

Determination of Electron-Microscope Parameters using a Neural Net

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Off-Axis-Electron-Holography [1] has proven a powerful tool in high-resolution electron microscopy, because it supplies the information for after the fact aberration correction by computer.

The process of image generation in electron optics can be described by mean of the complex wave transfer function $\exp(i\chi(\vec{q}))$ in Fourier space. The object wave $o(\vec{r}) = a(\vec{r})e^{i\phi(\vec{r})}$, in Fourier space described by $O(\vec{q}) = FT(o(\vec{r}))$, with space frequency \vec{q} and FT the Fourier transformation, is distorted in the image plane. The image wave originates from $B(\vec{q}) = e^{i\chi(\vec{q})}O(\vec{q})$ resulting in the real space image wave $b(\vec{r}) = FT^{-1}(B(\vec{q}))$. In electron holography, the complex image wave $b(\vec{r})$ is available, therefore, the object wave can be reconstructed if the wave transfer function is known.

There are different ways to find the transfer function. In crystalline specimens, the method of analysing crystal reflections [2] looks promising to find the coefficients of the transfer function. In the case of an amorphous and thin specimen, the analysis of the diffractogram is well established [3]. If the assumption of weak phase objects holds, the intensity distribution $I_d(\vec{q})$ in the diffractogram is described by

$$I_d(\vec{q}) = \sin^2(\chi(\vec{q})).$$

There are some well known techniques [4] to detect the parameters of the transfer function by analysing the intensity. The pitfall is that none of this processes uses all the information available in the diffractogram, and therefore, the optimum precision is not reached.

We investigated the application of neural networks to determine the wave transfer function. To concentrate the information, the intensity of the diffractogram is projected into the space $S = \text{span}(S_1 \dots S_n)$, with the basis vectors $S_i(q)$ (fig. 1) and the scalar product

$$\langle A, B \rangle = \int_{q=0}^{q=q_{\max}} A(q)B(q) dq.$$

The resulting scalar products $P_i = \langle I_d, S_i \rangle$ contain most of the information in the diffractogram and are used as input in a fed-forward neural net.

During training of the network, simulated diffractograms resulting from well known transfer functions are projected on S and fed to the net. The a-priori known result is fed back to the used backpropagation neural network to train the interconnections of the neurons. After some thousand training cycles, the net responds to the input signal in the correct way.

We trained the net with a defocus D_z in the range $D_z \in \{160 \dots 180 \text{ nm}\}$ and a spherical aberration C_s in the range $C_s \in \{1.5 \dots 1.6 \text{ mm}\}$. After training, we tested the output of the net with new simulated diffractograms, not part of the trainingset. The difference between output

of the net and simulation parameter C_s , is plotted over the absolute value of D_z and C_s of the input. The resulting error is shown in figure 2. In the central region, the error in C_s is below $10\mu\text{m}$. At the border of the training area, the error is larger due to the typical fact in neural net behaviour that they are good for interpolation but worse in extrapolation.

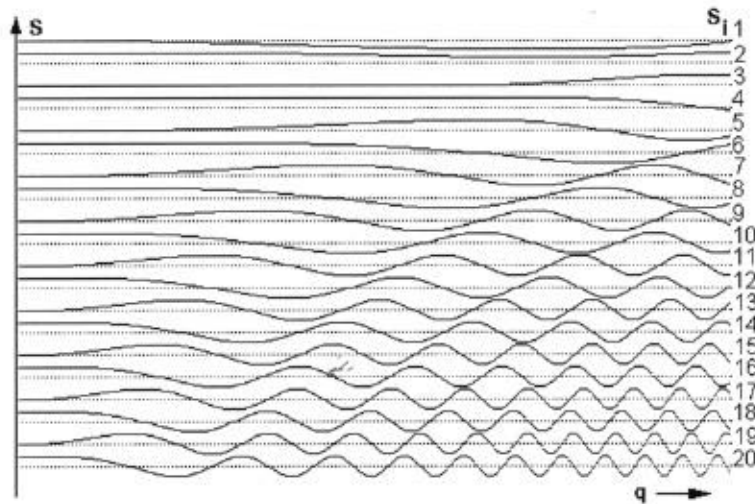


Fig. 1: Basis system for analysis of diffractograms. The set of 20 basisvectors was used as a mathematical coordinate system to reduce the input space of the neural network

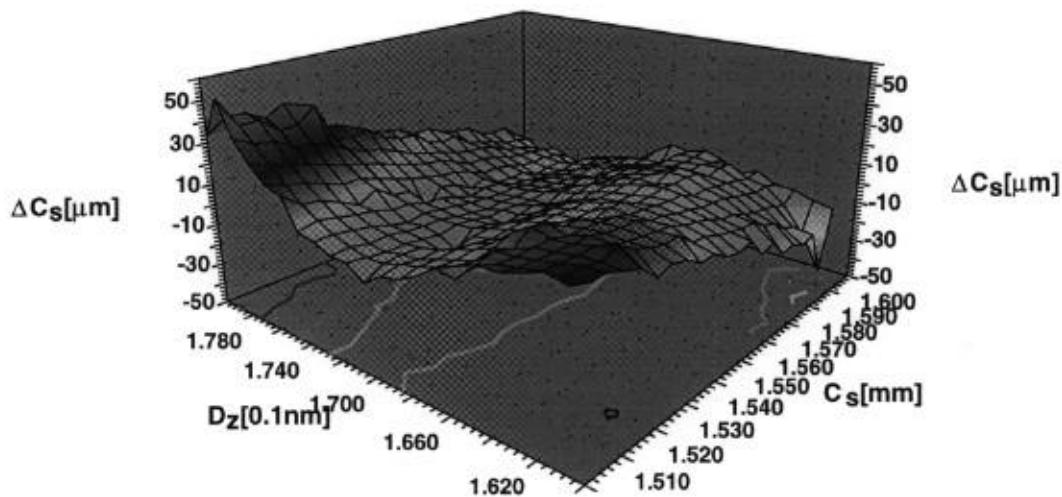


Fig. 2: The error of the neural net determining spherical aberration. In the center of training the error surface is nearly flat and with an error below 0.01mm .

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The financial support obtained from DFG is gratefully acknowledged.