-2}) = 2.24$, which gives $\theta_0 = 7.46^\circ$. This is equivalent to 0.42 Å in the tangential plane at $r' = 3.19$ Å. Contrary to the radial resolution, angular resolution improves with increasing $r'$ as the holographic signal becomes more localized.

3.2. Point scatterer chain

In experimental patterns of white beam x-ray absorption anisotropy, one can observe distinct minima corresponding to densely packed atomic rows [9]. This effect is closely related to axial...
channelling observed in electron scattering experiments [29]. Although analysis of channelling patterns provides information about lattice sites it is blind to local structure. In this work, in order to highlight the sensitivity of white-beam XFH to local structure, the simple absorber–scatterer system from the previous section can be extended to a chain of point scatterers.

For simplicity, consider an equally spaced scatterer chain (its schematic view is shown in figure 4(a)). The inter-atomic distance and the number of scatterers have been set to \( l = 3.19 \, \text{Å} \) and \( N = 100 \), respectively. The chain is aligned along the \( z \)-axis. The absorption anisotropy for the chain was calculated as

\[
\chi_{\text{Chain}} = \sum_{n=1}^{N} \chi_{\delta}(\theta, r = nl),
\]

where for clarity the dependence of \( \chi_{\delta} \) on \( r \) was explicitly shown. The wavelet transform profiles of \( \chi_{\text{Chain}} \) along the chain axis are presented in figure 4(b). Despite poor radial resolution the position of the first scatterer is visible and can be determined. The signals from further scatterers blend into a smooth curve. However, their contamination to the signal of the first scatterer is not severe. In the case of the Gumbel approximation only numerical calculations for a finite chain can be considered. In the Lorentzian case, an analytic result for an infinite chain can be obtained.

Figure 4. Wavelet transforms of a white beam hologram calculated for a chain of point scatterers. (a) Schematic view of the considered chain. (b) Wavelet transform \( \tilde{\chi}_{\text{Chain}} \) along the chain calculated using the Gumbel (blue squares) and Lorentzian (red circles) approximations. The circles were shifted by 0.5 for a better presentation. The solid line is the approximate analytic formula given by (20). The dashed curves show \( \tilde{\chi}_{\delta} \) for the first three scatterers. The vertical dashed lines mark the positions of the first five scatterers.
Our calculation gives

\[
\tilde{\chi}_{\text{Chain}}(r) = \sum_{n=1}^{\infty} \tilde{\chi}_n(r, nl) = -\frac{\pi r_e \sqrt{r/r_0}}{2k_0 l r} \text{Im} \left[ \psi_0(x) - \psi_0(\bar{x}) \right],
\]

where \(x\) is given by

\[
x = 1 + \frac{r(\beta^2 - 2i\beta - 1)}{l(\beta^2 + 1)}
\]

and \(\psi_0\) is the polygamma function \([23]\). As demonstrated in figure 4(b), the analytic result confirms numerical findings even for \(N \to \infty\). Thus, the CSWT of a white beam hologram of a point scatterers chain is sensitive to the nearest neighbour along the chain.

4. Visualization of the local structure in GaN crystals

4.1. Generation of white beam holograms

In this section, the accuracy and limitations of white-beam XFH are explored by studying gallium nitride. The choice of GaN was made as when doped with magnetic ions (transition metals or rare earth impurities) it becomes a diluted magnetic semiconductor (DMS) \([30]\). DMSs are a class of materials with interesting magnetic properties and promising applications in semiconductor spin transfer electronics. In order to determine their electronic and magnetic properties the distribution of dopants and their surroundings in the crystal matrix must be precisely known.

First, consider absorbing atoms occupying gallium sites. Wurtzite GaN has two non-equivalent Ga sites, which both contribute to the x-ray absorption anisotropy (see figure 5(a)). The x-ray absorption anisotropy was calculated in real space as a linear superposition of
Figure 6. White beam x-ray holography for a wurtzite GaN crystal. (a) White beam x-ray hologram of GaN calculated for a cluster with a radius of 100 Å. The left half of the hologram has noise added to it. The inner dashed circle marks the θ value of 25° while the outer dashed circle the value of 88°. (b) Projection of the wurtzite GaN crystal as seen from the two non-equivalent absorbing Ga sites. The size of atoms (balls) is proportional to their atomic number and inversely proportional to the distance from the absorbers. Double occupancy atoms are common for both non-equivalent Ga sites. Both images are in the equal area projection.

