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Adaptive-window angular spectrum algorithm for near-field ptychography

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ABSTRACT

Near-field ptychography provides advantages over far-field ptychography that large field-of-view (FOV) can be imaged with fewer diffraction images, and with weaker requirements on the detector dynamic range and beam coherence, which has drawn attention recently. However, the propagation distance of traditional angular spectrum (AS) method is limited and the reconstruction of the smallest resolvable object detail is restricted by the sensor's pixel size. To this end, we propose an adaptive-window angular spectrum (AWAS) algorithm to solve both problems by adding the window adaptively associated with the propagation distance and avoid the extra computations via extra scaling factors. Meanwhile, it features validity for the independent sample size and the sample number on the observation plane. This algorithm is strictly deduced from the Rayleigh–Sommerfeld formula and based on the linear convolution, which can be evaluated by fast Fourier transform effectively. The burden of calculations is comparable to traditional AS method. The performance has been achieved both in two-dimensional and three-dimensional near-field ptychography with simulations and experiments. This method will make near-field ptychography more practical and can be used in X-ray or electron-microscopy and other computational imaging techniques.

1. Introduction

Ptychography is a coherent diffractive imaging technique that produces wide field-of-view (FOV), quantitative phase images at a resolution limited only by the angular extent of the detector [1–3]. By recording overlapped diffraction patterns, the overlap results in a large degree of data redundancy, which can be used to recover the complex-valued information of object, decompose the coherent states and calibrate the system errors by advanced iterative algorithms [4–10]. This lensless method has been successfully demonstrated in the visible light [11,12] and electron regimes [13,14], and has earned considerable popularity in the X-ray community [15,16], where high-quality, high-resolution optics are challenging to manufacture.

Recently some researchers focus on the near-field ptychography since it provides advantages over far-field ptychography that large FOV can be imaged with fewer diffraction images, and with weaker requirements on the detector dynamic range and beam coherence [17–20]. The diffraction patterns will directly show the blurry contours of the samples. Additionally, the Fresnel numbers are significantly higher than in those far-field ptychography [20]. However, there are two drawbacks when normally using the angular spectrum (AS) algorithm for diffraction propagation, compared with using the fast Fourier transform (FFT) in the far-field ptychography. On the one hand, the sampling problem of the chirp function makes the AS method only valid for quite near-field simulation, otherwise the simulated patterns will be distorted and there will be some grid noise and the signal-to-noise ratio (SNR) will decrease [21,22]. Generally in ptychography, the smaller the size of the probe is, the better the sampling is [23,24]. And the probe needs to be clipped into a patch as small as possible for fast calculation. However, the probes cannot be tailored too small in order to assure the sampling requirements of the AS method. Otherwise the SNR will decrease. Accordingly, unnecessary computations will be introduced. On the other hand, the AS method cannot permit the independent sample size and the calculation window size on the source and observation plane due to the nature of FFT [25]. Thus the resolution of near-field ptychography is restricted by the sensor's pixel size, which is far from the resolution limit of ptychography.

Generally, there are two main kinds of methods for propagating wave fields between parallel planes [26]. The first kind is based on the integration in the spatial domain including the single Fourier-transform-based Fresnel method (SFT-FR) [27], the convolution-based Rayleigh–Sommerfeld method (CV-RS) [28], etc. In general, these simulation methods are not suitable for the near-field and cannot be used for

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the propagation between the tilted planes. Another kind of method is associated with the AS propagation, which can be used for the propagation between the tilted planes and for the near-field simulation [26]. Therefore, the AS method is more widely used in near-field ptychography since different illumination modes can be also used, however, it is not an all-round method due to the two drawbacks above. Adding a fictitious window (zero interpolation) is a good way to solve the former problem. But it increases the sampling numbers, which will result in unnecessary calculations and increase the calculation burden [21]. A multi-step relay-operated method [29] has been proposed, however, it causes a different error especially in long distance propagation, since the cascaded sampling windows used are equivalent to diffraction by the cascaded aperture. Another way is to limit its pass band, termed BLAS method [22], whereas it will reduce the effective sampling numbers with the increasing of propagation distance. It just relieves the problem and does not solve the problem fundamentally [21]. Besides, these methods all suffer from the second drawback. While Claus et al. [30] proposed a fictitious spherical lens with adjustable magnification to solve the second problem successfully. But it needs to adjust the magnification during the process and requires more iterations, which is not easy to achieve and time-consuming. Subsampling, or using extra scaling factor to adjust the pixel size is also a means to implement the different intervals of observation plane [31]. But they introduce more computations and cannot solve the former problem. The propagation distance cannot be arbitrary value. Xiao et al. [25] proposed a BLAS with selective scaling of observation window size and sample number via extra scaling factor, which can solve both problems to a certain degree but cannot solve the problems completely due to the nature of BLAS method [21].

