Ultramicroscopy 192 (2018) 29–36

Contents lists available at ScienceDirect

Ultramicroscopy

journal homepage: www.elsevier.com/locate/ultramic

Lateral position correction in ptychography using the gradient of intensity patterns

Priya Dwivedi*, A.P. Konijnenberg, S.F. Pereira, H.P. Urbach

Optics Research Group, Department of Imaging Physics, Delft University of Technology, Lorentzweg 1, Delft, 2628CJ, Netherlands

ARTICLE INFO

Article history:
Received 17 July 2017
Revised 22 February 2018
Accepted 12 April 2018
Available online 14 April 2018

ABSTRACT

Ptychography, a form of Coherent Diffractive Imaging, is used with short wavelengths (e.g. X-rays, electron beams) to achieve high-resolution image reconstructions. One of the limiting factors for the reconstruction quality is the accurate knowledge of the illumination probe positions. Recently, many advances have been made to relax the requirement for the probe positions accuracy. Here, we analyse and demonstrate a straightforward approach that can be used to correct the probe positions with sub-pixel accuracy. Simulations and experimental results with visible light are presented in this work.

1. Introduction

Coherent Diffractive Imaging (CDI) is a lensless imaging technique which uses far-field diffraction intensity patterns to reconstruct the image of an object. Ptychography is a form of CDI, where multiple far-field diffraction patterns corresponding to overlapping illuminated regions of the object are collected, and the object is reconstructed [1]. For the reconstruction of the object, the Ptychographical Iterative Engine (PIE) [2] is used of which many different variants have been developed [3–6]. PIE has been found to be robust if the a priori information such as the illumination probe function and the lateral probe positions are accurately known [7]. Several methods exist which can overcome the requirement for the accuracy of the a priori information. For example, Extended PIE (ePIE) can reconstruct the object as well as a poorly defined probe function [3]. However, ePIE has been found to be sensitive to the probe positioning errors, especially in applications involving short wavelengths such as X-rays and electron beams [8]. For these short wavelengths, the required accuracy in the probe positions should be in some cases of the order of 50 pm [9]. Since this is difficult to achieve experimentally, some new developments in the probe position corrections have been made.

The non-linear (NL) optimization approach was the first method that has been used to correct the probe positions [10]. However, this approach can easily lead to local minima which can be far from the required global minimum since several parameters (update of the object, the probe function and the probe positions) are used in the NL optimization routine. Improvements have been made in the NL optimization approach by combining it with ePIE and difference map (DM) [11]. In this reference, the authors have used the ePIE and DM to update the object and the probe function, whereas the probe positions have been corrected using the NL optimization. One drawback of this method is that the probe positions can not be corrected to sub-pixel accuracy. Other methods based on the genetic algorithm and a drift-based model were also explored [12,13]. In yet another study, the “annealing approach” “based on trial and error” was used, but at the cost of being computationally expensive [14]. Finally, there is a successful method that uses the cross-correlation between two consecutive object estimates for each probe position [9]. This approach has corrected the probe positions to sub-pixel accuracy using the additional sub-pixel registration method [15].

Here, we analyse and demonstrate an alternative algorithm to correct the probe positions with sub-pixel accuracy that is quite straightforward to implement [16]. This paper is organized as follows: In Section 2 we describe our method for the probe position correction. In Section 3, the robustness of the method will be verified by evaluating the simulation results. In Section 4, we show the experimental results. Finally, in Section 5, we present the conclusions.

2. The algorithm

In ptychography, the diffraction intensities $I^j(\mathbf{u})$ for different probe positions $j = 1,2,\ldots,J$ with respect to the object are recorded in the camera. Here, J is the number of diffraction patterns. If the

* Corresponding author.
E-mail address: p.dwivedi@tudelft.nl (P. Dwivedi).

