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Fourier Analysis of Ronchigram and Aberration Assessment

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A shadow image obtained from amorphous/non-periodic materials has been used for a manual alignment of a scanning transmission electron microscope (STEM), and proposed to measure aberrations quantitatively [1]. A Ronchigram, a shadow image obtained from crystal materials in STEM, can also be used to check an alignment quality [2-4]. It was shown that a Fourier transform of a Ronchigram might be used to measure aberrations [5-7]. This report revisits Fourier analysis of a Ronchigram to give a more concrete mathematical foundation.

We will confine here to a weak phase object and ignore interference between scattered waves. Thus, it will be enough if we consider an interference term between the center beam and +g reflection, and amplitude of the two-beam Ronchigram may be given

$$\Phi(\vec{k},\vec{r}_o) = \exp(2\pi i\vec{k}\vec{r}_o)\left[A(\vec{k})\exp\left\{\tfrac{2\pi}{\lambda}i\chi(\vec{k})\right\} + iQ(\vec{g})\exp(-2\pi i\vec{g}\vec{r}_o)A(\vec{k}-\vec{g})\exp\left\{\tfrac{2\pi}{\lambda}i\chi(\vec{k}-\vec{g})\right\}\right], \quad (1)$$

where r_o is a probe position, $\chi(\vec{k})$ a wave aberration function and $Q(\vec{g})$ a structure factor for a reflection g. By neglecting a second order term an observed Ronchigram (intensity) is given

$$R(\vec{k},\vec{r}_o) = \Phi(\vec{k},\vec{r}_o)\cdot\Phi^*(\vec{k},\vec{r}_o) \approx A(\vec{k}) + if_g(\vec{k}-\tfrac{1}{2}\vec{g},\vec{r}_o) - if_g^*(\vec{k}-\tfrac{1}{2}\vec{g},\vec{r}_o), \quad (2)$$

where

$$f_g(\vec{k},\vec{r}_o) \equiv A(\vec{k}+\tfrac{1}{2}\vec{g})A(\vec{k}-\tfrac{1}{2}\vec{g})Q(\vec{g})\exp(-2\pi i\vec{g}\vec{r}_o)\exp\left\{\tfrac{2\pi i}{\lambda}\left[\chi(\vec{k}-\tfrac{1}{2}\vec{g})-\chi(\vec{k}+\tfrac{1}{2}\vec{g})\right]\right\}. \quad (3)$$

Then, we will get a Fourier transform of a two-beam Ronchigram as

$$\Psi(\vec{h},\vec{r}_o) \equiv FT\left[R(\vec{k},\vec{r}_o)\right] = a(\vec{h},\vec{r}_o) + i\left[F_g(\vec{h},\vec{r}_o) - F_g^*(-\vec{h},\vec{r}_o)\right]\exp(\pi i\vec{g}\vec{h}), \quad (4)$$

where $a(\vec{h},\vec{r}_o)$ is an Airy disk, and $F_g(\vec{h},\vec{r}_o)$ is a Fourier transform of $f_g(\vec{k},\vec{r}_o)$. Figure 1 shows a two-beam Ronchigram and its Fourier transform, where you can see a pair of comet-shaped spot due to spherical aberration. Each comet comes from $F_g(\vec{h},\vec{r}_o)$. It was shown that the position from the origin changes with defocus and two-fold astigmatism, but the shape remains constant and the angle of the comet tail that is always 60˚ [5]. However, the reason of the comet shape remains unresolved.

When we consider a symmetric three-beam case, namely the center beam and +g and –g reflections, using Friedel's law for $Q(\vec{g})$ the Ronchigram may be written as

$$R(\vec{k},\vec{r}_o) = \Phi(\vec{k},\vec{r}_o)\cdot\Phi^*(\vec{k},\vec{r}_o) \approx A(\vec{k}) + if_g(\vec{k}-\tfrac{1}{2}\vec{g},\vec{r}_o) - if_g^*(\vec{k}-\tfrac{1}{2}\vec{g},\vec{r}_o) + if_g^*(\vec{k}+\tfrac{1}{2}\vec{g},\vec{r}_o) - if_g(\vec{k}+\tfrac{1}{2}\vec{g},\vec{r}_o) \quad (5)$$

and its Fourier transform for the three-beam Ronchigram results:

$$\Psi(\vec{h},\vec{r}_o) = a(\vec{h},\vec{r}_o) + i\left[F_g(\vec{h},\vec{r}_o) - F_g^*(-\vec{h},\vec{r}_o)\right]\left\{\exp(\pi i\vec{g}\vec{h}) - \exp(-\pi i\vec{g}\vec{h})\right\}. \quad (6)$$

Thus, the Fourier transform of a symmetric three-beam Ronchigram shows fine straight fringes perpendicular to the scattering vector, ***g***, due to the last terms in the curly brackets. The origin of these fringes was attributed to the presence of two identical sets of fringes in the Ronchigram [5].

