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An improved iterative wave function reconstruction algorithm in high-resolution transmission electron microscopy

W.Q. Ming, J.H. Chen*, Y.T. He, R.H. Shen, Z.K. Chen

College of Materials Science and Engineering, Centre for High Resolution Electron Microscopy, Hunan University, Changsha 410082, China

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ABSTRACT

Exit wavefunction reconstruction is a powerful image processing technique to enhance the resolution and the signal-to-noise ratio for atomic-resolution imaging in both aberration uncorrected and corrected transmission electron microscopes. The present study aims to improve the performance of the iterative wavefunction reconstruction algorithm in comparison not only with its conventional form but also with the popular commercial Trueimage software for exit wavefunction reconstruction. It is shown that by implementing a wave propagation procedure for refining its image alignment, the iterative wavefunction reconstruction algorithm can be greatly improved in accurately retrieving the wavefunctions while keeping its original advantages, which allow the reconstruction be performed with less images and a larger defocus step in the data set of through-focus image series. In addition, calculations of this algorithm can be accelerated drastically by the graphic processing unit (GPU) hardware programming using the popular computer unified device architecture language, whose computing speed can be 25–38 times as fast as a central processing unit (CPU) program.

1. Introduction

It is well-known that coherent aberrations of object lens are main factors limiting the point resolution of a modern high-resolution transmission electron microscope (HRTEM) [1–3]. Two fundamental methods have been proposed to remove or diminish these factors. The first way is to use aberration corrector devices directly and thus far many great achievements have been made in this approach [3–14]. For a HRTEM instrument at 200 kV, employing an aberration corrector only, the point resolution can be improved from 2.4 Å to 1.4 Å [9,10], whereas with the aid of chromatic aberration corrector and monochromator, the information limit can further be improved drastically down to 0.64 Å [7,11,12]. However, as an important issue, the expenses of this hardware approach is still very high, especially for low-energy HRTEM [13,14]. In addition, the image contrast can sometimes be difficult to interpret even for images acquired at the traditional Scherzer imaging and the negative spherical aberration (Cs) imaging, as well as at the channeling contrast imaging conditions, since for some material's structures misleading-contrast spots may still appear in these atomic resolution images due to the non-linear interference [10,15].

Another way to remove the effect of lens aberrations for achieving atomic-resolution images is to deal with the electron waves retrieved by posterior image processing algorithms, such as through-focus exit wave reconstruction (TF-EWR) technique [16–22] and beam tilt series exit wave reconstruction technique (BT-EWR) [23–25]. In this method, once the wavefunction in the image plane is retrieved and the lens aberrations are measured, one may then correct the aberrations in the wavefunction at the image plane, so as to restore the exit wavefunction at the bottom surface of the specimen with the resolution limit of the microscope. The advantages of obtaining the exit-wavefunction are two folds: (1) The phase-image of the aberration-corrected complex wavefunction can be interpreted as the projected potential of the specimen, so long as the specimen is thin (a quasi weak-phase object) and the aberrations are removed in the reconstructed wave. In other words, the phase-image is more a linear image effect, whereas the direct imaging intensity even under an optimum defocus is always sum of the linear image effect and the non-linear image effect, the later can be obviously seen even for thin specimens in an aberration-corrected HRTEM [10,15]. (2) The signal-to-noise ratio in the obtained complex wavefunction is high and therefore it is a good dataset for further quantitative image analysis. In addition, these posterior image processing techniques work well for both the aberration corrected and the uncorrected HRTEM. In an aberration corrected TEM, performing TF-EWR is much simpler, since much less aberrations will exist in the recorded images [10].

Among the existing algorithms for EWR, some of them are more widely used than the others due to their limitations in practice. For

* Corresponding author.
E-mail address: jhchen123@hnu.edu.cn (J.H. Chen).

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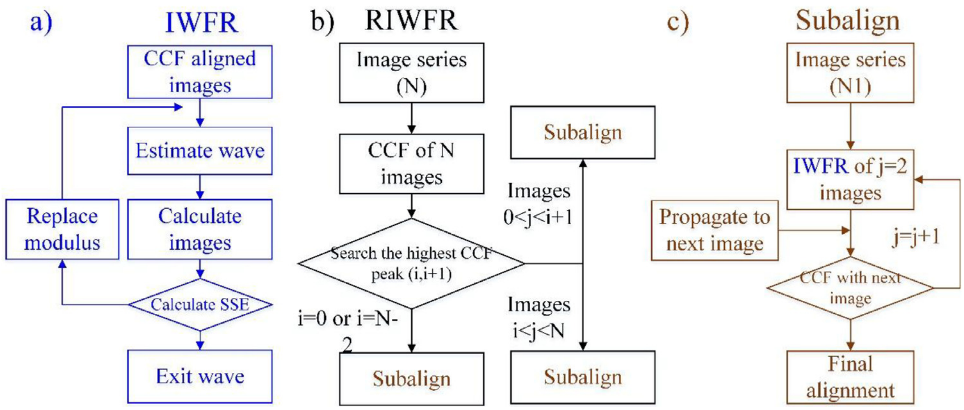

Fig. 1. (a) The data flow in the standard IWFR algorithm. (b,c) The flow chart of the alignment procedure in RIWFR algorithm. SSE in (a) is the short for the sum squared error calculated to indicate the convergence of the IWFR procedure.

