Tilt Series Reconstruction and Parallax Problem

Kazuo Ishizuka *

* HREM Research Inc. 14-48 Matsukazedai, Higashimastuyama, Saitama 355-0055 JAPAN

Introduction

The recent development of a *hardware* aberration corrector for transmission electron microscope has significantly improved the attainable resolution [1]. On the other hand, aberration can be *a posteriori* corrected, when we reconstruct complex wave function from a series of through-focus images taken with a non-Cs corrected microscope [2,3]. Importantly, a focal series reconstruction (FSR) gives an aberration-corrected *complex* wave function at the specimen exit surface, while a hardware aberration corrector gives only *intensity* distribution of the wave function. However, aberration corrected image obtained by using hardware or software is ultimately limited by the partial coherence of electrons (information limit).

Tilt Series Reconstruction

A promising method to improve resolution beyond the information limit is a tilt series reconstruction (TSR), where several images are recorded with different beam tilt [4]. Figure 1 compares the normal incidence (left) and tilted incidence (right). The orange-colored arrow shows the incident beam direction. Here, the optic axis is vertical in both figures. Thus, if we tilt the incident beam direction, we can collect information from higher diffraction angles with the same or less amount of wave aberration than the normal incident case.

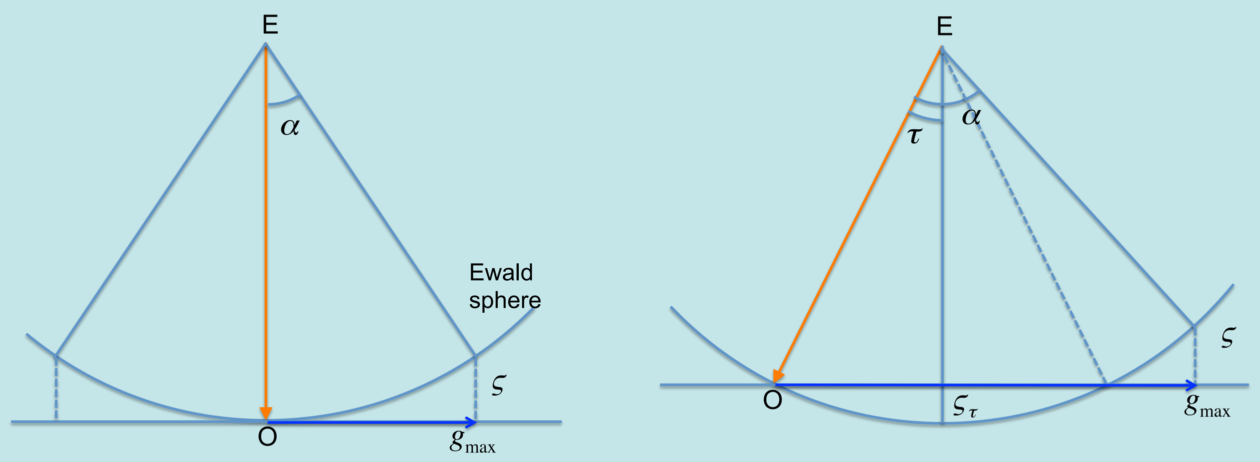

Figure 1 Comparison between the normal incidence (left) and tilted incidence (right). The orange-colored arrow shows the incident beam direction. Here, the optic axis is vertical. Thus, if we tilt the incident beam direction, we can collect information from diffractions with the same or less amount of wave aberration than the normal incident case,

However, information collected from a single tilted illumination is asymmetric (directional) in Fourier space as shown in Figure 2 (left). This asymmetry will be alleviated by collecting information from a tilt series, where the azimuth of the incident beam direction is changed as shown in Figure 2 (right). Since this is an 'aperture synthesis', we can improve resolution substantially. The sophisticated TSR procedure including a short focal series has been already developed [5], and is commercially available [6].