The presence of two identical patterns shifted by $\pm\frac{1}{2}\vec{g}$ is mathematically shown in Eq. (5).

The Fourier transform $F_g(\vec{h},\vec{r}_o)$ may be given by a far field distribution of $f_g(\vec{k},\vec{r}_o)$. Then, the comet shape will be determined by a gradient of a wave front controlled by the phase term. We may note that the total spot displacement may be estimated as a sum of gradients of constituent aberrations. Thus, the shift of a spot position due to spherical aberration will be given by

$$\nabla\chi_{40}(\vec{k}-\tfrac{1}{2}\vec{g})-\nabla\chi_{40}(\vec{k}+\tfrac{1}{2}\vec{g})=-2c_{40}(\vec{k}\vec{g})\vec{k}-c_{40}(k^2+\tfrac{1}{4}g^2)\vec{g} \quad . \tag{7}$$

where $c_{40}=C_s\pi\lambda^3/2$. Now, to simplify the argument we will define the new axis of coordinates, where the x-axis aligns the scattering vector ***g***, and the origin is placed at the comet head, namely $\left(c_{40}(\frac{1}{2}g_x)^2g_x,0\right)$. Then, the x and y components of the above gradient are respectively given by

$$X=c_{40}g_x\left(3k_x^2+k_y^2\right);\ Y=c_{40}g_x\left(2k_xk_y\right). \tag{8}$$

The position of the comet tail corresponds to the caustic determined by these coordinates. In order to verify this statement, we consider the angle α corresponding to (X, Y) using the polar coordinates for $\vec{k}$, namely $k_x=r\cos\theta, k_y=r\sin\theta$,

$$R=\tan\alpha=\frac{Y}{X}=\frac{\sin 2\theta}{2\cos^2\theta+1}$$

It is easily shown that R has an extremum at $\theta=\pm 60°$, and then $\alpha=30°$. Thus, the comet angle is 60˚ as observed by Boothryod [5]

The same argument on the shift of a spot position due to defocus and two-fold astigmatism gives the identical results derived from $\chi(\vec{k}-\vec{g})-\chi(\vec{k})$ [5-7]. However, it becomes clear from the argument for spherical aberration that the phase term $\chi(\vec{k}-\frac{1}{2}\vec{g})-\chi(\vec{k}+\frac{1}{2}\vec{g})$ in Eq. (3) is more fundamental for Fourier analysis of the Ronchigram.

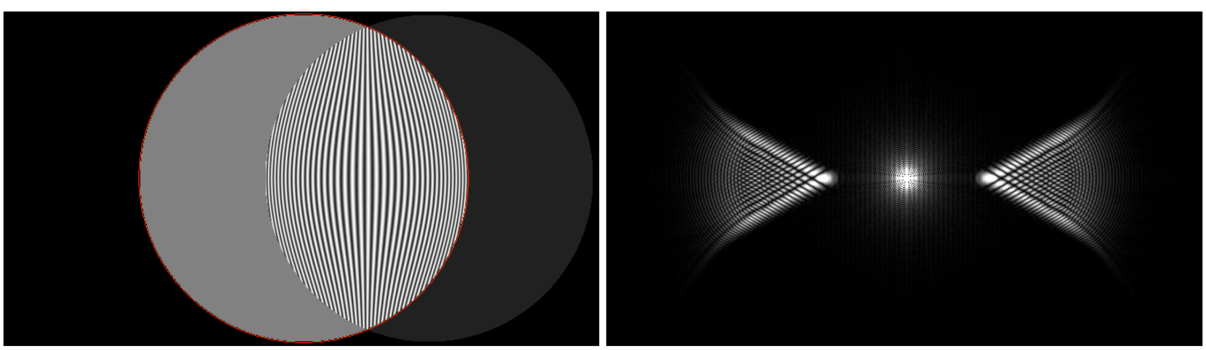

Figure 1. Two-beam Ronchigram (left) and its Fourier transform. This is a kinematical simulation and wave aberration is considered. 100 kV, Cs = 3.1 mm, defocus = 350 nm, g = 3.07 nm^{-1}.

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