AUTOMATIC ANALYSIS OF DIFFRACTION FRINGE PATTERNS IN ELECTRON MICROSCOPY

M. Blunck
Bremer Institut für Betriebstechnik (BIBA)
University of Bremen
P.O. Box 330440
West Germany

A method for the analysis of transmission electron microscopy diffractograms for determination of the phase contrast transfer function (PCTF) is presented. This is accomplished by pattern recognition methods together with a nonlinear regression method using apriori knowledge about diffractogram shapes and results in an automatic computation of defocus and astigmatism parameters. Other applications, e. g. for Interferometry fringe analysis is possible, whenever the fringes can be described in a similar way.

INTRODUCTION

The imaging process in Electron Microscopy can be described in terms of the Linear Optical Transfer Theory[1] by means of the optical transfer function of the whole system or it's Fourier transform. For weak-phase objects following equation for the wave function holds (for the one-dimensional case) [2]

$$\begin{aligned}\Psi_{(x)} &= \left\{\left[\left(\Phi_{0(x)} \otimes exp\left(-\frac{ikx^2}{2\delta f}\right)\right)\right.\right.\\ &\qquad \left.\left.\otimes\, exp\left(-\frac{ikx^2}{2z}\right)\right] exp\left(\frac{ikx^2}{2f}\right)\right\}\\ &\qquad \otimes\, exp\left(-\frac{ikx^2}{2z_i}\right)\end{aligned}$$

where the first term represents the object function, the second the defocus effect, the third the path to the lens, the fourth the lens itself, and the fifth the path to the image plane.

The relationship between the two-dimensional object function and the image function can also be described in the Fourier domain by a linear operator [3].

$$\begin{aligned}\Phi_{i(\mathbf{r})} &= H\left\{\Phi_{0(\mathbf{r})}\right\}\\ &= H\left\{\int \Phi_{0(\mathbf{r}')}\delta(\mathbf{r}-\mathbf{r}')d\mathbf{r}'\right\}\\ &= \int \Phi_{0(\mathbf{r}')} H\delta(\mathbf{r}-\mathbf{r}')d\mathbf{r}'\end{aligned}$$

where δ is the delta function and $H\{\delta(\mathbf{r}-\mathbf{r}')\}$ is the system's PSF.

Provided that the system is linear and space-invariant it follows that

$$\Phi_{i(\mathbf{r})} = \int \Phi_{0(\mathbf{r}')} \cdot k(\mathbf{r}-\mathbf{r}')d\mathbf{r} = \Phi_{0(\mathbf{r})} \otimes k(\mathbf{r})$$

or

$$\Phi_{I(\mathbf{u})} = \Phi_{0(\mathbf{u})} \cdot K_{(\mathbf{u})}$$

in the Fourier Domain, where $K_{(\mathbf{u})}$ is the optical transfer function of the system. By deconvolution, the object function can be separated from the PSF, which gives the relation between object and image function for all spatial frequencies.

According to Scherzer[4], following relation between aperture and defocus holds for weak-phase objects

$$K_{(\vartheta)} = exp\left[-\frac{2\pi i}{\lambda}\left(\frac{\delta f}{2}\vartheta^2 - \frac{c_s}{4}\vartheta^4\right)\right]$$

where ϑ is the diffraction angle, δf the defocus and c_s the aperture coefficient of the lens.

This equation must be further extended due to the only partial coherent illumination in the high resolution area and the energy distribution of the electron bean, which produces the chromatic error.

$$K'_{(\vartheta)} = K_{(\vartheta)} \cdot G_1(c_c(\Delta U, \Delta I)) \cdot G_2(\alpha_B)$$

The transfer function for weak-phase contrast is then given by [5]

$$\begin{aligned}K_{ph} &= -2sin\left[\frac{\pi}{2}\left(c_s \cdot R^4 \cdot \lambda^3 - \delta f \cdot R^2 \cdot \lambda\right)\right]\\ G_1 &= exp\left[-\left(\frac{\pi}{4(ln2)^{1/2}} \cdot c_c\lambda R^2 \cdot \frac{\Delta U}{U}\right)^2\right]\\ G_2 &= \left[1 + \left(\pi k\frac{T}{2.45E_b} \cdot c_c\lambda R^2\right)^2\right]^{-1}\end{aligned}$$