Holograms were generated on a spherical θ–φ angular mesh of 401 × 801 points. In experiments, in order to avoid the simultaneous recording of absorption and emission anisotropy [31], it is convenient to locate the detector around the pole. This limits the accessible angular range. For grazing angles the effective spectrum approximation becomes invalid due to beam hardening effects. Hence, θ was limited to an approximately 25–88° range to mimic the experimental geometry. A Poisson-like noise corresponding to 10^7 photons per pixel was added to the data.

A white-beam x-ray hologram calculated for a 100 Å radius cluster is shown in figure 6(a). The real space nature of such a hologram is evident when one compares figure 6(b). Even though the projections of atomic planes are clearly visible, the signal from nearest neighbours is concealed by features resulting from long-range order, similar to Kikuchi bands observed in electron diffraction [32].

4.2. Straightforward wavelet analysis

Once the holograms have been generated the CSWT can be applied. The wavelet transform space should resemble a 3D image of the local atomic structure around the absorbing atoms at
Figure 7. Straightforward wavelet analysis of the white-beam x-ray hologram of GaN. A 2D $r-\theta$ slice of the wavelet transform space for the (120) plane. White circles mark the expected positions of atoms up to 10 Å and their radius is inversely proportional to their distance from the central atom. The nearest-neighbour nitrogen and gallium atoms have been marked with arrows. In the part on the left side of the white vertical line the nearest-neighbour nitrogens have been subtracted. Note that the straightforward application of the wavelet transform to white beam x-ray holograms yields a real-space image with very poor quality.

Ga sites. Locally, it corresponds to a convolution of $\tilde{\chi}_\delta$ from figure 3 with $\rho(r)$ averaged over the two non-equivalent absorbing sites. An example slice of the wavelet transform of the x-ray hologram from figure 6(a) along the (120) atomic plane is presented in figure 7. For a better presentation the $\sqrt{r}$ scale is used and only the positive values of the transform are shown while the negative ones are set to zero. The transform has been computed from 1 to 20 Å. For $r$ smaller than 1 Å the small angle approximation becomes invalid, and thus the transform has not been computed in that region.

The reconstructed image of the structure shows signals from atoms as well as a number of artefacts. The signal from the heavy nearest-neighbour Ga atoms is strong, clearly visible and localized around the expected position. On the other hand, the signal from light N atoms is very weak and displaced from its expected position. To show this effect and to inspect the sensitivity to light atoms the nearest-neighbour N atoms have been subtracted by hand from the original signal. The result of this subtraction is presented in the left part of the hemicircle in figure 7. Note that the absence of nitrogen is hardly visible.

Apart from the signals from atoms a generally large number of artefacts arise in the transform space. Their intensity can be easily estimated by analysing the inner cone of the transform which corresponds to the excluded regions in the simulated x-ray absorption anisotropy patterns. This region should be free of atomic signals. In contrast to this the magnitude of the artificial signal is comparable to the signal from nearest atoms. The reason for this is the non-orthogonality of the wavelets used. In other words, the wavelet transform for single atoms has a cone-like shape (figure 3(a)) and the overlapping of such cones produces the unwanted effects.
4.3. Inverse windowed wavelet transform

It has been previously shown that the quality of the local structure image can be improved by performing the inverse wavelet transform for a limited range of scales [11]. This transform is defined as

\[
F(\hat{k}) = C_\psi \int_0^{\infty} \bar{\chi}(\hat{k}, s) w(s) \frac{ds}{s^2},
\]

(22)

where \(C_\psi = k_0 r_0 / [\pi \arctan (\beta^{-1})]\) and the window function \(w(s)\) is given by

\[
w(s) = \begin{cases} 1, & s_c \leq s \leq s_b, \\ 0, & \text{elsewhere}. \end{cases}
\]

(23)

\(s_c = (r_c/r_0)^{-1/2}\) and \(s_b = (r_b/r_0)^{-1/2}\) define the section in the radial direction from the absorber for which the inverse transform is calculated. \(r_b\) is required to lie in the range \(r_0 \leq r_b < r_c\). For local structure imaging it is set to the smallest possible value for which the small angle approximation is valid, namely \(r_0\) yielding \(s_b = 1\). \(r_c\) can be referred to as the cutoff distance. For \(w(s) = 1\), expression (22) corresponds to the standard inverse wavelet transform and \(F(\hat{k}) \simeq \chi(\hat{k})\).

