Electron crystallograhy via local TEM parameter determination for mixed type potentials using inverse object retrieval

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Electron crystallography and electron microscope tomography are new techniques to enhance structure investigations via local object analysis. However, in contrast to X-ray techniques this has the disadvantage that an ill-posed inverse problem for the highly nonlinear dynamical theory has to be solved. The retrieval of local object information can be directly performed from the electron microscope exit wave function without using trial-and-error iterative matching, as demonstrated e.g. to analyze variations within the lateral object extension for thickness and beam orientation, which is equivalent to local bending of the object [1, 2]. Fig. 1 schematically shows the different steps in analyzing the object structure directly (clockwise) or with trial-and-error techniques. In the following is of special interest that the parameterization of a mixed total scattering potential enables an extension of the structure retrieval procedure described earlier in detail (cf. [1, 2] and references therein) to reconstruct local structural variations. Object retrieval always requires the solution of the inverse scattering problem, which can be gained by linearizing the solution of the dynamical theory and constructing regularized and generalized inverse matrices, which may be summarized as follows.

Starting e.g. from an electron hologram, where all reflections **g** up to the maximum resolution are separately reconstructed, the moduli and phases for each **g** of the experimental exit plane wave Φ^{exp} are determined as function of the lateral pixel position (i,j). Theoretical waves Φ^{th} are then calculated using the dynamical scattering matrix M for an a priori model characterized by the number of beams and the scattering potential V. With a suitable experimentally predetermined a priori beam orientation $\mathbf{K}_o$ and sample thickness t_o as a free parameter, a perturbation approximation yields both Φ^{th} and M as linear functions of the parameter to be retrieved. Its analytic form enables the inverse solution yielding directly for each image pixel (i,j) the local thickness t(i,j), the local beam orientation $\mathbf{K}$(i,j), the variation of the potential V, and further data included into the parameter space. The enhancement [2] of the reconstruction algorithm includes second order perturbation and mixed type potentials. Here the optical potential matrix V is replaced by a mixture of different but constant matrices V^k representing different structures, compositions, defect regions etc. Additional parameter q_k describe the local variation via $\mathsf{V}(i,j) = q_k(i,j)\ \mathsf{V}^k$. The inverse solution reads now

$$[t, \mathbf{K}, q_1,q_2, ...]= [t_o, \mathbf{K}_o, q_{o1},q_{o2}, ...]+\mathsf{M}_{inv}(\Phi^{exp}-\Phi^{th}),$$

where the coefficients of the new V^k describe only additional a priori information, but the q_k increase the space of the unknown parameter to be reconstructed for each pixel (i,j).

In a mathematical sense the inverse problem is ill-posed and needs special techniques to get well-posed. A generalized inverse matrix, as e.g. $\mathsf{M}_{inv} = (\mathsf{M}^T\mathcal{C}_1\mathsf{M}+\gamma\mathcal{C}_2)^{-1}\mathsf{M}^T$, avoids the ill-posedness, but the generalized solution is now ill-conditioned. As pointed out in different previous analyses (cf. e.g. [3, 4] and references therein), a suitable regularization of the retrieval procedure via the regularization parameter γ and the smoothing matrices $\mathcal{C}_1$, $\mathcal{C}_2$ requires the control of the confidence and stability region, as well as the avoiding of modeling errors. As shown in Fig. 2 (left panel), the regularization smoothes the solution, this is of advantage for increasing the stability of the algorithm. However, it increases the fit error, which reduces drastically the confidence region. This holds true also for the new parameter space including the q_k of the mixed type potential as demonstrated in Figure 2 (right panel). However, the modeling errors are increased by the additional parameter to be retrieved. Due to couplings of the thickness with the mean absorption potential, of the tilt offset with the mean scattering potential, and of the q_k with each other, an artificial degeneracy of the solution occurs. The problem may be solved by a further iteration process including and varying additional a priori start configuration whenever the retrieved data go beyond the limits of the confidence region.

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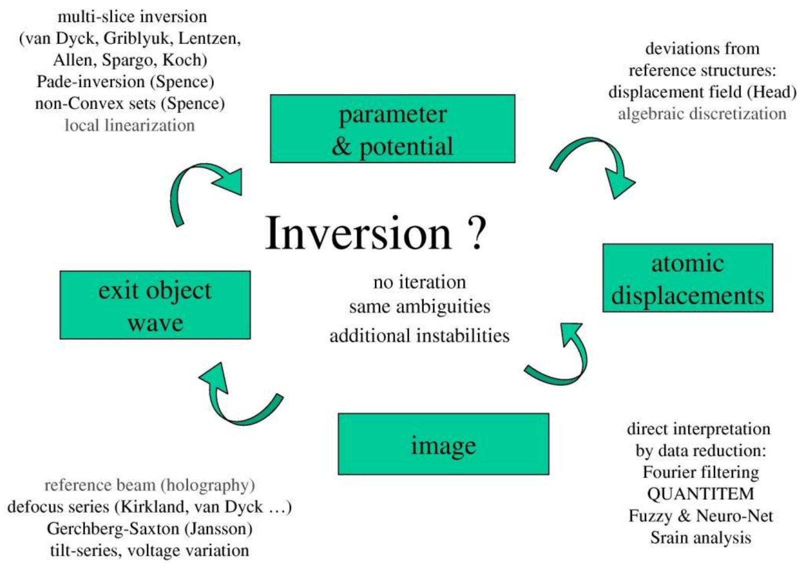

Figure 1. At least three different steps have to be inverted solving direct object retrieval in EM (clockwise) instead applying the trial-and-error technique (counter-clockwise): Step 1 of the inversion is solved by replacing the image by a hologram or a defocus series, which makes the problem linear, and finding the exit object wave by inverse Fourier transform. Step 2 yields the object structure directly from the exit wave, the real challenge of inversion. Step 3, the analysis of lattice defects, has no explicit solution yet. For details of different wave and data retrieval methods and respective references cf. [2].

