Sub-Wavelength Coherent Diffractive Imaging based on Sparsity

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***Abstract*—We propose and experimentally demonstrate a method of performing single-shot sub-wavelength resolution Coherent Diffractive Imaging (CDI), i.e. algorithmic object reconstruction from Fourier amplitude measurements. The method is applicable to objects that are sparse in a known basis. The prior knowledge of the object's sparsity compensates for the loss of phase information, and the loss of all information at the high-spatial frequencies occurring in every microscope and imaging system due to the physics of electromagnetic waves in free-space.**

I. Introduction

Coherent Diffractive Imaging (CDI) is an imaging technique where intricate features are algorithmically reconstructed from measurements of the freely-diffracting intensity pattern ([1], [2]). In CDI, an object is illuminated by a coherent plane wave (LASER light), and the far-field diffraction intensity is measured. That is, the measurements correspond to the absolute value squared of the Fourier components. Recent advances in making lasers in the x-ray regime and in the extreme ultraviolet have made this technique very important for a variety of applications, among them structural biology: mapping out the structure of proteins that cannot be crystalized. However, the physics underlying the propagation of electromagnetic waves acts as a low-pass filter, effectively truncating high Fourier components, and thereby setting a fundamental limit on imaging systems: the finest feature that can be recovered in imaging microscopes is larger than one half of the optical wavelength (the so-called diffraction limit). This stringent limit naturally also limits CDI: the resolution in all current work on CDI is limited by the diffraction limit [3]. Over the past decades, several techniques were developed for sub-wavelength imaging, but none of them works as actual imaging: they all involve scanning or integration over very many acquired images generated by sub-wavelength light sources. These methods include Scanning Near-Field Microscope ([4], [5]), scanning a sub-wavelength "hot spot" ([6], [7], [8]), or ensemble-averaging over multiple experiments with fluorescent particles ([9], [10], [11], [12]). Due to the nature of theses technique – which rely on scanning or averaging - they cannot be used for real-time imaging of dynamics processes (say, a chemical reaction that evolves with time). On the other hand, CDI, being a 'single shot' imaging technique, is suitable for ultra-fast imaging, but it lacks sub-wavelength resolution. Here, we present and demonstrate experimentally a method to enhance CDI resolution beyond the diffraction limit, based on prior knowledge that the object is sparse in a known basis.

II. Problem Formulation

In a typical, plane-wave CDI setting, an object is illuminated by a coherent plane wave, and the far field diffraction pattern intensity is measured. The measured diffraction intensity, in the paraxial approximation, is proportional to the magnitude of the object's Fourier transform, up to the cut-off frequency $1/\lambda$, where λ is the wavelength of the light [3]. Therefore, mathematically, the sub-wavelength CDI problem becomes the problem of recovering a 2D signal from only the magnitude of its truncated Fourier transform. Up to spatial coordinate scaling and normalization, the above relation can be written as:

$$I(j,k) = |LFb|^2(j,k), \tag{1}$$

where I is the measured far-field intensity, F is the 2D Fourier transform operator, L is a low-pass filter with a cutoff frequency of $1/\lambda$, and b is the sought 2D object. The operator $|\cdot|$ here stands for element-wise absolute value.

Inverting Eq.1, i.e. finding b from I, L, F is an ill-posed problem, both because the high frequency information is lost due to the coupling of high spatial frequencies to evanescent waves, and due to the loss of phase information - since only the far-field (Fourier) magnitude is measured. The problem at hand, therefore, is phase-retrieval of a 2D object, combined with bandwidth-extrapolation. In order to invert this ill-posed problem, some additional information is needed, e.g. prior knowledge on the sought signal.

In this work, we focus on objects that can be represented compactly in a known basis, i.e. $b = Ax$ where A is a known basis and x is a sparse vector, namely, containing a small number of nonzero elements. In this case, Eq. 1 can be rewritten as (For simplicity, the indices (j,k) are dropped from now on):

$$I = |LFAx|^2, \tag{2}$$

and the prior knowledge of the sparsity of x adds information that helps the inversion of Eq. 2. The sparsity prior has been used for sub-wavelength imaging [13], but only when the Fourier phase was also known, yielding a linear problem. Since the measurements in our setting are not linear in the unknown (but quadratic), standard linear sparse inversion algorithms cannot be used, and a method to find a sparse solution to a set of quadratic equations is required.

