Accuracy of Local TEM Parameter Determination for Mixed Type Potentials using Inverse Object Retrieval

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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, too. The retrieval of local object information can be performed directly 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. Always the object retrieval 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 **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 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. The regularization smoothes the solution, which 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 1. 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.

References

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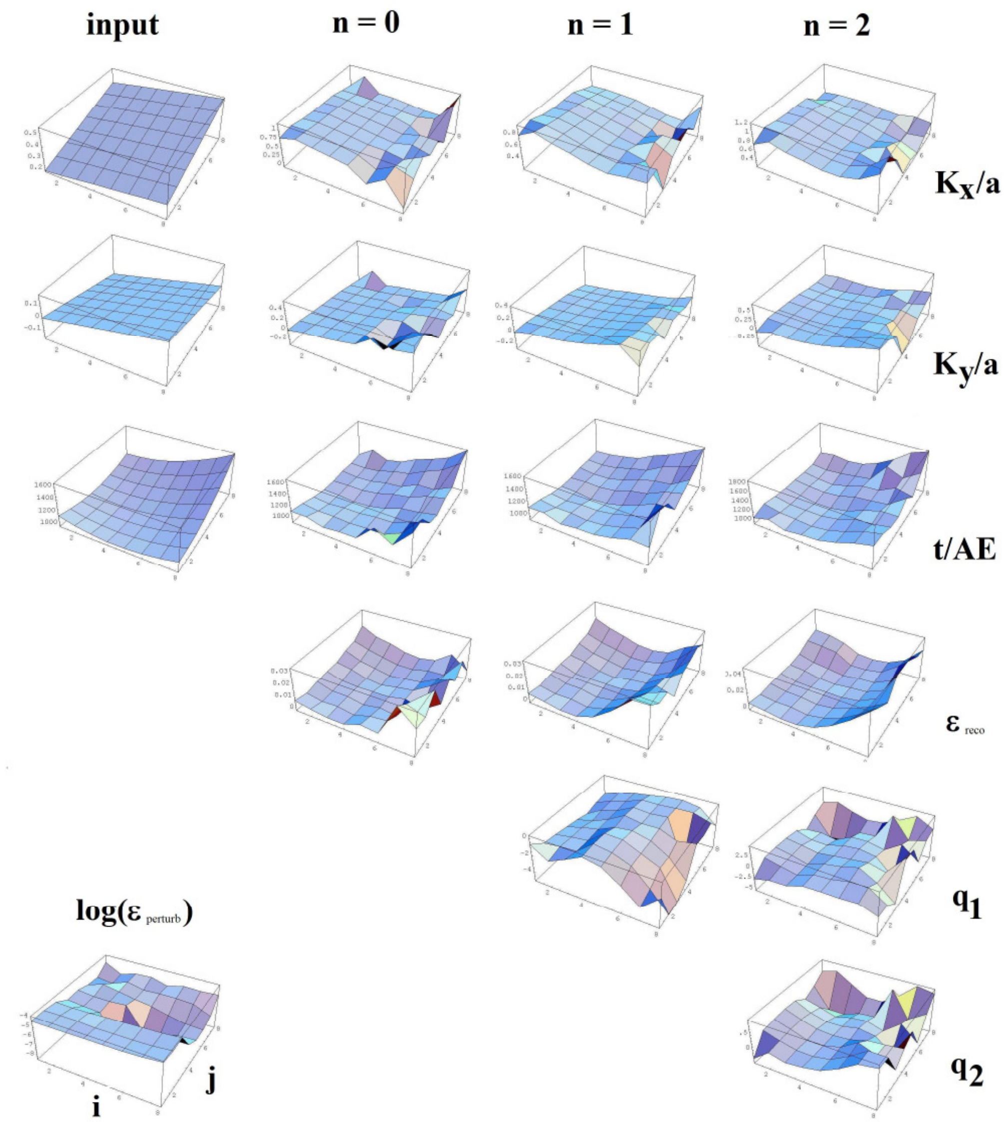

Figure 1. Retrieval of the local, pixelwise (i,j), orientation (Kx, Ky), thickness t, and coefficients q1, q2 of a simulated object with mixed type potential as given in “input”. Using increasing number of V^k (n=0, 1, 2) the retrieval show different modeling errors characterized by the overall error ε_{reco}, which is coupled to the extension of the parameter space and the validity of the perturbation approximation (cf. its $\log(\varepsilon_{perturb})$ error in the inset).