The influence of dynamic scattering on potential and mean-free-path measurements in medium resolution electron holography

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The electrostatic potential within a material is a key quantity influencing almost all properties of the material: On the atomic length scale electrons in a solid can be regarded as moving in the mean field of the other constituents (Hartree-Fock approximation), forming orbitals and chemical bonding. On a macroscoscopic length scale potential differences are key elements of electric devices, like pn-junctions, thermoelements, condensators, piezoelements, etc. A detailed knowledge of potential distributions thus yields important insight in the functionality of the materials. In this respect the within a certain volume averaged electrostatic potential V_0 can be regarded as a fingerprint quantity. Medium resolution electron holography provides direct access to V_0 through the following relationship to the reconstructed phase shift

$$\varphi(x,y) = \sigma \int_0^{t(x,y)} V_0(x,y,z)\,dz, \tag{1}$$

where σ is the interaction constant and t denotes the thickness. Similarly, the reconstructed amplitude A provides information about the inelastic mean free path length λ_{in} through

$$\lambda_{in}(x,y) = -t(x,y) / \left(2\ln\left(A(x,y)/A_0\right)\right), \tag{2}$$

where A_0 is the vacuum amplitude[1]. Both relationships are only strictly valid under kinematic scattering conditions. Deviations, which are referred to as dynamical effects, can be reduced by choosing special imaging conditions, i.e. tilting away from the zone axis.

We report on a detailed analysis of dynamical scattering effects under medium resolution holographic imaging conditions based on analytic scattering theory and explicit numerical calculations. Special emphasis is put on the validation of various tilt formalism used in the standard high-energy, small angle scattering approximations (Bloch wave / Multislice) obtained by testing against numerical forward integration of the original Klein-Gordon-scattering. A systematic underestimation of the mean inner potentials, derived by means of the phase object approximation (1), is obtained both for very thin layers of several atomic layers as well as thick samples. The deviations strongly depend on the scattering potential, i.e. the atomic species within the material. Correction tables approximately valid for very thin and thick specimen are derived (fig 1).

The incorporation of thermal motion in elastic scattering theory leads beside a phase modification also to damping terms in the reconstructed amplitude[2], adding to inelastic effects described in (2). This additional damping depends strongly on the scattering potential (fig 2) and the temperature, eventually leading to a systematic underestimation of λ_{in}, in particular when compared to EELS measurements. Consequently, the combination of cryo-TEM techniques with off-axis electron holography can significantly reduce the damping through thermal motion.

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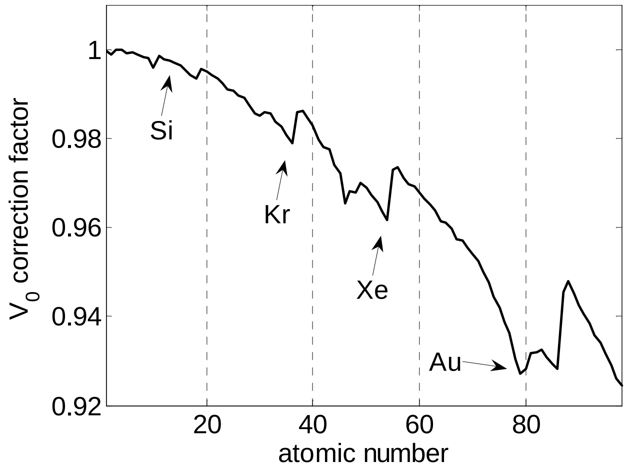

Figure 1. Single atomic dynamical correction factor table. The accurate V_0 is obtained by multiplying the measured V_0 with the dynamical correction factor. Corrections for complex materials are obtained by averaging over all atoms contained in one chemical unit.

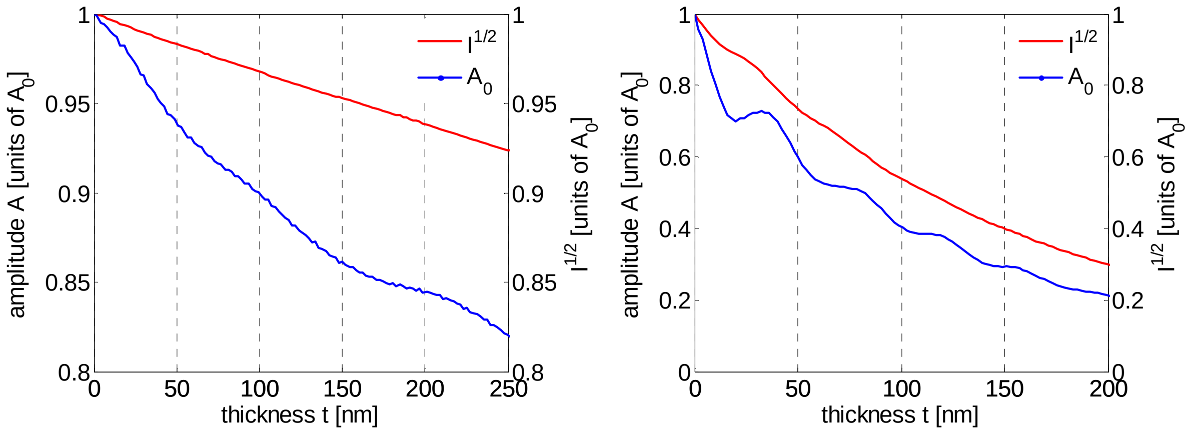

Figure 2. Thickness dependent damping of the total side band intensity (straight red line) and reconstructed zero beam amplitude (dotted blue line) in (a) Si and (b) Au as introduced by incorporating thermal motion into off-axis holographic imaging. Simulation details: Multislice algorithm, 200 kV acceleration voltage, specimen tilt 10° around [6,10,0] away from [0,0,1].

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