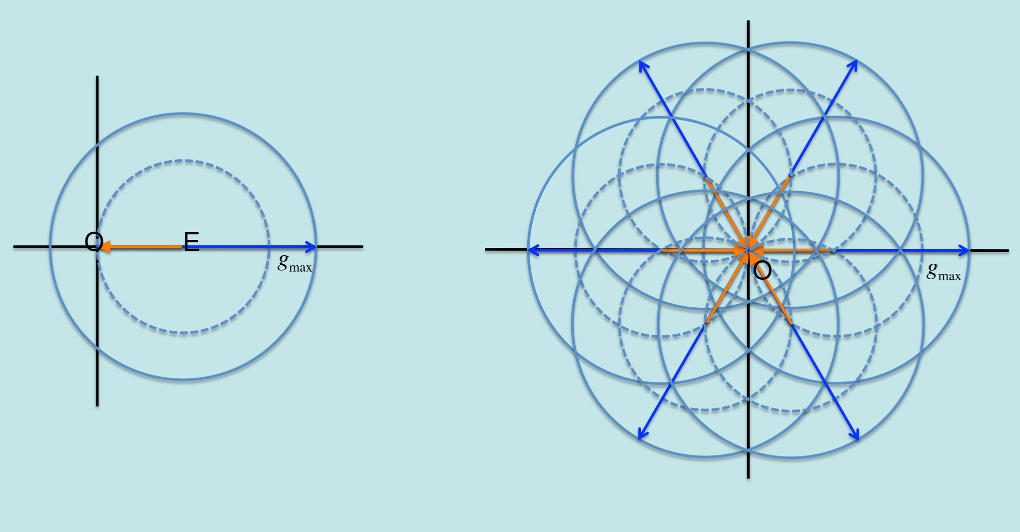

Figure 2 Information collection in Fourier space with single tilted beam (left) and multiple tilted beams (right). The former collects information asymmetrically in Fourier space, while the six tilted beams collect information nearly symmetrically.

However, it has been argued that the use of tilted illumination introduces a serious limitation on a specimen thickness by a parallax problem [7]. We will study the previous discussion for the geometric parallax, and derive a new estimate of an allowable specimen thickness in the case of the tilted illumination.

Geometrical Parallax

Under a normal illumination the atom at the top surface will be projected onto the atom at the bottom surface (Figure 1_left). However, under the tilted illumination the atom at the top surface will be projected onto the bottom surface displaced by s relative to the equivalent atom at the bottom surface (geometrical parallax) (Figure 1_right). Here, the displacement is approximated by $s=t.\tau$, where t is the specimen thickness and τ a tilt angle. In order to resolve a periodicity d the geometrical parallax s may be limited by $d/2$. Thus, a maximum thickness imposed by the geometrical parallax will be $d/2\tau$. The same conclusion has been derived using the phase shift between the points on the top and bottom specimen surfaces due to a beam tilt [7]. We may note however that this geometrical parallax is independent of an accelerating voltage (or a wavelength), and allows a sample of *infinite* thickness for a normal incident (τ=0) as shown in Figure 5.

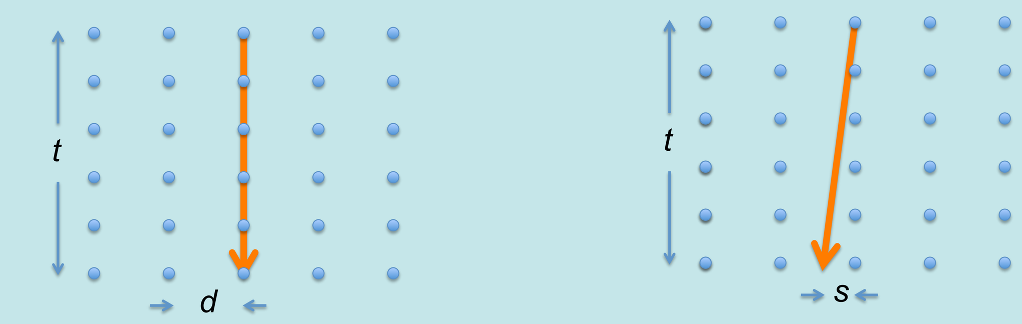

Figure 3 Geometrical parallax. In the case of the normal illumination there is no displacement of the top atom projected onto the bottom surface. Contrary to this, under the tilted illumination the atom at the top surface will be projected onto the bottom surface displaced by s relative to the atom at the bottom surface. This displacement gives an upper limit of the sample thickness.

