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Measurement of Off-Axial Aberration

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Abstract. High-resolution observation of a large field of view with a high quality detector is important for single particle analysis or in-situ experiments. Consequently, evaluation of aberrations that depend on position in the field of view, (off-axial aberrations) is required. We report the experimental measurement of off-axial aberrations including higher order components in several optical conditions together with the corresponding off-axial phase maps.

1. Introduction

Owing to the development of a high quality cameras with a large number of pixels, high resolution observations in both materials science and life science over a large field of view is becoming important in transmission electron microscopy (TEM). Atomic-resolution observation of two-dimensional materials and in-situ studies in the TEM require optimization of the electron-optical conditions over a large field of view, for example to understand point defects, dislocations and distortions of the lattice [1]. High-resolution image recording for single particle analysis with wide field of view cameras is also necessary to image a suitably large number of particles for reconstruction. However, when recording high-resolution TEM data with a large field of view, off-axial aberrations increase in the peripheral area, corrupting the data. Consequently, high-quality imaging is guaranteed only at the center axis of the image. Evaluation of off-axial aberrations is hence required to optimize the optical conditions for wide field of view imaging.

Measurement of off-axial aberrations using diffractogram from different positions in the experimental image field of view has been previously reported [2]. In this study, we define the off-axial aberrations, and extend the measurement of these to defocus and two-fold astigmatism up to 4th rank. Features arising from off-axial aberrations are discussed using the simulated patterns of diffractograms and compared to experimental measurements using an off-axial aberration phase map.

2. Measurement of off-axial aberrations

Aberrations including a spatial vector, $\mathbf{r} = (x, y)$ are defined as off-axial aberrations (Fig.1(b)), whereas aberrations that are described by only a complex angle, $\omega = \alpha \cdot \exp(i\theta)$ are defined as axial aberrations (Fig.1(a)), where α is the amplitude of the angle and θ is the azimuth. The total wave aberration function, W_{total} is described by summation of the axial and off-axial aberrations, as;

$$W_{total} = W_{axial} + W_{off\ axial} \quad (1)$$



where W_{axial} is the axial wave aberration function and $W_{off\ axial}$ is the off-axial wave aberration function.

The axial wave aberration function can be rewritten as;

$$W_{axial} = \sum_{m,n} \frac{1}{m+n} \text{Re}(C_{m,n} \bar{\omega}^m \omega^n) \quad (2)$$

where $\bar{\omega} = \alpha \cdot \exp(-i\theta)$ is the complex conjugate of ω .

The off-axial aberration wave function is given by;

$$W_{off\ axial} = \sum_{m,n,s,t} \frac{1}{m+n} \text{Re}(K_{m,n,s,t} \bar{\omega}^m \omega^n \bar{r}^s r^t) \quad (3)$$

where $\mathbf{r} = |r| \cdot \exp(i\theta_r)$ is a complex position, $|r|$ is amplitude of the complex position and θ_r is the azimuth of the complex position. In order to extend measurements to higher orders of off-axial aberration coefficients, a dimensionless parameter can be conveniently introduced to give the same unit for all coefficients. Hence, a dimensionless angle, $\boldsymbol{\gamma}$ is introduced as a parameter for the spatial position and consequently the off axial wave aberration function, $W_{off\ axial}$ can be rewritten as;

$$W_{off\ axial} = \sum_{m,n,s,t} \frac{1}{m+n} \text{Re}(K_{m,n,s,t(r_0)} \bar{\omega}^m \omega^n \bar{\boldsymbol{\gamma}}^s \boldsymbol{\gamma}^t) \quad (4)$$

where the complex dimensionless position $\boldsymbol{\gamma}$ at r_0 ; r_0 is a standard length; $\boldsymbol{\gamma} = |\boldsymbol{\gamma}| \cdot \exp(i\theta_\gamma)$ with $|\boldsymbol{\gamma}| = |r|/|r_0|$, which is the amplitude of the complex dimensionless position and $\theta_\gamma = \theta_r$ is the azimuth of the complex position. The geometrical order, N of the axial aberrations is $N = m + n - 1$, and R is a rank including the off-axial aberrations with $R = N + s + t$ [3]. The off-axial aberration coefficient of $K_{m,n}$ at r_0 for an axial aberration $C_{(m+n)}$ can be described by summation of each rank of the off-axial aberrations as,

$$K_{m,n} = \sum_{s,t} K_{m,n,s,t(r_0)} \bar{\boldsymbol{\gamma}}^s \boldsymbol{\gamma}^t \quad (5)$$

Hence, each coefficient (vector) of the off-axial aberrations for (m, n, s, t) at r_0 is the term corresponding to complex position of $\bar{\boldsymbol{\gamma}}^s \boldsymbol{\gamma}^t$ defined as $K_{m,n,s,t(r_0)}$. For the data reported, $\boldsymbol{\gamma}$ is defined at $r_0=100$ nm whence an off axial aberration coefficient corresponds to a value of the axial aberration 100 nm away from the centre of the axial position with a unit of length in this case.

