3D Lensless Diffraction Imaging
3D 無透鏡繞射顯微術

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Abstract

CDI is a "lensless" technique for reconstruction of the image of nanoscale structures. The main advantage of a typical CDI experiment is that this technique can be applied without using any lens to focus the coherent beam so that the measurements are not affected by aberrations and the resolution limited by wavelength. CDI involves collecting the diffracted wave of sample in the far-field and using the algorithm to reconstruct the sample image.

In this work, we started from the basic concepts of diffraction to the knowledge of CDI reconstruction. Then, we did the numerical simulations, using the phase retrieval algorithm, HIO algorithm and ePIE algorithm, for reconstructing the sample image. Which showed the effectiveness of both HIO algorithm and ePIE algorithm. Afterwards, we put it into practice, built an optical system. With the phase retrieval algorithm and optical system, we developed a lensless microscope, which its resolution up to several micrometers.

Motivation

The traditional microscope is Optic Microscope, while Optic Microscope's resolution is only about micron level, because of the limit of diffraction. To get higher resolution image, we can use Coherent diffraction imaging (CDI) technique, which is a "lensless" technique for 2D or 3D reconstruction of the image of nanoscale structures. In this research, we use matlab to test the program of CDI Algorithm, and reconstruct the image.

Introduction

1. Diffraction

Diffraction is the main concept of this work. Diffraction refers to various phenomena that occur when a wave encounters an obstacle or opening. Diifraction can be generally divided into Fraunhofer diffraction and Fresnel diffraction. The Fraunhofer diffraction occurs when the diffraction pattern is viewed at a long distance from the diffracting object (in the far-field region). Fresnel diffraction, in contrast, the diffraction pattern created near the object (in the near field region)[1].

2. CDI reconstruction

The main advantage of a typical CDI experiment is that this technique can be applied without using any lens to focus the coherent beam so that the measurements are not affected by aberrations and the resolution limited by wavelength. CDI involves collecting the diffracted wave of sample in the far-field and using the algorithm to reconstruct the sample image. However, we have deal with the phase problem, losing the phase information when doing measurements by detector arrays.

3. Phase retrieval algorithm

The concept of Phase retrieval algorithm is we assume the missing phase as the initial phase, with the amplitude and initial phase of diffraction pattern, we do the IFFT to obtain the sample. Then, we replace the amplitude by the known amplitude, and with the do the FFT again. We do the above step over and over again until it saturated, which is defined as the difference between the current diffraction amplitude and the measure amplitude to be smaller than the value we set.

One of the Phase retrieval algorithm is the Hybrid Input Output (HIO) Algorithm. Each iteration of the HIO algorithm consists of several steps summarized as follows:

- Step1: Set the initial phase multiply with $\sqrt{I(k)}$, get the initial $\psi'(\mathrm{k})$.
- Step2: Apply IFFT to $\psi'(\mathrm{k})$, take the wave function into real space and get $\psi'(\mathrm{r})$.
- Step3: Put $\psi'(\mathrm{r})$ into the equation below, S is the boundary. Get $\psi(\mathrm{r})$.

$$\Psi_n(\mathrm{r}) = \begin{cases} \psi'_{n-1}(\mathrm{r}) & , if\ r\epsilon S\ and\ real[\psi_{n-1}(\mathrm{r})] \geq 0 \\ \psi_{n-1}(\mathrm{r}) - \beta\psi'_{n-1}(\mathrm{r}) & , otherwise \end{cases}$$

- Step4: Apply FFT to $\psi(\mathrm{r})$, take the wave function into k space and get $\psi_n(k)$. Then, keep the phase of $\psi_n(k)$ and multiply with the original amplitude of diffraction$\sqrt{I(k)}$, generate the new wave function $\psi'_n(k)$. The equation shows below:

$$\psi'_n(k)=\sqrt{I(k)} \times \frac{\psi_n(k)}{|\psi_n(k)|}. \text{ Get } \psi'_n(k).$$

- Step5: Repeat the step2-step4 until the difference of the amplitude of $\psi(\mathrm{r})$ in step3 smaller than the value we set, which is defined as saturation.

4. Extended Ptychographic Iterative Engine (ePIE)

Extended Ptychographic Iterative Engine (ePIE) is a different algorithm to deal with phase problem, which is developed by J. M. Rodenburg and H. M. L. Faulkner. The main difference of ePIE algorithm is it collects more than one diffraction patterns through changing the position of probe sample. With multiple diffraction patterns, ePIE has better accuracy of the retrieved image.