Physical Parallax

Physical parallax may be argued as a limit of the specimen thickness, with which a projection approximation will be satisfied. We discuss here physical parallax by taking into account kinematical scattering with a thin sample of thickness t. Figure 4 illustrates the Ewald construction for a tilted illumination, where we assume the diffraction plane (the zero order Laue zone) is parallel to the specimen slab. Here, τ is the tilt angle, λ* (=1/λ) the radius of the Ewald sphere, g_{max} the resolution limit. The intersection between the Ewald sphere and the diffraction plane gives the Laue circle (orange circle), whose center is located at A, and ζ and ζ_τ correspond to excitation errors (distances between the diffraction spot center and the Ewald sphere) at the scattering vectors g_{max} and g/2, respectively. We may note that under kinematical approximation the scattering distribution in Fourier space will elongate approximately by $1/t$ perpendicular to the specimen slab. Thus, the optimum tilt angle in terms of the kinematical scattering is given at $\zeta = \zeta_\tau$.

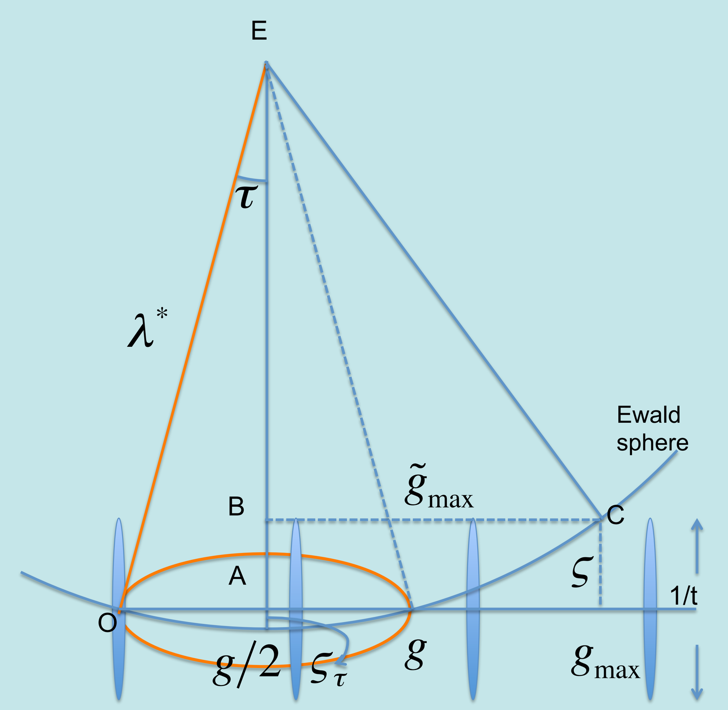

Figure 4 Ewald construction for a tilted illumination. Here, τ is the tilt angle, λ* the radius of the Ewald sphere, g_{max} the resolution limit, ζ and ζ_τ excitation errors. The scattering distribution in reciprocal space elongates perpendicular to the specimen slab.

The following two equations will be observed, when we apply Pythagorean theorem to the triangles ΔEOA and ΔECB :

$$\left(\lambda^* - \varsigma_\tau\right)^2 + \left(g/2\right)^2 = \left(\lambda^*\right)^2 \quad \text{and} \quad \left(\lambda^* - \left(\varsigma_\tau + \varsigma\right)\right)^2 + \tilde{g}_{max}^2 = \left(\lambda^*\right)^2$$

where $\tilde{g}_{max} = g_{max} - \left(g/2\right)$. Then, for small angle scattering they respectively reduce to the following two approximations:

$$\left(g/2\right)^2 \approx 2\varsigma_\tau\lambda^* \quad \text{and} \quad \tilde{g}_{max}^2 \approx 2\left(\varsigma_\tau + \varsigma\right)\lambda^*$$

Using these approximations and the two simple relationships: $\tau \approx \lambda\left(g/2\right)$ for a small tilt angle, and $2\zeta \le 1/t$ for the excitation error at g_{max} for a tilt angle less than the optimum tilt ($\zeta_\tau \le \zeta$), we finally get the expression for the maximum thickness as a function of the beam tilt τ and the resolution g_{max}: $\boxed{t \le 1\big/\left(\lambda g_{max}^2 - 2g_{max}\tau\right)}$

This is a general formula, and gives a correct thickness limit $t \le 1/\lambda g_{max}^2$ for the normal incidence (τ=0) (Figure 1). Figure 5 shows the maximum sample thickness given by physical parallax as well as the geometrical parallax. We may note that physical parallax decreases, and thus the maximum sample thickness increase, when the tilt angle is increased up to the optimum tilt angle, where $\zeta = \zeta_\tau$.