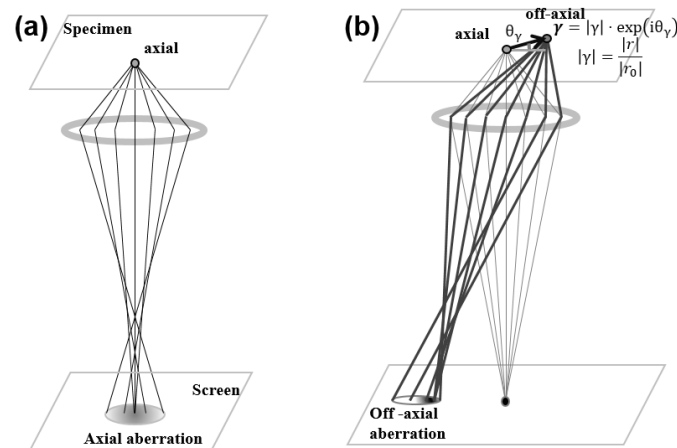


Figure 1. (a) Schematic diagram of (a) axial aberrations. (b) off-axial aberrations.

Table 1: Off-axial aberration coefficients. Using corresponding axial aberration notations, \mathbf{O}_2 denotes defocus, \mathbf{A}_2 denotes two-fold astigmatism, \mathbf{P}_3 denotes axial coma, and \mathbf{A}_3 denotes three-fold astigmatism.

Off-axial aberration $K_{m,n,s,t(r_0)}$				
Axial aberration	Off-axial aberration	2 nd rank	3 rd rank	4 th rank
\mathbf{O}_2	$\text{Re}[\mathbf{O}_2 \bar{\boldsymbol{\gamma}}^s \boldsymbol{\gamma}^t]_{(r_0)}$	$\mathbf{O}_2 \boldsymbol{\gamma}_{(r_0)}$	$\mathbf{O}_2 \boldsymbol{\gamma} \bar{\boldsymbol{\gamma}}_{(r_0)} \cdot \mathbf{O}_2 \boldsymbol{\gamma}^2_{(r_0)}$	$\mathbf{O}_2 \boldsymbol{\gamma}^2 \bar{\boldsymbol{\gamma}}_{(r_0)} \cdot \mathbf{O}_2 \boldsymbol{\gamma}^3_{(r_0)}$
\mathbf{A}_2	$\mathbf{A}_2 \bar{\boldsymbol{\gamma}}^s \boldsymbol{\gamma}^t_{(r_0)}$	$\mathbf{A}_2 \boldsymbol{\gamma}_{(r_0)} \cdot \mathbf{A}_2 \bar{\boldsymbol{\gamma}}_{(r_0)}$	$\mathbf{A}_2 \boldsymbol{\gamma} \bar{\boldsymbol{\gamma}}_{(r_0)} \cdot \mathbf{A}_2 \boldsymbol{\gamma}^2_{(r_0)} \cdot \mathbf{A}_2 \bar{\boldsymbol{\gamma}}^2_{(r_0)}$	
\mathbf{P}_3	$\mathbf{P}_3 \bar{\boldsymbol{\gamma}}^s \boldsymbol{\gamma}^t_{(r_0)}$		$\mathbf{P}_3 \boldsymbol{\gamma}_{(r_0)} \cdot \mathbf{P}_3 \bar{\boldsymbol{\gamma}}_{(r_0)}$	
\mathbf{A}_3	$\mathbf{A}_3 \bar{\boldsymbol{\gamma}}^s \boldsymbol{\gamma}^t_{(r_0)}$		$\mathbf{A}_3 \boldsymbol{\gamma}_{(r_0)} \cdot \mathbf{A}_3 \bar{\boldsymbol{\gamma}}_{(r_0)}$	

Table 2: Coefficients of off-axial defocus and off-axial two-fold astigmatism

Symmetry → Rank ↓	0	1	2	3	0	1	2	3	4
	Off-axial defocus				Off-axial two-fold astigmatism				
2		$O_{2\gamma(r_0)}$				$A_{2\gamma(r_0)}$		$A_{2\bar{\gamma}(r_0)}$	
3	$O_{2\gamma\bar{\gamma}(r_0)}$		$O_{2\gamma^2(r_0)}$		$A_{2\gamma^2(r_0)}$		$A_{2\gamma\bar{\gamma}(r_0)}$		$A_{2\bar{\gamma}^2(r_0)}$
4		$O_{2\gamma^2\bar{\gamma}(r_0)}$		$O_{2\gamma^3(r_0)}$					

