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Diffractogram tableaux by mouse click

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Abstract

A computer program written in "Java" is presented, which calculates the diffractogram tableaux and the wave aberrations of electron microscopes. This program can be used interactively for alignment and measuring the optical data of any electron microscope. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Since the beginning of electron microscopy, the alignment of electron microscopes has been an important electronic and optical problem. One reason of this is obvious: it is impossible to manufacture electron microscopes with the necessary nanometer accuracy. Nowadays electron microscopes are equipped with powerful software that aligns the instruments automatically. These procedures, running in black boxes, are of course very convenient for the operator. The procedure proposed here does not claim to compete with those. It is an interactive procedure based on an understanding of the wave aberration and phase-contrast transfer function of the electron microscope. This iterative method promotes the understanding of electron microscope optics. It is "open source" and can be adjusted to satisfy users' demands. This paper can be regarded as a supplement to the early paper [1], where the so-called coma-free alignment with the aid of optical diffractograms was introduced. In that paper an optical procedure for creating diffractogram tableaux is described. At that time—a quarter of a century ago—the recording of a set of images from which the diffractogram tableau could be constructed required about 1 day of hard work, not including the laborious evaluation of the recorded data. Moreover, in the 1970s, computers were much slower and one could hardly envisage the incorporation of this digital procedure into the software of an electron microscope. The diffractogram tableau as a method was not very practical at that time. It was a method that came too early for the available technology and it took decades to become a generally accepted technique. The

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calculation of the diffractogram tableau that needed several hours in 1978 can now be performed in <1 s. We offer a "Java" computer program for calculating diffractogram tableaux. The program is available in the INTERNET [2]. It is designed to run in most common web-browsers. The speed of this program makes it practical to measure the current optical aberrations of the electron microscope by changing the parameters of the calculated diffractogram tableau step by step till it matches the appearance of the measured diffractogram tableau.

2. The idea of aligning electron microscopes using diffractogram tableaux

The only purpose of aligning and adjusting an electron microscope is to minimise its parasitic aberrations, e.g., the correction of the two-fold astigmatism is one of the first tasks one learns in electron microscopy. Every electron microscopist is familiar with the "stigmator". Nobody will doubt the necessity of this correction because two-fold astigmatism does obviously disfigure the image. But this correction alone will not provide a correct alignment if the two-fold astigmatism is caused by a beam tilt. In this case turning the knobs of the stigmator means turning the wrong knobs. The problem is to decide whether the astigmatism is caused by a deviation from the ideal rotational symmetry of the objective lens field or whether it is caused by a small tilt of the primary beam. In most cases, the two-fold astigmatism is caused by both, a beam tilt and an asymmetry of the objective lens. One may use the diffractogram tableau method to solve this problem. Modern electron microscopes should have a computer-controlled routine available, quickly showing the current diffractogram tableau of the instrument. This routine is nearly as simple as the fast Fourier transformation showing a single power spectrum. This experimental diffractogram tableau may then be evaluated and corrected by comparison with calculated diffractogram tableaux using the Java computer program described in the following paragraph.

3. The "Java" computer program

The "Java" computer program [2], named "diffractogram tableau" may be a help for electron microscopists. The electron microscopists can insert the current parameters of their electron microscope and in about 1 s, the node lines of the related diffractogram tableau are shown as a computer plot on the screen. This computer program has some essential advantages:

1. A measured diffractogram tableau can be analysed by approximating the computer plot diffractogram tableau step by step to it. Of course this needs some practice, but it can be learned quickly although there are 8 parameters, which influence the diffractogram tableau strongly and in different ways.
2. The effect of each aberration coefficient can be studied separately.
3. No mathematical effort is needed. The mathematics is hidden in the "black box" of the program, but of course the source code is available, and can be accessed by a mouse click.
4. These computer diffractogram tableaux are applicable to any electron microscope regardless of its acceleration voltage and aberration coefficients, since normalised parameters are used.
5. The "wave aberration" of the current electron microscope is shown on the screen as a phase plate rather like a geographical map [3]. The lines here are "isophases".
6. The program can be changed by any user to adapt it to his special needs.

Moreover this program can be used as a teaching aid for learning the optical behaviour of electron microscopes.

4. Demonstration and discussion of some typical diffractogram tableaux

At first, the defocus D is normalised by the so-called scherzer unit $\sqrt{C_S\lambda}$ and the space frequency R is normalised by $1/\sqrt[4]{C_S\lambda^3}$, the reciprocal of the unit glaser. Hence the tilt angle of the illumination for recording the diffractogram tableau is normalised by $1/\sqrt[4]{C_S/\lambda}$. C_S is the coefficient of spherical aberration of the objective lens and λ the de Broglie wavelength of the electrons.

