THE OPTIMUM C$_S$ CONDITION FOR HIGH-RESOLUTION TRANSMISSION ELECTRON MICROSCOPY

Michael A. O'Keefe

National Center for Electron Microscopy, MSD, LBNL B72, Berkeley, CA 94720

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High-resolution electron microscopists are familiar with the concept of an "optimum defocus" for obtaining high-resolution transmission electron microscope images. Scherzer[1] recognized that it is possible to balance the phase changes imposed by the spherical aberration of the TEM objective lens by adjustments to lens defocus. Selection of this focus condition maximizes the same-phase transfer of structural information carried by electrons scattered from the specimen. The upper limit of spatial frequencies transferred with the same phase change determines the resolution of the microscope. The resolution and "optimum defocus" depend only on the electron wavelength of the microscope and the spherical aberration coefficient, C$_S$, of its objective lens. Reduction of C$_S$ is the major route to improved resolution.[2]

With the advent of electron-optical systems able to generate negative spherical aberration (usually called "C$_S$ correctors"[3]), it has now become feasible to zero-out objective lens C$_S$ in the high-resolution transmission electron microscope. Under the condition of zero C$_S$, it is possible to generate high-resolution images that are projections of the specimen charge density at a resolution determined by the defocus setting of the microscope objective lens.[4] However, instead of tuning out spherical aberration completely, it may prove experimentally advantageous to retain a small residual amount of spherical aberration in order to allow generation of the familiar "projected-potential" image that is obtained at the Scherzer defocus condition. It can be shown that there is an optimum value for the residual C$_S$ that maximizes information transfer to the best resolution and depends only on the information limit of the microscope. In analogy with the practice of speaking of the optimum defocus condition as the "Scherzer condition", this optimum C$_S$ condition could be called the "Rose-Haider condition".

Since we can adjust C$_S$, we can extend the phase contrast transfer function (CTF) crossover to any spatial frequency we wish. Thus there is no need to use the usual extended "optimum defocus" of $-\sqrt{(1.5C_S?)}$ and we can choose optimum defocus to be one Scherzer unit of $-\sqrt{(C_S?)}$ to avoid the familiar "dip" in the extended CTF. C$_S$ is optimized when the crossover of the CTF falls at the information limit of the microscope. The optimum CTF can be derived from the lens phase given by the usual $?(u) = pe?u^2 + pC_S?^3u^4/2$, where e is defocus. At crossover, $? = 0$ and we get $u^2 = -2e/(C_S?^2)$. Thus at the Scherzer defocus condition of $e = -\sqrt{(C_S?)}$, CTF crossover occurs at $u_x = \sqrt{2}C_S^{-1/4}?^{-3/4}$. On the other hand, the information limit of the microscope is determined by the temporal-coherence damping envelope, and is usually defined[5] as the spatial frequency at which this envelope drops to $1/e^2$. At the information limit, $\exp\{-p^2?^2?^2u^4/2\} = \exp\{-2\}$, giving the limit $u_? = (p??/2)^{-1/2}$. Equating u_x with $u_?$, the optimum value of C$_S$ is then given as $C_{Sopt} = p^2?^2/?$, where $?$ is the root mean square (rms) value of the (assumed gaussian) spread of focus.

The spread of focus, $? = C_C\sqrt{\{(s^2(V)/V^2 + 4s^2(I)/I^2 + s^2(E)/E^2\}}$, is computed by summing, in quadrature, rms values of high-voltage ripple, lens current ripple and the proportion of energy spread in the electron beam, then multiplying by the chromatic aberration coefficient.[5] Older FEG-TEMs often have rms ripple values of 10^{-6} (1ppm); FWHH energy spreads are 0.7eV, equivalent to rms values of s(E)=0.7/2.355=0.3eV. At the start of the NCEM one-Ångstrom microscope (OÅM) project[6], similar values for a CM300FEG/UT gave a projected $?$ of 36Å, with the CTF shown in fig.1a. The corresponding C$_S$-optimized case (fig.2a) shows same-phase transfer to 1.1Å for $C_{Sopt} = p^2?^2/? = 0.068mm$.