Diffraction patterns at different positions in a field of view were simulated using second rank off-axial defocus and off-axial two-fold astigmatism (Fig.2). Figure 2(a) shows diffraction patterns of segmented areas from the full field of view with off-axial defocus, $O_{2\gamma(100nm)} = (100nm, 0)$ and axial defocus, $O_2 = -100$ nm. The defocus with position in the field of view is determined by the off-axial defocus and the defocus becomes close to zero at the right hand side. Figure 2(b) shows diffraction patterns from segmented areas with $O_{2\gamma(100nm)} = (0, 100nm)$, where the defocus at the lower part is close to zero. The position dependence of defoci due to the off-axial defocus $O_{2\gamma(100nm)} = (0, 100nm)$ shows a 90° rotation relationship to the off-axial defocus $O_{2\gamma(100nm)} = (100nm, 0)$. Figs. 2(c) and 2(d) show diffraction patterns from segmented areas with off-axial two-fold astigmatism, $A_{2\gamma}$ and $A_{2\bar{\gamma}}$, respectively. The two-fold astigmatism becomes larger toward the edge of the field of view, and the azimuth of the two-fold astigmatism changes depending on position. A map of $A_{2\bar{\gamma}}$ shows an overall three-fold symmetry, since the symmetry of the pattern in the field of view is $|m-n| + |s-t|$ in the case of off-axial defocus and off-axial two-fold astigmatism. Table 3 lists examples of measured coefficients for the off-axial aberrations using experimental diffraction patterns at a 200kV using JEM-ARM300F.

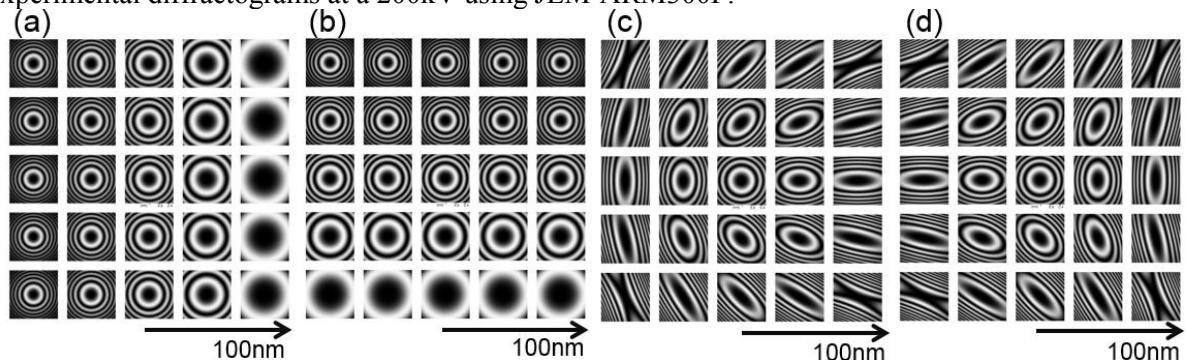


Figure 2. Diffraction patterns from segmented areas with a width of 200 nm (a) $O_{2\gamma(100nm)} = (100nm, 0)$, (b) $O_{2\gamma(100nm)} = (0, 100nm)$, (c) $A_{2\gamma(100nm)} = (100nm, 0)$ (d) $A_{2\bar{\gamma}(100nm)} = (0, -100nm)$.

Table 3. Measured values of off axial aberration coefficients. ($r_0=100$ [nm])

Rank	Off-axial aberration	Amplitude	Azimuth	Rank	Off-axial aberration	Amplitude	Azimuth
2	$O_{2\gamma(r_0)}$	8.620 nm	-102.00°	2	$A_{2\gamma(r_0)}$	1.9067 nm	-156.65°
3	$O_{2\gamma\bar{\gamma}(r_0)}$	-0.3148 nm		2	$A_{2\bar{\gamma}(r_0)}$	1.1012 nm	-18.94°
3	$O_{2\gamma^2(r_0)}$	0.4245 nm	-24.02°	3	$A_{2\gamma^2(r_0)}$	0.7866 nm	165.90°
4	$O_{2\gamma^2\bar{\gamma}(r_0)}$	0.1341 nm	177.86°	3	$A_{2\gamma\bar{\gamma}(r_0)}$	0.5034 nm	12.55°
4	$O_{2\gamma^3(r_0)}$	0.0264 nm	-67.50°	3	$A_{2\bar{\gamma}^2(r_0)}$	0.5401 nm	-92.60°
3	$P_{3\gamma(r_0)}$	407.66 nm	-30.10°	3	$A_{3\gamma(r_0)}$	5.963 nm	61.76°
3	$P_{3\bar{\gamma}(r_0)}$	50.907 nm	-77.95°	3	$A_{3\bar{\gamma}(r_0)}$	13.317 nm	154.36°

