MEASUREMENT OF THE ENERGY-SPREAD CONTRIBUTION TO INFORMATION TRANSFER LIMITS IN HR-TEM

Michael A. O'Keefe*, Peter C. Tiemeijer° and Maxim V. Sidorov

*National Center for Electron Microscopy, LBNL, Berkeley, CA 94720, USA
°FEI Electron Optics, PO Box 80066, 5600 KA Eindhoven, The Netherlands
Advanced Micro Devices, P.O. Box 3453, M/S 32, Sunnyvale CA 94088, USA

MEASUREMENT OF THE ENERGY-SPREAD CONTRIBUTION TO INFORMATION TRANSFER LIMITS IN HR-TEM

Michael A. O'Keefe*, Peter C. Tiemeijer° and Maxim V. Sidorov

*National Center for Electron Microscopy, LBNL, Berkeley, CA 94720, USA
°FEI Electron Optics, PO Box 80066, 5600 KA Eindhoven, The Netherlands
Advanced Micro Devices, P.O. Box 3453, M/S 32, Sunnyvale CA 94088, USA

Sub-Ångstrom TEM of materials at intermediate voltages requires the use of techniques such as focal-series reconstruction or electron holography (until correction of spherical aberration becomes routine). Consequently, the information limit of the intermediate-voltage microscope becomes more significant than its native (Scherzer) resolution. With a Scherzer resolution of 1.7Å, but a sub-Ångstrom information limit, the one-Ångstrom microscope (OÅM) project[1] at the NCEM is able to generate resolution below 0.8Å.[2-3] This resolution comes from using the Philips/Brite-Euram computer software by Coene and Thust[4-5] to process experimental focal series of images (containing sub-Ångstrom information) obtained with a modified CM300FEG-UT. The sub-Ångstrom resolution produced by the OÅM has been used to image structures containing light atoms[1-3, 6], as well as ceramics[7] and structures within semiconductor devices.[8]

HRTEM resolution is defined by the first zero in the phase-contrast transfer function (CTF) at optimum defocus. Microscope information limit d comes from damping of the CTF by the temporal coherence envelope $\exp\{-\frac{1}{2}\pi^2\lambda^2\Delta^2\mathbf{u}^4\}$, where λ is electron wave-length, $|\mathbf{u}|$ is spatial frequency, and Δ is spread of focus. Information limit $d = \sqrt{(\pi\lambda\Delta/2)}$ is the inverse of the spatial frequency $|\mathbf{u}|$ at which E $(\mathbf{u})$ falls to $1/e^2$ (fig.1).

Spread of focus is usually estimated from $= C_C\sqrt{\{(^2(E)/E^2 + ^2(V)/V^2 + 4^2(I)/I^2\}}$.[1-3] C_C is the chromatic aberration coefficient and (E)/E, (V)/V, and (I)/I are fractional root-mean-square (rms) variations in beam energy spread, high voltage, and lens current over the time of image acquisition. However, E and V terms have contributions that add linearly as well as quadratically.[9] In practice, total beam energy spread (combined E and V terms) can be measured with a spectrometer such as a Gatan Image Filter (GIF), then computed by adding rms lens current ripple in quadrature and applying C_C. The problem is to get the best estimate of the actual energy spread from the GIF measurements. For the OÅM, GIF measurements of the beam-energy spread fall from 0.93eV FWHH at 4kV extraction voltage to 0.6eV FWHH at zero (fig.2a).

From the GIF, energy spread is $E_{GIF} = \sqrt{\{E_i^2 + V_n^2 + G_{ab}^2 + G_{psf}^2 + G_n^2\}} + G_{180} + V_r + E_B$ where E_i is the intrinsic gun spread; V_n is HT noise; G_{ab}, G_{psf}, and G_n are GIF aberrations, point-spread function and noise; G_{180} is the contribution from 180Hz stray fields; V_r is HT ripple and E_B is the Boersch contribution. The FEI ZrO_2/W Schottky gun at 1800K has intrinsic energy spread at zero extraction voltage of 0.37eV FWHH.[10] High-tension (HT) noise contributes 0.1eV, as does the HT ripple. The Boersch effect is 0.1eV at 4kV. GIF aberrations and noise each contribute 0.2eV, and the point-spread function from 2-pixel broadening is about 0.1eV at 0.05eV/pixel. 180Hz stray fields from the microscope surroundings typically contribute in the range of 0.01 to 0.05eV.

From these values, E_{GIF} is 0.60 to 0.64eV at zero extraction voltage, and 0.93 to 0.97eV at 4kV. The lower values agree with measurements from the OÅM GIF (fig.2a) allowing us to estimate the actual beam spread. At 4kV, $E_{beam} = \sqrt{\{E_i^2 + V_n^2\}} + V_r + E_B = 0.85eV$ FWHH. From this value we are able to form the rms energy spread, add it to the lens current ripple, and compute the OÅM spread of focus as 19.6Å and the information limit as 0.78Å (fig.2b). This information limit has been confirmed experimentally.[2-3] According to the above analysis, the beam energy value to be used in deriving the spread of focus for the experimental microscope beam can be estimated from the GIF measurement via $E_{beam} = \sqrt{\{(E_{GIF} - G_{180} - V_r - E_B)^2 - G_{ab}^2 - G_{psf}^2 - G_n^2\}} + V_r + E_B$.

