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Global optimized reconstruction of off-axis electron hologram using genetic algorithms

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Abstract

The Genetic Algorithms (GAs), a novel numerical reconstruction method of off-axis electron hologram is presented. As an example, an off-axis electron hologram of electric microfields induced by charged latex particles has been reconstructed successfully by using GAs method, and then a reconstructed image with high quality was obtained in this paper. Compared with other methods (filtering process and neural net) shows that applying GAs to numerical reconstruction, global optimum result can be obtained.

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Keywords: Electron hologram; Numerical reconstruction; Super-pixel; Genetic Algorithms

1. Introduction

Holography was first proposed by Gabor in 1948 as a way to correct aberration and improve resolution of electron microscopes [1]. Since the microstructure of materials can be provided by means of electron holography, the electron holography has been received more attention. In electron holography, the reconstruction method is a key technique. Generally, the numerical reconstruction methods, such as the filtering process method in Fourier space and neural network method in real space, were often used for reconstructing electron holograms [2,3]. However, there are some shortcomings in these methods, for instance, the information contained in the autocorrelation is not used in filtering process, and the complex training procedure of a neural network is necessary to anti noise in neural net method. Alternative method to overcoming these shortcomings, the Genetic Algorithms(GAs), a new numerical reconstruction method of electron holograms in real space, is presented and described in this paper.

The Genetic Algorithms (GAs) developed by Holland [4] is a novel direct search optimization method based on principles of "natural selection" and "survival of the fittest" from natural evolution. By simulating natural evolution, GAs can effectively search and easily solve complex problems in the given problem domain. Furthermore, by emulating biological selection and through the "reproduction", "crossover" and "mutation" iterative process, GAs

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can search the global optimum result, which is frustrated in other search methods [5]. On the other hand, the entire information was used and the training procedure of neural net was not needed in the GAs reconstruction process of off-axis electron hologram, so it is a more effective method comparing with filtering process and neural net method.

As an example, an off-axis electron hologram of electric microfields induced by charged latex particles has been reconstructed successfully by using GAs method, and then a reconstructed image with high quality was obtained in this paper.

2. Recording an off-axis electron hologram

The research of electron holography includes two main parts: the recording and reconstruction of the electron hologram.

The schematic diagram of the set up for recording an off-axis electron hologram is shown in Fig. 1. In off-axis electron holography, only a part of electron beam emitted from field-emission gun transmits the object (specimen) and is modulated by the object specimen with the complex transmittance, while the other part of the incident electron beam (wave) is not influenced by the object specimen and can be used as a reference wave; the wave exiting the specimen is called the object wave $O(\vec{r}) = a(\vec{r})\exp\{i\varphi(\vec{r})\}$, where $\vec{r}$ denotes a two-dimensional vector in the object plane. The object lens conveys a magnified image of the object wave into the image plane. The image wave is expressed as $b(\vec{r}) = A(\vec{r})\exp\{i\phi(\vec{r})\}$; correspondingly, reference wave $R(\vec{r}) = 1\times\exp(-2\pi i\vec{q}\cdot\vec{r})$, here the amplitude of the reference wave is assumed to have an amplitude of unity. $\vec{q}$ is the fringe space frequency.

In order to record an electron hologram, an electron biprism is mounted between the back focal plane and the image plane of the objective lens, as sketched in Fig. 1. This biprism deflects both the object wave and reference wave towards the image plane and leads to a superposition of both waves in the image plane, which yields an interference pattern, i.e. an electron hologram in the image plane. The intensity of electron hologram can be recorded as

$$I(\vec{r}) = 1 + A^2(\vec{r}) + 2A(\vec{r})\cos(2\pi\,\vec{q}\cdot\vec{r} + \phi(\vec{r})) \quad (1)$$

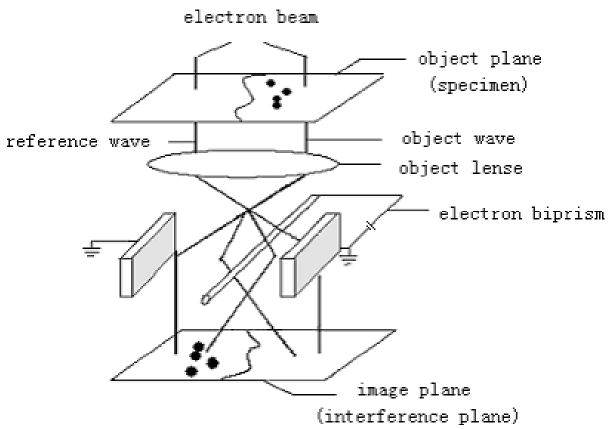


Fig.1. Schematic diagram of the set up for recording an off-axis electron hologram.