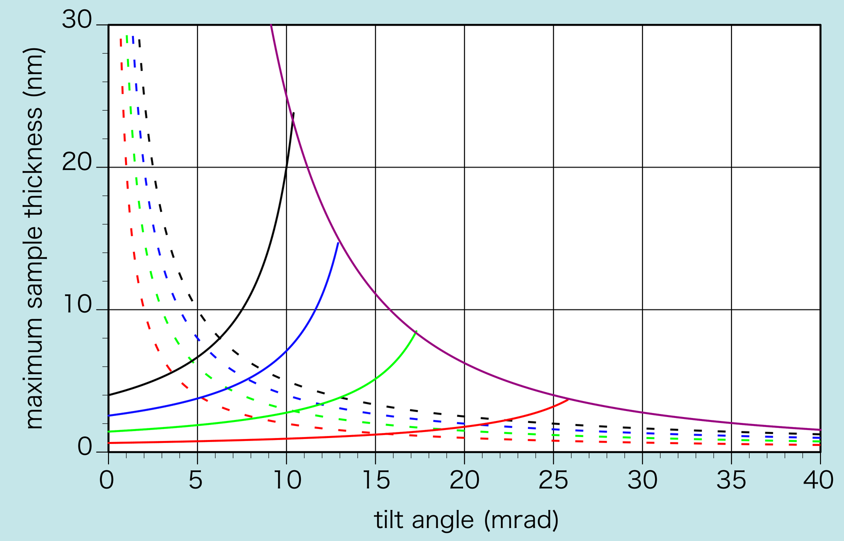

Figure 5 Maximum sample thickness for 200 kV electrons. Broken and solid lines correspond to geometrical parallax and physical parallax, respectively. Black, blue, green and red lines correspond to the resolutions d = 0.10, 0.08, 0.06 and 0.04 nm (α = 25.0, 31.3, 41.7 and 62.5 mrad), respectively. You may note the complete difference of the maximum thicknesses estimated from geometrical parallax and physical parallax.

At the optimum tilt angle the maximum thickness is given as $t \le \left(3+2\sqrt{2}\right)\big/\lambda g_{max}^2$, and the optimum tilt is given $\alpha = \lambda g_{max} = \left(1+\sqrt{2}\right)\tau_{opt}$. Thus, for the same resolution the TSR can be applied to a 5.8-times thicker sample than the FSR. Even when we improve resolution twice of the FSR using the TSR, we can still use a 1.5-times thicker sample than the FSR.

For the tilt angle larger than the optimum tilt the maximum thickness will be determined by the excitation error ζ_τ as $1/t \cong 2\varsigma_\tau = \lambda\left(g/2\right)^2 = \tau^2/\lambda$. Thus, after the optimum tilt for each resolution g_{max}, the maximum thickness is inversely proportional to the square of the tilt angle. Thus, it is not a good idea to use the tilt angle larger than the optimum tilt for each resolution.

The geometrical parallax ($d/2\tau$) will be obtained for the high accelerating-voltage limit, where the Ewald sphere becomes flat plane. Here, $\varsigma_\tau = \tau\left(g/2\right)$ and $\varsigma = \tau g_{max}$. Thus, the maximum thickness is given by $1/t \cong 2\varsigma = 2\tau g_{max} = 2\tau/d$.

Conclusions

We have derived the formula for physical parallax due to a tilted illumination by taking into account kinematical scattering. Physical parallax decreases with the tilt angle up to the optimum tilt angle for a given resolution contrary to geometrical parallax. Even when we improve resolution twice of the FSR using the TSR, we can still use a 1.5-times thicker sample than the FSR. These conclusions may be surprised in terms of the geometrical parallax. However, the TSR collects information on a diffraction plane over a wider area by an aperture synthesis. Then, using the Fourier projection theorem the TSR will give a better projection of a sample. Thus, the parallax due to sample thickness may not be a limiting factor for the TSR.

References

[1] M. Haider et al., Ultramicroscopy 75 (1998) 53.
[2] W.J.M. Coene et al, Ultramicroscopy 64 (1996) 109.
[3] R.R. Meyer et al., Ultramicroscopy 92 (2002) 89.
[4] A.I. Kirkland et al., Ultramicroscopy 57 (1995) 355.
[5] R.R. Meyer et al., Ultramicroscopy 99 (2004) 115.
[6] FTSR (Plug-in for DigitalMicrograph), www.hremresearch.com
[7] S.J. Haigh et al., Phil. Trans. R. Soc. A367 (2009) 3577.

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