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Quantitative Relation Between Differential Phase Contrast Images Obtained by Segmented and Pixelated Detectors

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In scanning transmission electron microscopy (STEM), differential phase contrast (DPC) imaging has been developed to measure electromagnetic fields in materials. The incident beam is deflected due to Coulomb or Lorentz forces, shifting the transmitted bright field disk on the detector plane. The deflection angle can be measured using an azimuthally segmented detector. This simple description is valid only when electromagnetic field is uniform inside the electron probe, otherwise electron distribution inside the disc is varied. Quantitative measurement of electromagnetic fields is possible within the weak phase object approximation (WPOA) by using the phase contrast transfer function (PCTF) given in the early papers on DPC [1,2]. Recently it was indicated that measuring the center of mass (CoM) of electron distribution in the transmitted bright field disk with a pixelated detector is a proper way to quantify the field under the phase object approximation [3]. Applying this method, the field distribution convolved with probe-intensity function is obtained. While accurate CoM is not measurable with a segmented detector, an approximation method was recently proposed [4]. Here we calculate the PCTFs for segmented and pixelated detectors based on the (approximated) CoM method and obtain the quantitative relation between DPC images acquired by the two types of detectors.

Under the WPOA, intensity in DPC images is described as $I_{\mathrm{DPC}}(\boldsymbol{r}) = \mathcal{F}^{-1}[\sigma V_{\mathrm{prj}}(\boldsymbol{q})\beta(\boldsymbol{q})]$, where $\boldsymbol{r}$ and $\boldsymbol{q}$ denote coordinates in real and reciprocal space respectively, σ is a proportional constant and $V_{\mathrm{prj}}(\boldsymbol{q})$ is a Fourier transformation of a projected potential function $v_{\mathrm{prj}}(\boldsymbol{r})$. $\beta(\boldsymbol{q})$ is a PCTF given as below [2],

$$\beta(\boldsymbol{q}) = \frac{i}{\Omega_0} A(\boldsymbol{K}_\perp) D(\boldsymbol{K}_\perp)\big(A(\boldsymbol{q}-\boldsymbol{K}_\perp)\exp\big[-\mathrm{i}\big(\chi(\boldsymbol{q}-\boldsymbol{K}_\perp)-\chi(\boldsymbol{K}_\perp)\big)\big] - A(\boldsymbol{q}+\boldsymbol{K}_\perp)\exp\big[\mathrm{i}\big(\chi(\boldsymbol{q}+\boldsymbol{K}_\perp)-\chi(\boldsymbol{K}_\perp)\big)\big]\big)\mathrm{d}^2\boldsymbol{K}_\perp,$$

where $\boldsymbol{K}_\perp$ denotes a wavenumber component perpendicular to the illumination axis, $A(\boldsymbol{K}_\perp)$, $D(\boldsymbol{K}_\perp)$ and $\chi(\boldsymbol{K}_\perp)$ denote the condenser aperture function, the detector response function and the aberration function, respectively. This description is valid for both segmented and pixelated detectors. Fig. 1 shows the schematics of each type of detector. Accurate CoM of electron intensity is measurable with a pixelated detector. In contrast, it is impossible to know detailed electron distribution inside each segment in a segmented detector. Here, distributions in each segment are assumed to be uniform [4]. Based on the (approximated) CoM method, the detector response functions for α-component (α denotes x or y) of DPC imaging with pixelated and segmented detector are defined as $D_\alpha^{\mathrm{pix}}(\boldsymbol{K}_\perp) = K_{\perp\alpha}$ and $D_\alpha^{\mathrm{seg}}(\boldsymbol{K}_\perp) = \{K_{\perp\alpha}\}_{\mathrm{CoM},j}$ (if $\boldsymbol{K}_\perp$ lies within the jth segment) respectively, where $K_{\perp\alpha}$ denotes α-coordinate of $\boldsymbol{K}_\perp$ and $\{K_{\perp\alpha}\}_{\mathrm{CoM},j}$ denotes CoM of the jth detector segment [4]. In the case of DPC, the PCTFs is purely imaginary. Taking into account the formula $\mathcal{F}\big[\partial_\alpha v_{\mathrm{prj}}(\boldsymbol{r})\big] = 2\pi i q_\alpha V_{\mathrm{prj}}(\boldsymbol{q})$, DPC image intensity can be rewritten using a real PCTF $\beta'(\boldsymbol{q}) = -i\beta(\boldsymbol{q})/q_\alpha$ as below

$$I_{\mathrm{DPC},\alpha}(\boldsymbol{r}) = \mathcal{F}^{-1}\left[\frac{\sigma}{2\pi}\mathcal{F}\big[\partial_\alpha v_{\mathrm{prj}}(\boldsymbol{r}_p)\big]\beta'_\alpha(\boldsymbol{q})\right].$$