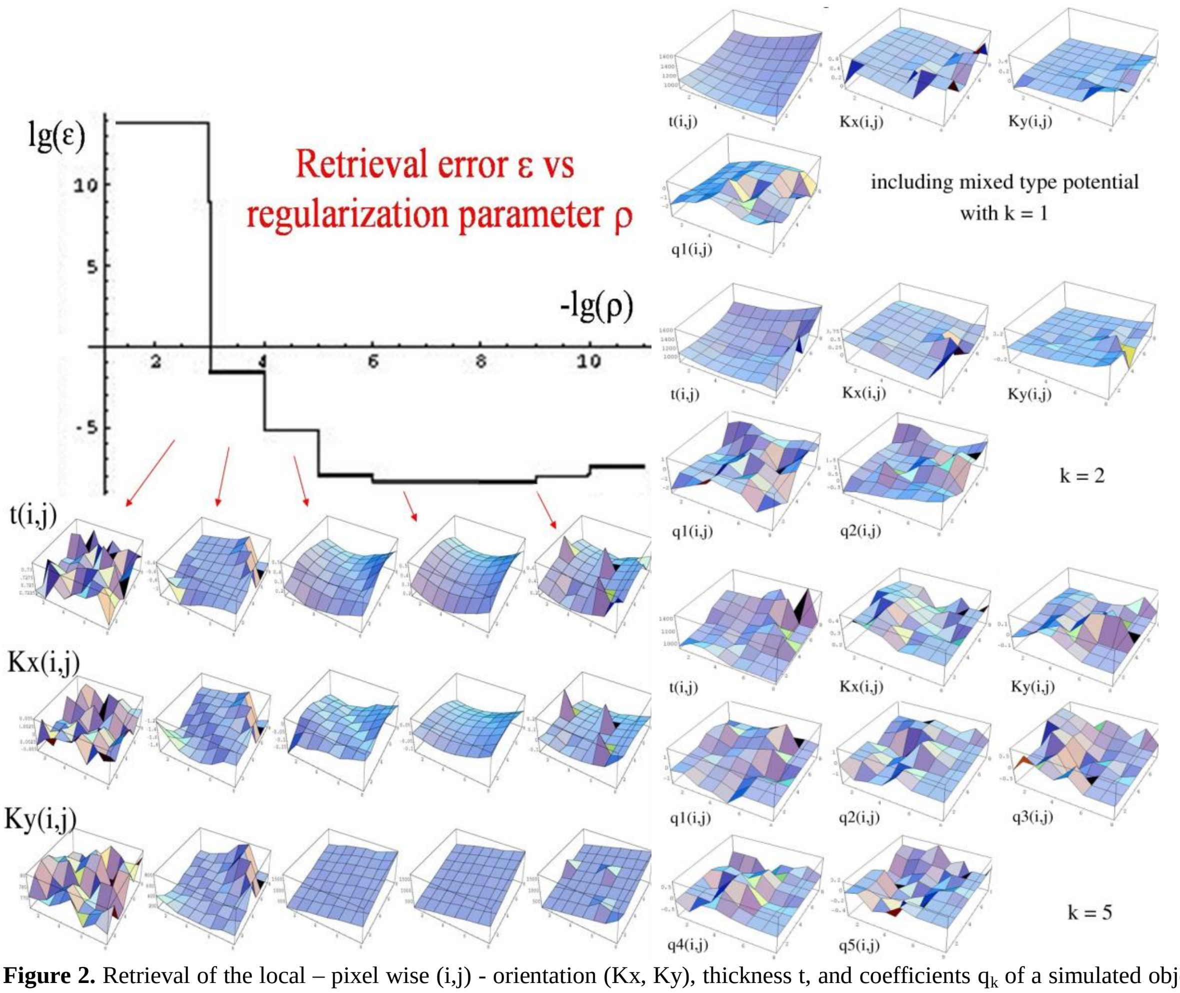

Figure 2. Retrieval of the local – pixel wise (i,j) - orientation (Kx, Ky), thickness t, and coefficients q_k of a simulated object with mixed type potential $q_k V^k$: Only for a small confidence region of the regularization parameter ρ (approximately 10^{-6} to 10^{-8}) the overall retrieval error ε is small (approximately 10^{-8}) resulting in perfect non-disturbed retrieval of the test data (for the case k=0, left panel). However, using increasing number k=1, 2, 5 of V^k the retrieval show different modeling errors characterized by increasing noise and larger number of pixels with disturbed reconstructed K, t or q_k (right panel).