HRTEM at Half-Ångstrom Resolution: from OÅM to TEAM

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Transmission electron microscopy (TEM) at sub-Ångstrom resolution is important for nano-technology. As researchers design and build artificially-structured nano-materials such as semi-conductor devices, ceramic coatings, and nanomachines that operate at the atomic level, the require-ment for "seeing" what has been built becomes more crucial. Identifying atom positions requires appropriate resolution, the ability to separate distinct objects in images [1]. Heavy (metal) atoms are routinely imaged in TEM specimens at resolutions from 2Å to 1.5Å. Better resolution (near 1Å) is required to "see" lighter atoms such as carbon [2], nitrogen [3] and lithium [4]. Scherzer resolution [5] is set by spherical aberration (C_S) to about 1.5Å for uncorrected mid-voltage TEMs, and 1Å at high-voltage (>1MV). With C_S corrected, the information limit of the TEM controls resolution.

The one-Ångstrom microscope (OÅM) project at LBNL exceeds one-Ångstrom resolution at lower voltage [6] by using a combination of a modified CM300FEG-UT with computer software [7,8] able to correct C_S and generate sub-Ångstrom images from experimental image series. Following the success of the OÅM in demonstrating that a resolution of 0.78Å is possible with this technique [9], a proposal was made to reach resolutions of 0.5Å [10]. The TEAM (transmission electron achromatic microscope) will be a TEM using hardware correction of C_S [11] with a monochromator to improve its information limit beyond that of the OÅM by improvement of the electron-beam energy spread. Correction of chromatic aberration would allow a range of electron energies to be focussed together.

Improvement of the TEM information limit, $d_\Delta = \sqrt{(\pi\lambda\Delta/2)}$, requires reduction in the spread of focus, $\Delta = C_C\sqrt{\{(\sigma^2(E)/E^2 + 4\sigma^2(I)/I^2\}}$. Here λ is wavelength, C_C is the coefficient of chromatic aberration, and $\sigma(E)$ and $\sigma(I)$ are the root-mean-square (rms) variations in the beam energy and lens current respectively. Beam energy spread (in FWHH) is $E_{beam} = \sqrt{\{E_i^2 + V_n^2\}} + V_r + E_B$, where E_i is the intrinsic gun spread, V_n is HT noise, V_r is HT ripple, and E_B is the Boersch contribution [12]. For the TEAM to reach a resolution of 0.5Å requires that its information limit be at or below 0.5Å. Extensions of methods employed (and expertise gained) in the planning and implementation of the successful OÅM project [2] have been used to determine appropriate parameters for the TEAM [13].

For the OÅM, measured energy spread [12] is 0.86eV (FWHH), giving a $\sigma(E)/E$ of 1.21ppm (rms). Lens current ripple $\sigma(I)/I$ is 0.3ppm (rms), for a spread of focus of $\Delta = 19.6$Å at $C_C = 1.45$mm, and a demonstrated information limit of 0.78Å [9]. A monochromator added to the OÅM specifications would provide an information limit of 0.55Å at an easily attained energy spread of 0.2eV. However, no amount of reduction in energy spread would be able to produce 0.50Å. At this level of energy spread, current ripple is the major contributor to the spread of focus, Δ, and a reduction in $\sigma(I)$ from the OÅM's 0.3ppm to 0.2ppm would be necessary to lower the information limit to 0.50Å (Table 1).

We can lower Δ by reducing either the energy spread or current ripple. However, reducing energy spread with a monochromator also reduces beam current. Alternatively, reduction in lens current ripple allows for much more beam current. Ideally, to allow a good beam current and have balanced contributions from energy spread and current ripple, $\sigma(E)/E$ should be at least twice the $\sigma(I)/I$; then $E_{beam} > 4.7\times10^{-3} E.\sigma(I)/I$ eV, where E is in keV. At 300keV and $\sigma(I)/I = 0.2$ppm, the balanced E_{beam} would be 280meV (Fig.1) to give 0.50Å information limit (Fig.2). Lower accelerating voltages require lower lens current ripple and correspondingly lower energy spreads (Table 1).

