Coherence and sampling requirements for diffractive imaging

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Abstract

Coherent Diffractive Imaging (CDI) allows images to be reconstructed from diffraction patterns by solving the non-crystallographic phase problem for isolated nanostructures. We show that the Shannon sampling of diffraction intensities needed in CDI requires a coherence width about twice the lateral dimensions of the object, and that the linear number of detector pixels fixes the energy spread needed in the beam. The Shannon sampling, defined by the transform of the periodically repeated autocorrelation of the object, is related to Bragg scattering from an equivalent crystal, and shown to be consistent with the sampling of Young’s fringes established by scattering from extreme points in the object. The results are relevant to the design of diffraction cameras for CDI and plans for femtosecond X-ray diffraction from individual proteins.

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The coherent diffractive imaging method (CDI) in X-ray [1], optical, and electron diffraction [2] uses the hybrid input–output (HiO) algorithm [3] (also referred to as oversampling), to solve the phase problem for the continuous distribution of intensity scattered from an isolated object [4,5]. Phase information has been found to be encoded in the diffracted intensity if it is sampled finely enough, and this may be extracted using iterative algorithms. Striking atomic-resolution images of individual carbon nanotubes have recently been obtained in this way [6], and soft X-ray images of isolated objects reconstructed from their diffraction patterns alone [7]. Applications to cryoelectron microscopy from monolayer proteins have also been proposed [8]. These were reconstructed from diffraction patterns without the aberrations and resolution limits of a lens-based imaging system. The recording time in these experiments depends on source brightness and coherence angle, which in turn control the radiation dose. In this letter we give the relationship between data sampling and illumination conditions for optimum results in diffractive imaging, which minimize the...
radiation dose yet provide adequate coherence. The requirements for chromatic coherence are also reviewed.

As shown in Fig. 1, we consider the simplified one-dimensional case of a compact object of width \( W \) whose autocorrelation function has width \( 2W \). The Fraunhoffer diffraction pattern is recorded in the far-field using a detector with pixel spacing \( \Delta Z \). The first-order pixel subtends angle \( \alpha \) at the sample. We assume an incoherently filled source subtending angle \( \theta_c \) at the sample. We assume small angles throughout, and that the detector pixel spacing has been chosen to satisfy the Shannon sampling theorem for the diffracted intensity. This spacing optimally samples the Fourier Transform of the autocorrelation function of the object, allowing it to be reconstructed at any point.

The Van–Cittert–Zernike theorem gives the transverse coherence width at the sample as \( X_c = \lambda/\theta_c \). The question arises as to whether \( X_c \) should set equal to the width \( W \) of the object or to the width \( 2W \) of its autocorrelation function. Experimentally, the space outside the support (boundary) of the object (between \( W \) and \( 2W \)) has been filled either by an optically transparent medium (forming a zero-density region of “known” object pixels, or by an opaque mask, of similarly “known” density (e.g. if the sample fills an aperture hole). In the second case one is considering the significance of coherent illumination of the opaque mask, which cannot contribute to the diffraction pattern. For given source brightness, the choices \( X_c = W \) and \( X_c = 2W \) result in a increase in exposure time by a factor of four in two dimensions for the same dose, and so have important experimental consequences.

As shown in the figure, the angle subtended at the sample by the first-order detector pixel is \( \alpha \). In the single-scattering approximation, the diffracted intensity at each pixel is the modulus squared of the sum of the complex amplitudes due to scattering from each independent source point, that is, for each value of \( \theta_c \). The experimental requirement for diffractive imaging fixes the pixel separation \( \Delta Z = L\alpha = L\lambda/(2W) \), where \( L \) is the distance between sample and detector, and the value of \( \alpha \) has been chosen according to the Shannon sampling theorem, applied to the diffracted intensity, as discussed further below.

Illumination from source point \( S_0 \) produces a diffraction pattern centered on detector pixel \( D_o \), to which must be added the intensities of patterns excited by neighboring source points. In the weak scattering approximation, a change of illumination angle produces only a simple translation of the pattern. If the illumination semiangle equals \( \alpha \), however, the first-order Shannon sample excited by source point \( S_c \) coincides at \( D_1 \) with the zero-order sample excited from source point \( S_1 \). Since these source points are statistically independent, the coherence required for diffractive imaging will thus be lost if \( \theta_c > \alpha \). Using \( X_c = \lambda/\theta_c \) and \( \alpha = \lambda/(2W) \) we find that

\[ X_c > 2W \]

is the spatial coherence condition for diffractive imaging. This applies for both transparent and opaque material outside the support of the sample.