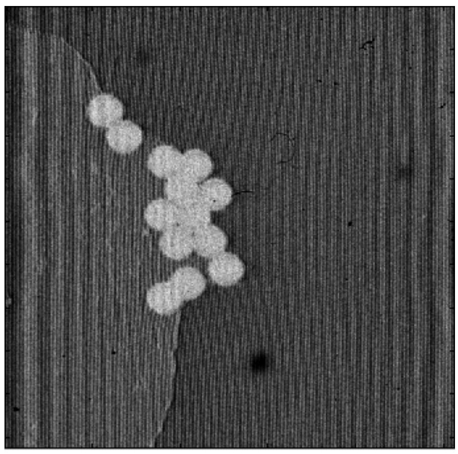


Fig 2. Hologram of electrostatic microfields of charged latex particles.

Fig. 2 shows the electron hologram of electrostatic microfields induced by charged latex particles, which was recorded by the electron microscopy Philips EM 400 T equipped with a field-emission electron gun worked at 100 KV [6], and the electron hologram is stored by 512×512 matrix.

From wave electron optics, the phase variety of the object wave can be described by formula (2) when it passes electric field.

$$\Delta \phi(x, y, z) = \frac{\pi}{\lambda U} \int_l V(x, y, z) dz \tag{2}$$

where V is the static electric potential; U is the accelerating potential of electron wave, and λ is the wavelength of the electron wave. Consequently, the equiphase line in reconstruction plane is the equipotential line in electric field.

3. Numerical reconstruction of an off-axis electron hologram, using a Genetic Algorithm

Based on holography's physical principle, numerical reconstruction of off-axis electron hologram is that: two basic parameters, amplitude and phase, of object wave should be retrieved by using various numerical calculating methods (such as filtering process, Neural Net method, general optimization method and Genetic Algorithms etc.)

Genetic Algorithms is an optimization search method that can obtain global optimum result. As the general constrained optimization problem, its mathematic programming form is:

$$\begin{cases} \min f(\vec{x}) \\ a_i \le x_i \le b, \quad i = 1,2,3...,n. \quad \text{explicit constraint} \\ g_j(\vec{x}) \le 0, \quad j = 1,2,3,...m. \quad \text{implicit constraint} \end{cases} \tag{3}$$

where $\vec{x} = (x_1, x_2, \cdots, x_n)^T$ is search arguments vector, $f(\vec{x})$ is objective function. From formula (1), we can see that the optimization problem is an extreme value problem of the objective function $f(\vec{x})$ defined in the n-dimensional space R^n of search arguments vector.

In the GAs, each gene, which can be expressed as a string of bits codes, is corresponding to a component of search arguments vector $\boldsymbol{x}$ in the general optimization method. A chromosome of an individual is corresponding to a search arguments vector $\boldsymbol{x}$, i.e. a coordinate point in the n-dimensional search space, so one chromosome is combined by n genes. The fitness is defined to evaluate the quality of a chromosome in GAs. Thus, the fitness is corresponding to an objective function in the optimization method. The chromosome with higher fitness (i.e. smaller objective function value) can be reproduced into next generation.

The computation of optimization search using GAs starts with a population of individuals generated by randomness in a given range, and performs a selection of individuals based on their fitness. Specifically, a number of coordinate points (K points) are selected as a set of individuals in the n-dimensional search space, i.e. there are K=*PopSize* individuals in the population. It means that there are K candidate solutions. In our computation, K=*PopSize* =80.

