Phase Shifts at twin boundaries at medium resolution – A dynamic scattering simulation study

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The phase shift of the object exit wave is known to be a very sensitive indicator for electric and magnetic fields at nanometer level [1]. Hence electron holography reconstructing phase information is suited for investigating potential distributions in materials in principle. Ferroelectric domain boundaries are supposed to contain potential jumps [2] and provide an interesting object for electron holographic studies. Nevertheless, experimental conditions suffer from uncertainties in object or illumination tilt over the range of several mrad also inducing modulations of the reconstructed image wave, which may not be interpreted as electric fields as shown by simulations in this work.

A simple structure model consisting of a 90°-PTO-twin boundary with non-relaxed atomic positions (Figure 1) is composed for full dynamic scattering simulations with SEMI [3] in this contribution. The width of one domain is about 28.5 nm and the simulation was performed up to a thickness of about 117.2 nm. The object potential is based on free atomic potentials according to A. Weickenmeier and H. Kohl [4] of the contributing atoms. Periodic boundary conditions are applied in all three dimensions. Object tilt is introduced by beam tilt, which is however limited by the small angle approximation [5]. To regard medium resolution conditions, a smooth aperture with a radius of 0.3/nm is multiplied to the Fourier transform of the simulated wave.

A variation of beam tilt over the range of 15 mrad is leading to a chaotic amplitude and phase behavior and pretending potential jumps like the ferroelectric one when treating the phase as a projected potential (Figure 2). This effect is just due to the dynamical scattering of electrons at the lattice potential, amplified by the discontinuity of the crystal structure at the boundary. This can be understood as an intrinsic delocalization of the wave at the boundary influencing the further propagation through the material. Investigations for large tilt angles indicate a vanishing global jump; local variations at the boundary remain though.

This contribution exhibits that potential investigations at boundaries can be very critical when the effects of dynamical scattering and uncertainties in the microscope are not taken into account. It also provides a counterexample of the common criterion for kinematical conditions: A considerable phase modulation due to dynamical scattering can be existent (Figure 3), even if nearly no modulations in amplitude are formed.

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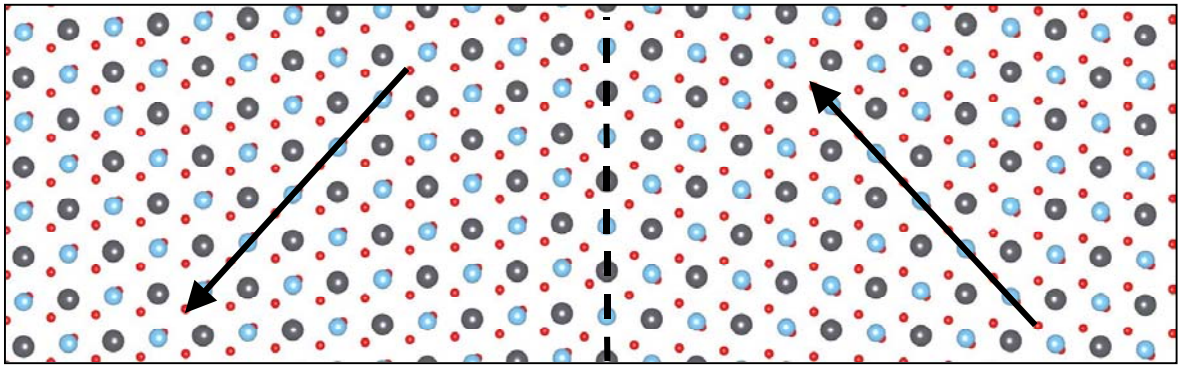

Figure 1. Cutout of the structure model: Lead atoms in gray, Titanium atoms in blue, Oxygen atoms in red. Twin boundary denoted as dashed line. Ferroelectric polarization indicated with black arrows.

