Electron Microscope Object Reconstruction: Retrieval of Local Variations in Mixed Type Potentials

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Applying parameterization of a mixed total scattering potential a simple extension of the structure retrieval procedure is possible to reconstruct local variations of the object potential, too. As described earlier in details [1-4] the retrieval of local object information can be performed directly from the electron microscope exit wave function without using trial-and-error iterative matching. The algorithm allows the direct analysis of variations within the lateral object extension of object thickness and beam orientation or equivalently local bending of the object. In principle, extensions are possible also to include changes of the scattering potential, local structural variations and special lattice defects into the reconstruction algorithm. 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.

The retrieval procedure may be summarized as follows. Starting e.g. from an electron hologram, where all reflections **g** 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). Moduli and phases up to the maximum resolution are necessary to get sufficient a priori data. 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 represented by the potential coefficients V^o_g. With a suitable experimentally predetermined trial average beam orientation $\mathbf{K}_o$ and a sample thickness t_o as a free parameter, a perturbation approximation yields both Φ^{th} and M as linear functions of parameters to be retrieved.

The analytic form of the equations enables the inverse solution

$$[t, \mathbf{K}, V_g, ...] = [t_o, \mathbf{K}_o, V^o_g, ...] + \mathsf{M}_{inv}(\Phi^{exp} - \Phi^{th}),$$

thus yielding directly for each image pixel (i,j) the local thickness t(i,j), the local beam orientation $\mathbf{K}$ (i,j), and the variation of the potential V as well as further data included into the parameter space. However, an enhancement of the reconstruction algorithm is possible: The application of mixed type potentials simplifies the reconstruction algorithm and allows to overcome some limitations using a local variable V. The optical potential matrix V is replaced by a mixture of different but constant matrices V^k representing different structures or composites or defect regions etc. Additional parameter q_k are introduced to describe the local variation. With $\mathsf{V}(i,j) = q_k(i,j)\,\mathsf{V}^k$ the inverse solution is then replaced by

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

where the new V^k_g as coefficients of 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).

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In mathematical sense the inverse problem is ill-posed and needs special techniques to get well-posed. A generalized inverse matrix, as e.g. $\boldsymbol{M}_{inv} = (\boldsymbol{M}^T\boldsymbol{C}_1\boldsymbol{M}+\gamma\boldsymbol{C}_2)^{-1}\boldsymbol{M}^T$, avoids the ill-posedness of the mathematical problem, but the generalized solution is now ill-conditioned. As pointed out in different previous analyses (cf. [5] and references therein), a suitable regularization of the retrieval procedure via the regularization parameter γ and the smoothing matrices $\boldsymbol{C}_1$, $\boldsymbol{C}_2$ requires the control of the confidence and stability region, as well as the avoiding of modeling errors. The confidence region may be discussed considering the error of the fit for synthetic models using a Likelihood measure, showing that the thickness is an uncritical parameter (cf. Fig. 1). The linearization 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. The problem may be solved by an additional iteration process varying the a priori start configuration whenever the retrieved data go beyond the limits of the confidence region. This holds true also for the new parameter space including the q_k of the mixed type potential. In addition the difficulty in the retrieval of the potential is avoided which arise because the thickness is coupled with the mean absorption potential and a tilt offset couples with the mean scattering potential. Due to these couplings an artificial degeneracy of the solution occurred, the mixed type potential, however, removes this coupling degeneracy via the restricted freedom in applying the a priori information.

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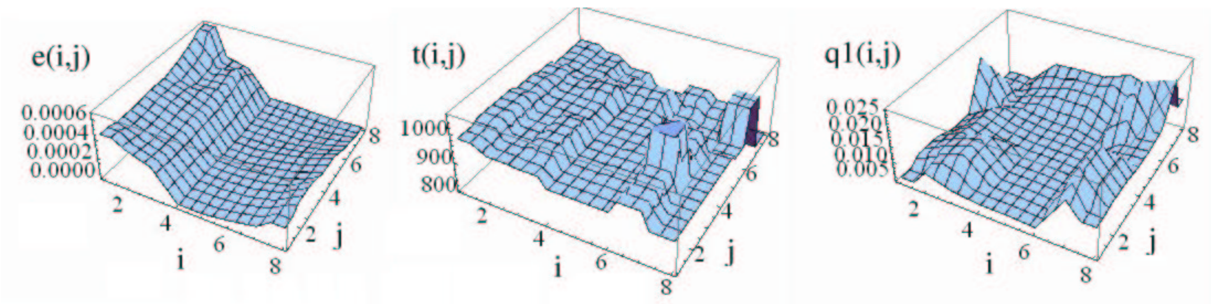

Figure 1. Error e(i,j) of incident data (Likelihood measure of the difference between reconstructed vs. simulated Φ^{exp} for varying K(i,j) in a hypothetic model) and its influence to the reconstructed thickness t(i,j) and parameter q1(i,j) of the mixed potential used, which both should be constant (t=999 and q1=0) for the data used to check the confidence range.

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