In the reconstruction procedure by GAs, the electron hologram is needed to divided into some square areas with same size[3], and then is used as a basic calculating unit for optimization search to reconstruct the image wave $b(\vec{r})$ at a particular pixel position $\vec{r}$ .This square area is called a Super-pixel. In this paper, each super-pixel is composed of 7×7 pixels of electron hologram shown in Fig. 3. Since the object wave function and then the image wave function are continuum function, the variation of intensity of wave distribution is provided with continuity. So the intensity at the position of a particular pixel in the image wave distribution is related to the neighbouring pixel surrounding area.

In the present case, the amplitude $A(\vec{r})$. And phase $\phi(\vec{r})$ of the image wave at the centre of the super-pixel are taken as search parameters, and the square difference between the image wave intensity calculated formula (1) at position $\vec{r}$**,** named the calculated value, and that of measured hologram pattern, named the experimental value, is taken as an objective function.

In the calculation, the numerical hologram matrix can be represented as I_H (512×512), and super-pixel is composed of 7×7 pixels, so the whole hologram is composed of 506×506 super-pixels, and represented by super-pixel compound matrix I_S (506×506); where $I_S(1,1) = I_H(1{:}7, 1{:}7)$, $I_S(1,2) = I_H(1{:}7, 2{:}8)$. That is

$$I_S(i, j) = I_H(i : i+6, j : j+6) \tag{4}$$

where $i=1,2,\ldots 506$; $j=1,2,\ldots,506$ are the row and column of super-pixel matrix I_S respectively.

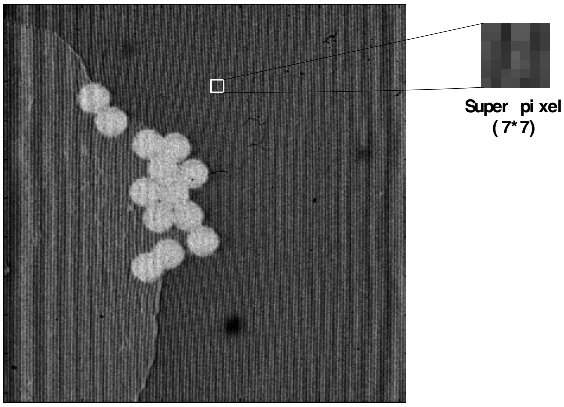


Fig 3. Sketch map of super pixel.

So, the objective function is:

$$f_{i,j} = \sum_{m=-3}^{3}\sum_{n=-3}^{3} W\,[1 + A_{i,j}{}^2 + 2A_{i,j}\cos(2\pi\vec{q}\cdot\vec{r} + \phi_{i,j}) - I_H(i+3+m, j+3+n)]^2 \tag{5}$$

and the corresponding fitness function is:

$$F_{i,j} = \frac{1}{\sum_{m=-3}^{3}\sum_{n=-3}^{3} W[1 + A_{i,j}{}^2 + 2A_{i,j}\cos(2\pi\vec{q}\cdot\vec{r} + \phi_{i,j}) - I_H(i+3+m, j+3+n)]^2 + \varepsilon} \tag{6}$$

where W is Hanning function, given by formula (7), used as weight factor to highlight centre pixel in a super-pixel, and ε is a small positive number in order to avoid the denominator of the fitness function being zero. The fitness function is written as the formation of reciprocal of the objective function, which accords with the target that the higher the fitness function, the lower the value of the objective function.

$$W = \frac{1}{18}[1 + \cos(\frac{x^2 + y^2}{18}\pi)] \tag{7}$$

where x, y are the coordinates relative to centre pixel of the super-pixel.

The task is now to find the optimum estimate for the complex value of the image wave $b(\vec{r})$ in the centre of super-pixel, i.e. to find the optimum estimate for the search parameters of the complex image wave $b(\vec{r})$. It should be carried out to fit a simulated hologram pattern calculated from formula (1) to the measured experiment intensities for each pixel.

In our case, the search parameters $A(\bar{r})$ and $\phi(\bar{r})$ correspond to 2 genes composing a chromosome in the GAs optimization search. That is one chromosome of each individual includes 2 genes. One population is composed of a set of individuals.

