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Coded diffraction system in X-ray crystallography using a boolean phase coded aperture approximation

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ABSTRACT

Phase retrieval is a problem present in many applications such as optics, astronomical imaging, computational biology and X-ray crystallography. Recent work has shown that the phase can be better recovered when the acquisition architecture includes a coded aperture, which modulates the signal before diffraction, such that the underlying signal is recovered from coded diffraction patterns. Moreover, this type of modulation effect, before the diffraction operation, can be obtained using a phase coded aperture, just after the sample under study. However, a practical implementation of a phase coded aperture in an X-ray application is not feasible, because it is computationally modeled as a matrix with complex entries which requires changing the phase of the diffracted beams. In fact, changing the phase implies finding a material that allows to deviate the direction of an X-ray beam, which can considerably increase the implementation costs. Hence, this paper describes a low cost coded X-ray diffraction system based on block–unblock coded apertures that enables phase reconstruction. The proposed system approximates the phase coded aperture with a block–unblock coded aperture by using the detour-phase method. Moreover, the SAXS/WAXS X-ray crystallography software was used to simulate the diffraction patterns of a real crystal structure called Rhombic Dodecahedron. Additionally, several simulations were carried out to analyze the performance of block–unblock approximations in recovering the phase, using the simulated diffraction patterns. Furthermore, the quality of the reconstructions was measured in terms of the Peak Signal to Noise Ratio (PSNR). Results show that the performance of the block–unblock phase coded apertures approximation decreases at most 12.5% compared with the phase coded apertures. Moreover, the quality of the reconstructions using the boolean approximations is up to 2.5 dB of PSNR less with respect to the phase coded aperture reconstructions.

1. Introduction

X-ray crystallography is a technique that allows to determine the atomic position of a crystal in a three-dimensional (3D) space from diffraction patterns [1]. These X-ray diffraction patterns are measured by locating the crystal in a goniometer that gradually rotates while it is exposed to a monochromatic beam of X-rays. The crystal rotation results in a diffraction pattern since the X-ray wavelength is on the same order as the intern atomic distances of the crystalline structure. In general, optical sensors that measure the intensities of the diffraction patterns are not able to measure the phase. Then, the phase of the signal is typically recovered using a retrieval algorithm that builds a 3D model of the molecular structure of the crystal under study [2]. Recently, coded apertures have been successfully employed in phase retrieval [3]. To date, coded apertures have been widely applied to improve the performance of sensors [4], generate uniformly redundant arrays to create images without employing lenses [5], and to apply compressive sensing theory in hyperspectral imaging [6–8]. Particularly, in the phase retrieval approach, the coded aperture modulates the signal before being diffracted and captured at the sensor, as shown in Fig. 1. Specifically, the modulation pattern either changes the phase of the signal or blocks the beams before being diffracted. The percentage of diffracted X-rays that passes through the coded aperture is known as the transmittance. Moreover, the choice of the beams to be modulated is typically performed in a random manner [8]. In addition, modulating the signal

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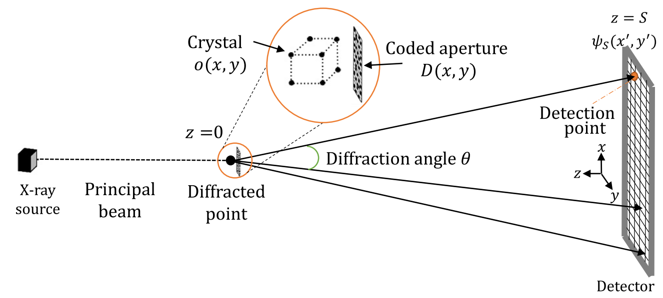

Fig. 1. Theoretical schematic representation of a coded diffraction system. A coded aperture is introduced in front of the sample. The traditional size of a sample in X-ray crystallography is 0.43 mm [10].

before diffraction can be obtained using a phase coded aperture after the sample [9] as shown in Fig. 1.

On the other hand, state of art methods described in [2,11–13] recover the phase from coded X-ray diffraction patterns by applying techniques such as convex programming, matrix completion, and non-convex formulations [14]. However, a practical implementation of a phase coded aperture in an X-ray application is not feasible, since it is computationally modeled as a matrix with complex entries which in practice requires changing the phase of the diffracted beams. In fact, changing the phase implies finding a material that allows to change the direction of an X-ray beam, which drastically increases the implementation costs [15].

