

Correction of the object wave using iteratively reconstructed local object tilt and thickness

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Object data can directly - without using trial-and-error matching - be retrieved from electron microscope exit waves, as e.g. reconstructed by holography [1, 2]. Such a inverse retrieval of local data, e.g. thickness, orientation and potential, as a basis of a general object reconstruction, can be gained by linearizing, regularizing and generalizing the scattering problem. Figs. 1 shows the basic idea of trial-and-error versus inverse solution schemes and Fig. 2 the reconstruction of thickness and orientation at an Ge-CdTe interface applying different scattering potential for the Ge and the CdTe regions.

The inverse solution starts from moduli (A) and phases (P) of the set of plane waves Φ^{exp} at the exit surface (cf. Fig.1). Exit waves Φ^{th} are calculated using the dynamical scattering matrix M for an a priori model with a suitable scattering potential and by assuming a trial average beam orientation (K_{x_0} , K_{y_0}) predetermined by the experiment (upper arrow, direct trial-and-error formalism). With the sample thickness t_0 as a free parameter, a perturbation approximation yields both the moduli and phases of the plane wave amplitudes as linear functions of the object thickness t and orientation (K_x , K_y). The analytic form of the equations (cf. lower arrow, linearized inverse from scattering matrix M and its derivative δM) yields directly for each image pixel (i, j) the local thickness t_{ij} and local beam orientation $(K_x, K_y)_{ij}$. However, as pointed out in different previous analyses of the stability of the retrieval procedure (cf. the summaries in [3-5]) it requires the knowledge of the confidence region, conditions for stability, and restrictions due to modeling errors. The ill-posed inverse matrix is transformed by generalizing and regularizing to a well-posed but ill-conditioned one, which is equivalent to a least square (maximum-likelihood) minimization $\|\Phi^{\text{exp}} - \Phi^{\text{th}}\|_{+\gamma} \|\Omega\| = \text{Min}$ or to pixel smoothing, controlled and optimized by the regularization parameter γ and the constraint Ω .

However, to reduce further the modeling errors and to extend the confidence region the start values and the assumptions for the underlying scattering model may be varied iteratively as demonstrated in Fig. 3, where the first subsequent iterative reconstruction yields noise reduction.

1. K. Scheerschmidt, Lecture Notes in Physics 486 (1997) 71-85.
2. K. Scheerschmidt, Journal of Microscopy 190 (1998) 238-248.
3. K. Scheerschmidt, Microsc. Microanal. 9, Suppl.6 (2003) 56-57.