We emphasize that our values are estimates for the NCEM OÅM and depend strongly on age and condition of the Schottky emitter[10], on microscope environment (noise and stray fields)[11], and on alignment of the GIF (especially focus and stray field compensation).
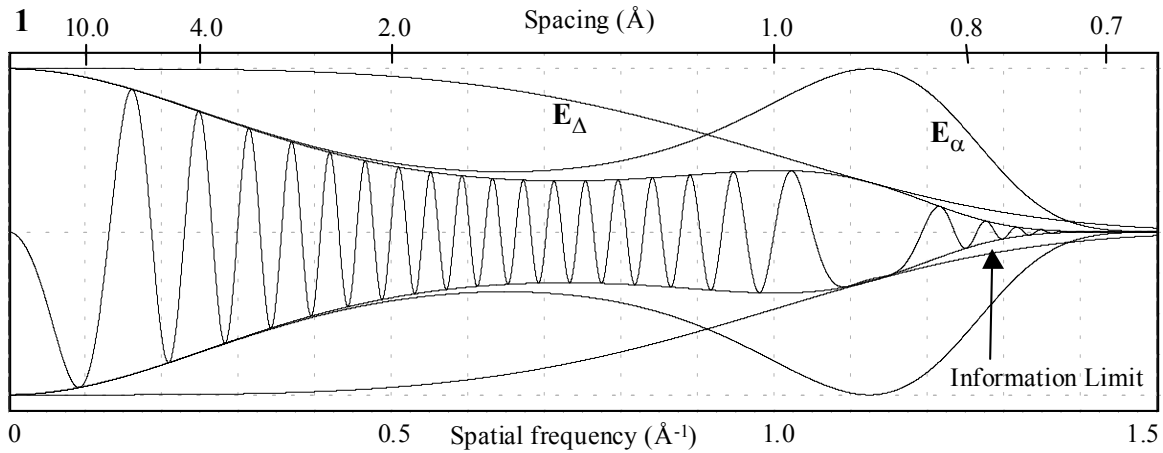
Fig.1. Phase-contrast transfer function (ctfExplorer[12]) for the OÅM at alpha-null defocus[13] for 0.89Å transfer. Spatial coherence damping (E_α) depresses mid-range frequencies. Temporal coherence damping (E_Δ) sets the OÅM information limit at 0.78Å (marked) for 20Å spread of focus (computed from the energy spread measured on the OÅM GIF).
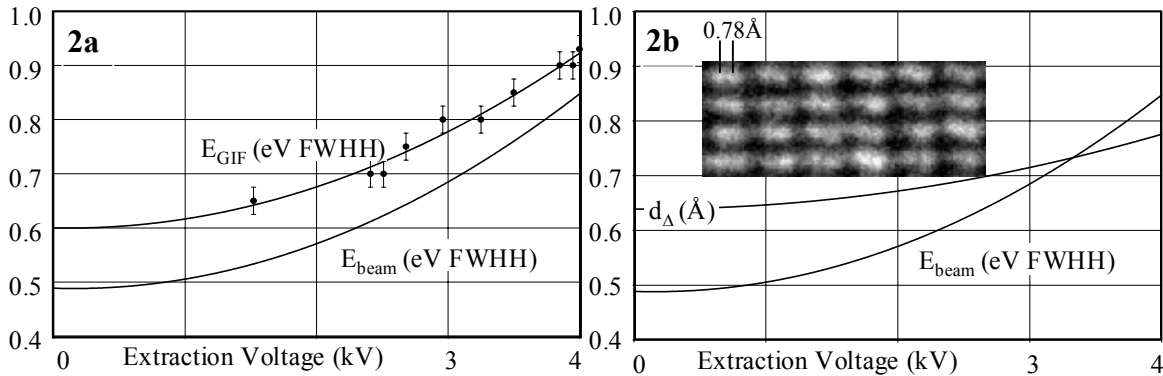

Fig.2(a) Energy spread measured on the OÅM GIF is E_{GIF} = 0.93eV at 4kV, 0.65eV at 1.5kV and extrapolates to 0.6eV at zero extraction voltage. Beam spread, computed from $E_{beam} = \sqrt{\{(E_{GIF} - G_{180} - V_r - E_B)^2 - G_{ab}^2 - G_{psf}^2 - G_n^2\}} + V_r + E_B$, is about 1eV lower.
(b) Information limit d (Å) falls from 0.78Å at 4kV to 0.72Å at 3kV. The OÅM image of silicon in [112] orientation (insert) shows the 0.784Å separation of the Si atoms.[2-3]

References
1. O'Keefe, M.A. et al. (2001) *Ultramicroscopy* **89** 4: 215-241.
2. O'Keefe, M.A. et al. (2001) *59th Ann. Proc. MSA, Long Beach, California*, 898-899.
3. O'Keefe, M.A., Nelson, E.C., Wang, Y.C., Thust, A. (2001) *Phil. Mag. B* **81**, 1861.
4. Coene, W.M.J., Thust, A., Op de Beeck, M, Van Dyck, D. (1996) *Ultramicr.* **64**, 109.
5. Thust, A., Coene, W.M.J., Op de Beeck, M, Van Dyck, D. (1996) *Ultramicr.* **64**, 211.
6. Kisielowski, C. et al. (2001) *Ultramicroscopy* **89**, 4: 243-263.
7. Ziegler, A., Kisielowski, C., Ritchie, R.O. (2002) *Acta Mat.* **50**, 565-574.
8. Principe, E. et al. (2002) to be published.
9. Tiemeijer, P.C. (1999) *Ultramicroscopy* **78**, 53-62.
10. Fransen, M.J. et al., (1999) *Advances in Imaging and Electron Optics* **III**, 91.
11. Turner, J.H., O'Keefe, M.A., Mueller, R. (1997) *55th Ann. Proc. MSA,* 1177.
12. Sidorov, M.V. (2002) *60th Ann. Proc. MSA, Quebec, Canada.*
13. O'Keefe, M.A. (2001) *59th Ann. Proc. MSA, Long Beach, California,* 916-917.

email: maok@lbl.gov