Therefore, this paper proposes to approximate a phase coded aperture as a boolean pattern, that can be used in a low cost coded diffraction system. Specifically, the proposed coded diffraction system with boolean (block–unblock) approximations of the phase coded apertures is presented. In addition, this paper presents an algorithm to obtain the boolean coded aperture approximations, which can be easily implementable on a real diffraction system such as that on [16]. Moreover, this work uses the SAXS/WAXS X-ray crystallography software to simulate the diffraction patterns of a real crystal structure called *Rhombic Dodecahedron* [17,18]. Furthermore, this paper develops a modified version of the Truncated Wirtinger Flow Algorithm to recover the phase using boolean coded diffraction patterns [19]. Several simulations were performed to recover the phase using the boolean coded aperture approximations and the set of simulated diffraction patterns. Moreover, simulation results show that the performance of the coded boolean system approximation decreases up to 12.5% in terms of PSNR compared with the performance of the phase coded aperture. The quality of the image reconstructions were measured in terms of the Peak Signal to Noise Ratio (PSNR). Results show that the quality of the reconstructions using the boolean approximations is up to 2.5 dB of PSNR less with respect to the phase coded aperture reconstructions. The main contributions of this paper are summarized as follows

- A coded diffraction system that employs a boolean phase coded apertures is described, along with an iterative algorithm to obtain the boolean approximations of the phase coded apertures. Also, given that the coded aperture is boolean, the proposed system can be easily implemented.
- A modified version of the Truncated Wirtinger Flow (TWF) algorithm is presented in order to recover the phase from boolean encoded measurements. Moreover, since the TWF algorithm requires several truncation parameters, this work used a Bayesian framework in order to determine the optimal truncation values.

2. Theoretical background

This section explains the phenomenon occurring in a coded diffraction system, including the phase retrieval problem and the diffraction theory. The Fourier transform pair is defined as

$$\mathcal{F}\{f(x,y)\} = F(k_x,k_y) = \iint_{\infty}^{-\infty} f(x,y)\mathrm{e}^{ik_x x + ik_y y} dx dy, \tag{1}$$

$$\mathcal{F}^{-1}\{F(k_x,k_y)\} = f(x,y) = \frac{1}{4\pi^2}\iint_{-\infty}^{\infty} F(k_x,k_y)\mathrm{e}^{-ik_x x - ik_y y} dk_x dk_y, \tag{2}$$

where (x,y) and (k_x,k_y) represent the spatial and the frequency indexing variables, respectively.

2.1. Scalar diffraction theory

In general, the amplitude $\psi_p(x',y';z=S)$ of a diffracted field $\psi_0(x,y)$ at distance $z=S$ can be found by solving the *Helmholtz equation* for $\psi_p(x',y';z=S)$, obtained by replacing $\psi_p(x',y';z=S)$ into the scalar wave equation as explained in [15]. Then, the amplitude $\psi_p(x,y;z=S)$ is obtained as

$$\psi_p(x',y';z=S) = \mathcal{F}^{-1}\{\mathcal{F}\{\psi_{p0}(x,y)\}\mathcal{H}(k_x,k_y;z=S)\}, \tag{3}$$

where the transfer propagation function $\mathcal{H}(k_x,k_y;z)$ at a distance $z=S$ is defined as

$$\mathcal{H}(k_x,k_y;z=S) = \exp\left(-ik_0\sqrt{1-\left({k_x}^2/{k_0}^2+{k_y}^2/{k_0}^2\right)S}\right), \tag{4}$$

where $i=\sqrt{-1}$, and k_0 is the wave number. Further, the amplitude ψ_p calculated by Eq. (3) corresponds to the Angular Spectrum zone, because the Fresnel number B satisfies that $B \gg 1$ [20]. The Fresnel number is given by $B=\frac{a}{S\lambda}$, where a is the characteristic size of the diffracted field ψ_0 and λ is the wavelength of the X-ray source [15].

On the other hand, when the Fresnel number satisfies $B \ll 1$, Eq. (3) becomes the far field diffraction known as the Fraunhofer approximation, which is modeled as

$$\psi_p(x',y';z=S) = \tau\mathcal{F}\{\psi_0(x,y)\}, \tag{5}$$

where $\tau = \frac{ik_0}{2\pi S}\exp(\frac{-ik_0}{2S}(x^2+y^2+2S^2))$. Note that the magnitude of the right hand side of Eq. (5) mainly depends on the Fourier transform of the field $\psi_0(x,y)$ [15]. The next subsection presents the diffraction process in an X-ray crystallography diffraction system and the relation with the Fraunhofer approximation.

2.2. Phase retrieval problem from coded measurements

The measurements $I(x',y')$ captured at the detector in a traditional X-ray crystallography diffraction system correspond to the magnitude of the Fraunhofer diffraction of the object under analysis $o(x,y)$, which can be approximated as

$$I(x',y') = |\mathcal{F}\{o(x,y)\}|^2. \tag{6}$$

Further, from Eq. (6) the typical phase retrieval problem aims to recover the phase of the signal $\mathcal{F}\{o(x,y)\}$ from the measurements $I(x',y')$. Then, introducing a coded aperture $D(x,y)$ which modulates the signal $o(x,y)$ before being diffracted, as shown in Fig. 1, implies that coded measurements can be modeled as

$$\bar{I}(x',y') = |\mathcal{F}\{D(x,y)o(x,y)\}|^2. \tag{7}$$

In general, the modulation of the signal before being diffracted as modeled in Eq. (7) is not possible in real X-ray crystallography architectures, because the coding element needs to be the same size as the crystal, which in practice is on the order of 0.43 mm [10]. One strategy to implement the coded aperture $D(x,y)$ is to use an equivalent phase coded aperture $P(k_x,k_y)$ instead of using the coded aperture $D(x,y)$ [21], which will be explained in Section 3.