Fig. 1 shows the diffractogram tableau of the electron microscope at a defocus of 1 scherzer unit. Explanations of parts of the figure are:

(a) List of parameters here all are zero except for the defocus and the tilt.
(b) The corresponding diffractogram tableau, the power spectrum in the centre shows the circular node lines associated with the oscillating phase contrast transfer function. The radius of the inner circle is $\sqrt{2}$. Note the symmetry of the diffractogram tableau with respect to the central diffractogram, this is an indication, that the electron microscope is well aligned. The power spectra at the periphery show a two-fold astigmatism and an additional defocus due to the beam tilt.
(c) Shows the beautiful axial symmetry of the wave aberration. The radius of this phase plate, the maximal normalised space frequency is 2. The grey steps show the changing values of the phase shift with increasing space frequency: the grey values are measured in units of 2π, therefore 0.4 means a phase $0.4 \times 2\pi = 0.8\pi$.

Fig. 2 shows a typical diffractogram tableau when the electron microscope is not correctly aligned. The parameters are the same as in Fig. 1 except for the axial coma constant $B = 0.5$. Explanations of parts of the figure are:

(a) This axial coma causes the "one-fold" asymmetry of the diffractogram tableau. The aberration axial coma occurs when the illuminating beam is tilted relative to the optical axis. There are several aberrations caused by tilting the beam, e.g. a defocus, a two-fold astigmatism and a shift of the image. All these aberrations can be compensated, but the axial coma due to beam tilt remains. The axial coma disfigures the image, although it does not influence the central power spectrum. This demonstrates the necessity of recording images with tilted illumination and calculating diffractogram tableaux. If such a one-fold asymmetry of the diffractogram tableau occurs, a realignment is absolutely imperative. The necessary stepwise alignment procedure is described in the paper [4].
(b) Shows the accompanying wave aberration. The wave aberration shows also the one-fold asymmetry. The red zone indicates that the wave aberration is running out of range, phase $\geqslant 4.4\pi$.

Fig. 3 shows a typical diffractogram tableau obtained experimentally. Electron microscopes are afflicted more or less by a series of different aberrations. The parameters used in Fig. 3 are:

Defocus	$D = 2.7$
Two-fold astigmatism	A2 = 0.23
Azimuth of two-fold astigmatism (deg)	alfa2 = −88
Radius of the tableau	tilt = 1.1
Axial coma	B = 0.68
Azimuth of axial coma (deg)	beta = −75
Three-fold astigmatism	A3 = 0.06
Azimuth of three-fold astigmatism (deg)	alfa3 = 13.

Explanations of parts of the figure are:

(a) the diffractogram tableau and
(b) the wave aberration.

The three-fold astigmatism is also visible in the diffractogram tableau but not in a single member, e.g., the central power spectrum. The three-fold astigmatism can be corrected by a hexapole-field that can be realised either by a dodecapole (twelve-pole) element or by the usual octopole stigmator, adding appropriate currents to produce a three-fold field [5].

5. Conclusion

The use of diffractogram tableaux for measuring and correcting electron-optical aberrations is essential for achieving high-resolution images with modern electron microscopes. The diffractogram