In general, the GAs that yields good results in many practical problems are composed of these operations: reproduction, crossover and mutation [4]. The practical operation steps of GAs are summarized as follows:

(1) Initialization and calculation of fitness

First, we code the chromosome (individual) by a string of bits codes (binary character string) and then create *K=PopSize* individuals randomly in the search space and divide the chromosome of each individual into 2 gene strings, then each pair of genes are transformed into a set of corresponding $A(\bar{r})$ and $\phi(\bar{r})$ by decoding.

For this paper, every individual is represented by the size of 19 bits' random binary character string, where the front 9 bits denote $A(\bar{r})$, and the rest of 10 bits are $\phi(\bar{r})$. In the meanwhile, the binary character string must be decoded to its corresponding value. On the consideration of relative intensity and normalization, $A(\bar{r})$ and $\phi(\bar{r})$ can be confined in: $0 \le A \le 1$, $-\pi \le \phi \le \pi$.

After that, calculating the value of fitness for every individual according to equation (6). Search for optimized $A(\bar{r})$ and $\phi(\bar{r})$ of super-pixel's centre pixel with entire population in certain generation. That is to get best individual as population's evolution before ending point. Executing the same procedure to every super-pixel of super pixel compound matrix, the global optimized results can be obtained.

(2) Selection and Reproduction

Some individuals are selected according to a given method. In our work, the roulette wheel selection method is chosen. It is based on the fitness of each individual: the higher the fitness of individual, the greater probability of being selected, and then they are copied and placed into the new generation.

Reproduction is a basic operation in GAs, making the superior individuals able to reproduce to the next generation.

(a) Crossover

"Crossover" is a main method to produce new individuals in GAs. Select two individuals within the generation in the probability of $Pc = 0.55$ and determine a crossover site, and then carry out a swapping operation of the string bits to the right hand side of the crossover site of both individuals. There are many ways of implementing this crossover, for example having a single crossover point or many crossover points. These crossover points are selected randomly.

(b) Mutation

"Mutation" is another way to produce new individuals in GAs. After crossover has occurred, each child produced by the crossover undergoes mutation with a probability $Pm = 0.15$. The mutation operator will guarantee diversity within the population, while avoiding finding a local optimal result.

(3) Replacing and inserting process

Take new individuals with higher fitness to replace the individuals with lower fitness in the original population to form a new generation population.

The flowchart of the GAs search process for the optimization is shown in Fig. 4.

