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Strategies for Aberration Control in Sub-Angstrom HRTEM

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With the upcoming transmission electron microscopes equipped with a monochromator it is possible to access the sub-Angstrom resolution regime on a routinely basis. Apart from the high demands on the instrumental stability and on the specimen quality, the precise measurement and the correction of residual higher-order aberrations is a primary challenge in order to be able to take advantage of the extra resolution offered by such microscopes. Just in the same way as the resolution jump enabled by field emission guns in the early nineties required a precise correction of axial coma, two- and threefold astigmatism, the resolution jump enabled now by monochromators requires the control of many more aberrations than have been considered so far. A graphical overview of aberrations, which are expected to play a role in the resolution regime around 0.8 Angstrom, is given in Fig. 1.

While the introduction of a hardware corrector for the spherical aberration (C_S) yields a drastic improvement in the image quality, our experience with the C_S corrected CM200 FEG instrument installed in Jülich shows that a parallel integration and even a further development of software solutions is helpful or even necessary in order to fully overcome the aberration problem.

Firstly, the aberration measurement software, which is based on a diffractogram analysis and which is currently delivered with the CEOS hardware corrector [1], is by far not robust and precise enough for a corrector alignment aiming at a target resolution around 0.8 Angstrom. Moreover, error limits, which are traditionally given only for single aberrations (see e.g. Ref. 1) are no longer realistic in the case of a large ensemble of potential aberrations as is shown in Fig. 1. For this purpose we developed a new software suite for ultra-precise aberration measurement, which includes numerous novel insights and approaches for the recognition of diffractograms as well as a correct error propagation analysis. First experiments with the new software running in parallel with the CEOS software on the Jülich microscope show a drastic improvement by a full order of magnitude in the precision of the diffractogram recognition. Due to this essential progress in the software methodology a reliable corrector alignment for target resolutions well below one Angstrom is now possible for the first time.

Secondly, the fact that aberrations, which can be potentially corrected by hardware, may vary with time, and the fact that many higher-order aberrations cannot be corrected by hardware at all, suggest to combine an incomplete hardware correction with an a-posteriori software correction via phase-retrieval methods. A comparison of a C_S corrected image with the corresponding phase image, which was retrieved by focal-series reconstruction, is shown in Fig. 2. Apart from the improvement of the signal-to-noise ratio, the a-posteriori elimination of residual aberrations from the retrieved wave function leads to an apparent improvement of the optical quality, allowing for a direct interpretation of the atomic details belonging to the imaged defect structure [2].

References

[1] S. Uhlemann and M. Haider, *Ultramicroscopy* 72 (1998) 109.
[2] K. Tillmann, A. Thust and K. Urban, *Microsc. Microanal.* 10 (2004) 185.

