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Inversion of dynamic scattering: Determination of local object thickness and orientation

K Scheerschmidt

Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle (Saale), Germany; schee@mpi-halle.de

ABSTRACT: Electron microscope structure analysis is usually based on the trial-and-error image matching between simulated contrasts and the experiment. A quantitative analysis requires the accurate knowledge of the local thickness and orientation of the samples, which is difficult to include pixelwise into the iterative procedure. In principle, electron holography allows the aberration-free reconstruction of the complex wave function in amplitudes and phases at the exit surface of a crystal. This implies the possibility of directly retrieving object information, the inverse solution can be gained by linearizing the scattering problem yielding an analytical solution of the dynamical theory with respect to the local sample thickness and orientation.

1.INTRODUCTION

The imaging of crystal defects by high-resolution transmission electron microscopy (HREM) or with the help of the electron diffraction contrast technique is well known and routinely used. However, a direct and phenomenological analysis of electron micrographs is mostly not possible, thus requiring the application of image simulation and matching techniques. To perform image simulations interactively and in a more quantitative manner implies the availability of a lot of additional facilities, e.g., precise microscope alignment and optimization of imaging, as well as an analysis of the validity of the approximations used.

Alternatively it is of importance that the reverse problem can be solved, i.e. the direct retrieval of the specimen structure from the electron micrographs. This analysis is based on the knowledge of the complex electron wave at the exit plane of an object reconstructed for single reflections by electron holography (Lichte 1991 and 1998, Orchowski and Lichte 1997) or other wave reconstruction techniques. In principle, it enables directly the retrieval of the local thickness and orientation of a sample (Scheerschmidt 1997 and 1998) as well as the refinement of potential coefficients or the determination of the atomic displacement fields, caused by a crystal lattice defect (Scheerschmidt and Knoll 1994).

2. TRIAL-AND-ERROR HREM-IMAGE INTERPRETATION

The HREM image contrast is determined by two processes: First, by the electron interferences owing to the interaction process of the electron beam with the almost periodic potential of the matter and, second, by the interference of the plane waves being transferred by the microscope. The most laborious part of the simulation process is the computation of the electron wave function at the exit plane of the specimen, which demands the solution of the dynamical scattering problem. The correct description of the imaging process has to include the microscope instability and a nonlinear transfer which is given by the autocorrelation of the wave spectrum weighted with the transmission cross-correlation coefficient.

Repeating the image modelling by varying both the model and the imaging parameters up to coincidence with the experiment is called the image matching technique. The scheme is shown in Fig. 1: A priori information of the experiment leads to a start model and an initial parameter set. It is important to have suitable criteria to analyze the similarity of experimental and simulated images. A good strategy of varying model and parameter (simulated annealing, genetic algorithm) are necessary and sufficiently precise structure modelling of the object has to be using preferentially molecular dynamics structure relaxations. Nevertheless, the whole process is equivalent to an inverse problem as discussed below, with the same difficulties in finding proper solutions.