III. Solution Method

The problem of sub-wavelength CDI can be viewed as consisting of two sub-problems: Phase retrieval, and bandwidth extrapolation. The problem of phase retrieval, i.e. recovering a signal from the magnitude of its Fourier transform arises in applications such as holography and crystallography, and there has been a vast amount of work dealing with it ([14], [15]). Usually, some prior knowledge about the object is used (e.g. known support or known real-space megnitude), and the different constaints are imposed iteratively. These techniques have been used in the context of CDI [2], but their application has always been limited to the information contained within numerical aperture of the system.

Here, we devise a phase-retrieval method that can also deal with the loss of high-requencies, by using the prior knowledge that the sought object is sparse in a known basis. The two problems are not handled separately, but rather solved as a combined optimization problem. The logic of the technique is as follows: An iterative thresholding method is used in order to solve Eq. 2 while using the sparsity information. The method attempts to find a solution to the following problem:

$$\begin{aligned} \text{min} \quad & ||x||_0 \\ \text{subject to} \quad & \left|\left|I - |LFAx|^2\right|\right|_2^2 \leq \epsilon \\ & x \geq 0 \end{aligned} \tag{3}$$

The non-negativity constraint on corresponds to the assumption that the real-space object contains no phase information, which is the case we consider in this work. The thresholding method is described in detail in [16], and briefly below. First, an initial support of the vector is approximated from the blurred real-space image. Then, the following two steps are repeated iteratively:

1. Solve the minimization problem:

$$\begin{aligned} \text{min} \quad & \left|\left|I - |LFAx|^2\right|\right|_2^2 \\ \text{subject to} \quad & x \geq 0 \end{aligned} \tag{4}$$

This is a non-convex problem, and in practice we use the L-BFGS method [17] to find a local minimum.

2. Remove the weakest element of x from the support, i.e. set it to zero. This element is constrained to remain zero in the following iterations. Go-to step 1.

The iterations continue as long as the constraint $\left|\left|I - |LFAx|^2\right|\right|_2^2 \leq \epsilon$ can be satisfied. Note that this requires knowledge of the noise level ϵ in the measurements, which might be approximated from knowledge or calibration measurements in the optical system. In addition, a stopping criterion may be defined by analyzing the reconstruction error $\left|\left|I - |LFAx|^2\right|\right|_2^2$.

