

A Practical Solution for Elimination of Artificial Image Contrast in Cs-corrected TEM

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The recent development in spherical aberration (Cs) correction of magnetic lenses has caused a great improvement in point-to-point resolution of high-resolution transmission electron microscopy (HRTEM) up to the information limit, and various applications have enabled progress of structure analysis at an atomic level [1,2]. The objective of ultimate high resolution in TEM is to reproduce potential distribution as a continuous function that have maxima corresponding to atom positions in materials. Unfortunately, artificial contrast maxima always appear at positions where no atom exists in current HRTEM images. The artificial contrast is coming from the following two problems based on imaging theory of phase contrast, and cannot be solved even by Cs correction established presently. It is considered that improvement of resolution without solving the problems is somehow difficult and may cause misleading results in atomic-level analyses of unknown structures.

The first one of the two problems is existence of non-linear image components in HRTEM images. They are formed by interference between diffracted beams and do not correspond to actual atomic arrangements, as well known as half-spacing lattice fringes of gold [3]. We proposed recently a simple and practical method to eliminate the non-linear components by using Cs-corrected TEM [4]. In two Cs-corrected TEM images taken at defoci of the same magnitude and opposite signs, image contrasts of linear components are inverted exactly due to perfect inversion of the phase contrast transfer function (PCTF). On the other hand, it is proved that non-linear components are influenced by absolute values of the defoci, that is, exactly the same non-linear components are formed in the two images. Therefore, a subtractive operation of the two Cs-corrected images makes elimination of the non-linear components. This idea is illustrated schematically in Fig. 1. It has been proved that this method is applicable to also 2-dimensional lattice images [4].

The second problem is the imperfectness of a kind of phase plate formed by the defocused objective lens (Scherzer method). The actual PCTF is partly flat only in limited frequency regions, and resultant images are composed of improper Fourier coefficients. To solve the problem, a compensation technique by image processing called "image deconvolution" has been tried since 1980s [5]. The method is based on an idea that a flat PCTF can be recovered by a deconvolution operation of a HRTEM image by inverse Fourier transform of the actual PCTF. Analyses of unknown structures by this method, however, have been rather difficult owing to the next two points: 1) A PCTF in a conventional TEM has some zero-crossings, which induce divergence in the deconvolution process; and 2) A deconvolution process without elimination of nonlinear components induces an improper increase of the nonlinear components and the resultant artificial images [6]. Here, it should be noted that these two difficulties can be proved by using a Cs-corrected PCTF without zero-crossings and the above subtractive method.

In this study we propose and demonstrate a simple and elegant method to solve the problem of the artificial image contrast by a combination of "image subtraction" for elimination of non-linear components and improved "image deconvolution" for proper compensation of non-flat PCTFs [7]. Figs. 2(a) and (b) are experimental Cs-corrected images of silicon along a $\langle 110 \rangle$ direction at 4 nm over- and underfocus. In the overfocus image, atomic columns appear as bright spots and hexagons as shown by white lines are formed by adjacent six atomic columns alike in the schematic diagram (Fig. 2(d)). Bright spots, however, appear also at the center of the hexagons where no atomic column exists (white arrow). In the underfocus image, atom columns appear as dark spots. Their positions, however, shift slightly from the actual positions and the hexagons have been deformed. In the image processed by a combination of image subtraction and deconvolution (Fig. 2(c)), atomic columns appear only at the actual positions.

It can be concluded that the present image subtraction & deconvolution (ISD) method is extremely useful for imaging real positions of atomic columns so far as kinematical approximation in electron diffraction does almost hold.

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References

- [1] N. Tanaka, et al., J. Electron Microsc. 52 (2003) 69-73.
- [2] J. Yamasaki, et al., J. Electron Microsc. 53(2) (2004) 129-135.
- [3] J.C.H. Spence, Experimental HREM, Clarendon Press, Oxford, 1981, p.126.
- [4] J. Yamasaki, et al., J Electron Microsc. 54(3) (2005) 209-214.
- [5] F.S. Han, et al., Acta Cryst. A42 (1986) 353-356.
- [6] C.Y. Tang, et al., Ultramicroscopy 106 (2006) 539-546.
- [7] J. Yamasaki, et al., Microsc. Microanal. 14 (2008) 27-35.

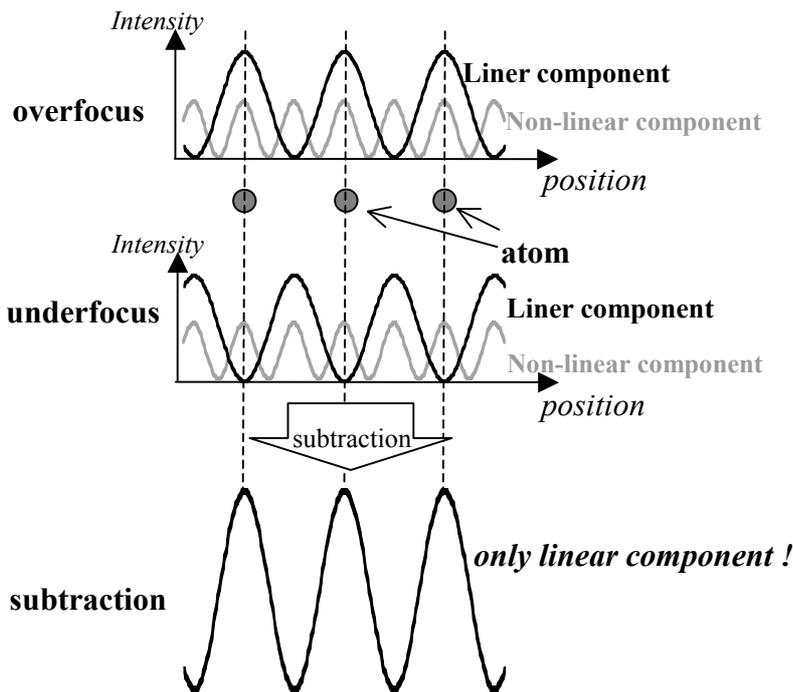


Fig. 1. Schematic illustration for elimination of non-linear components by a subtractive operation between C_s -corrected defocused images.

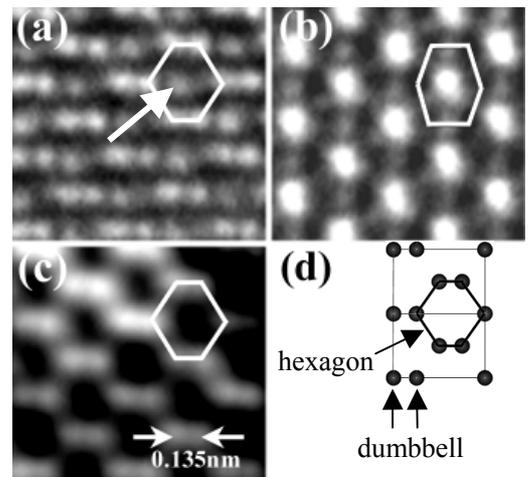


Fig. 2. C_s -corrected images of silicon along a $\langle 110 \rangle$ direction at 4 nm overfocus (a) and underfocus (b). The image processed by a combination of image subtraction and deconvolution (c). Schematic diagram of atomic positions (d).