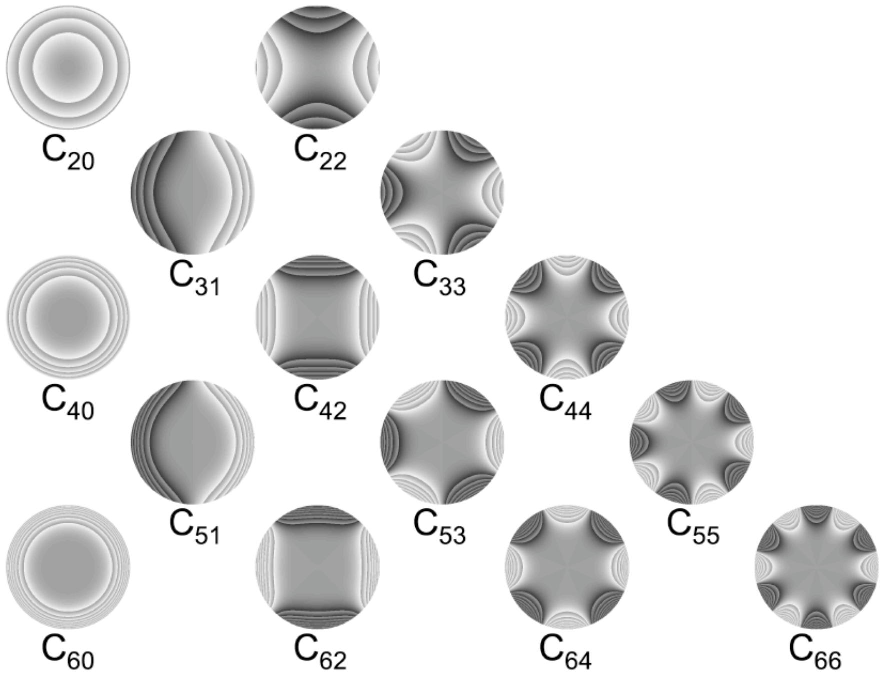

FIG. 1. Schematic wave optical display of aberrations in Fourier space up to the sixth order of the spatial frequency g. The notation C_{mn} is chosen in such a way that the index m denotes the order of the spatial frequency, whereas n denotes the rotational symmetry. Bright areas indicate a positive phase, dark areas a negative phase, discontinuities highlight multiples of π. E.g. C_{20} denotes the defocus, C_{22} the 2-fold astigmatism, C_{40} the spherical aberration, C_{mm} in general a m-fold astigmatism.

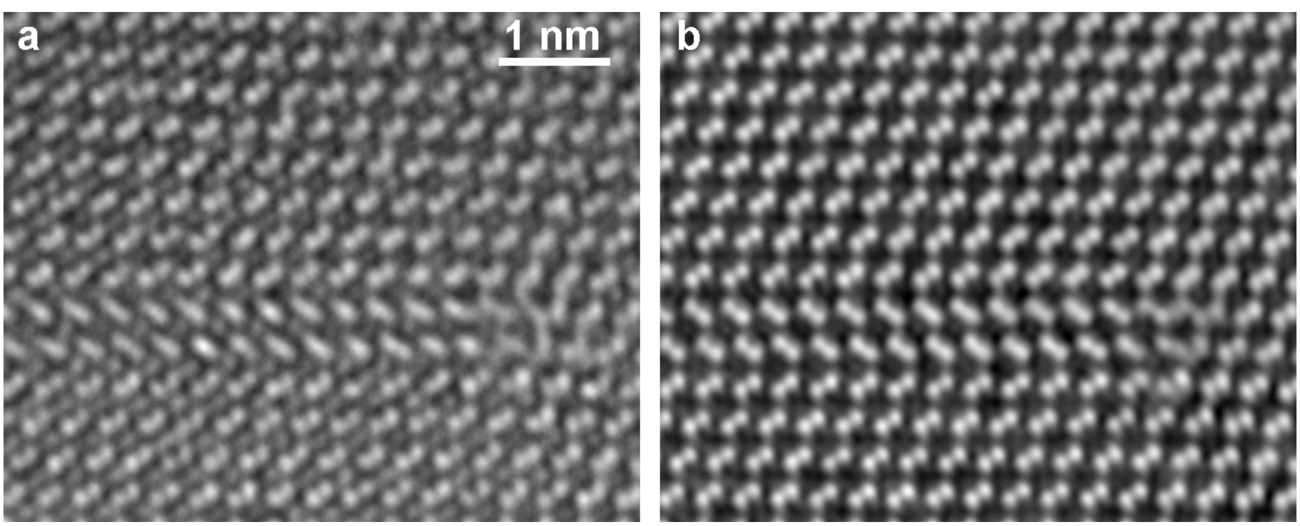

FIG. 2. (a) Image of a stacking fault in GaAs taken with a C_S corrected microscope under bright atom contrast conditions. (b) Phase reconstructed from a focal series after a-posteriori software correction of residual aberrations C_{20}, C_{22}, C_{31}, C_{33} and C_{40}. The artificial kidney-shaped distortion of the dumbbell contrast and the blurred appearance of the fault, as observed in (a), are absent in the phase.

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