The proceeds of extended PIE algorithm can be described by several steps summarized as follows:

- Step 1: Set the initial guess of the object $O_j(r)$ in real space
- Step 2: $\psi_j(\mathrm{r}) = O_j(\mathrm{r})P_j(\mathbf{r} - \boldsymbol{R_{s(j)}})$.
- Step 3: $\psi_j(\mathrm{u}) = \sqrt{I_{s(j)}(u)}\,\frac{\mathcal{F}[\Psi j(\boldsymbol{r})]}{|\mathcal{F}[\Psi j(\boldsymbol{r})]|}$
- Step 4: $\psi_j{}'(\mathrm{r}) = \mathcal{F}^{-1}[\Psi j(\boldsymbol{u})]$
- Step 5:

$$O_{j+1}(\boldsymbol{r}) = O_j(\boldsymbol{r}) + \alpha \frac{P_j^*\left(\mathbf{r} - \mathbf{R}_{\boldsymbol{s}(\boldsymbol{j})}\right)}{\left|P_j(\mathbf{r} - \mathbf{R}_{\boldsymbol{s}})\right|_{max}^2} \left(\psi_j{}'(\mathbf{r}) - \psi_j(r)\right),$$

$$P_{j+1}(\boldsymbol{r}) = P_j(\boldsymbol{r}) + \beta \frac{O_j^*\left(\mathbf{r} - \mathbf{R}_{\boldsymbol{s}(\boldsymbol{j})}\right)}{\left|O_j\left(\mathbf{r} - \mathbf{R}_{\boldsymbol{s}(\boldsymbol{j})}\right)\right|_{max}^2} \left(\psi_j{}'(\mathbf{r}) - \psi_j(r)\right).$$

The constant α can be adjusted to alter the step-size of the updating procedure, and the parameter β is similar to α in the update function.

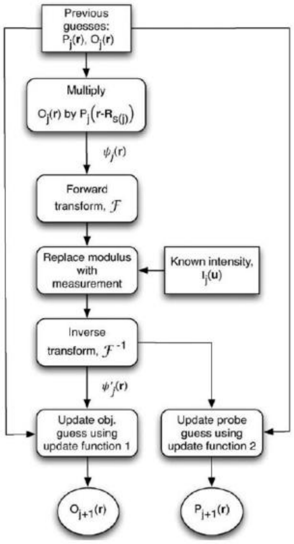


Figure 1: The flowchart of ePIE algorithm [4].

Experimental results

1. System Design

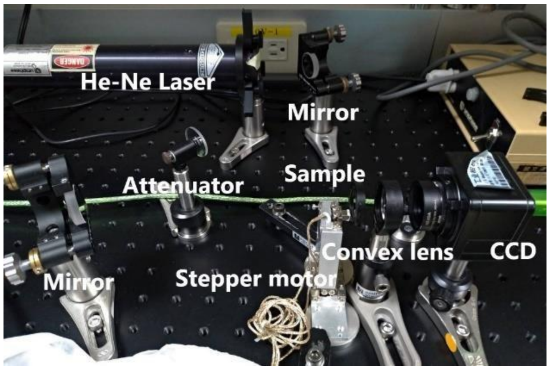


Figure 2: The structure of optical system

Figure 3: R1L1S1N (sample)

Fig 2 is the structure of optical system. We used He-Ne Laser as the light source, which wavelength is 632.8nm. With attenuator and polarizer, we can weaker the intensity of Laser, avoid the diffraction pattern being too saturate, which can result to collect diffraction pattern incompletely.

We used R1L1S1N as our sample, which is designed for calibration of imaging systems and microscope stages. The R1L1S1N negative pattern is ideal for collimators and other illuminated test equipment.