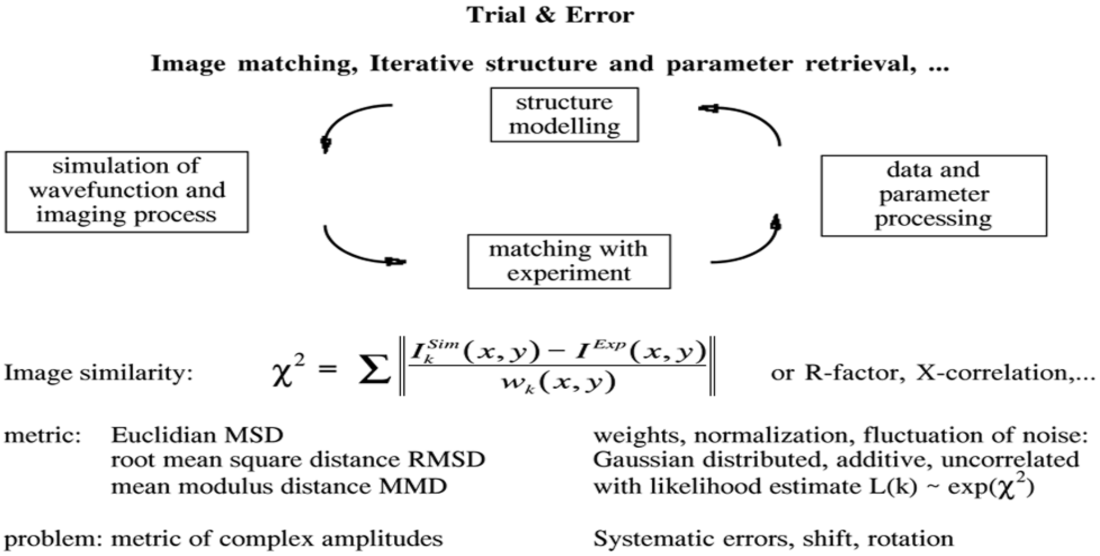

Fig. 1: Scheme of trial-and-error image matching

3. WAVE AND OBJECT RECONSTRUCTION

Holography with electrons offers one of the possibilities of increasing the resolution by avoiding the microscope aberrations (Lichte 1991 and 1998, Orchowski and Lichte 1997). It also enables the complete complex object wave to be restored. Using a Möllenstedt-type electron biprism (cf. the ray path in Fig. 2) a reference wave outside the object mutually overlaps with the object wave in the image plane creating additional interference fringes, viz. the hologram. Its intensity is modulated by the amplitude of the object wave, whereas the fringe position is variied by the phase, thus containing maximum object information due to coherent electrons.

A Fourier transform of the intensity distribution of the hologram (cf. spectrum FT in Fig. 2) generates three distinct spectral patterns if the carrier frequency is sufficiently high. In the central region of the spectrum the zero peak and the autocorrelation are obtained, representing the conventional diffractogram of the object intensity, completely identical with that obtained from a corresponding HREM micrograph. Thus no phase information is contained in the reconstruction of the autocorrelation (cf. HREM in Fig. 2). The sidebands represent the Fourier spectrum of the complete complex image wave and its conjugate, respectively, from which the object wave (cf. WAVE) can be reconstructed by separating, centring, and applying the inverse Fourier transform including a reciprocal Scherzer filter.

In addition, the wave reconstruction can be applied to each reflection separately (cf. amplitudes/phases in upper/lower row of SINGLE REFLECTION in Fig. 2), which enables the next step, the object retrieval (Scheerschmidt 1997 and 1998). In its simplest form, the basic solution of the dynamical theory is linearized by a series expansion in terms of deviations from a given set of start values of, e.g., the sample thickness t, the incident beam direction (K_x,K_y), the lattice potential. Using a perturbation approach the linearized plane wave amplitudes at the exit face of the object may be expressed in analytic form $\Phi(t,K_x,K_y,\ldots)=\Phi(t_o,K_{xo},K_{yo},\ldots)+M\cdot[t-t_o,K_x-K_{xo},K_y-K_{yo},\ldots]$. Comparing the theoretical with the experimental amplitudes and phases for each reflection and at each image pixel yields a linear equation system for the sample thickness, beam orientation etc. Analyzing the equations enable the inverse solution $[t,K_x,K_y, \ldots]=M_{inv}\cdot(\Phi^{exp}-\Phi)$. Here, however, the inverse matrix M_{inv} has to be a generalized and regularized one, e.g., the Moore-Penrose inverse. This difficulty is due to the fact that the problem is overdetermined with respect to the unknowns but underdetermined if the noise is included. While direct problems are mostly properly posed, i.e. they are characterized by the existence, stability and uniqueness of a solution, inverse problems are improperly or ill-posed, so that they can be solved only in a least-square minimization of a suitable vector norm $||\Phi^{exp}-\Phi||+\gamma||W||=Min$, which is equivalent to a Maximum-Likelihood method. The resulting solution is now well-posed but perhaps ill-conditioned, which is controlled and optimized by an additional constraint and a regularization parameter γ.

