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Coded aperture design for solving the phase retrieval problem in X-ray crystallography

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ABSTRACT

X-ray crystallography is an experimental technique used in material analysis that allows to measure the atomic positions of the elements present in a crystal. This technique is based on the X-ray diffraction patterns that provide electronic and elastic properties of the crystal of interest. Thus, the crystal can be uniquely identified by means of the phase of its diffraction patterns that are also used to analyze the material of interest. The phase of the X-ray cannot be directly measured; however, it can be recovered from the intensity of diffraction patterns. A recent work has shown that the phase signal can be recovered more efficiently when the acquisition architecture includes an optical element, known as coded aperture, such that the underlying signal is recovered from coded diffraction patterns. A coded aperture is an element that modulates the X-ray diffraction patterns by blocking some X-ray beams. The structure and the number of coded projections are crucial inasmuch they determine the quality and the acquisition time of the X-ray signal. This paper presents the analysis of a coded X-ray Crystallography system, and the design of the spatial structure of the coded aperture, such that the images are recovered with high PSNR (Peak Signal to Noise Ratio) using the minimum number of coded projections. The simulations indicate that the designed coded apertures obtain a reduction of up to 50% in the number of coded projections and an increase in the PSNR of up to 2 dB when the results are compared with the reconstructed images by using random non-designed coded aperture structures. All simulations were carried out on a set of diffraction pattern images, obtained by using the SAXS/WAXS X-ray crystallography software to simulated the diffraction patterns of a real crystal structure, called Rhombic Dodecahedron.

1. Introduction

X-ray crystallography is a technique that allows to determine the atomic positions represented in the three-dimensional space of a crystal [1]. For measuring X-ray diffraction, the crystal is located in a goniometer that gradually rotates while being exposed to a monochromatic beam of X-rays. Given that the wavelength of X-rays is in the same order as the interatomic distances of the crystalline structure, the rotation of the crystal results in a diffraction pattern. The intensities of the reflections in the diffraction patterns are measured by an optical sensor. However, these sensors cannot measure directly the phase of the diffraction patterns. For this reason, a recovering algorithm is used to retrieve the phase of the signal. The recovered phase is used to make a three-dimensional model of the molecular structure of a crystal. Moreover,

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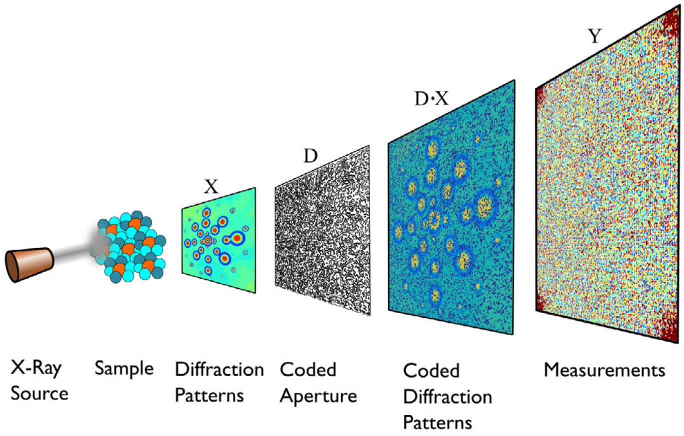

Fig. 1. Coded diffraction pattern system. The X-ray source illuminates the sample, resulting in the diffraction patterns $\mathbf{X} \in \mathbb{C}^{n\times n}$. The coded aperture $\mathbf{D} \in \mathbb{C}^{n\times n}$ blocks some of these diffraction patterns and the sensor data $\mathbf{Y} \in \mathbb{R}^{n\times n}$ receives the measurements.

the measurements that arrive to the detector are approximated to the modulus of the Fourier transform, following the Fraunhofer diffraction [2].

Based on the solution of the electronic density function, the middle positions of the atoms in the crystal can be determined, just like its chemical bonds; the unusual electronic and elastic properties of a material provide information about the chemical interactions and processes, to serve as a basis for the design of medicines against illness [3] and development of new materials [4].

The most traditional algorithms to solve the phase retrieval problems are based on the Error-Reduction method [5], however the rate of convergence of this algorithm is considerable slow [2,5]. Therefore, a recent work has shown that the phase can be recovered more efficiently from measurements acquired with architectures including an optical element known as coded aperture [2]. This element modulates the X-ray diffraction pattern before being measured in the sensor as shown in Fig. 1. The signal is modulated by changing its phase or blocking some diffracted beams. The selection of modulated beams is conventionally performed in a random fashion. The percentage of diffracted X-rays that passes through the coded aperture is known as transmittance [6].

Some applications of coded apertures include improvement in the performance of sensors [7], uniformly redundant array for creation of images without lens [8], Hadamard transformation in spectroscopy [9] and compressive hyperspectral imaging [10,11]. Moreover, coded apertures are used for the reconstruction of Raman spectroscopy imaging based on compressive sensing [6], using fewer measurements than those required by traditional Shannon–Nyquist sensing procedures.

Several methods have been developed to recover the phase from coded X-ray diffraction patterns. Some of them include convex programming techniques such as PhaseLift [2], by solving a convex optimization problem inspired by the recent literature on matrix completion [12], non-convex formulations of the phase retrieval problem via Wirtinger Flow (WF) [13], Truncated Wirtinger Flow (TWF) [14], Truncated Amplitude Flow (TAF) [15] and Reshaped Wirtinger Flow (RWF) [16]. In addition, these works have proposed coded aperture designs that help in obtaining the reconstruction of the phase. Despite the fact that these coded apertures have been designed to recover the phase from diffracted beams, its physical implementation in a real architecture is impractical, because it requires changing the phase of a diffracted beam [17,18], and finding a material allowing these changes is highly expensive. Remark that in [17] was only established that is possible to recover the phase by using block–unblock coded apertures, but it does not guarantee the convergence of the reconstruction algorithm from boolean encoded measurements, which is proved in this paper. Further, in this work theoretical details about the optimal boolean coded aperture design to solve the phase retrieval problem are presented.

This paper presents the analysis of different designs of block–unblock coded apertures that allow the phase recovery from coded X-ray diffraction patterns. These coded apertures are also known as boolean, and their modulation on the signal consist only in allow a few diffracted beams to pass. Furthermore, the construction of these coded apertures is feasible and it is possible to use them in a real coded diffraction pattern system. Also, the optimal transmittance and spatial distribution for the use of these coded apertures are also determined.

This work develops a modification of the TWF algorithm to reconstruct in order to retrieve the phase from boolean encoded diffraction patterns, by using a set of synthetic images. This set of diffraction was obtained by using the SAXS/WAXS X-ray crystallography software, to simulated the diffraction patterns of a real crystal structure called, Rhombic Dodecahedron. This modification permits to get closer to an implementation of a real coded diffraction patterns system. Moreover, different simulations vary the transmittance value and calculate the Peak Signal to Noise Ratio (PSNR) to measure the quality of image reconstructions. Simulations show that the proposed method attains a higher performance to recover the phase in comparison with the state-of-art methods. Also, these numerical results suggest that the optimal coded aperture transmittances, for the four tested designs are 70%, 50%, 50% and 70% respectively, which results in up to 24.00 dB of PSNR.