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# Stability of object parameters retrieved by inverse solutions of electron diffraction

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Object data can directly be retrieved from the electron microscope exit wave function without using trial-and-error iterative matching [1, 2]. Such a retrieval of local data, e.g. thickness, orientation and potential, as a basis of a general object reconstruction, can be gained by linearizing the scattering problem and constructing regularized and generalized inverse matrices. However, as pointed out in different previous analyses of the stability of the retrieval procedure (cf. the summaries in [4, 5]) it requires the knowledge of the confidence region, the conditions for stability, and the restrictions due to modeling errors.

The retrieving procedure may again be summarized in short (see Fig. 1): Starting e.g. from a hologram, all reflections are separately reconstructed yielding the moduli (A) and phases (P) of the set of plane waves $\Phi^{exp}$ at the exit surface. Exit waves $\Phi^{th}$ are calculated using the dynamical scattering matrix M for an a priori model characterized by the number of beams and the scattering potential, and by assuming a suitable trial average beam orientation ($K_{xo}$, $K_{yo}$) predetermined by the experiment. With the sample thickness $t_O$ 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 enable the inverse solution $[t,K_x,K_y, ...]=M_{inv}\cdot(\Phi^{exp}-\Phi^{th})$, thus yielding directly for each image pixel (i,j) the local thickness $t_{ij}$ and local beam orientation $(K_x,K_y)_{ij}$.

The ill-posedness of the inverse problem (overdetermination with respect to the unknowns, underdetermination if noise is included) needs to generalize and regularize the inverse matrix $M_{inv}=(M^TC_1M+\gamma C_2)^{-1}M^T$, which is equivalent to a least square (maximum-likelihood) minimization $\|\Phi^{exp}-\Phi^{th}\|+\gamma\|\Omega\|=Min$. The resulting solution is now well-posed but ill-conditioned, which may be controlled and optimized by the regularization parameter $\gamma$ and the constraint $\Omega$, i.e. pixel smoothing via $C_{1,2}$. Figure 2 demonstrates the smoothing of the regularized inverse solution as a function of the regularization parameter $\gamma$. The retrieval error $\varepsilon$ (deviation of t and K over all pixel) has a minimum with $\gamma$ for the best fit of test data, the noise increase for smaller $\gamma$, however, depending on pixel smoothing, and modelling errors occur for larger $\gamma$. Figure 3 shows the confidence behavior (overall error $\varepsilon$ in Fig. 3a) and the retrieval of t and $(K_x,K_y)$, cf. Fig. 3b, c, resp., for simulated test data as a function of the steps in iteratively enhancing the a priori start values ($K_{xo}$, $K_{yo}$). If the first start data are within a certain convergence region (cf. curves i for different pixel smoothing $C_{1,2}$), the correct solution is always found with high precision, whereas out of the region (cf. curves ii) the retrieval remains instable.

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.
4. K. Scheerschmidt, WAVES 2003, Proc. 6th Int. Conf, Math. Num. Aspects Wave Prop., Eds.: G. C. Cohen and P. Joly, Springer Vlg.,2003, 607-612.

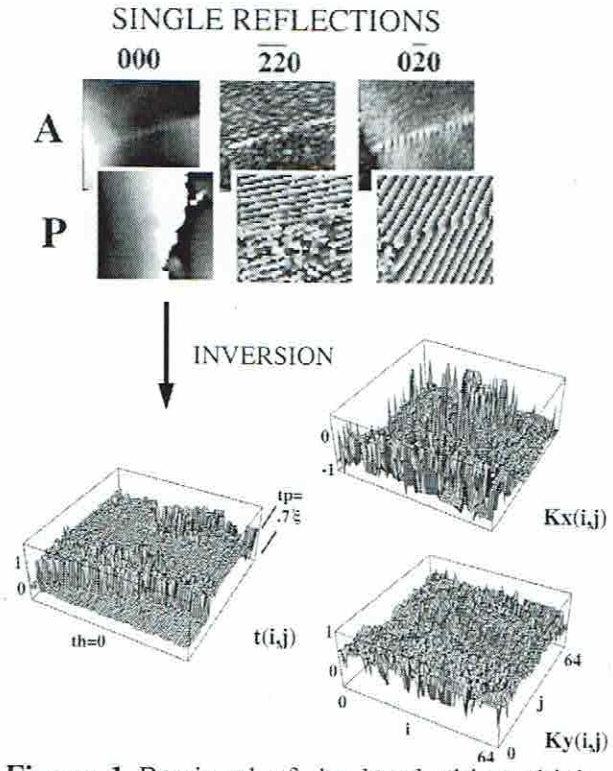


**Figure 1** Retrieval of the local object thickness t(i,j) and bending K(i,j) starting with single reflections of experimentally reconstructed exit waves of a Au grain boundary.