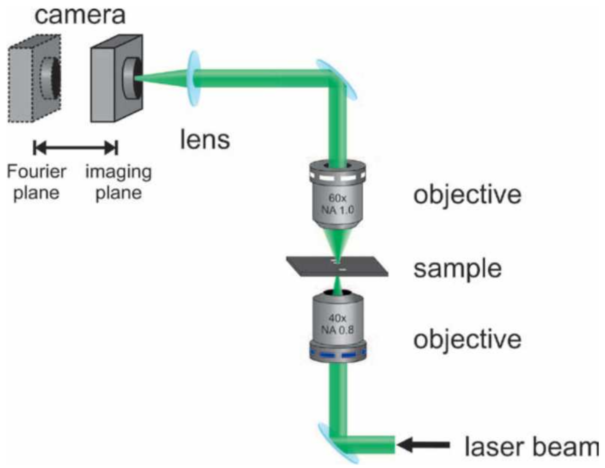

Fig. 1. Experimental setup

IV. Experimental Results

We demonstrate sparsity based sub-wavelength CDI experimentally, using the setup shown in Fig. 1. A coherently illuminated microscope (532nm LASER) is used to image arrangements of sub-wavelength holes, 100nm in diameter, in a 100nm thick Chrome layer covering a transparent substrate of fused silica. The imaging setup consists of a water-immersed objective (NA=1) and a lens imaging onto a 1002×1002 pixel CCD camera. The camera can be moved so that either the real-space (blurred) magnitude of the object is measured, or its truncated Fourier magnitude (Fig. 1). Two different patterns are imaged and recovered experimentally. The first, a star of David, is shown in Fig. 2. Figure 2a shows the Scanning-electron-microscope image of the sample. Figure 2b shows the measured real-space image using our microscope, featuring the blur caused by the diffraction limit. The measured truncated Fourier magnitude is shown in Fig. 2c. The basis for reconstruction is taken as 100nm circles on a grid, and the reconstructed image is shown in Fig. 2d. The circles are recovered with the correct locations, and their recovered amplitude is close to constant - which is consistent with the illumination used for the imaging, which had approximately constant intensity across the sample.

In order to demonstrate our ideas on a non-symmetric sample, exhibiting a truly complex Fourier transform, a second pattern, comprising of a 'random' distribution of twelve 100nm circles, is also recovered. Figure 3a shows the measured blurred real-space image, and Fig. 3b shows the measured truncated Fourier spectrum. The sparse sub-wavelength object is recovered (Fig. 3c) from its truncated Fourier spectrum, using our method, and the SEM image of the true object is shown in Fig. 3d. The reconstruction basis used here is the same as in Fig. 2, namely, 100nm circles on a grid.

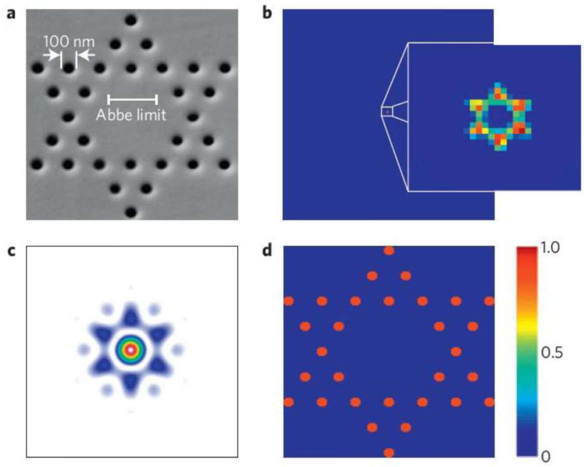

Fig. 2. a) Scanning Electron Microscope (SEM) image of the sample. b) Real-space imaging, blurred due to diffraction limit. c) Measured Fourier magnitude. d) Sparse reconstruction

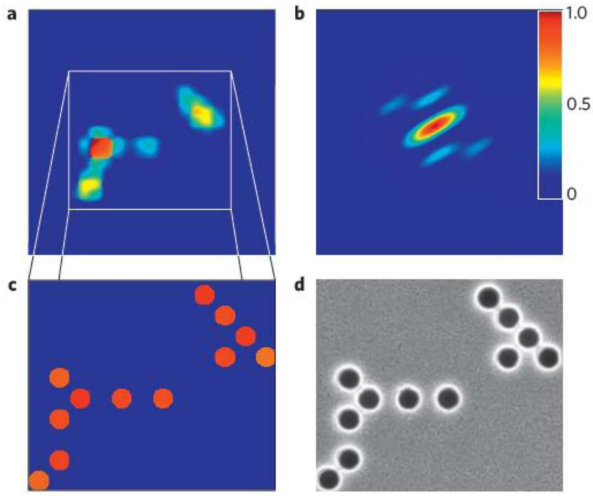

Fig. 3. a) Real-space imaging, blurred due to diffraction limit. b) Measured Fourier magnitude c) Sparse reconstruction d) Scanning Electron Microscope (SEM) image of the sample.

V. Conclusion

In this work, we have presented a technique facilitating the reconstruction of sub-wavelength features, along with phase retrieval, at an unprecedented resolution for single-shot experiments. This work opens the way for ultrafast sub-wavelength coherent diffractive imaging: ultrafast phase retrieval at the sub-wavelength scale. Fundamentally, sparsity-based concepts can be implemented in all imaging systems and achieve sub-wavelength resolution without additional hardware, given only that the image is sparse in a known basis. For example, sparsity-based methods could considerably improve the CDI resolution with x-ray free electron laser [18], without hardware modification.

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