3. Experimental measurement of off-axial aberrations

Figs. 3(d-f) show off-axial phase maps from experimental measurements. Figs.3(a-c) were recorded by changing the excitation of the transfer lens (TL) between two multipoles in the TEM corrector. Fig.3(a)

was recorded using a weaker excitation of the TL, and Fig.3(c) with a stronger excitation. The TL excitation used to record Fig.3(b) is intermediate between that used to record Figs.3(a) and 3(c). In general, specimen or local bending introduces a defocus change across the field of view, artificially resulting in second rank off-axial defocus. To distinguish genuine electron-optical off-axial aberrations from this specimen effect, the second rank off-axial defocus was set to zero in the phase maps shown in Figs.3(d-f). From these measurements, the value of a $A_{2\bar{\gamma}}$, which has three-fold symmetry, shows a significant difference (Table 4). The off-axial aberrations cause a change of the two-fold astigmatism at the periphery of the field of view demonstrating that optimization of $A_{2\bar{\gamma}}$ is important for a double hexapole TEM corrector.

Table 4: Measured values of off axial aberrations. ($r_0=100$ [nm])

Off-axial aberration	Setting 1(Figs.3(a) and 3(d))		Setting 2(Figs.3(b) and 3(e))		Setting 3(Figs.3(c) and 3(f))	
	Amplitude	Azimuth	Amplitude	Azimuth	Amplitude	Azimuth
$A_{2\gamma(r_0)}$	1.81 nm	142.59°	1.83 nm	-125.38°	2.67 nm	-110.61°
$A_{2\bar{\gamma}(r_0)}$	4.38 nm	72.71°	1.04 nm	101.96°	2.70 nm	-131.97°

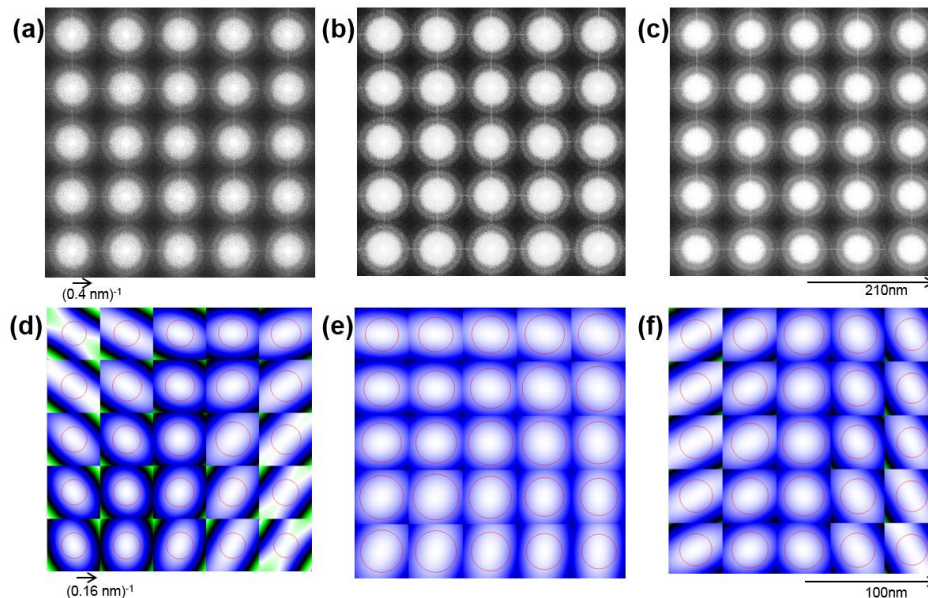


Figure 3. (a-c) 5x5 diffractogram maps from segmented areas. (d-f) Off-Axial Phase Map for different TL excitations. An offset, $O_2 = -5$ nm is used to visualize the off-axial two-fold astigmatism in the phase maps. Red circles denote the $\pi/4$ phase limit within each local area.

4. Conclusion

Measurement of off-axial aberrations including those of higher rank was reported using diffractograms calculated from different positions in a wide field of view. Experimental measurements have been reported for several optical settings. For the measurements reported off-axial two-fold astigmatism, $A_{2\bar{\gamma}}$, with a three-fold symmetry across the field of view is clearly evident in images recorded using a double-hexapole TEM corrector.

References

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