$\beta'_\alpha(\boldsymbol{q})$ can be regarded as a PCTF for the partial derivative of projected potential with respect to α. Therefore, quantitative relation between the two types of DPC is given as below

$$I^{\mathrm{pix}}_{\mathrm{DPC},\alpha}(\boldsymbol{r})/\beta'_{\mathrm{pix}}(\boldsymbol{q}) = I^{\mathrm{seg}}_{\mathrm{DPC},\alpha}(\boldsymbol{r})/\beta'_{\mathrm{seg}}(\boldsymbol{q}).$$

Fig. 2 shows examples of PCTF $\beta'_\alpha(\boldsymbol{q})$ and simulated DPC of single Si atom for segmented and pixelated detectors. Because the PCTF for a segmented detector is lower than pixelated one, field strength measured by a segmented detector underestimates the field. Validity of the relation for realistic specimen case with finite thickness and thermal diffuse scattering will be discussed in the presentation.

References

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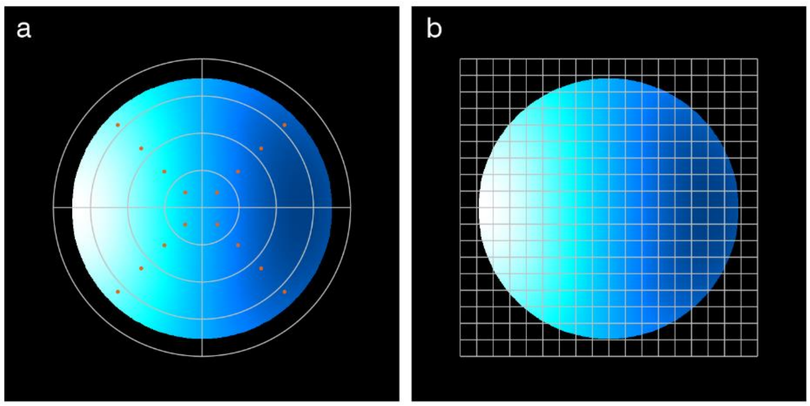

Figure 1. Schematics of segmented detector (a) and pixelated detector (b) with a simulated transmitted bright field disk pattern. CoMs of each segment are indicated by red points.

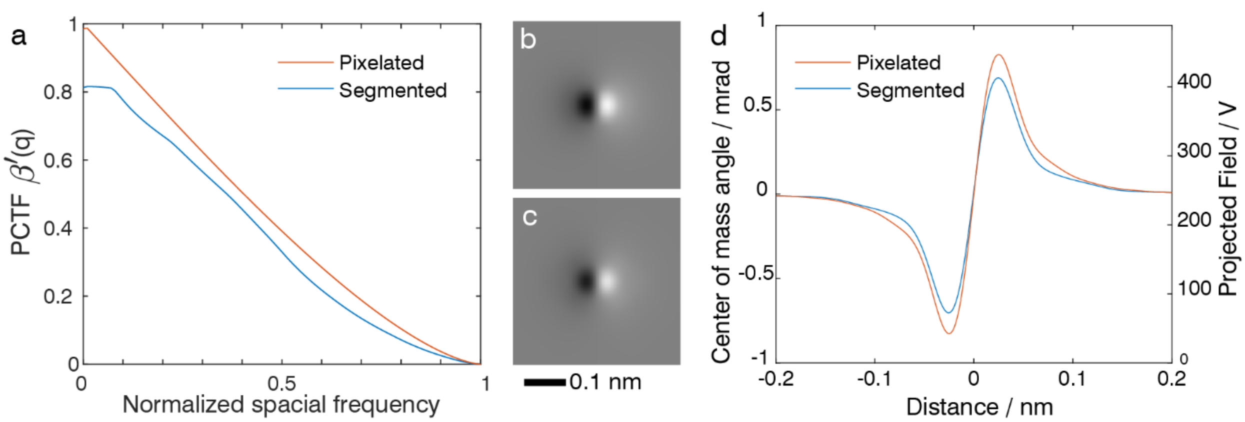

Figure 2. (a) PCTFs $\beta'(\boldsymbol{q})$ for segmented and pixelated detectors. The special frequency is normalized by the information limit. The aberrations were assumed to be zero. (b,c) Simulated DPC images (x component) of Si single atom with pixelated and segmented detectors, respectively. (d) Line profiles of the each DPC images along the lateral direction. The simulation was carried out with accelerating voltage of 300 kV and convergence semi-angle of 24 mrad. Geometric relation between a segmented detector and transmitted bright field disk is shown in Fig. 1a. The mean squared displacement of Si atom was assumed to be 0.0063 Å^2. Only elastic scattering was taken into account.

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