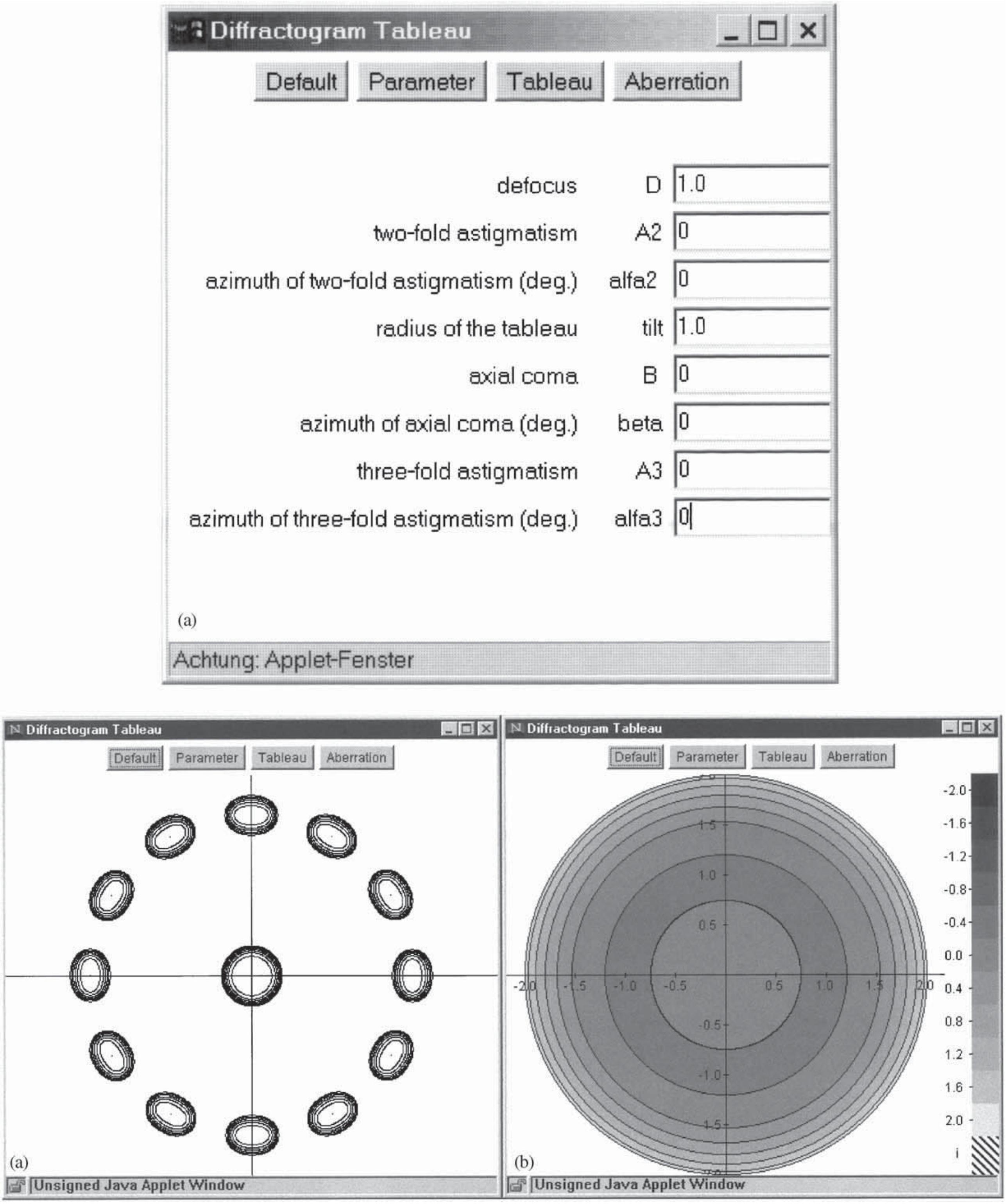

Fig. 1. (a) Optical parameters of an image recorded at defocus 1 scherzer unit, which are just the parameters of the diffractogram tableau and the wave aberration shown in (b) and (c).

