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Depth-related contrast in aberration-corrected confocal STEM

N. de Jonge, A.R. Lupini, K. van Benthem, A.Y. Borisevich and S.J. Pennycook
Condensed Matter Science Division, Oak Ridge National Laboratory, PO Box 2008, Oak Ridge, TN 37831-6030, USA

Probe convergence angles in aberration-corrected scanning transmission electron microscopy (STEM) are sufficiently large that the depth of focus becomes less than the sample thickness. This effect can be used to obtain depth sensitivity. Several definitions can be used for the depth resolution of the 3D confocal STEM [1]. Similarly to incoherent light optics, for systems with negligible aberrations the intensity *I(z)* at a position *z* on the optic axis obeys the equation [2]:

$$I(z) = \left(\frac{\sin\left(\pi \frac{\alpha^2}{2\lambda} z\right)}{\pi \frac{\alpha^2}{2\lambda} z} \right)^2 I_0 \qquad 1$$

where α is the probe semi-angle and λ is the electron wavelength. The depth resolution then can be defined using a vertical equivalent of the Rayleigh criterion, leading to the expression:

$$dz = 2\frac{\lambda}{\alpha^2} \cong 2\frac{\delta}{\alpha} \qquad 2$$

where δ is the transverse resolution. For the 300 keV aberration-corrected VG Microscopes' HB603U at ORNL typical numbers are d_{50} = 0.8 Å, α = 22 mrad, λ =1.9 pm and thus the depth resolution is *dz* = 7.9 nm. This number is close to the experimentally obtained half-width for single platinum atoms on a thin carbon support [1]. Expression (2) is defined for point sources of scattering. In reality objects are not point sources of scattering, but may be extended, i.e., consist of an extended array of atoms whose internal arrangement we do not always need to resolve. The contrast in dark field STEM is formed by the number of electrons that are scattered outside the electron beam onto the detector due to interaction with a certain atom, as defined by the partial scattering cross section. The cross section is a function of the local density, the atomic number and the atomic mass in the volume of interest. For many samples, beam damage already occurs at the radiation doses needed for high-resolution images, limiting the achievable resolution.

Another important aspect is the depth precision. The position *z* of single small objects spaced much further apart vertically in a sample than *dz* can be determined with significantly higher precision than the actual depth resolution, similar as in confocal light microscopy [3]. When a beam is defocused by a certain amount of *dh*/2, the radius *r* of the spot irradiating the object increases to approximately $\alpha dh/2 + r$ and the current density *J* on the object is reduced with respect to imaging in focus by:

$$J = \eta J_0 \qquad 3$$

Following geometrical considerations η is given by:

$$\eta(\alpha dh/2 + r)^2 = r^2 \qquad 4$$

$$\Leftrightarrow \alpha^2 dh^2 + \alpha r dh + r^2 = r^2/\eta \qquad 5$$

Solving this equation and neglecting negative solutions for *dh,* gives the expression:

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$$dh = \frac{2r}{\alpha}\left(\frac{1}{\sqrt{\eta}} - 1\right) \quad 6$$

The depth precision dh_{50} can be found by replacing $2r$ by d_{50} ($\cong \delta$):

$$dh_{50} = \frac{d_{50}}{\alpha}\left(\frac{1}{\sqrt{\eta}} - 1\right) \cong \frac{\lambda}{\alpha^2}\left(\frac{1}{\sqrt{\eta}} - 1\right) \quad 7$$

We need to define a criterion for the difference of the signal from the particle imaged at two different z positions to be detectable. Typically, a small point-like object of the order of one pixel will be detectable when the signal-to-noise ratio S is 5 or larger [3]. The detection is associated with Poisson statistics, such that $S = N/\sqrt{N}$, with total amount of counts N. The required minimum signal-to-noise ratio relates to the confidence level of the measurement. An object spanning a multiple of pixels can be detected with a lower signal-to-noise ratio with satisfying confidence level. However, care should be taken which pixels are selected to belong to the object and which are not. Assuming a linear relation between the current density and the signal in the detector we can write η as:

$$\eta = 1 - 1/S \quad 8$$

which finally gives the depth precision on single particles as:

$$dh_{50} = \frac{\lambda}{\alpha^2}\left(\frac{1}{\sqrt{1 - 1/S}} - 1\right) \quad 9$$

This equation shows that the depth precision can be much better than the actual depth resolution for a good signal-to-noise ratio. In practice the signal-to-noise ratio cannot be increased without limit, due to radiation damage, differences in the local mass density of the samples, beam noise, scan noise, additional detector noise and environmental noise. In a recent publication [4] it was indeed shown that the depth precision on small objects that are well-separated in space was significantly better than the depth resolution when detected with a good signal-to-noise ratio. The depth precision on individual hafnium atoms in a silicon oxide matrix amounted to better than 0.5 nm, a factor of at least 15 smaller than dz [5].

We will discuss the actual achievable depth precision as a function of the experimental parameters and perform a statistical analysis of the required value of S as a function of the number of pixels in the object. Furthermore we will derive an expression for the relation between the depth precision and the maximal electron dose to which the sample can be exposed during the imaging before beam damage occurs. We will discuss deconvolution and 3D visualization strategies and we will present several applications and examples of 3D confocal STEM.

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