2. numerical simulations

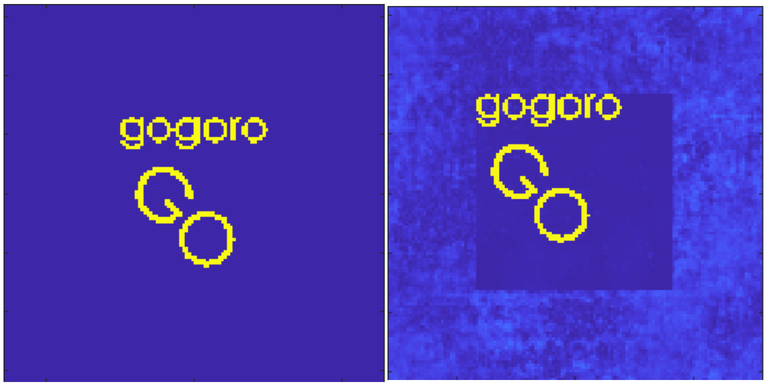


Figure 4: numerical simulation of HIO (a) Sample image (b) Retrieved image

For the simulation of HIO algorithm, the left image of Figure 4 is the sample image, and the right image is the retrieved image after 100 iterations of HIO algorithm. We can find that the density region is retrieved well.

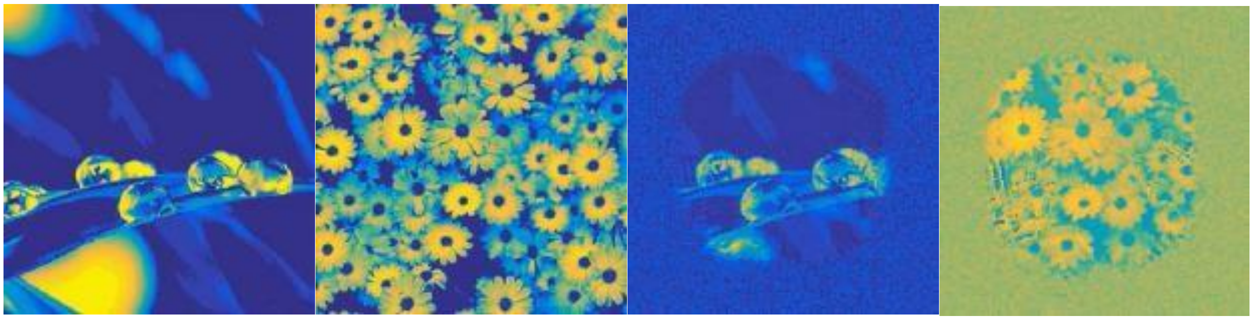


Figure 5: numerical simulation of ePIE

(a) Sample amplitude (b) Sample phase (c) retrieved image amplitude (d) retrieved image phase

For the simulation of ePIE algorithm, we obtain 25 diffraction patterns by moving the probes beams by the sequences. Then, using the ePIE algorithm and the 25 diffraction patterns of $|A_D|^2$ to retrieve both A_o, φ_o and A_p, φ_p. From the result of the ePIE simulation which shows above, we can find that the amplitude and phase which are close to the center of the image can be retrieved perfectly. The retrieved images are similar as the sample image. While the retrieved region of the image is only around the center, which is result from the probe positions s(j) were around the center. If we want to retrieved the complete image, we need to gain more diffraction patterns and the probe position s(j) can cover the hole image.

3. Sample testing of Optical System

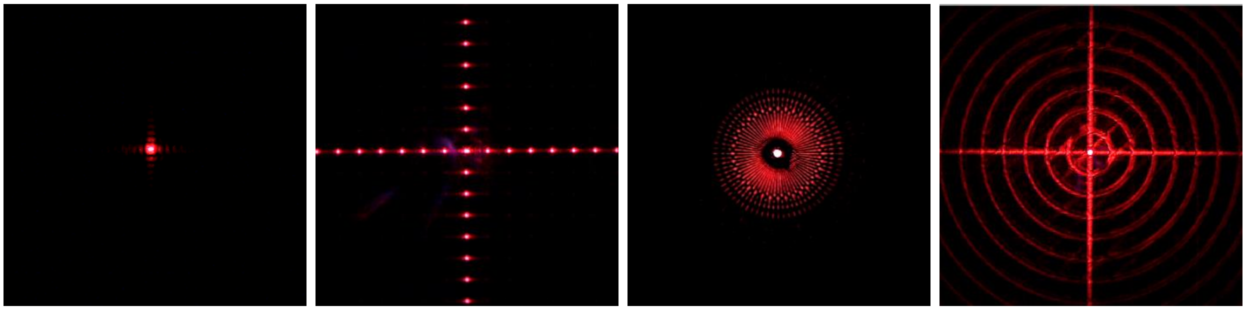
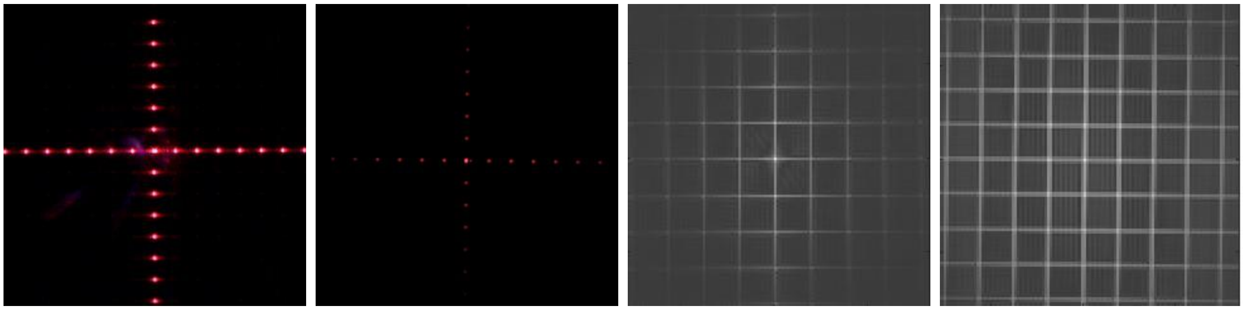