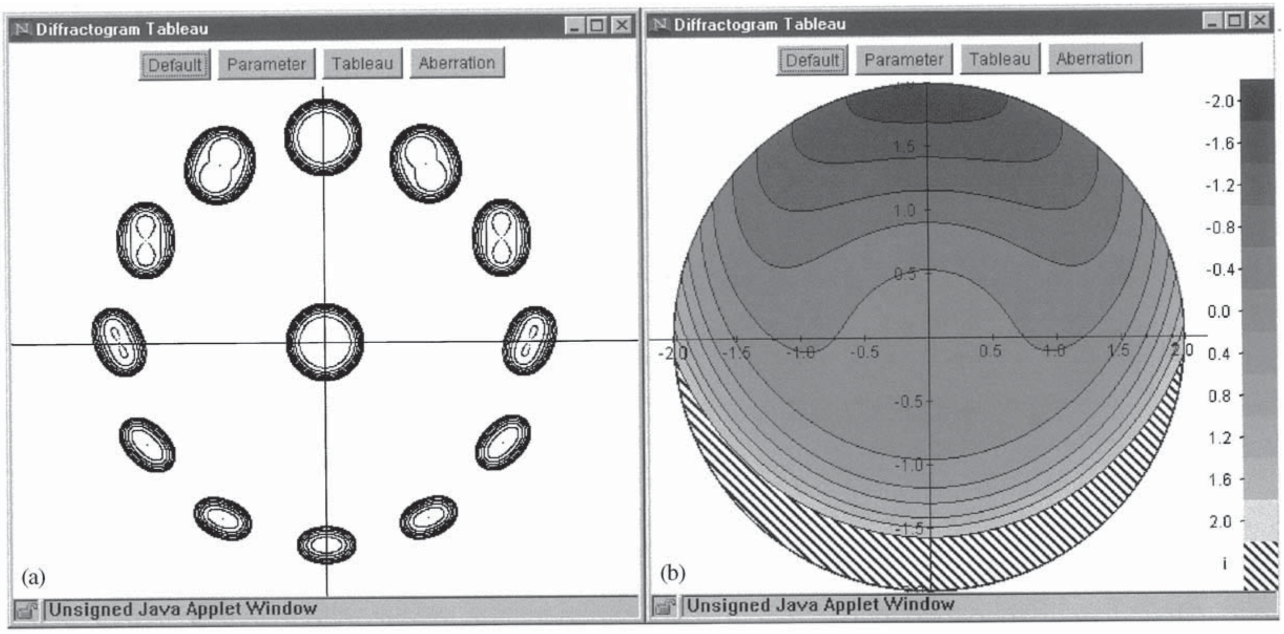

Fig. 2. (a,b) Diffractogram tableau and the wave aberration at defocus 1 scherzer unit for a misalign electron microscope. The beam tilt causes in this case an axial coma $B = 0.5$.

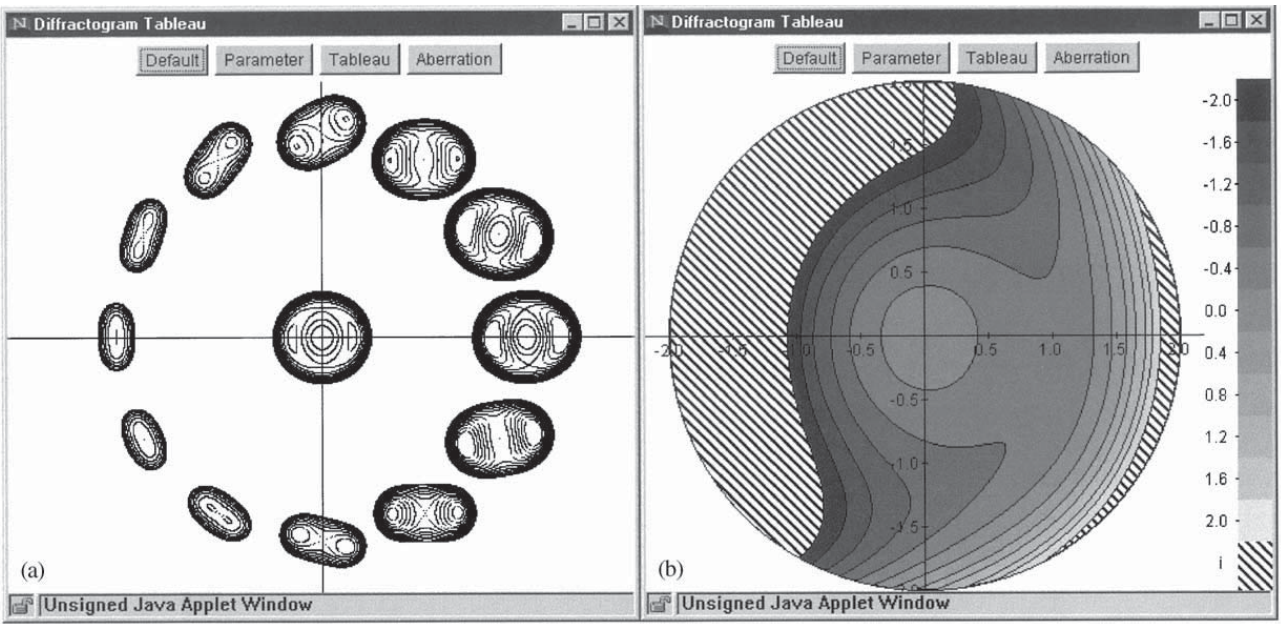

Fig. 3. (a,b) The diffractogram tableau and the wave aberration of an electron microscope that we found in practice before the correct alignment. These parameters determined from the diffractogram tableau, we put as defaults.

tableau method is now recognised as a powerful tool. A highlight of the application of diffractogram tableaux was the measurement of the optical characteristics of the first electron microscope corrected for the spherical aberration [6]. Although instrumental alignment is more conveniently performed by a computer routine designed for this task, the study of diffractogram tableaux is important to understand how such alignment can be achieved. These tableaux will be valuable elements in training courses for electron microscopists. More information in this field of aberrations of electron microscopes is described in Refs. [3,5–9].

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