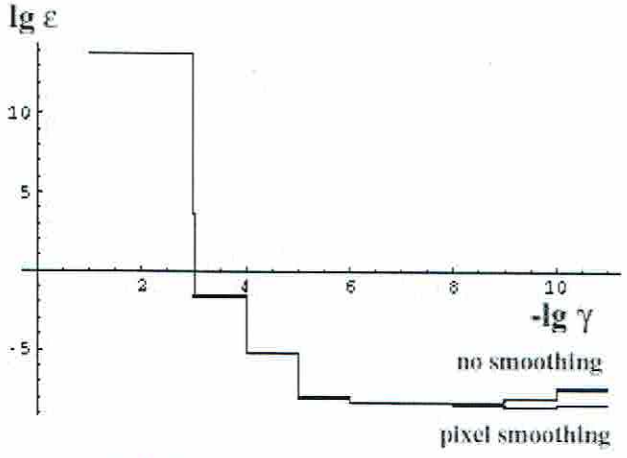


**Figure 2** Influence of the regularization parameter γ to the overall retrieval error ε for a simulated test object.

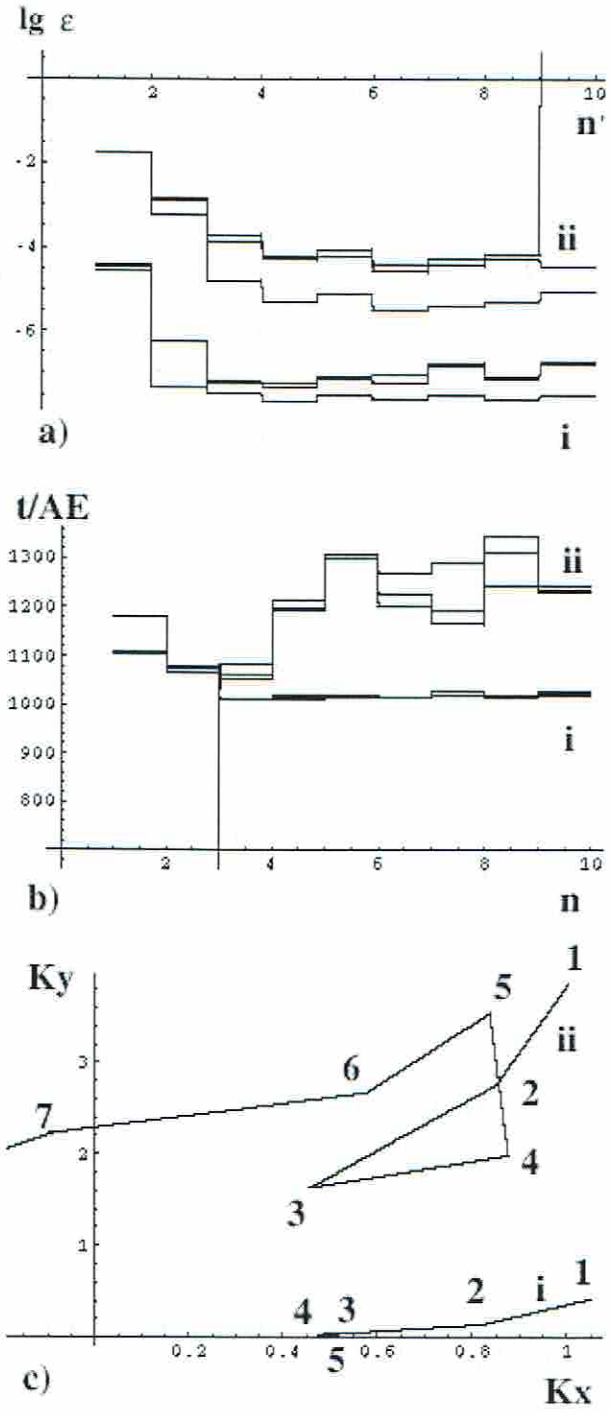


**Figure 3** Confidence behavior (cf.text): a) ε, b) t, c) $(K_x,K_y)$, for simulated test data as a function of the steps n iteratively enhancing the a priori start values $(K_{xo}, K_{yo})$.