For the Philips EM301 ($c_s = 3.4mm, c_c = 3.1mm, \frac{\Delta U}{U} = 3 \cdot 10^{-6}, U = 100kV, T = 2800K$) the transfer function for $\delta f = 112$ is shown in Figure 1. The oscillation of the PCTF with spatial frequency yields positive or negative contrast for object details having different spatial frequency ranges, so electron micrographs at high-resolution are not easy to interpret. Especially annoying is the lack of image details which spatial frequencies fall onto the zero-crossings of the PCTF. This can be overcome by construction of inverse filters for amplitude and

AVC 1988 doi:10.5244/C.2.37

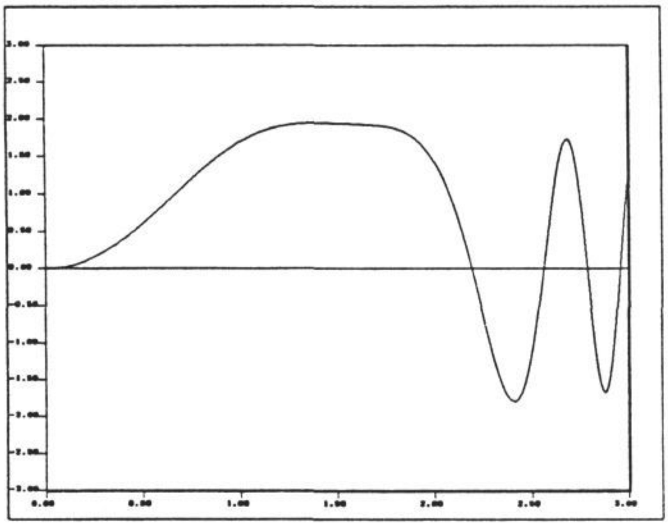

Figure 1: *PCTF of Phillips EM301,* $\delta f = 112$

phase [6], which has been done at the Dept. of Physics at the University of Bremen [7,8]. The first step in this procedure is the precise determination of defocus for all azimuth angles.

ACQUISITION OF FRINGE DATA POINTS

A typical Thon-Diffractogram [9] of a carbon foil is shown in Figure 2. The elliptical fringes represent different PCTFs for all azimuth angles [7]. In case of no axial astigmatism the fringes would be circles. In general, the images are noisy and the fringes are not closed. Fourier transform approaches have been tried but the results turned out difficult to interprete and the method itself is time-consuming. For this reasons, a local approach in the spatial domain has been choosen:
Projections of the image in x and y produce histograms which are smoothed first by standard moving average methods. Then, from their maxima the centre of the concentric fringe system is calculated. Profiles through the centre are taken, using alternatively a two-dimensional average, respectively some sort of 'tangent' operator, see Figure 3. The resulting histograms are evaluated for the minima, which give the limits for the application of a center-of-gravity operator which is applied to the non-smoothed data to determine the center line of the fringe. Its output is labeled with respect to the fringe number. At last, the corresponding x and y coordinates in the images are computed from the labeled output.
Now, a set of data points representing center lines of fringes is available and can be used for fitting.

APPROXIMATION OF QUADRATIC CURVES

Given a quadratic function:

$$f_{x,y} := c_1 x^2 + c_2 xy + c_3 y^2 + c_4 x + c_5 y - 1 = 0$$

with

$$z^i := \left[x_i^2, x_i y_i, y_i^2, x_i, y_i\right]^T$$

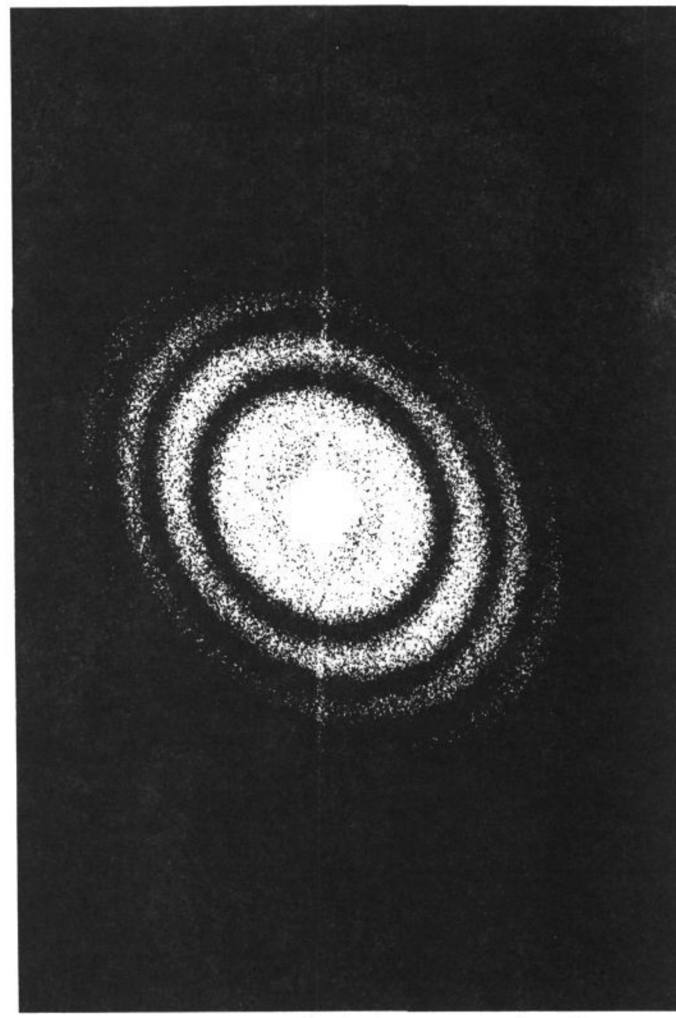

Figure 2: *Thon-Diffractogram of a carbon foil*

as the data vector and

$$c^n := [c_1^n, c_2^n, c_3^n, c_4^n, c_5^n]^T$$

the coefficient vector for which

$$\sum_{i=1}^{n} (1 - c^T \cdot z^i)^2$$

must be minimized, i.e.

$$\frac{\partial f}{\partial c} = 2 \sum_{i=1}^{n} \left[(1 - c^T z^i)(-1) z^{i^T}\right] = 0$$

hence

$$\sum_i z^{i^T} = \sum_i (c^T z^i) z^{i^T} = c^T (\sum_i z_k^i z_l^i)_{k,l}$$

Let

$$A := \begin{pmatrix} z^1 \\ . \\ . \\ . \\ z^n \end{pmatrix} = \begin{pmatrix} x_1^2 & x_1 y_1 & y_1^2 & x_1 & y_1 \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ x_n^2 & x_n y_n & y_n^2 & x_n & y_n \end{pmatrix}$$

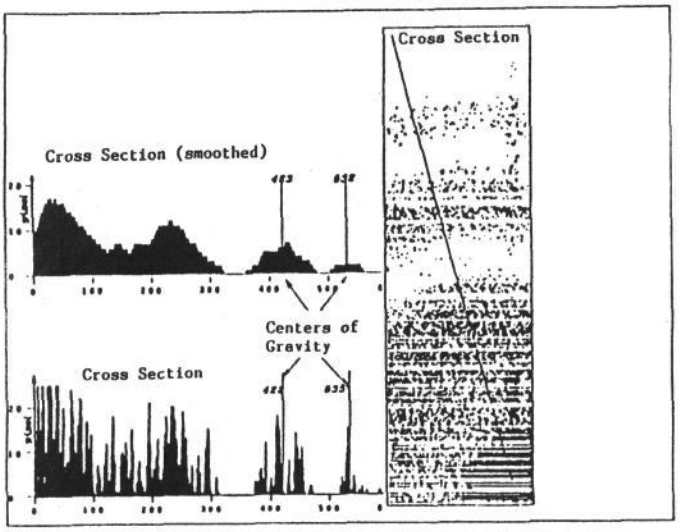

Figure 3: *Cross section through fringe pattern, determination of center lines*

and $B := A^T \cdot A$, then

$$\sum_i z_k^i z_l^i = \sum_i a_{ik} a_{il} = \sum_i a_{ki}^T a_{il}$$

and

$$\sum_i z^{i^T} = c^T B \Rightarrow \sum_i z^{i^T} B^{-1} = c^T$$

Since $B^T = B$, transposing results to

$$(B^{-1})^T \cdot \sum_i z^i = B^{-1} \cdot \sum_i z^i = c$$

Let

$$Z := \sum_i z^i = \begin{pmatrix} \sum x^2 \\ \sum xy \\ \sum y^2 \\ \sum x \\ \sum y \end{pmatrix}$$