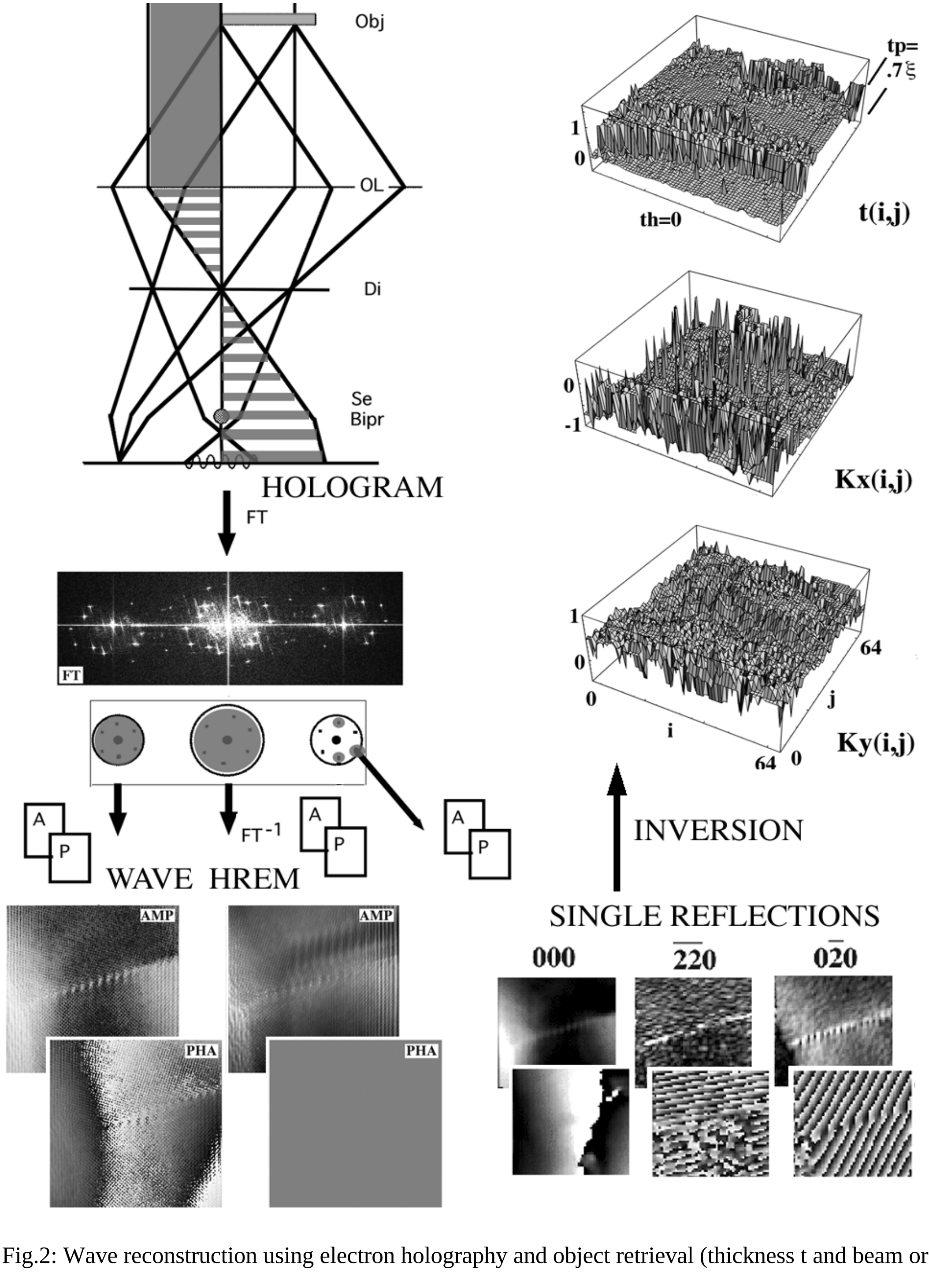

Fig.2: Wave reconstruction using electron holography and object retrieval (thickness t and beam orentation K)

Fig. 3 demonstrates the smoothing of the regularized inverse solution as a function of the regularization parameter and the dependencies of the ambiguities on the initial conditions, implying the criteria for the validity of the perturbation approximation. Such systems of linear algebraic equations are a conceptionally simple mathematical model for inverse problems of the first kind and equivalent to the determination of unknown parameters of an object with known interaction. If one includes additionally the determination of unknown lattice defects in the retrieval procedure, one gets an inverse problem of the second kind, directly related to the analysis of black boxes. Here much more a priori information is necessary to avoid modelling errors and to overcome the difficulties resulting from missing data as well as to transform the system to an inverse problem of first kind.

