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Estimation of the Electron Beam Energy Spread for TEM Information Limit

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Sub-Ångstrom TEM of materials is becoming routine now that the techniques of focal-series reconstruction and electron holography have become available to retrieve the electron wave at the specimen exit-surface to very high resolution. A recent third advance is correction of spherical aberration. As a consequence of these developments, emphasis has shifted from microscope resolution to information limit. With a sub-Ångstrom information limit, the one-Ångstrom microscope (OÅM) project[1] at the NCEM uses a modified CM300FEG-UT with computer software[4-5] to generate resolution below 0.8Å[2-3] from experimental image series containing sub-Ångstrom information. 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 and information limit are defined for linear transfer of spatial frequencies (diffracted beams) from the specimen exit-surface wave to the image. Linear transfer is described by the familiar phase-contrast transfer function (CTF). The microscope information limit d_Δ comes from damping of the contrast transfer function by temporal coherence factors. The damping envelope is $\exp\{-\frac{1}{2}\pi^2\lambda^2\Delta^2\mathbf{u}^4\}$, where λ is electron wavelength, $|\mathbf{u}|$ is spatial frequency, and Δ is the spread of focus parameter (standard deviation of a Gaussian distribution of defocus). The information limit d_Δ is the inverse of the spatial frequency $|\mathbf{u}|_\Delta$ at which $E_\Delta(\mathbf{u})$ falls to $1/e^2$, so $d_\Delta = 1/|\mathbf{u}|_\Delta = \sqrt{(\pi\lambda\Delta/2)}$. To reach an information limit of d_Δ by focal reconstruction requires Δ to be less than $2d_\Delta^2/(\pi\lambda)$. At 300keV, spread of focus is 20Å for $d_\Delta = 0.78$Å (fig.1).

Spread of focus is usually estimated from $\Delta = C_C\sqrt{\{(\sigma^2(E)/E^2 + \sigma^2(V)/V^2 + 4\sigma^2(I)/I^2\}}$, where C_C is the chromatic aberration coefficient and $\sigma(E)/E$, $\sigma(V)/V$, and $\sigma(I)/I$ are the fractional root-mean-square (rms) variations in beam energy spread, high voltage, and lens current over the time of image acquisition[1-3]. However, the E and V terms have contributions that add linearly as well as quadratically. In practice, total beam energy spread (including both the E and V terms) can be measured with a spectrometer such as a Gatan Image Filter (GIF), then Δ 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).

Energy variation can be estimated by including all contributions – linearly or quadratically as appropriate[9]. For the GIF measurement, the expected value 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 OÅM CM300 was built to what have become Tecnai specifications for beam and lens current. For the FEI ZrO_2/W Schottky gun at 1800K, intrinsic energy spread for zero extraction voltage is 0.37eV FWHH[10]. High-tension (HT) noise contributes 0.1eV, as does the HT ripple. Boersch effect is close to 0.1eV at 4kV and to 0 at zero. GIF aberrations and noise can both contribute approximately 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 have the effect on the GIF of an apparent contribution in the range of 0.01 to 0.05eV.

At zero extraction voltage, $E_{GIF} = \sqrt{\{0.37^2 + 0.1^2 + 0.2^2 + 0.1^2 + 0.2^2\}} + (0.01 \text{ to } 0.05) + 0.1 + 0.0 = 0.60 \text{ to } 0.64$eV. At 4kV, $E_{GIF} = \sqrt{\{0.65^2 + 0.1^2 + 0.2^2 + 0.1^2 + 0.2^2\}} + (0.01 \text{ to } 0.05) + 0.1 + 0.1 = 0.93 \text{ to } 0.97$eV. In both cases, the lower values agree with the measurements from the OÅM GIF (fig.2a). This agreement allows us to form a good estimate of the actual beam spread by summing without GIF contributions. At 4kV the energy spread in the beam will be $E_{beam} = \sqrt{\{E_i^2 + V_n^2\}} + V_r + E_B = 0.85$eV 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 to be used in deriving the spread of focus can be estimated from the GIF measurement via $E_{beam} = \sqrt{\{(E_{GIF} - G_{180} - V_r - E_B)^2 - G_{ab}^2 - G_{psf}^2 - G_n^2\}} + V_r + E_B$.

