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Subset geometric phase analysis method for deformation evaluation of HRTEM images

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ABSTRACT

Geometrical phase analysis (GPA) is typically a powerful tool to investigate the deformation in high resolution transmission electron microscopy images and has been used in various fields. The traditional GPA method using the fast Fourier transform, referred to as global-GPA (G-GPA) here, is based on the relationship between the displacement and the phase difference. In this paper, a subset-GPA (S-GPA) is introduced for further improvement. The S-GPA performs the windowed Fourier transform block by block in the image. The maximum strain measurement scale of the GPA method is theoretically analyzed on the basic of the phase spectrum extraction process. The upper limit is one third of the atomic spacing. The results of various numerical simulations verified that the S-GPA method performs better than the traditional G-GPA method in both the homogeneous and inhomogeneous deformation conditions, with the evaluation parameter of calculation reliability of S-GPA 10% higher than G-GPA. Specifically, the measurement accuracy of S-GPA is about three times higher than the G-GPA when calculating small strain (less than 2000με). For the large strain (greater than 150000με), the measurement accuracy of S-GPA is about 50% higher than that of the G-GPA. Besides, the S-GPA method can significantly eliminate the phase filling effect, while the G-GPA cannot. The S-GPA method has been successfully applied to analyze the strain field distribution in an lnGaAs/InAlAs supperlattice heterostructure.

1. Introduction

High resolution transmission electron microscopy (HRTEM) enables to image crystal structures at an atomic resolution. During the last decades, many efforts have been paid in order to obtain quantitative information from HRTEM images [1]. In principal, the interpretation of HRTEM images is rather difficult since the image contrast depends on several parameters (such as specimen thickness, composition, surface contamination, specimen damage due to ion milling and the imaging conditions, like defocus and other microscope parameters) and since the lattice fringes do not necessarily correspond to the atomic configuration [1,2]. A lot of efforts have been focused on these parameters by many researchers all over the world [3–6].

Actually and fortunately, an effective method was put forward and has been successfully and widely used in the high resolution electron microscopy (HREM) image analysis. The aim of this paper is to ulteriorly study the geometrical phase analysis (GPA), which has become a powerful and indispensible tool in studying the deformations in HRTEM images. The traditional GPA method, referred to as global-GPA (G-GPA) here, is based on the relationship between the displacement and the phase difference. In the G-GPA method, regular atoms are used as deformation carriers. Hence, the G-GPA method can be divided into two branches owing the difference of the approach obtaining reference phase. One is self-reference, usually used in the HRTEM field and the reference phase is reconstructed from a uniform area in the original HRTEM image and the other is pre-reference, where an undeformed image can be obtained before the analyte deformed. In this case, the displacement can be measured by analyzing the lattices before and after deformation, and this technique has been utilized to measure the deformation at macro and microscales [7–14].

In the traditional G-GPA method, the fast Fourier transform (FFT) algorithm, employed for saving computational time [8,15], plays a crucial role as the phase information is extracted by it. However, when the deformation is non-uniform, particularly with strong distortion, the G-GPA method would fail to extract the deformation accurately as the FFT cannot extract the fundamental

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component with a wide frequency band [16], which could lead to a non-ignorable error in the obtained deformation field. In this paper, the windowed Fourier transform (WFT) algorithm [17,18], which is a local Fourier transform algorithm, has been employed and it is defined as subset-GPA (S-GPA) method. Different from the traditional G-GPA method, WFT element has a limited spatial extension due to the window function, and performs the transform in a small area of the image, where can be regarded as a region with uniform deformation. So the local frequency can be extracted more accurately and the inhomogeneous deformation field can be measured with high accuracy. Coincidentally, the name of the two methods defined in this paper are similar to the method of global digital image correlation (global-DIC) and subset digital image correlation (subset-DIC) method in the field of experimental solid mechanics [19,20]. Note that the measurement method, both G-GPA and S-GPA used in this paper are all the first case, self-reference, where the reference phase is directly extracted from the HRTEM images.

The maximum strain measurement range of GPA method is analyzed on the basic of the phase spectrum extraction process, with the upper limit 1/3. The simulation results shows that, compared with G-GPA, the S-GPA method can extract the strain field accurately in both homogeneous and inhomogeneous strain field. The measurement accuracy of S-GPA is about three times greater than that of G-GPA for the inhomogeneous small strain (less than 2000με) measurement whether the small strain is contained in a large non-uniform strain field or in a pure small inhomogeneous strain field. Furthermore, experiment result shows that the S-GPA can make the calculation without any phase filling effect. It is important to study the strain distribution of a strain-compensated lnGaAs/InAlAs multiple quantum well structures or other superlattice, because the compensated strain and non-mismatch in the interface is of great importance in semiconductor application. An application experiment was successfully conducted in studying the strain distribution of a strain-compensated lnGaAs/InAlAs using the S-GPA method.