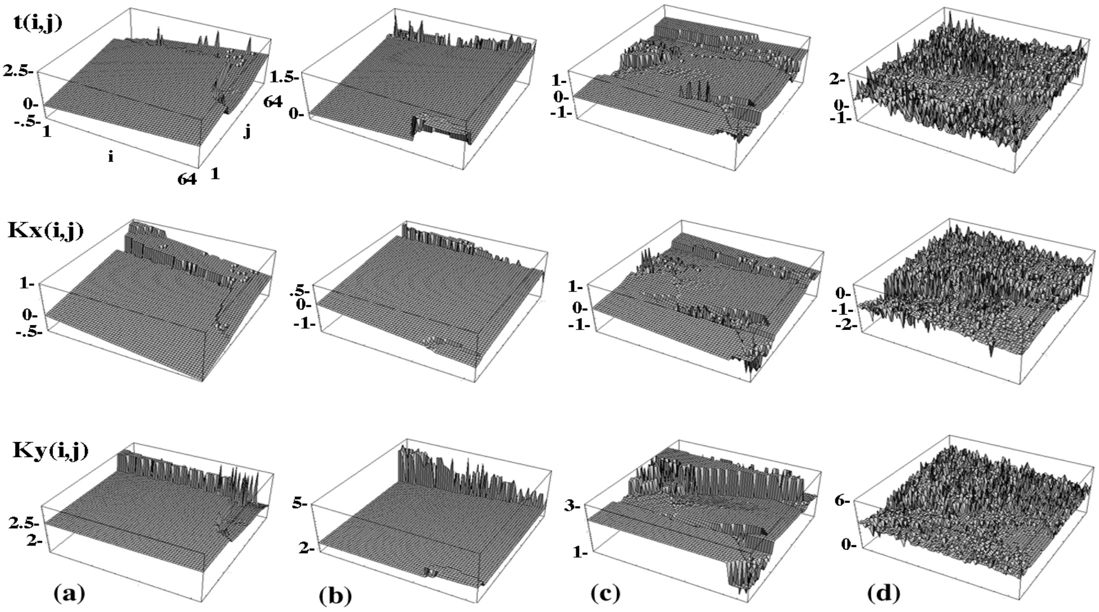

Fig. 3: Retrieval of object thickness t and beam orientation K for a simulated test object (constant $t=2.55\xi$, linearly varying $K=f(i,j)$ of pixel i,j) for different retrieval parameter differences: $\delta K=(0,0)$, $\delta t=1.5\xi$, $\gamma=10^{-19}$ (a); $\delta K=(0,0)$, $\delta t=1.5\xi$, $\gamma=10^{-6}$ (b); $\delta K=(-1.2,0)$, $\delta t=1.5\xi$, $\gamma=10^{-19}$ (c); $\delta K=(-.2,0)$, $\delta t=7.5\xi$, $\gamma=10^{-8}$ (d).

4. CONCLUSIONS

With the advances on the microscope design, HREM has become routine with a resolution much better than 0.2nm. The atomic imaging, however, requires further instrumental improvements as to the point resolution, or using object wave reconstruction methods as, e.g., the holography to avoid phase changes and transfer zeros up to the information limit of the microscope. For an improved and more quantitative interpretation the imaging conditions should be determined most precisely. Furthermore, the trial-and-error retrieval procedure needs quantitative similarity criteria and a very good object modelling. The images in extremely thin areas present the electron density distribution and small defects as two-dimensional projections, i.e. information seems irretrievably lost. Nevertheless, irrespective whether there exists a unique solution, the image matching should be overcome, which requires additional information via the wave phases, or different projections. Thus, object retrieval as the solution of the inverse problem should be searched for and extended to the analysis of defects, too.

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