Figure 6: Diffraction patterns of different targets

(a) 10um Grid Pattern (b) 100um Grid Patterns (c) star sector (d) concentric circle



(a) (b) (c) (d)

Figure 7: (a)(b) different intensity of 100um Grid's diffraction patterns
(c)(d) retrieved image of (a)(b) (partial enlargement)

According to Figure 7, which shows the diffraction patterns and retrieved image of 100um Grid pattern, we can find that the original image can be retrieved perfectly, which resulted from the simple structure of grid pattern in our we opinion. Also, Figure 7 shows two different intensity of diffraction patterns, which retrieved image are slightly different, (c) seems to be not retrieved as completely as (d). Which is because of the saturate problem when CCD collects the intensity of light, as the intensity of laser being higher than the range of CCD can collect, the intensity will be defined as the maximum value, known as saturate condition. This condition will result to the diffraction pattern collects incompletely, making the phase retrieval be harder than the normal condition.

Conclusions

We have demonstrated the numerical simulation of the phase retrieval algorithm. By the simulation result, we can find that with intact diffraction patterns, CDI reconstruction technique is an effective to observe nanoscale structure. After that, by using the stepper motor, CCD camera, and other apparatus, we successfully built an optical system – a lensless microscope.

While in the practical experiment, we find that there are some limitation and deviation of CDI reconstruction technique. Such as spatial noise, which will affect the accuracy of diffraction patterns, making the final retrieved image be different from the sample. Also, the resolution of camera and the wavelength of Laser will change the size of pixels, which will affect the accuracy of retrieved image. The more pixels of the diffraction pattern, the more accuracy of the final retrieved image. In spite of some limitations of CDI, with complete and accurate diffraction pattern, CDI is still an effective and reliable method to recover original image.

For the further study, adding spatial filter to the optical system to eliminate the noise, using different wavelength of Laser and high resolution of detector are the ways for the further research. hoping to improve the accuracy and resolution of CDI reconstruction technique.

Reference

[1] 趙凱華、鍾錫華，《光學》第二章 p. 202

[2] Rodenburg, J. M., & Faulkner, H. M. L. (2004). A phase retrieval algorithm for shifting illumination. Applied Physics Letters, 85(20), 4795.

[3] J. M. Rodenburg and H. M. L. Faulkner. *Appl. Phys. Lett.*, **85**, 4795, (2004).

[4] Maiden, A. M., & Rodenburg, J. M. (2009). An improved ptychographical phase retrieval algorithm for diffractive imaging. Ultramicroscopy, 109(10), 1256–1262.

Thoughts

在修習這項專題的一開始，我對光學的知識只停留在最基礎的層面，對於專題內容的了解也算是片面而已，但藉由修習光學相關的課程、跟教授進行一次又一次的討論以及自己去閱讀 paper 跟網路上的資料，漸漸建構起專題所需要的相關知識，也更了解這項專題所要達到的目標。

在專題進行的過程中，學習到許多不同面向的知識，像是能進行數值運算的 Matlab，用來控制硬體的 Labview，以及跟本項專題最息息相關的光學知識。而與此同時，藉由這次的專題經驗，也對我自行查找資料以及閱讀文獻的能力有大大的提升，相信對未來進行研究能有所幫助，也感謝教授的指導。