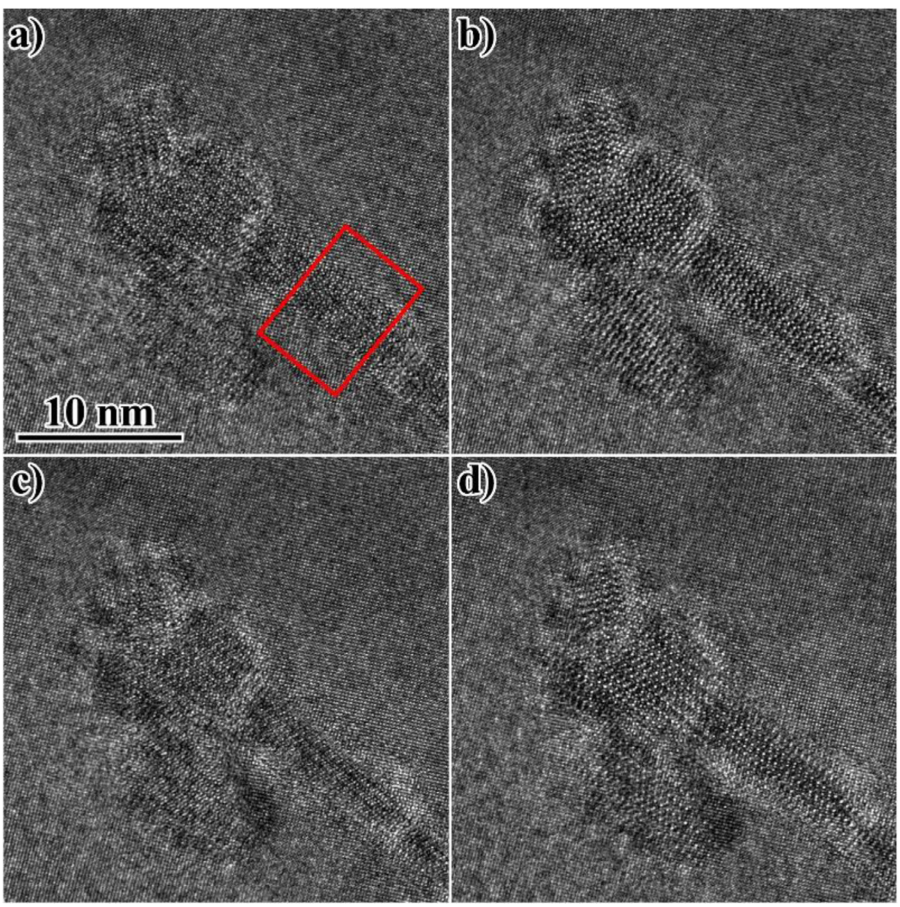

Fig. 2. The 1st, 7th, 13th, 19th images of the first focal series of typical S-precipitates formed in a 2000 series Al alloy, which is referred as Series 1 in Table 1. These images are taken along the $[001]_{Al}$ direction.The voltage is 200 kV, and the defocus step is set −4.77 nm (verified value). Only the area selected by the red rectangle will be displayed with high magnification for demonstrating the reconstruction results in the coming figures.

performing the BT-EWR, it is often difficult to precisely distinguish the specimen drift and the beam tilt induced image displacement [26,27], which limits its extensive application in practice. On the contrary, TF-EWR technique has been widely investigated [17–21] and successfully applied to determining unknown structures in materials science [28–38]. Thus far the most widely applied program for TF-EWR is the Thermal Fisher (FEI) Trueimage software based on the parabola method (PAM) [18] and maximum likelihood method (MAL) [17]. Other algorithms have also been proposed and studied, such as the wiener filter method [22] and iterative wave function reconstruction method (IWFR) [19,20]. The PAM and wiener filter methods filter the non-linear imaging information that are much weaker than the linear imaging information and serve as the initial wavefunction for further iterative refinement using algorithms such as the MAL algorithm, which is an effective method to search for the global minimum of error in the reconstructed wavefunctions at the image plane, but normally consumes much longer time than other algorithms.

The iterative wave function reconstruction (IWFR) algorithm was firstly proposed by Allen in 2004, based on the wave propagation in free space [19]. Although its calculation complexity is much lower, the IWFR algorithm has been demonstrated to have similar performance with the MAL algorithm, even when less images (e.g., 5 images) are used for reconstruction [29,30]. In addition, this algorithm only iterates very few times before reaching convergence. Hence, it sounds theoretically and should be very promising for practical application, provided that accurate image alignment of the TF-series of images can be