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Determination of object thickness and orientation from electron holograms by iterative inverse retrieval methods

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For the quantitative interpretation of atomic resolution micrographs the accurate knowledge of thickness and orientation is indispensable. Electron holography, in principle, allows the aberration-free reconstruction of the complex wave function (amplitudes and phases) at the exit surface of a crystal up to the microscope information limit /1/. This implies the possibility of directly retrieving object information as, e.g., the local object thickness and orientation /2/ as well as the shifted positions of the atomic scattering centres /3/ instead of using trial-and-error simulation techniques. The inverse solution can be found by using the a priori information from the diffraction (e.g. range of the posiible incident beam orientations and thicknesses, lattice potential, diffracted beams), calculating the respective scattered intensities and phases via the dynamical theory in a sufficiently dense net of the parameter space, and fitting the experimental data using a least square minimization. However, an analytical solution of the special problem of retrieving the local sample thickness and orientation is directly given by applying the perturbation approximation to perfect crystals, and by using regularized and generalized matrices to invert the resulting linearized problem.

Figure 1 demonstrates the three main steps of the retrieving procedure for a $\Sigma 13$ grain boundary in gold /2/. Starting from the hologram (Fig. 1a) all reflections are separately reconstructed (here nine reflection pairs owing to the grain tilt). A Gaussian filtering is applied to reduce the noise, and for each reflection the moduli and phases of the plane waves are determined (the most important ones are shown in Fig. 1b). A nine-beam case in terms of Bloch waves is solved numerically for this special diffraction geometry assuming an a priori beam orientation K_0 predetermined by the experiment, and with the sample thickness t as a free parameter. The perturbation approximation yields both the moduli and the phases of the plane wave amplitudes as linear functions of the object thickness and orientation, and can directly be retrieved using a generalized inversion of this functionality. The corresponding iteration procedure yields local thickness t(i,j) and bending $K_{xy}(i,j)-K_0$ of the object for each image pixel (i,j). Figure 1c shows the result of the t(i,j)-reconstruction using the moduli and phases of Fig. 1b without numerically stabilizing the iteration procedure, which is reflected by the noise. Nevertheless, there are two distinct regions of thickness values t(i,j) for the hole ($t\approx 0$) and the plateau ($t\approx 0.7\xi$, extinction distance ξ of the 220 reflections). The interface region itself is present as a modelling error.

From the mathematical point of view such inverse problems are ill-posed. Additional information is necessary to render the solutions stable and continuous. Smoothing the data or the first derivatives and regularizing the generalized inverse solution may drastically reduce the influence of noise and outliers. The ambiguities, however, cannot be corrected in this way /4/. Figure 2 demonstrates the influence of the regularization on a synthetically generated object wave, for which a constant thickness $t=2.5\ \xi$ and a linearly bent sample, i.e. a linearly varying beam orientation, were assumed. The reconstruction reflects the assumptions made with different noise applying regularization parameters of $\gamma=10^{-5}$ and 10^{-4} in Figs. 2a and b, respectively. The resulting different $\log(\chi^2)$ measures (1,3=numerical error and regression, 2=standard deviation) as functions of the regularization parameters in Fig. 2c show the existence of maximum confidence regions.

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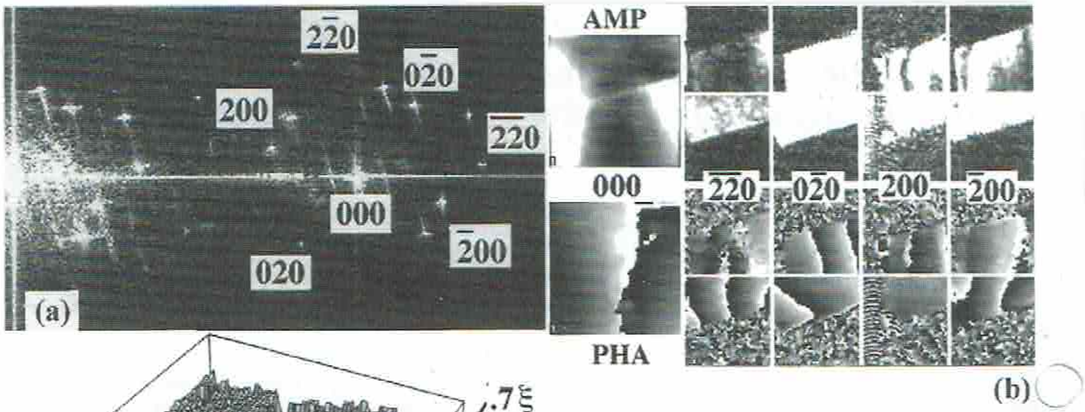

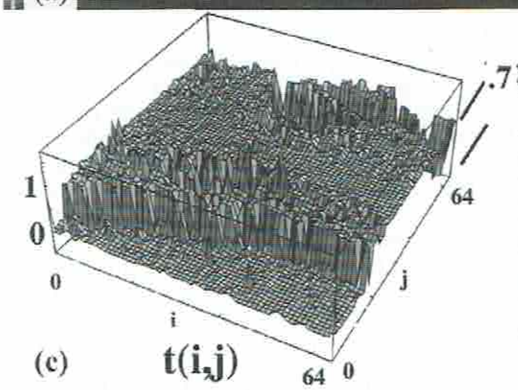

Fig.1: Sideband of an experimental hologram of a Au grain boundary (a), reconstructed plane wave amplitudes (AMP) and phases (PHA) of the most important reflections (b) for both grains, and the retrieved thickness (c)

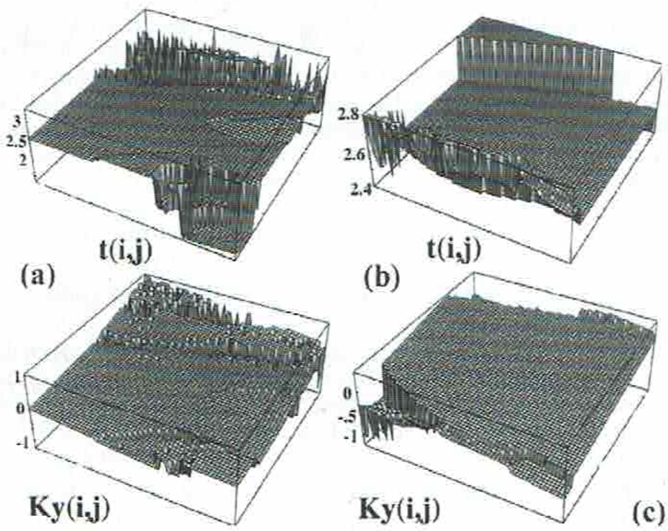

Fig.2: Retrieval of thickness t/ξ and beam tilt Ky for a simulated object wave and different regularizations (a,b; see text); confidence tests versus regularization γ (c)