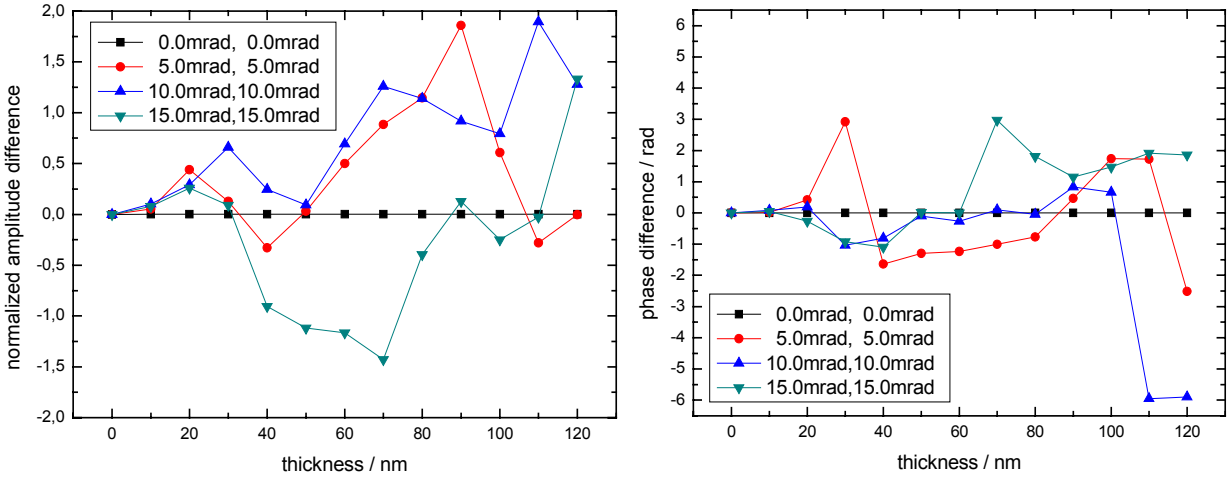

Figure 2. Mean amplitude difference (left) and mean phase difference (right) between adjacent domains in dependence on specimen thickness of certain beam tilts.

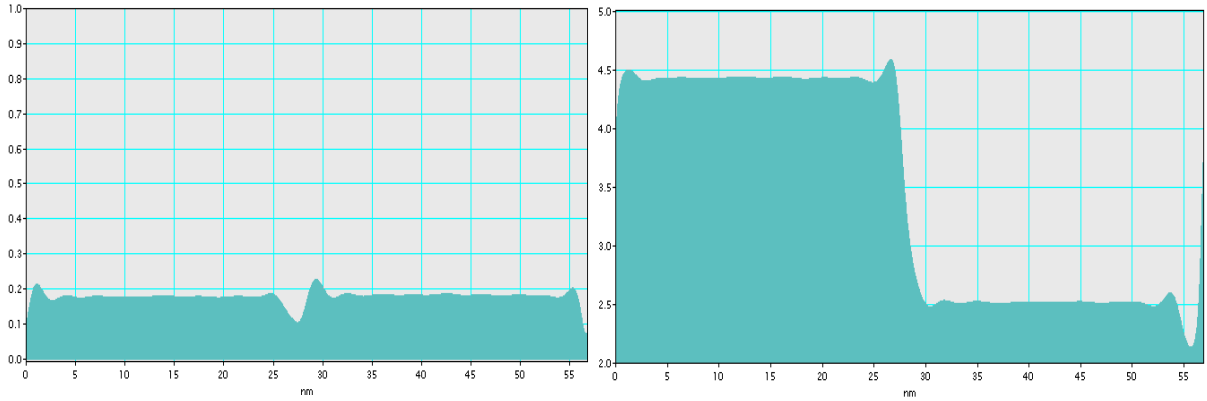

Figure 3. Profile of amplitude and phase (in rad) across the domain boundaries at 110 nm thickness and at beam tilt of (15.0, 15.0) mrad (see green lines in Figure 2). Sameness in amplitude doesn't mean that dynamical effects are negligible.

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