The table shows improvements necessary to reach 0.5Å information limit. A 300keV TEAM with the OÅM's C_C of 1.45mm would also require 0.2ppm (rms) current ripple, and would be allowed an energy spread of 0.28eV (fig.1). Of course, it is possible to move from the balance point to trade energy spread for lens current ripple. An information limit of 0.5Å can be achieved over a range of lens current ripple (fig.3). At 300kV, a lens ripple of 0.25ppm rms would require an energy spread of 0.2eV, whereas a lower lens ripple of 0.1ppm would allow an energy spread of 0.37eV and a correspondingly better beam current. Values are smaller at lower voltages (fig.3), but a reduction in lens ripple will still allow the energy spread to be increased to provide improved beam current.

Objective lens current ripple is a critical parameter, since significant gains in the allowable energy spread (and thus beam current) can be made by reducing the lens current ripple as much as possible. Requirements are not formidable; a reduction from the 0.3ppm of the OÅM to 0.2ppm provides a 0.5Å limit for a 300keV TEAM with 0.28eV energy spread. However, lens ripple in the range of 0.05ppm to 0.1ppm maximizes the energy spread at all voltages (fig.3) – to almost 0.4eV at 300keV.

A C_C corrector is not required for a TEAM to reach 0.5Å at 300keV (or 200keV). At lower voltage, a TEAM would require strict limits on energy spread to reach the targeted 0.5Å resolution. No improvement in HT ripple or noise is required to improve the information limit *per se* since the monochromator determines the energy spread in the beam. However, improved HT ripple and noise will improve the beam current statistics (number of electrons passing through the monochromator) by placing more of the electrons closer to the center of the energy-spread distribution [14].

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TABLE 1. Improvements required to reach 0.5Å information limit as TEAM voltage is lowered.

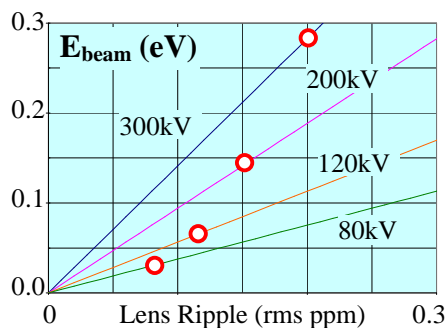| Energy (keV)	Beam spread (eV)	Lens ripple (ppm rms)	Focus spread (Å)	Info limit (Å)	Required improvement
300	0.86	0.3	19.6	0.78	current OÅM
300	0.20	0.3	9.6	0.55	200meV monochromator
300	0.28	0.2	8.2	0.50	2 in 10^7 lens ripple
200	0.15	0.14	6.2	0.49	Reduce voltage to 200kV
120	0.07	0.12	5.0	0.51	Reduce voltage to 120kV
80	0.035	0.09	3.8	0.50	Reduce voltage to 80kV

FIG. 1. Variation of balanced E_{beam} with σ(I)/I for the four accelerating voltages of 300kV, 200kV, 120kV and 80kV. 0.5Å points are marked.
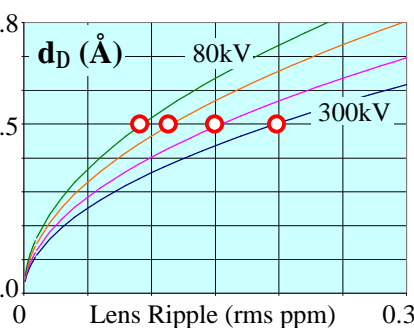
FIG. 2. Variation of information limit ($d_Δ$) with σ(I)/I for the four accelerating voltages. The 0.5Å points are marked.
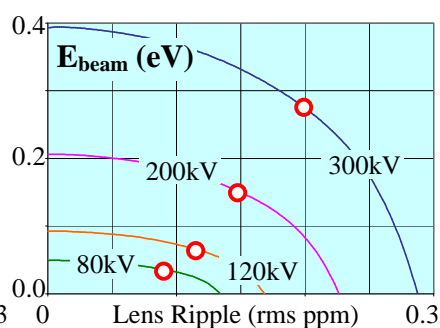
FIG. 3. Allowed E_{beam} for σ(I)/I at 0.5Å information limit and the four accelerating voltages. The balance points are marked.