For the purpose of the present work, let us rewrite (22) as

\[
F(\hat{k}) = C_\psi \int_\Omega \chi(\hat{k}') \left[ \int_0^{\infty} \psi_{k,s}(\hat{k}') w(s) \frac{ds}{s^2} \right] d\Omega
\]

\[
= C_\psi \int_\Omega \chi(\hat{k}') \psi_\hat{k}(\hat{k}') d\Omega.
\]

(24)

For the quantity in brackets and the wavelet family from (14), we obtain

\[
\psi(\theta) = \frac{1}{2q_0 \theta^2} \left[ e^{-q_0 \theta^2/s_c^2} \sin \left( \frac{q_0 \theta^2}{s_c^2} \right) - e^{-q_0 \theta^2/s_b^2} \sin \left( \frac{q_0 \theta^2}{s_b^2} \right) \right].
\]

(25)

The analytic formula (25) is of profound importance as it allows a fast and precise computation of \(F(\hat{k})\) in a single step. A two-step procedure involving subsequent application of (13) and (22) would require that at least tens of transformations had to be performed. Therefore, in the remainder of this paper an inverse wavelet transform will be always computed by means of (25).

The inverse windowed wavelet transform (IWWT) \(F(\hat{k})\) of the white beam x-ray hologram from figure 6(a) for \(r_c = 5\ \text{Å}\) is presented in figure 8(a). For a better presentation only the positive values are shown. A direct comparison with figure 6(b) enables one to establish a correspondence between \(F(\hat{k})\) and the real space projection of the local atomic structure. This is emphasized by the white circles and ellipses which mark the positions of atoms up to approximately 10 Å. For this small value of \(r_c\) the most intense spots correspond to nearest Ga atoms. The obtained image is nearly free of artefacts. The degree of their suppression (as compared to figure 7) is directly visible in the excluded region around the pole. Additionally, the signal from nearest N atoms is clearly visible even in the presence of noise. This is highlighted by a comparison with the data from which the nitrogen atoms have been removed by hand from the cluster.

For a more quantitative analysis, a profile along the (120) plane is shown in figure 8(b). The vertical lines with triangles mark the angular positions of atoms up to 5 Å. Their height is proportional to the atomic number and occupancy and inversely proportional to the distance...
Figure 8. Projections of GaN local structure obtained using the IWWT from white-beam x-ray hologram. (a) Projection around Ga atoms for \( r_c = 5 \) Å. White circles and ellipses mark the positions of atoms (cf figure 6(b)). In the part of the plot to the left of the white vertical line the nearest-neighbour nitrogens have been subtracted. (b) Angular profile along the white line. The solid line represents the signal from all the atoms, the dashed line the signal with the nearest nitrogens subtracted and the dotted line the signal with both nearest nitrogen and gallium atoms subtracted. Vertical lines with triangles mark the positions of atoms up to 5 Å and their height is proportional to the expected signal. Plots (c) and (d) are analogous to (a) and (b) but were computed for \( r_c = 10 \) Å. In (c) the atoms are marked up to 10 Å.

From the absorber. The most intense maxima in \( F(\hat{k}) \) coincide with the positions of scatterers. However, smaller peaks result from superposition of signals from few weaker scatterers. This can be easily checked by removing certain atoms, e.g. nearest-neighbour nitrogens (dashed line) or both nearest-neighbour nitrogens and galliums (dotted line).

For larger cutoff distances the structure of \( F(\hat{k}) \) becomes more complicated (the results for \( r_c = 10 \) Å are shown in figures 8(c) and (d)) as more atoms start to contribute to the signal. For example, the signal from double occupied Ga atoms (closest to the pole) becomes comparable with the nearest-neighbour Ga signal. Note that while the intensity of those maxima
is comparable with the intensity of peaks corresponding to the nearest Ga scatterers, the smaller angular size gives information on their larger distance from the absorber. Although projections of more atoms can be identified in figure 8(c), the inspection of the angular profile shows that their position is simultaneously affected and cannot be unambiguously determined if \( r_c \) is too large. This means that a comprehensive analysis is only possible when performed for different \( r_c \) values. The sensitivity of the results to the changes of the \( r_c \) can be directly estimated from (16).