2. Subset geometric phase analysis

2.1. Principles of geometric phase analysis

The G-GPA method was independently introduced by Takeda [21] and Hÿtch [22,23], and has already been successfully applied in the displacement/strain field analysis of crystal structures with high resolution electron microscopy. The processes of GPA are introduced briefly here and the detail can also be found in [22]. The technique is based upon centering a small aperture around a strong reflection in the Fourier transform of a crystal lattice image and performing an inverse Fourier transform. In the formulation, the relationship between the phase component P_g in the complex image and the local displacement of atomic planes $u(\vec{r})$ is written as [22]

$$\hat{P}_g(\vec{r}) = -2\pi\vec{g}\cdot u(\vec{r}) \tag{1}$$

where P_g is the phase in the image at position $\vec{r}=(x, y)$ and g is the reciprocal lattice vector of the lattice.

Considering the conventional type of images analyzed in the field of electron microscopy that the lattice always contains more than two crossed spatial frequencies, the displacement field can be derived as the matrix form (an orthogonal lattice formation is used here for derivation):

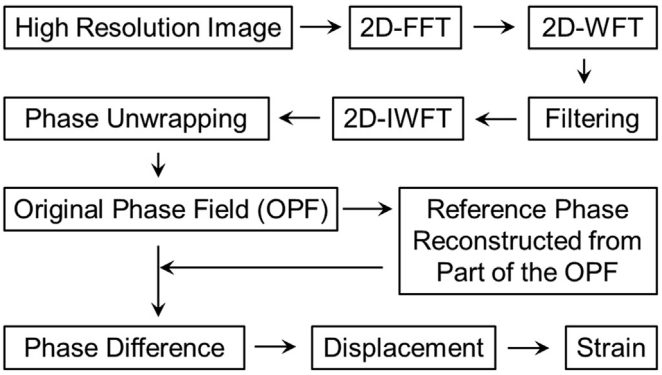

Fig. 1. The flow chart of the S-GPA method.

$$\begin{pmatrix} u(x) \\ u(y) \end{pmatrix} = -\frac{1}{2\pi}\begin{pmatrix} g_{1x} & g_{1y} \\ g_{2x} & g_{2y} \end{pmatrix}^{-1}\begin{pmatrix} \hat{P}_g(x) \\ \hat{P}_g(y) \end{pmatrix} \tag{2}$$

where the subscripts x and y represents the x and y directions respectively.

Then the strain components can be obtained from the displacement gradients as the matrix form:

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} \\ \varepsilon_{yx} & \varepsilon_{yy} \end{pmatrix} = \begin{pmatrix} \frac{\partial u(x)}{\partial x} & \frac{\partial u(x)}{\partial y} \\ \frac{\partial u(y)}{\partial x} & \frac{\partial u(y)}{\partial y} \end{pmatrix} = -\frac{1}{2\pi}\begin{pmatrix} g_{1x} & g_{1y} \\ g_{2x} & g_{2y} \end{pmatrix}^{-1}\begin{pmatrix} \frac{\partial P_{g_1}}{\partial x} & \frac{\partial P_{g_1}}{\partial y} \\ \frac{\partial P_{g_2}}{\partial x} & \frac{\partial P_{g_2}}{\partial y} \end{pmatrix} \tag{3}$$

where ε_{xx} and ε_{yy} are the direct strains in the x and y directions, ε_{xy} and ε_{yx} are the shear strains, respectively.

2.2. The theory of subset geometric phase analysis

Actually, according to the traditional Fourier theory, the 2-dimensional Fourier transform of a function $q(x, y)$ can be expressed as [24]

$$Q(\xi, \eta) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} q(x, y)e\{-i\xi x - i\eta y\}dxdy \tag{4}$$

where $Q(\xi, \eta)$ is the frequency spectrum, ξ and η represent the frequency components in the x and y directions, respectively.

As for the 2-dimensional windowed Fourier transform (2D-WFT), it can be expressed as [14,17]

$$Q(\mu, \upsilon, \xi, \eta) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} q(x, y)g(x-\mu, y-\upsilon)e\{-i\xi x - i\eta y\}dxdy \tag{5}$$

where $Q(\mu, \upsilon, \xi, \eta)$ represents the windowed Fourier spectrum of a small block; $g(x-\mu, y-\upsilon)$ is a window function (like Lorentzian, Gaussian, Cosine, Hanning, Hamming, or …) and Gaussian window is used in this paper; (μ, υ) is the coordinate of the center of the window. The target window changes with different pairs of μ and υ, therefore the WFT can be realized pixel by pixel. Also, it can be found that Eq. (5) is a local transform of Eq. (4).

Fig. 1 illustrates the process of the proposed S-GPA method. The 2-dimensional FFT (2D-FFT) is first employed to get the frequency spectrum of the captured high resolution image, followed by the 2D-WFT process. Actually, before the 2D-FFT procedure, it's reasonable to do appropriate spatial filter on the original high resolution image (such as median filter, winner filter, etc.). In this paper, only the simple median filter is used to filter the original image, which will not affect the subsequent computations. The 2D-WFT is performed in the region around the chosen diffraction point and then each frequency spectrum is filtered by a Gaussian window function. Afterwards, the 2-dimensional inverse