

## Determination of Aberration Center of STEM Ronchigram for Fully Automated Aberration Correctors

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One of the key technologies for aberration corrected electron microscopes is the computerized aberration recognition and feedback system to simultaneously adjust all the electron-optical elements, which consist of at least two multipoles, four-five round lenses, and more than four deflector pairs.[1] However the aberration measurement, the very first process for the correctors, still requires pre-alignment of the optical axis which depends on users' experiences. The axis alignment is typically based on the high-tension (HT) center, objective lens current (Obj) center, or coma-free axis alignment. In the case of aberration corrected microscopes, the coma-free alignment can be more generally expanded as "aberration-free" alignment, since the coma aberration in a conventional TEM (CTEM) is mostly induced from the decentering of the spherical aberration. In this study, we propose and demonstrate a new method to automatically determine the "aberration center", which we consider most important for high quality imaging. Mis-centering of HT or Obj axis basically induces blurring of the image (damping in contrast) due to the round chromatic aberration or instability while decentering of aberration center axis induces erroneous contrasts in imaging, or non-round beam shape in probe formation.

In general, displacement of the center of an aberration induces lower-order aberrations, which we call "decentering-induced secondary" (DIS) aberration.[2] Primary and DIS aberrations are summarized in Figure 1. To find the aberration-free center axis, we minimize DIS aberrations, assuming that the residual intrinsic aberrations are of higher orders. The fitness function to be minimized was set as a sum of the DIS aberration amplitudes with properly distributed weight values depending on the order of the aberrations. This algorithm to determine the aberration center is applied to the segmental Ronchigram autocorrelation method (SRAM) for STEM and is verified by finding the center of the Ronchigram using the SRAM method for aberration corrected STEM.[3]

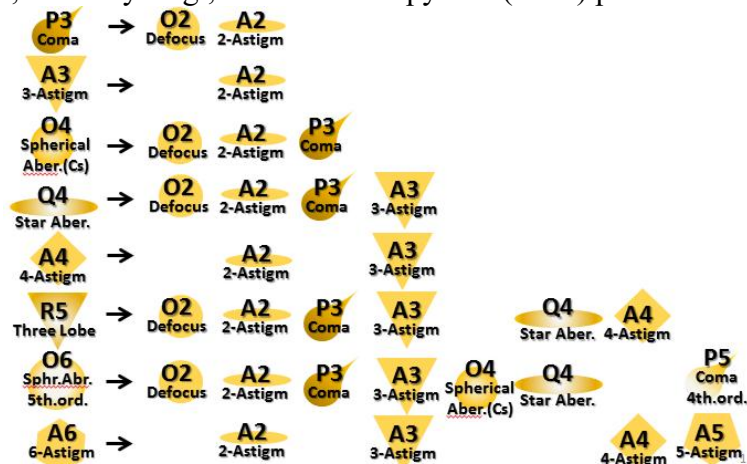
We checked the validity of our algorithm by calculating the fitness values from the simulated Ronchigram with different aberration conditions as well as experimentally by using the R005 microscope with asymmetric aberration correctors and amorphous germanium.[1]

Lower order DIS aberrations, especially for 3rd and 2nd wave(potential) orders, show multiple local minima in the fitness function while higher order DIS aberrations that originate from six-fold astigmatism or higher order spherical aberration tend to give a single minimum. By properly distributing the weight values including, proper convergence of the aberration center search was achieved. Because this center search depends on the accuracy of the aberration measurement, we took multiple steps to check the convergence to find the optimal center. Different aberrations were intentionally induced and tested. It was found that the center search converges faster when the residual aberrations are smaller. With large coma aberration, for instance, the search process gave an oscillative behavior along the azimuthal angle of the coma aberration.

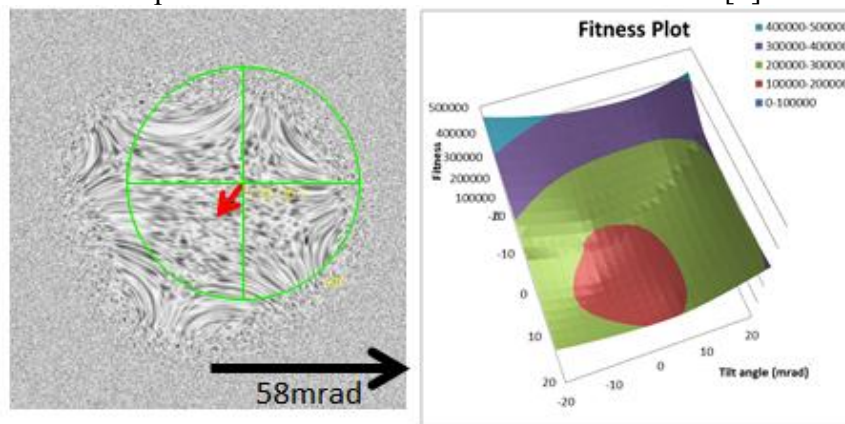
Our proposed method is based on the measured aberration values and requires only one set of images which are initially acquired to measure the aberration values. The center search procedure is therefore very fast. This method is generic and is applicable to any aberration measurements, such as Zemlin's diffractogram tableaux for TEM. The aperture alignment, which should be set to the aberration center and is critical for STEM observation, could also be automatized using this technique.

References:

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 [2] S J Haigh, H Sawada, A I Kirkland, Phil. Trans. R. Soc. A 367 (2009) p. 3755-3771.  
 [3] H Sawada, T Sannomiya, F Hosokawa, T Nakamichi, T Kaneyama, T Tomita, Y Kondo, T Tanaka, Y Oshima, Y Tanishiro, K Takayanagi, Ultramicroscopy 108 (2008) p.1467-1475.



**Figure 1.** Schematized relation of primary (left most column) and resulting decentering induced secondary aberrations. We adopted the aberration notation of the reference [3].



**Figure 2.** Simulated Ronchigram (left) with six-fold astigmatism, star aberration, and two-fold astigmatism. The initial center for SRAM calculation and the found optimal center are indicated by the green circle and the red arrow head respectively. The fitness function landscape (right) used to find the center shows a single minimum, corresponding to the optimal aberration center.