4.4. Dopants in GaN crystals

For the sake of simplicity, only impurity positions shown in figure 5(b) will be considered, i.e. substitutional sites at Ga and N positions as well as octahedral (O) and tetrahedral (T) interstitial positions. Note that for each position two non-equivalent sites exist, which are labelled 1 and 2.

In the case of the substitutional Ga sites, the x-ray holograms have already been generated in the previous section. White-beam x-ray holograms (\( \chi_N \), \( \chi_T \) and \( \chi_O \)) for the N, T and O sites are generated analogously for 100 Å radius clusters. The comparison of the N, T and O holograms with crystal geometrical projections and the corresponding IWWT images for \( r_c = 10 \) Å are shown in figure 9. In all cases the wavelet analysis produces images that can be interpreted as projections of the local atomic structure. There is a direct relation between all maxima visible in the IWWT data and positions of atoms in the nearest neighbourhood of the absorbing atom. Even the characteristic splitting of the strongest peaks in IWWT projection generated for T site (not visible for O site) has a structural origin and is due to the presence of scatterers in the next coordination shells. The fine differences in the images indicate the high sensitivity to the local structure.

It is useful to note the similarity between the local and long-range structures among the considered impurity locations. The comparison of the geometrical projections and holograms for the N and T sites shows that the long-range structure around these sites possesses similarities. Despite this, the wavelet analysis enables one to extract distinct images of the local structure. On the other hand, the comparison of images for the T and O sites depicts similarities between the local atomic structure and completely different features in the holograms corresponding to long-range order. The above results unequivocally indicate the sensitivity of white beam XFH to local structure.

5. Wavelet-based structure refinement

As shown in the previous section, wavelet analysis of white-beam XFH is capable of providing high-quality projections of the local structure. However, in real systems the structural analysis can be complicated by the presence of multiple impurity lattice sites. In fact, already the presence of two non-equivalent sites (such as in the case of GaN) introduces some ambiguity into the data analysis. As will be shown in the next section, such sites can be detected and the x-ray projections obtained using the direct application of wavelet transform from figure 9 can be used as the starting point of structure refinement.

5.1. Wavelet-assisted R-factor analysis: detection of multiple impurity sites

The ability to compute the IWWT in a fast single step, by means of (25), opens the way to another procedure for structural analysis of white-beam x-ray holograms by means of a
conventional R-factor (reliability factor) analysis. This trial-and-error procedure can be sped up by calculating reliability factors between IWWTs of an experimental x-ray hologram and of x-ray holograms calculated for small probing clusters. This overcomes the problem of generating x-ray absorption anisotropy for large clusters, for which the computation time scales with the third power of the cluster radius and is, therefore, time consuming. In addition, as seen in figure 9, IWWT acts as an image filter which suppresses noise in the data.

As an example, consider an impurity at T sites (figure 5(b)) and its holographic pattern which will represent the experimental data. In the first step of the procedure, IWWT is applied to the white-beam x-ray hologram characteristic of this site. For GaN, all interesting impurity
sites lie in the (120) plane. Therefore, in the second step, the (120) slice of the GaN unit cell (5.53 Å × 5.17 Å) from figure 5(b) is divided into a 35 × 32 grid. For other systems, an extension to a 3D mesh is straightforward. For each point of the grid a small probing cluster of radius 10 Å is generated. For each cluster a hologram and the corresponding IWWT are calculated. Then the following R-factor is calculated:

\[ R = \frac{\sum_i [(F_{\text{exp}})^i - (F_{\text{calc}})^i]^2}{\sum_i [(F_{\text{exp}})^i + (F_{\text{calc}})^i]^2}, \]

where \( F_{\text{exp}} \) is the ‘experimental’ IWWT image for the T impurity site and \( F_{\text{calc}} \) is the IWWT image of the small probing cluster. Index \( i \) runs through the pixels of the IWWT images. For a simplified description we used the most popular R-factor definition. It could be improved by introducing a \( \sin \theta \) weighting term or by modifications accounting for a 2D character of the data. For the sake of compatibility with the formalism of previous sections, a standard cross-correlation can be, in principle, also used.

The resulting 2D R-factor map is shown in figure 10(a). The lower the R-factor value, the more probable it is that the impurity occupies the corresponding position. The positions of the two non-equivalent T sites have been reconstructed properly and are given by the distinct minima. Their FWHMs are 0.96 and 0.83 Å in the horizontal and vertical directions, respectively. Thus, the obtained resolution is better than the value given by equation (16). R-factor analysis involves correlation of the signals from many atoms which yields an improved resolution.