Then for n datapoints
$c^n = B_n^{-1} Z^n =$

$$\begin{pmatrix} \sum x^4 & \sum x^3y & \sum x^2y^2 & \sum x^3 & \sum x^2y \\ \sum x^3y & \sum x^2y^2 & \sum x^2y^3 & \sum x^2y & \sum xy^2 \\ \sum y^2x^2 & \sum x^2y^3 & \sum y^4 & \sum y^2x & \sum y^3 \\ \sum x^3 & \sum x^2y & \sum xy^2 & \sum x^2 & \sum xy \\ \sum x^2y & \sum x^2x & \sum y^3 & \sum yx & \sum y^2 \end{pmatrix}^{-1}$$

$$\cdot \begin{pmatrix} \sum x^2 \\ \sum xy \\ \sum y^2 \\ \sum x \\ \sum y \end{pmatrix}$$

The matrix inversion is done by a modified Gauss-Jordan algorithm.

DEFOCUS CALCULATION

The last step is the assignment of the fitted curves with the corresponding defocus parameter. For this reason, first the intersections of the scanning profile with the determined curves are calculated and transformed to corresponding lengths in the image.
The PCTF is zero for disappearing sinus arguments, i.e. for $0.\pi, 2\pi \ldots$ Hence,

$$\delta f = c_s \cdot R_n^2 \lambda^2 - \frac{2n}{R_n^2 \lambda} \qquad n = 0, 1, 2, \ldots$$

for the period length $R = \lambda \frac{f}{x} V$, where λ is the wavelength of the laser used for diffraction (632.8 nm), f is the focal length of the diffraction device (1125 mm), and V is a combined magnification factor for the whole chain EM - diffraction device - scanner, which is calibrated by integration of a ruler in a test image.

Figure 4: *Ellipse fitting without use of center coordinates, ten datapoints used for approximation*

IMPROVEMENTS FOR ELLIPSE FITTING

In general, the approximation procedure does not guarantee for a special curve (e.g. an ellipse). Instead, for some sets of data points, better fitting hyperbolas are found. This can be overcome by using the known centre coordinates of the ellipses to replace two coefficients and the solution gets even smaller:

$$c^n = \begin{pmatrix} \sum(x^2 - 2xx_c) \\ \sum(xy - xy_c - x_c y) \\ \sum(y^2 - 2yy_c) \end{pmatrix} \cdot \begin{pmatrix} c_1 & c_2 & c_3 \end{pmatrix}$$

where the c_i are the columns

$$c_1 = \begin{pmatrix} \sum(x^2 - 2xx_c)^2 \\ \sum(x^2 - 2xx_c)(xy - xy_c - x_c y) \\ \sum(x^2 - 2xx_c)(y^2 - 2yy_c) \end{pmatrix}$$

$$c_2 = \begin{pmatrix} \sum(x^2 - 2xx_c)(xy - xy_c - x_c y) \\ \sum(xy - xy_c - x_c y)^2 \\ \sum(y^2 - 2yy_c)(xy - xy_c - x_c y) \end{pmatrix}$$

$$c_2 = \begin{pmatrix} \sum(x^2 - 2xx_c)(y^2 - 2yy_c) \\ \sum(y^2 - 2yy_c)(xy - xy_c - x_c y) \\ \sum(y^2 - 2yy_c)^2 \end{pmatrix}$$

The same procedure is recommended if only a part of an elliptical fringe is present. In this situation, often a hyperbola is found, or the best fitting ellipse is not the desired one, see Figure 5 and Figure 6.

SYSTEM REQUIREMENTS

The images have been taken by a high-resolution (2048 pixels) CCD-line scanner, which was also used for character recognition purposes and therefore produced a binary image. The run-length encoded image was transmitted to a UNIX workstation were final processing took place. Sometimes transmission errors occured, which resulted in wrong decoding of image parts. The method is resistant to such errors.