Recently, with lens current ripple at a negligible value of less than 0.1ppm, and an improved HT tank producing HT ripple of about 0.3ppm, OÅM beam values of 0.93eV FWHH have been measured with a GIF, representing the combined effects of HT ripple and energy spread. For negligible lens current ripple, the spread of focus is $? = C_C.s_E/E$, where s_E is the combined rms value. For the OÅM, $s_E = 0.93/2.355eV$ gives a 20Å spread of focus and an information limit of 0.78Å with focal-series reconstruction to this value.[7] A current OÅM CTF is shown in fig.1b; a C$_S$-optimized equivalent is shown in fig.2b for $C_{Sopt} = p^2?^2/? = 0.020mm$. Both figs.1b and 2b show clear transfer beyond 1Å.

Proposed C$_S$-corrected microscopes will usually be fitted with monochromators designed to reduce energy spread. With a spread of 200meV FWHH, a 300keV FEG-TEM could have a s(E)/E of 0.28ppm, which combines with the presently-attainable s(V)/V of 0.3ppm to give $?=6.2$Å, leading to an information limit of 0.44Å. C$_S$-optimized CTFs for $?=6.2$Å show clear transfer beyond 0.5Å (fig.2c). A CTF for the equivalent non-C$_S$-corrected microscope (fig.1c) shows that it does not reach the information limit at Scherzer focus (due to the minimal beam convergence of 0.1milliradian used in all the CTFs presented). However, such a microscope could follow procedures used by the OÅM, utilizing focal series to gather missing higher-frequency information out to the information limit.[5,6] The effect of beam convergence on the CTFs of C$_S$-optimized microscopes is of course negligible. By optimizing the C$_S$ of a monochromator-equipped FEG-TEM to the "Rose-Haider" condition, continuous microscopy at resolution levels beyond 0.5Å appears feasible.[8]