It must be emphasized that the values used here are estimates for the NCEM OÅM and will depend strongly on the age and condition of the Schottky emitter[10], on the microscope environment (noise and stray fields)[11], and on the alignment of the GIF (especially focus and stray field compensation).[14]

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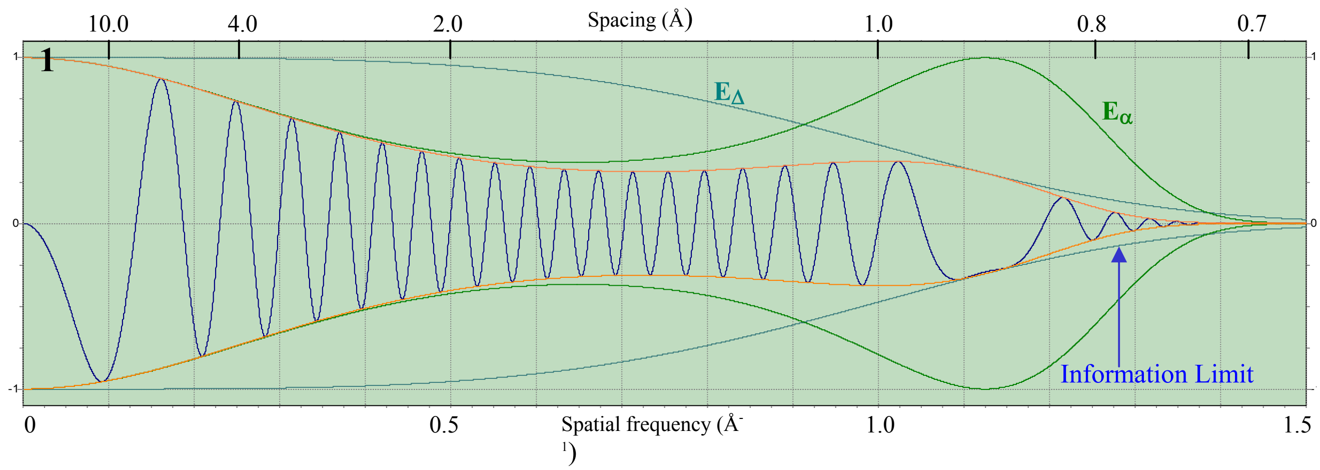

Fig.1. Phase-contrast transfer function (ctfExplorer[12]) plotted for the One-Ångstrom Microscope at alpha-null defocus[13] for 0.89Å transfer (wide band). Temporal coherence damping curve (E_Δ) shows that the OÅM information limit is 0.78Å (marked) at the 20Å spread of focus computed from the measured energy spread.

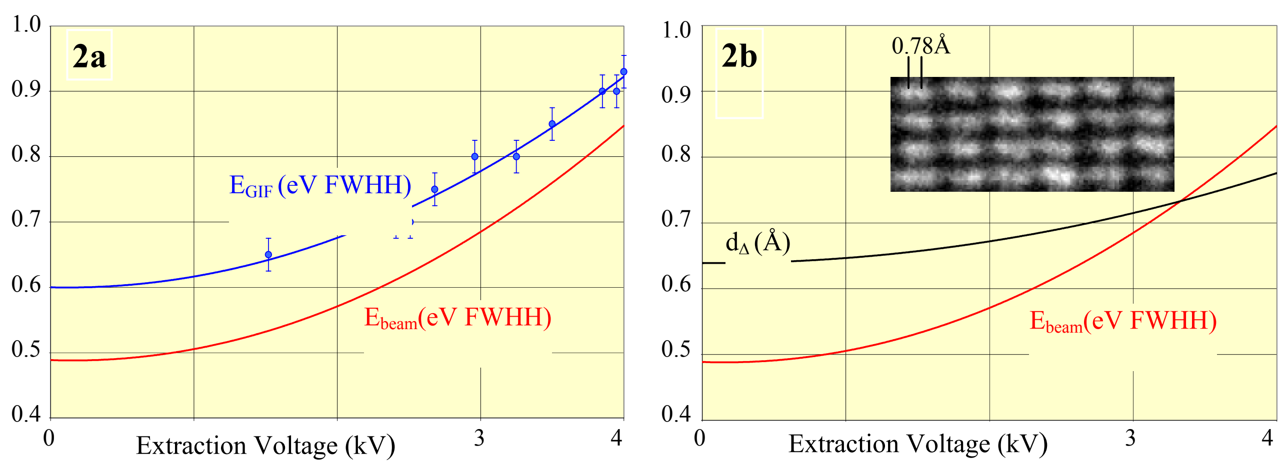

Fig.2(a) As extraction voltage is reduced, energy spread measured on the OÅM GIF falls from $E_{GIF} = 0.93$eV at 4kV to 0.65eV at 1.5kV. E_{GIF} extrapolates to 0.60eV at zero extraction voltage. Beam energy spread, computed from $E_{beam} = \sqrt{\{(E_{GIF} - G_{180} - V_r - E_B)^2 - G_{ab}^2 - G_{psf}^2 - G_n^2\}} + V_r + E_B$, is approximately 1eV lower. (b) As beam energy spread falls, information limit d_Δ(Å) falls from 0.78Å at 4kV to 0.72Å at 3kV. OÅM image of silicon in [112] orientation (insert) shows 0.784Å separation of Si atoms.[2-3]

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