

Electron Microscope Object Reconstruction: Confidence Criteria of Inverse Solutions

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The retrieval of local object information can be performed directly from the electron microscope exit wave function without using trial-and-error iterative matching [1,2]. The present algorithm allows the direct analysis of variations of the object thickness and the beam orientation, local bending, and changes of the scattering potential within the lateral object extension. In principle, extensions are possible also to include local structural variations and special lattice defects into the reconstruction algorithm. However, 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. Such an inverse scattering problem is in mathematical sense ill-posed and needs special techniques to get well-posed solutions.

The retrieval procedure may be summarized as follows. Starting e.g. from an electron hologram, where all reflections \mathbf{g} are separately reconstructed, the moduli and phases for each \mathbf{g} of the experimental exit plane wave Φ^{exp} are determined. 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_g^0 . With a suitable experimentally predetermined trial average beam orientation \mathbf{K}_{0xy} and a sample thickness to 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

$$[t, \mathbf{K}_{xy}, V_g, \dots] = [t_0, \mathbf{K}_{0xy}, V_g^0, \dots] + \text{Minv}(\Phi^{\text{exp}} - \Phi^{\text{th}}).$$

Thus yielding directly for each image pixel (i,j) the local thickness $t(i,j)$, the local beam orientation $\mathbf{K}_{xy}(i,j)$, and the variation of the potential as well as further data included into the parameter space.

A generalized inverse matrix, as e.g. $\text{Minv} = (M^T C_1 M + \gamma C_2)^{-1} M^T$, avoids the ill-posedness of the mathematical problem, but the generalized solution is now ill-conditioned. As pointed out in different previous analyses (cf. e.g. [3-6]), a suitable regularization of the retrieval procedure via the regularization parameter γ and the smoothing matrices C_1, 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. 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. In addition the retrieval of the potential couples the thickness with the mean absorption potential and a tilt offset with the mean scattering potential. Due to these couplings an artificial kind of degeneracy of the solution occur, which may be avoided by the additional assumption, that the mean inner potential must be the same within one object.

The enhancement due to the iteration of the start values and the restriction of the mean inner potential will be demonstrated applying the retrieval procedure to test objects and analyzing experimental holograms. Besides this, a critical revision of the underlying theoretical assumptions [7-9] with respect to approximations made in dynamical theory and scattering model is done to reduce the number of unknowns by coupling parameters via a priori dependencies.

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