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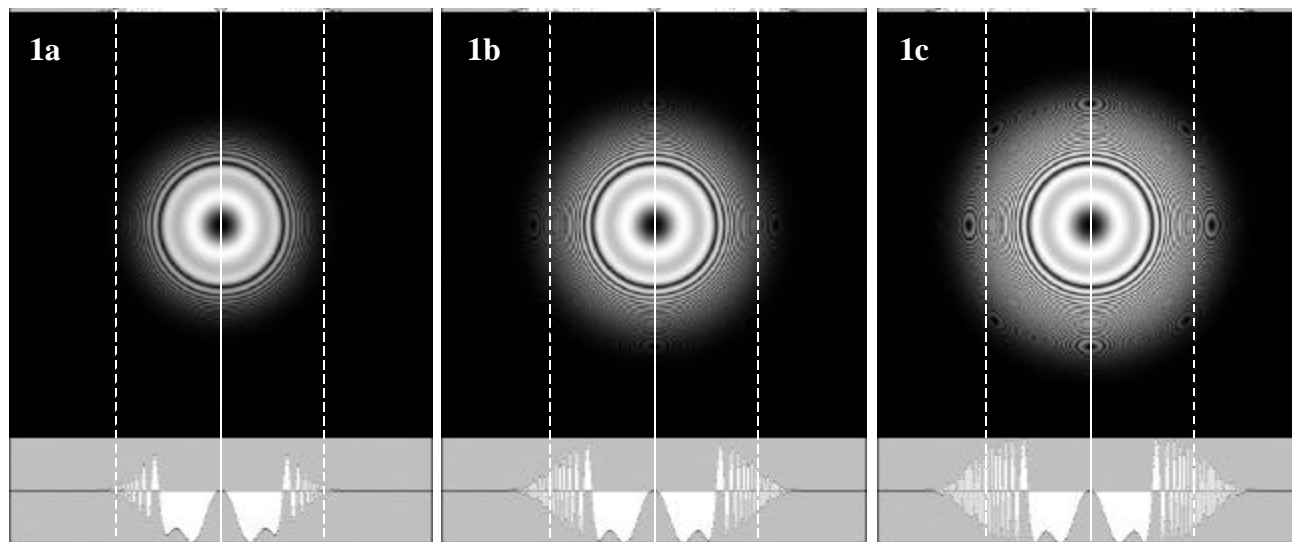
Figure 1.   Conventional FEG-TEM. All plots show the CTF below a two-dimensional intensity spectrum. Dashed lines show 1Å position. Plots for a CM300FEG-UT TEM with C_S=0.65mm at 300keV for a defocus of –430Å. (a) Typical mid-1990s spread of focus of ?=36Å, from an energy spread of 0.7eV FWHH and ripple of 1ppm, gives an information limit of 1.1Å. (b) CTF for NCEM one-Ångstrom microscope (OÅM) shows the current information limit of 0.78Å produced by a spread of focus of ?=20Å, computed from a measured 0.93eV FWHH. (c) CTF for a monochromated microscope with 200meV energy spread giving a spread of focus of ?=6.2Å and an information limit of 0.44Å.
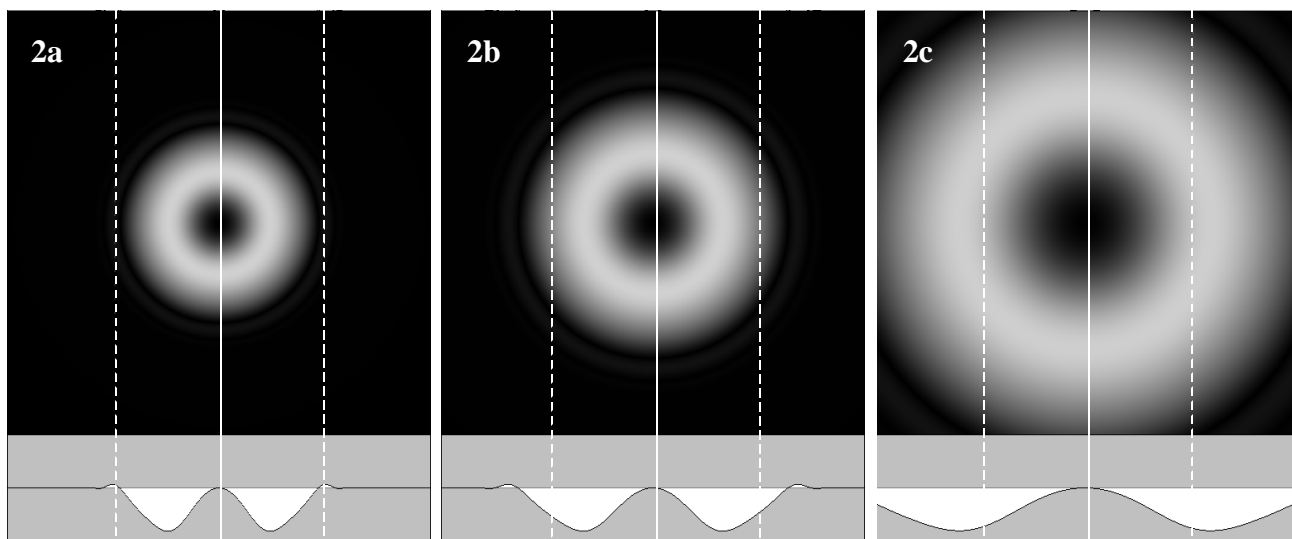

Figure 2.   Optimum-C_S FEG-TEM. Plots for hypothetical C_S-corrected TEMs with C_S set at $C_{Sopt} = p^2 ?^2/?$ at 300keV. All plots show characteristic "donut" diffractograms with same-phase transfer out to crossover at the information limit. (a) Spread of focus of ?=36Å and information limit of 1.1Å. (b) For parameters (0.93eV FWHH) corresponding to those of the NCEM one-Ångstrom microscope (OÅM) a C_S-corrected TEM has same-phase transfer to 0.78Å. (c) A mono-chromated microscope with 200meV energy spread has same-phase transfer to an information limit of 0.44Å.