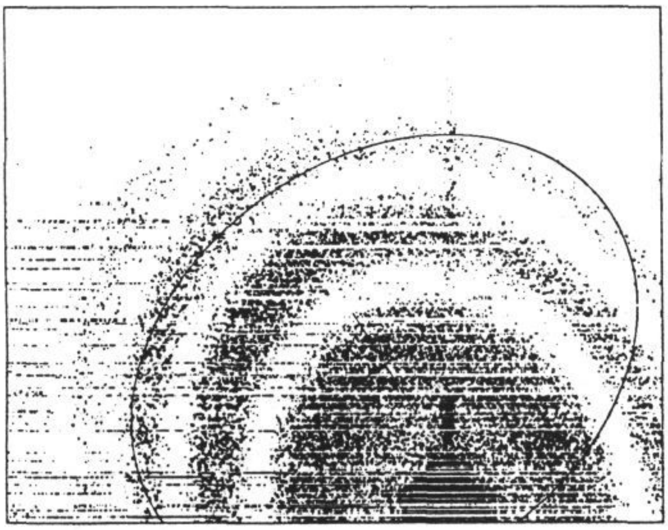

Figure 5: *Ellipse fitting using only six datapoints from the upper left part*

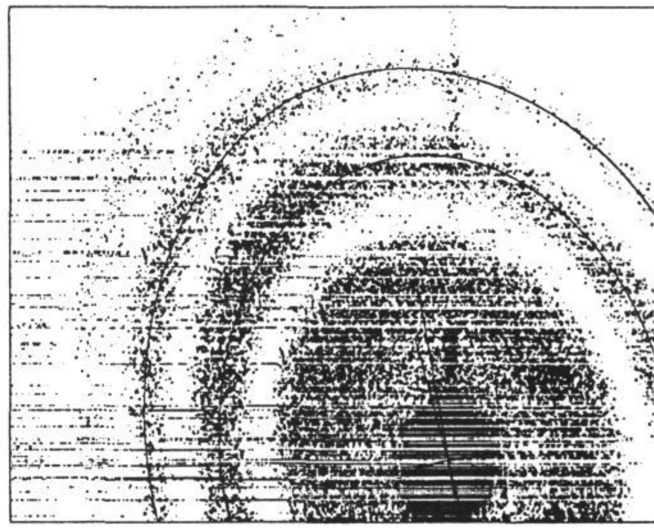

Figure 6: *Ellipse fitting using six datapoints from the upper left part and center coordinates*

SUMMARY

In contrast to other methods [10,11], the presented method can only process fringe patterns which can be described by quadratic functions. But this can be done very quickly, fully automatic, on noisy data, and with a high accuracy which stems from the knowledge about the class of curves to approximate.

REFERENCES

1. Hanszen, K.-J. "The optical transfer theory of the electron microscope: Fundamental principles and applications" in: *Advances in optical and electron microscopy* (R. Barer, V.E. Coslett, Eds.), Acad. Press NY, (1971).

2. Bethge, H., Heidenreich, J. (Eds.) *Elektronenmikroskopie in der Festkörperphysik* , Springer, (1982).

3. Andrews, H. C. *Computer techniques in image processing* , Acad. Press NY, (1970).

4. Scherzer, O. "The theoretical resolution limit of the electron microscope" *J. Appl. Phys* **20** (1949) pp. 20-29.

5. Formanek, H., Knapek, E. *Ultramicroscopy* **4** (1979) pp. 77-.

6. Halioua, M. et al. "Attainment of improved high-resolution electron microscopy images with gapless flat transfer functions" *Optik* **44** (1975)

7. Block, H., Boseck, S. "Bildgütekriterien und ihre Anwendung auf dünne Phasenobjekte im Elektronenmikroskop" *Optik* **75** No. 1 (1986) pp. 1-7.

8. Block, H. "Zur komplexen Phasenfilterung im kohärent optischen Prozessor *Optik* **78** No. 3 (1988) pp. 108-110.

9. Thon, F. in: *Electron Microscopy in Material Science* (U. Valdré, Ed.), Acad. Press NY, (1971).

10. Funnell, W. R. J. "Image processing applied to the analysis of interferometric fringes" *Appl. Opt.* **20** (1981) pp. 3245-3250.

11. Robinson, D. W. "Automatic fringe analysis with a computer image-processing system" *Appl. Opt.* **22** (1983) pp. 2169-2176.