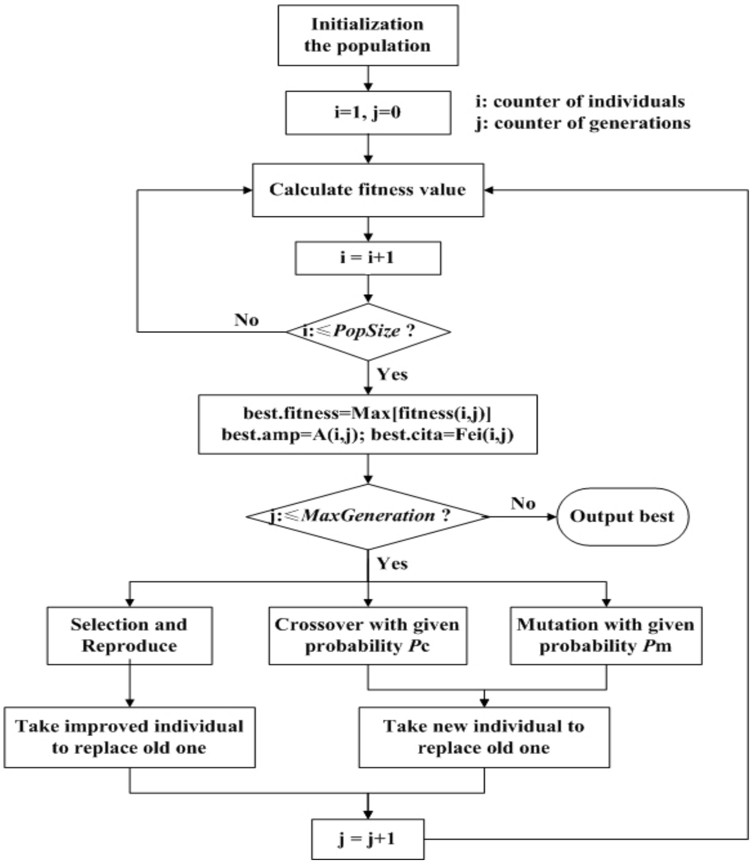


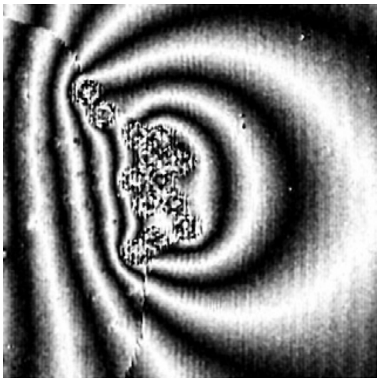
Fig. 4. Flowchart of GAs search process for the optimization.

4. Reconstruction results

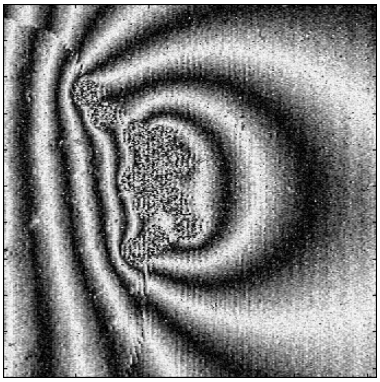
In our GAs reconstruction, the maximum number of iterations is *Max_Generation=50*. The reconstruction result by GAs is shown in Fig. 5 (a).

For comparing the quality of the reconstructed image, we also performed the reconstruction of example hologram using Filtering and Neural Net method. The reconstruction results by using Filtering and Neural Net method without anti-noise training and with anti-noise training are also shown in Fig. 5(b) and 5 (c,d), respectively. From Fig. 5, it can see that the GAs reconstructed image is much clear and better than the others.

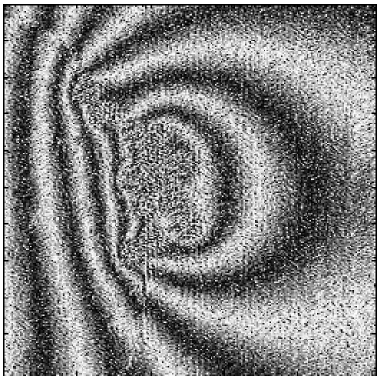
In the Filtering process, a numerical Fourier transform is performed. The Fourier spectrum is composed of three parts: one center band and two sidebands. After selecting one of the sidebands and moving it to the origin of Fourier space and then the reverse Fourier transform of the isolated sideband directly yields the image wave. Obviously, the amplitude information contained in the autocorrelation is not used by this procedure. However, the entire information (both centre and sideband information are used for amplitude in GAs. So the reconstruction image with high quality is obtained by using GAs method.



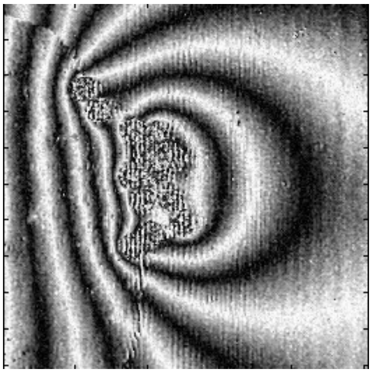
(a)Genetic Algorithms



(b) Filtering process



(c) Neural Net without anti-noise training



(d) Neural Net with anti-noise training

Fig. 5. Results of numerical reconstruction.

5. Discussion and conclusions

Compared with other numerical reconstruction method, GA has several advantages:

A. By making full use of the whole hologram, and avoiding loss of information in filtering process, one can get a more accurate reconstruction pattern.

B. Consequently, GAs search for the global optimum solution result.

C. GAs have good flexibility. If a neural net is equipped with the ability of anti-noise, the net should be trained with several grades of noise. When the reference wave changes, the net must be retrained. But, GAs just need to change the corresponding parameters.

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