

New concepts for quantifying the optical properties of modern high-resolution transmission electron microscopes

A.Thust, J. Barthel and R.E. Dunin-Borkowski

Ernst Ruska-Centre, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Email: A.Thust@fz-juelich.de

Keywords: HRTEM, aberration correction, information limit

Aberration corrected high-resolution transmission electron microscopes of the latest generation have a resolving power which reaches the sub-Angstrom regime on a routine basis. By using a monochromator or a corrector for the chromatic aberration (Cc-corrector) in addition to a corrector for the spherical aberration (Cs-corrector), sub-Angstrom resolution can be achieved not only at accelerating voltages of 200 – 300 kV, but also at substantially lower accelerating voltages below 100 kV. Based on our practical experience with the first Cs-corrected Philips CM200 prototype microscope, with a Cs-corrected FEI Titan 80-300 microscope, and very recently also with the Cs/Cc-corrected FEI PICO microscope installed at the Ernst Ruska-Centre, we find that the theoretical concepts for the description of the optical properties of such microscopes have not kept up with the rapid technical development of the recent years.

We consider here two important optical properties. First, we address the definition of the so-called information limit, which has served traditionally as a measure of the resolving power of a high-resolution microscope. Second, we address the optical stability of a microscope. While the information limit refers solely to the question of whether a certain object frequency can be transferred or not, the optical stability reflects the degree of control over the transfer of this object frequency and can therefore serve as a quality measure for the optical transfer. A comprehensive description of the performance of a high-resolution microscope is only possible by including statements about both of these complementary measures.

It is widely agreed to define the information limit $d_{\text{info}} = 1/g_{\text{info}}$ as the smallest object distance that is transferred linearly by a microscope. In recent decades, the partial temporal coherence was regarded as the dominant resolution limiting factor and it became common to set the frequency g_{info} equal to the spatial frequency g_t at which the temporal coherence envelope reaches a value of $1/e^2$ [1]. However, we showed by means of Young's-fringe measurements that linear contrast transfer can be limited by additional damping effects at spatial frequencies of $g < g_t$ [2]. Such additional damping effects, which are caused by the camera modulation transfer function and most likely also by high frequency mechanical, electrical and magnetic instabilities, can be described together by an effective product envelope with a cut-off frequency g_p . A situation where the linear contrast transfer terminates at a frequency $g_p < g_t$, and where the traditional formulation of the information limit simply as $g_{\text{info}} = g_t$ is inadequate, is presently also found on the PICO microscope. Whereas the temporal resolution limit g_t should extend up to $g_t \approx 27/\text{nm}$ at 300 kV, the true termination of the linear transfer is measured to be $g_p \approx 15/\text{nm}$, yielding a discrepancy of almost a factor of two between the familiar formulation and the measured value. If one chooses to maintain the definition of g_{info} as the termination of linear contrast transfer then a more complete formulation, which includes both temporal coherence and an effective product envelope, is:

$$g_{\text{info}} \leq \min [g_t, g_p]$$

The reason to establish a stability criterion in addition to a resolution criterion is based on the practical requirement that a microscopist should be able to acquire images using desired imaging conditions in a reproducible manner for as long as possible after the adjustment of all relevant optical aberrations. An estimate for the length of this timespan, which we refer to here as the lifetime τ of the total optical state, can be obtained by using the 2-fold astigmatism a_{22} as a representative aberration. The 2-fold astigmatism is well suited as a representative aberration for several reasons: First, the lifetime of the total optical state will in general be shorter or equal to that of the 2-fold

astigmatism state alone. Second, in contrast to the defocus, the 2-fold astigmatism is independent of small mechanical specimen movements parallel to the electron beam. Third, the 2-fold astigmatism is, in our experience, one of the most strongly fluctuating aberrations. Fourth, the 2-fold astigmatism can be monitored frequently over long time periods [3]. According to the well-accepted $\pi/4$ criterion, the maximum tolerable astigmatism deviation δ_{22} for a desired target frequency of $g_{\max} \leq g_{\text{info}}$ is $\delta_{22} = 1/(4 \lambda g_{\max}^2)$, where λ is the electron wavelength. The lifetime τ_{22} of the astigmatism state is then equal to the timespan between an initial astigmatism measurement and the earliest measurement that deviates by more than δ_{22} from the initial setting. By averaging over many independent τ_{22} values obtained either from an extended single experiment (see Fig. 1), or even from many such experiments, statistically representative average lifetime values $\langle \tau_{22} \rangle$ can be determined. The resulting average lifetime $\langle \tau_{22} \rangle$ is well suited as a benchmark parameter for the assessment of the optical stability of a microscope. We have determined the average lifetime $\langle \tau_{22} \rangle$ for various microscopes under different working conditions and have found that the $\langle \tau_{22} \rangle$ values typically lie between only a few tens of seconds and several minutes, depending on the microscope, the chosen accelerating voltage and the desired target resolution.