In this paper, an all-round AS method, termed adaptive-window angular spectrum (AWAS) algorithm is proposed to solve both problems and demonstrated in near-field ptychography as examples. Adding window is the most suitable method to solve the former problem compared with other methods due to three basic facts: (i) The input field needs to be doubled along both x- and y-axis in order to convert a circular convolution to a linear convolution [22]; (ii) FFT will broaden the spectrum of object, which will bring in the aliasing spectrum transmission, and adding window can avoid the artifacts [25]; (iii) The size of detector is usually larger than the object in practice. But adding window like other methods will introduce more computations in turn. So in our method, we introduce an extra scaling factor to bypass those unnecessary calculations, since they are all zeros. As for the second problem, we introduce another extra scaling factor to freely adjust the interval and window size on the observation plane like the method in Ref. [25]. This algorithm is strictly deduced from the Rayleigh–Sommerfeld formula [32] and based on the linear convolution, which can be evaluated by FFT effectively. The burden of calculations is comparable to traditional AS method. The performance has been achieved both in simulation and experiments and has been compared with the existing methods. Our method can not only be used in near-field ptychography, but also be used in other computational techniques, such as digital holography [33,34], Fourier ptychography [35–37].

2. Adaptive-window angular spectrum scheme

In the scalar diffraction theory, the accurate diffraction formula is the Rayleigh–Sommerfeld diffraction integral [32]. The coordinate system used in formulation is shown in Fig. 1.

$$U(x, y, z) = \iint U_0(x_1, y_1, 0) \exp(ikr) \frac{z}{r} \left(\frac{1}{r} - ik\right) dx_1 dy_1 \quad (1)$$

where $r = [(x-x_1)^2 + (y-y_1)^2 + z^2]^{1/2}$, k is the wave number, z is the propagation distance, (x_1, y_1) and $U(x_1, y_1, 0)$ are the coordinates and the input light field, (x, y) and $U(x, y, z)$ stand for the coordinates and the light field of observation plane, respectively. Consequently, the AS is formulated as follows:

$$U(x, y, z) = \mathcal{F}^{-1}\left\{\mathcal{F}\left\{U_0(x_1, y_1, 0)\right\} H(u, v, z)\right\} \quad (2)$$

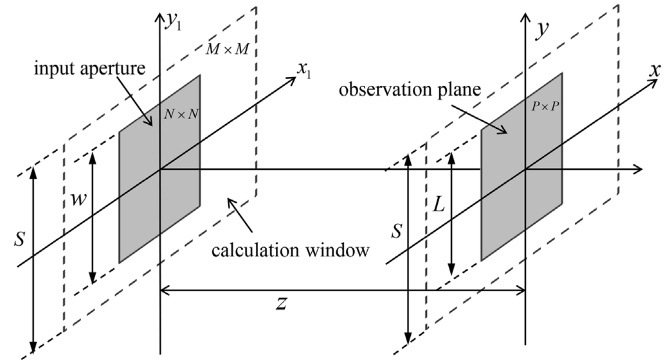

Fig. 1. Geometry of the wave propagation model.

where the transfer function $H(u, v, z)$ is given by

$$H(u, v, z) = \exp\left(i2\pi z\sqrt{\lambda^{-2} - u^2 - v^2}\right) \quad (3)$$

Note that there is a chirp function in the transfer function. In order to avoid the aliasing error, the propagation distance z needs to satisfy [26]

$$z \le \frac{W^2}{N\lambda} = \frac{N\Delta x_1^2}{\lambda} \quad (4)$$

where N is sampling number, W is the length of input aperture, Δx_1 is the pixel size of input aperture. Besides, the AS method of Eq. (2) is based on one time of forward and inverse FFT , which needs the same sample interval and calculation window size on the source and observation plane. One way to solve the former problem is to limit its pass band to retain those effective sampling points for long distance propagation [22].

$$H'(u, v, z) = H(u, v, z)\, rect\left(\frac{u}{2u_{limit}}\right) rect\left(\frac{v}{2v_{limit}}\right) \quad (5)$$

where $u_{limit} = \left[\lambda\sqrt{(2\Delta u z)^2 + 1}\right]^{-1}$, and the v_{limit} can be analogical. But it will reduce the effective sampling numbers with the propagation distance increasing. In order not to lose imaging precision, we let all the sampling numbers in the frequency domain are effective by adding windows. Then the sampling in the frequency domain should meet the requirement.

$$\Delta u = \frac{1}{S_1} = \frac{2u_{limit}}{N} \quad (6)$$

Thus the width of the calculation window size can be determined by the Eqs. (5) and (6) as follows.

$$S_1 = \frac{2\sqrt{2}zN\lambda}{\sqrt{-N^2\lambda^2 + \sqrt{N^4\lambda^4 + 64z^2N^2\lambda^2}}} \quad (7)$$

In addition, adding windows are necessary due to other three factors. First, the input field needs to be doubled along both x- and y-axis in order to convert a circular convolution to a linear convolution [22].

$$S_2 = 2W \quad (8)$$

Second, FFT will broaden the spectrum of object, which will bring in the aliasing spectrum transmission [25]. Thus the minimum window size also needs to satisfy

$$S_3 = W + L \quad (9)$$

And finally, the size of detector is usually larger than the object in practice. Adding windows are suitable to the real situations. Therefore, the calculation window needs to meet all these conditions from Eq. (7)