Apart from the true expected minima, fake minima arise in the R-factor map. These arise at positions in the (120) plane for which the probing clusters have a similar local structure to the T site. Such similarities are evident when one compares the IWWT images of the O and T positions from figure 9. Clearly, in the R-factor map from figure 10(a) there are two minima in

Figure 10. Precise reconstruction of the magnetic impurity position (T site) in the GaN matrix. (a) 2D R-factor map in the (120) plane (cf figure 5(b)). (b) \( c_i \) values obtained for the most intense minima with the general linear least-squares approach.
the O$_1$ and O$_2$ positions. Put in a different way, the R-factor analysis preceded by IWWT gives information only about the local atomic structure; thus sites with a similar local surrounding can be misinterpreted. These artefacts can be, however, easily rejected by using the long-range order information contained in the holograms as described below.

5.2. Linear regression

In general, impurities can occupy multiple positions and the anisotropy signal can be a complicated superposition of signals from each of these sites. The net signal can be written as

$$\chi_{\text{Impurity}} = \sum_{i=1}^{M} c_i \chi_i,$$

where $\chi_i$ is the hologram characteristic of the $i$th site and the $i$ index runs through all the $M$ impurity sites. The goal is to determine the $c_i$ coefficients. This can be done by applying the simple generalized linear least-squares \cite{33} method. Application of the generalized linear least squares gives the following equation:

$$\begin{pmatrix} A^T A \end{pmatrix} c = A^T b,$$

where the $i$th row (column) in matrix $A$ is filled with all the values of the anisotropy calculated for the $i$th site, i.e. $\chi_i$. The elements of the column vector $b$ are obtained in a similar manner from the experimental hologram. The column vector $c$ contains the unknown $c_i$ coefficients. The $c_i$ coefficients are found by inverting the $A^T A$ matrix, which has the size of $M \times M$. Consideration of all possible impurity positions in the unit cell could yield a singular matrix. However, we can limit ourselves to the most probable positions determined from R-factor maps.

Let us apply this linear regression scheme to the hologram for the T sites. Thus, $\chi_T$ will again represent the experimental data. Consider now the six most probable lattice sites which are visible in the R-factor map of figure 10(a). For each of these minima, large 60 Å clusters are generated and a set of holograms $\chi_1, \chi_2, \ldots, \chi_6$ is constructed. Here, for the calculation of $\chi_i$ we use a direct real space calculation; however, calculations in reciprocal space \cite{34} could also be used.

The normalized values of the $c_i$ coefficient for each of the considered sites are presented in figure 10(b). The correct T$_1$ and T$_2$ sites have almost equal contributions and the fake minima are ruled out. The uncertainties result from the presence of noise. Note that this approach could be used, e.g. for checking the preferential distribution of impurities on Ga$_1$ and Ga$_2$ sites indicated by electron paramagnetic resonance (EPR) results \cite{35}.

5.3. Determination of impurity displacements

The above results illustrate the general idea of the method. However, note that for the regular lattice position the linear least-squares method could be used right from the beginning, just by considering several most probable lattice site positions. Consider, thus, an example for which linear regression has to be ultimately preceded by the wavelet analysis.

Consider a dopant located at lattice sites, which either coincide with Ga sites or are displaced by a value of $d$ from the Ga site in the [001] direction. The detection of such shifted sites was reported, e.g. for Eu in GaN \cite{29} via electron channelling methods. Two non-equivalent sites of this type are marked as S$_1$ and S$_2$ in figure 5(b). Here, for the purpose of a
clear illustration, we used an exaggerated and relatively large shift of 0.4 Å. However, for the introduced noise level, a shift as small as 0.1 Å could be detected with the proposed procedure. For such sites, R-factor and linear regression procedures were used in a similar way as in the previous example. A comparison of the R-factor maps obtained for Ga and S ‘experimental’ holograms is shown in figures 11(a) and (b). The difference (the shift of dopant positions) between the two images is evident. The linear regression results are shown only for S sites. However, in both cases they yield correct site occupancies. It should be also underlined that the linear regression (contrary to IWWT analysis) is not sensitive to the local structure. For example, removal of the atoms from the first coordination shells did not influence the $c_i$ values (data not shown). This means that both approaches give complementary information about short- and long-range structures.