We consider now the sampling of the diffraction pattern in more detail. In Fig. 1, the largest angle between two rays arriving at the detector is \( W/L \). These rays make the finest Young’s fringes in the pattern, whose intensity has period \( \lambda L/W \). Now the sampling theorem requires two samples (spacing \( \Delta Z \)) per period of this intensity, hence \( 2\Delta Z = \lambda L/W \), or \( 2W = \lambda/\alpha \). This is the correct (Nyquist
or Shannon) sampling of the diffraction-plane intensity, and a twofold oversampling of the diffraction-plane wave amplitude. (Here we have applied Shannon’s theorem in reverse. Because the object’s autocorrelation function has compact support, it may play the role of a “bandlimited” spectrum, and so can be periodically extended without loss of information. The effect is to sample the diffracted intensity at intervals proportional to $1/(2W)$. We can derive this result in another way by using this fact that the diffracted intensity is the Fourier Transform of the autocorrelation function of the object, which has width $2W$ for an object of width $W$. Letting the lowest spatial frequency have this period $2W$, the condition that the corresponding first-order diffraction occur at angle $\alpha$ into the first-order pixel is again $2W = \lambda/\alpha$. In this way the oversampling method collects diffraction data coherently from a region larger than the object. The area outside the object is assumed known (e.g. transparent), and this known information compensates for the unknown phases in the diffraction pattern.

These arguments can be summarized more succinctly by noting that (i) Shannon sampling of the intensity corresponds to periodic extension of the object’s autocorrelation function with period $2W$. (ii) Just as Bragg diffraction is only possible (avoiding overlap of orders) with a beam divergence less than the Bragg angle, so diffractive imaging is only possible with a beam divergence less than the “Shannon angle”, which is half the Bragg angle.

The requirements on temporal coherence can be similarly estimated. We require that the coherence length $L_c = 2\lambda E/\delta E$ of the illuminating electron beam (or $L_c = \lambda E/\delta E$ for X-rays and light) be at least as great as the maximum path difference $\Delta = (XT - YT)$ between any pair of interfering rays. (Here $E$ is the energy of the electron or X-ray beam, and $\delta E$ the energy spread). Then $\Delta$, as shown, will be the path difference between rays from opposite extremities of the sample to the outer edge of the detector. Hence, in terms of a scattering angle $\theta = Z/L$, we require $L_c > W\theta_{\max}$, or $2E/\delta E > W\theta_{\max}/\lambda$. If the finest spatial frequency is $d_{\min} = \lambda/\theta_{\max}$, then we have $W/d_{\min} = 2E/\delta E$. Now the object reconstruction process will occur without loss of information if the linear number of pixels $N$ in the image equals that in the diffraction pattern. Then $W/d_{\min} = N = 2E/\delta E$. Hence, if spatial coherence (source size) is not limiting, the number of pixels is fixed by the energy spread in the beam. This result may readily be expressed in terms of the coherence volume $\Omega = A_cL_c = N\lambda X_c^2$, degeneracy and brightness [9].

Using the relevant expressions (e.g. $X_c = \lambda/(2\pi\theta_c)$ for a uniformly filled incoherent disk source subtending semiangle $\theta_c$ at the sample), these results may readily be extended to two dimensions.

The resolution in CDI for a phase object is a property of the object, and so cannot be easily defined. However, if the diffraction pattern contains significant information out to, say $U_{\text{max}} = d_{\min}^{-1} = \theta_{\max}/\lambda$, then we note that there will be two pixels per unit distance $d_{\min}$ in the object, if the number of pixels in the diffraction pattern and the image are equal. This is a result of periodic extension of the band-limited diffraction pattern (with period $2U_{\text{max}}$), which defines the sampling of the object.

To assist in isolating objects lying on a transparent substrate for diffractive imaging, coherent illumination may be focussed. Then the phase shift across an unaberrated, diffraction limited focussed probe is $\pi$ between center and first minimum. By using a sufficiently small illumination aperture, this diffraction limited probe may be made larger than the object, so that the contribution to the object phase shift from the illumination remains small, and a complex object is avoided. Such a probe spanning two objects allows inversion of complex images [10].

We have shown by simple arguments that the Shannon sampling of diffraction intensities needed in CDI requires a coherence width about twice the lateral dimensions of the object. This counterintuitive result means that, for example, an opaque mask surrounding an object must be coherently illuminated. We also show that the linear number of detector pixels fixes the energy spread needed in the beam. The Shannon sampling, defined by the transform of the periodically repeated autocorrelation of the object, is related to Bragg
scattering from an equivalent crystal, and shown to be consistent with the sampling of Young’s fringes established by scattering from extreme points in the object. These results fix the maximum permissible beam divergence and energy spread in CDI and hence the intensity and recording time at the critical damage dose for given source brightness. They are therefore relevant to the design of optical systems designed to minimize damage to radiation-sensitive materials, such as CDI of individual proteins irradiated by a femtosecond X-ray source.

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References