https://doi.org/10.1016/j.ultramic.2018.04.004

object and illumination probe functions are represented as $O(\mathbf{r})$ and $P(\mathbf{r})$, then

$$I^j(\mathbf{u}) = |\mathscr{F}\{O(\mathbf{r})P(\mathbf{r}-\mathbf{R}^j)\}(\mathbf{u})|^2, \quad (1)$$

where $\mathbf{R}^j = (X^j, Y^j)$ is the probe position vector, $\mathbf{r}$ and $\mathbf{u}$ represent the coordinate vector in the real and reciprocal space respectively, and $\mathscr{F}$ denotes the Fourier transform. We combine the well-known phase reconstruction method ePIE with our position correction method. That means, for the kth iteration and the jth probe position, we update the object $O_k(\mathbf{r})$ to $O_{k+1}(\mathbf{r})$ and the probe function $P_k(\mathbf{r})$ to $P_{k+1}(\mathbf{r})$ using the ePIE after which the probe position $\mathbf{R}_k^j$ is updated using our probe position correction method. We describe the probe position correction method below. Note that in this probe position correction method, we use the previous estimates $O_k(\mathbf{r})$ and $P_k(\mathbf{r})$ instead of $O_{k+1}(\mathbf{r})$ and $P_{k+1}(\mathbf{r})$ as this saves one extra Fourier transform to perform. The reason will be clear soon.

For the kth iteration, the diffracted far-field for the probe position $\mathbf{R}_k^j$ can be written as

$$\Psi_k^j(\mathbf{u}) = \mathscr{F}\{O_k(\mathbf{r})P_k(\mathbf{r}-\mathbf{R}_k^j)\}, \quad (2)$$

and the estimated intensity is

$$I_k^j(\mathbf{u}) = |\Psi_k^j(\mathbf{u})|^2. \quad (3)$$

For the object estimate $O_k(\mathbf{r})$ and probe estimate $P_k(\mathbf{r})$, the inaccuracy in the measurement intensity due to the error $(\Delta X_k^j, \Delta Y_k^j)$ in the probe position is given by:

$$\Delta I_k^j \approx \frac{\partial I_k^j}{\partial X_k^j}\Delta X_k^j + \frac{\partial I_k^j}{\partial Y_k^j}\Delta Y_k^j. \quad (4)$$

Here, $\frac{\partial I_k^j}{\partial X_k^j}$ and $\frac{\partial I_k^j}{\partial Y_k^j}$ are the derivatives of the estimated intensity with respect to the probe position along the x and y directions. We solve Eq. (4) for ΔX_k^j and ΔY_k^j where ΔI_k^j is assigned to $I^j - I_k^j$.

To calculate $\frac{\partial I_k^j}{\partial X_k^j}$ and $\frac{\partial I_k^j}{\partial Y_k^j}$, we have

$$\frac{\partial I_k^j}{\partial X_k^j} = 2Re\left\{\frac{\partial \Psi_k^j}{\partial X_k^j}\Psi_k^{j*}\right\}, \quad (5a)$$

$$\frac{\partial I_k^j}{\partial Y_k^j} = 2Re\left\{\frac{\partial \Psi_k^j}{\partial Y_k^j}\Psi_k^{j*}\right\}, \quad (5b)$$

and

$$\frac{\partial \Psi_k^j(\mathbf{u})}{\partial X_k^j} = \mathscr{F}\left\{O_k(\mathbf{r})\frac{\partial P_k(\mathbf{r}-\mathbf{R}_k^j)}{\partial X_k^j}\right\}(\mathbf{u}), \quad (6a)$$

$$\frac{\partial \Psi_k^j(\mathbf{u})}{\partial Y_k^j} = \mathscr{F}\left\{O_k(\mathbf{r})\frac{\partial P_k(\mathbf{r}-\mathbf{R}_k^j)}{\partial Y_k^j}\right\}(\mathbf{u}). \quad (6b)$$

We approximate the right hand side of the Eq. (6) as

$$\frac{\partial \Psi_k^j}{\partial X_k^j} = \frac{\Psi_k^j - \mathscr{F}\{O_k(\mathbf{r})P_k(\mathbf{r}-(\mathbf{R}_k^j+\mathbf{1}_x))\}}{|\mathbf{1}_x|}, \quad (7a)$$

$$\frac{\partial \Psi_k^j}{\partial Y_k^j} = \frac{\Psi_k^j - \mathscr{F}\{O_k(\mathbf{r})P_k(\mathbf{r}-(\mathbf{R}_k^j+\mathbf{1}_y))\}}{|\mathbf{1}_y|}, \quad (7b)$$

where $\mathbf{1}_x$ and $\mathbf{1}_y$ are the vectors along the x and y directions and the magnitudes are the lengths of a pixel along the x and y directions, respectively.