References

- [1] M. A. O'Keefe, Ultramicroscopy **47** (1992) 282.
- [2] J. Barthel and A. Thust, Phys. Rev. Lett. **101** (2008) 200801.
- [3] J. Barthel, A. Thust, Ultramicroscopy **111** (2010) 27.

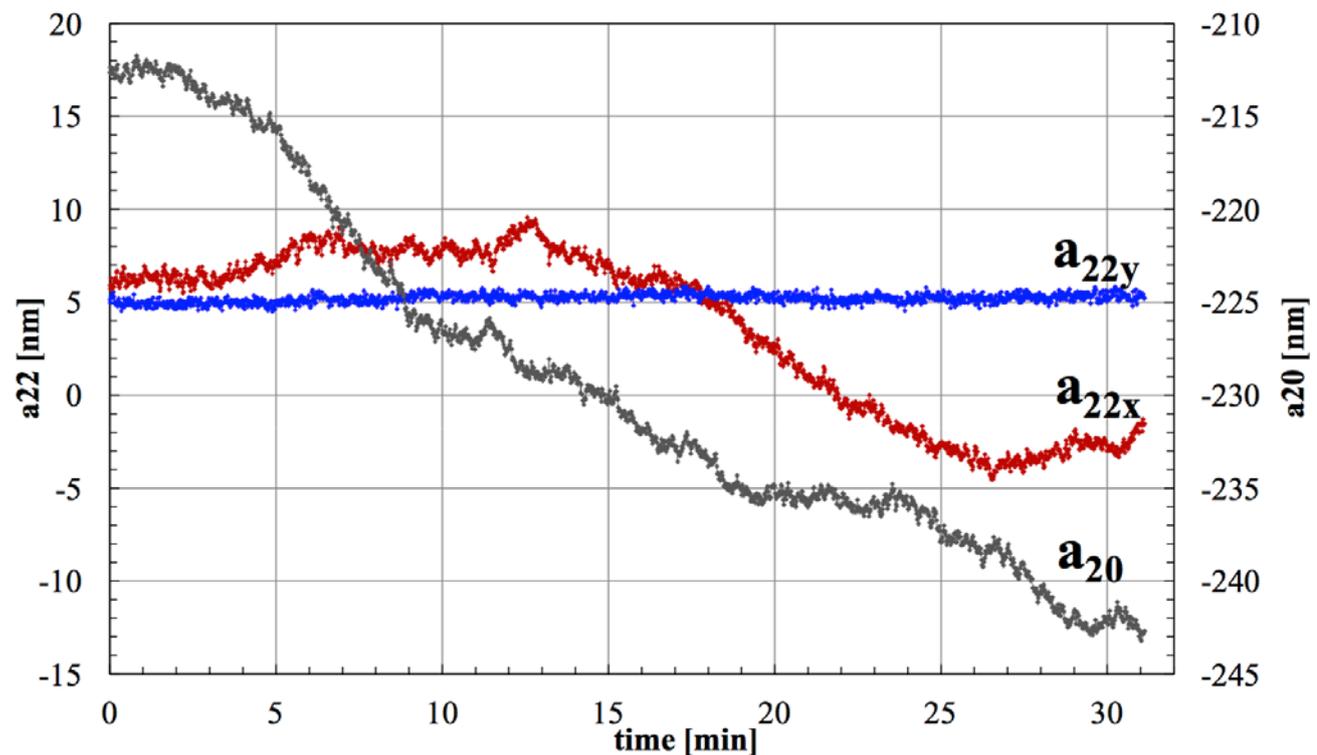


Figure 1. Long-time monitoring of the defocus a_{20} and the 2-fold astigmatism a_{22} of the PICO microscope operated at 300 kV accelerating voltage. A coupling between the strong fluctuations of the defocus a_{20} and of the astigmatism x-component a_{22x} is observable. The astigmatism x-direction coincides with the “strong” quadrupole direction of the Cs/Cc-corrector and the observed optical fluctuations can be correlated with fluctuations of the quadrupole power supplies. For a target resolution of 0.065 nm, which is equal to the information limit at 300 kV accelerating voltage, a maximum astigmatism variation of $\delta_{22} = 0.5$ nm is tolerable according to the $\pi/4$ criterion. For the half-hour measurement shown here one obtains an average lifetime of $\langle \tau_{22} \rangle = 28$ seconds.