6. Summary and outlook

In this work we have discussed the unique properties of white beam x-ray fluorescence holography with an emphasis on future applications. Introduced analytical models and realistic simulation allowed for a detailed description of wavelet-transformed holograms, which can be directly interpreted as projections of the local structure around absorbing atoms. Fast computation of the IWWT enabled us to propose a wavelet-assisted method for the location of dopants relative to the crystal matrix, which works for multiple lattice sites and is sensitive to small shifts from regular lattice positions. Both approaches are complementary and give different kinds of information about local and long-range structure.

The information provided by the white beam variant of XFH makes it potentially suited for analysis of interesting structural phenomena in doped systems such as distortions around impurities or aggregation of dopants in magnetic semiconductors or oxides with the formation of secondary crystallographic phases [36, 37]. White beam XFH is used in cases where the use of charged particles is not possible, e.g. when an external electric or magnetic field is applied.

As yet, the potential of the wavelet method used in this work has not been fully exploited. The usage of an orthogonal wavelet family [38] should reduce the number of artefacts in the
wavelet transform space and allow exact 3D imaging of the local structure. This could be done in harmonic space in analogy with the recent approach demonstrated for XFH [39]. The R-factor analysis could be extended by introducing additional parameters of the structure-like local distortion of the lattice around dopants. As compared to standard x-ray or electron diffraction, this kind of analysis will be simplified since white-beam holograms are linear with respect to the structural model [26].

The main limitation of white-beam XFH is weak signal. However, the recent synchrotron beam experiment with fluorescence detection at a hard x-ray wiggler indicates the possibility of interesting applications. The use of an extremely powerful and hard white x-ray beam from a 40 m-long array of damping wigglers planned at PETRA III [22] would make it possible to perform high-resolution imaging even for very diluted samples. On the other hand, preliminary results indicate that white-beam x-ray holography can also be recorded with chemical sensitivity using a laboratory-based experimental setup described in [40]. In such a case a combination of the presented approaches will be necessary to improve the low spatial resolution limited by the use of relatively low-energy x-ray beams.

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Appendix

The calculation of white-beam x-ray holograms in real space is a numerically involving process and requires a significant amount of time for large clusters. In order to facilitate a fast computation, the following approximations of (5) are used.

Firstly, atomicity is assumed which implies \( \rho(\mathbf{r}) = \sum_j \rho_j(\mathbf{r}) \) where the sum runs over atoms in the crystal cluster. Then for a real valued \( \rho(\mathbf{r}) \), formula (5) can be rewritten as

\[
\chi(\hat{k}) = -2r_e \sum_j \text{Re} \left[ \int_0^\infty N(k) \int_V \frac{\rho_j(\mathbf{r})}{r} e^{i k r_j} \, dV \, dk \right].
\]  

(A.1)

Secondly, by introducing the atomic scattering factor \( f(\mathbf{k}) \) the equation reads

\[
\chi(\hat{k}) = -2r_e \sum_j \text{Re} \left[ \int_0^\infty N(k) f_j(\hat{k}, \mathbf{k}) \frac{e^{i k r_j}}{r_j} \, dk \right].
\]  

(A.2)

Formula (A.2) neglects spherical wave and near-field effects. Such effects have been thoroughly studied and widely used [17, 41–43]. Generally, these effects fall rapidly with \( (kr)^{-1} \) and the contribution of such effects to our hard x-ray regime is neglected.

In general terms, only a numerical integration over \( dk \) is possible which practically excludes generation of holograms for large clusters. This problem can be efficiently solved by using the following approximation:

\[
\chi(\hat{k}) = -2r_e \sum_j f_j(\hat{k}, \mathbf{k}) \text{Re} \left[ \int_0^\infty N(k) \frac{e^{i k r_j}}{r_j} \, dk \right].
\]  

(A.3)
Figure A.1. Verification of the approximated generation method of white-beam x-ray holograms. Comparison of holographic profiles for single Ga (a) and N (b) scatterers. Dashed lines correspond to (A.2) while solid lines to (A.3). Atoms are separated by 3.19 Å and the spectrum from figure A.1 is used.

where $\bar{k}$ is a characteristic value of $N(k)$, e.g. its mode, and the integral over $k$ has an analytic form.

Finally, in order to demonstrate the accuracy of the used approximations, white-beam x-ray holograms were calculated for different scatterers and are shown in figure A.1. The agreement between exact and approximate calculations fully justifies the proposed approximation.

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