The following steps are performed to calculate the error and update the probe positions.

1. Calculate the difference ΔI_k^j between the measured intensity I^j and the estimated intensity I_k^j given by $\Delta I_k^j = I^j - I_k^j$.
2. Calculate $\frac{\partial \Psi_k^j}{\partial X_k^j}$ and $\frac{\partial \Psi_k^j}{\partial Y_k^j}$ using Eq. (7).
3. Calculate $\frac{\partial I_k^j}{\partial X_k^j}$ and $\frac{\partial I_k^j}{\partial Y_k^j}$ using Eqs. (5).

Note that in Eq. (4), ΔI_k^j, $\frac{\partial I_k^j}{\partial X_k^j}$, and $\frac{\partial I_k^j}{\partial Y_k^j}$ are vectors whose components correspond to the values at the pixels. Given an intensity measurement consisting of N pixels, we can thus rewrite Eq. (4) as a matrix equation

$$\begin{bmatrix}\Delta I_k^j(1)\\ \Delta I_k^j(2)\\ \vdots\\ \Delta I_k^j(N)\end{bmatrix} = \begin{bmatrix}\frac{\partial I_k^j}{\partial X_k^j}(1) & \frac{\partial I_k^j}{\partial Y_k^j}(1)\\ \frac{\partial I_k^j}{\partial X_k^j}(2) & \frac{\partial I_k^j}{\partial Y_k^j}(2)\\ \vdots & \\ \frac{\partial I_k^j}{\partial X_k^j}(N) & \frac{\partial I_k^j}{\partial Y_k^j}(N)\end{bmatrix}\begin{bmatrix}\Delta X_k^j\\ \Delta Y_k^j\end{bmatrix}. \quad (8)$$

From this equation, we want to find $(\Delta X_k^j, \Delta Y_k^j)$. Because there are more equations than variables, there may be no solution $(\Delta X_k^j, \Delta Y_k^j)$ to this equation. Therefore, we calculate the least-squares solution which is given by

$$\begin{bmatrix}\Delta X_k^j\\ \Delta Y_k^j\end{bmatrix} = (A_k^{jT}A_k^j)^{-1}A_k^{jT}\begin{bmatrix}\Delta I_k^j(1)\\ \Delta I_k^j(2)\\ \vdots\\ \Delta I_k^j(N)\end{bmatrix}, \quad (9)$$

where

$$A_k^j = \begin{bmatrix}\frac{\partial I_k^j}{\partial X_k^j}(1) & \frac{\partial I_k^j}{\partial Y_k^j}(1)\\ \frac{\partial I_k^j}{\partial X_k^j}(2) & \frac{\partial I_k^j}{\partial Y_k^j}(2)\\ \vdots & \\ \frac{\partial I_k^j}{\partial X_k^j}(N) & \frac{\partial I_k^j}{\partial Y_k^j}(N)\end{bmatrix}, \quad (10)$$

and A_k^{jT} is the transpose of A_k^j. Note that $A_k^{jT}A_k^j$ is a 2×2 matrix, so the computation of its inversion is computationally inexpensive. Finally, the update equation for the probe position (X_k^j, Y_k^j) is given by

$$X_{k+1}^j = X_k^j - \beta\Delta X_k^j, \quad (11)$$

$$Y_{k+1}^j = Y_k^j - \beta\Delta Y_k^j. \quad (12)$$

Here, β is a feedback parameter which defines the step size of the update in the probe positions. Choosing smaller β in general leads to accurate correction but the computation time is larger. The value of β can be chosen as 1, 0.5 or 0.1.

To compare our approach with NL optimization method, the derivatives in NL optimization approach are calculated using discrete Fourier Transform whereas we are using finite difference method. On comparing the computational time of our approach with the cross-correlation (CC) method [9], we have found that each iteration of our method is less computationally expensive than CC method. Here, in the probe position correction part, we are using two Fourier transforms whereas the CC method uses three Fourier transforms. Additionally, the CC method requires an optimization in each iteration to find the cross-correlation peak. Furthermore, in the section 3.4, we have carried out an actual comparison between CC method and proposed method.