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A Relativistic Formalism and the Small Angle Approximation of Elastic Electron Scattering in TEM

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A main part of the electrons scattered at the specimen in Transmission Electron Microscopy (TEM) are elastically scattered. The scattering is commonly described by a so-called relativistically corrected Schrödinger equation [1]. The original derivations of this equation from the Dirac equation are rather involved and lengthy. We will present a short derivation, which furthermore will shed some additional light on the approximations necessary. In the quadratic form of the Dirac equation

$$\left[E^2 - 2EV + V^2 - ie\hbar c\vec{E}\cdot\vec{\alpha}\right]\Psi = \left[c^2\vec{p}^2 + m_0^2c^4 + e\hbar c^2\vec{B}\cdot\vec{\sigma}\right]\Psi . \quad (1)$$

the different parts of the spinor Ψ couple through terms containing the electric field $\vec{E}$ and magnetic field $\vec{B}$. The examination of those parts yields that they are small within the electromagnetic potentials produced by a standard specimen in TEM. The magnetic part on the other hand does produce a different phase shift of a spin down and spin up electron within the magnetic field of the objective lens, which is, however, normally not accessible by the experiment since different electrons superpose incoherently. Consequently the coupling terms can be neglected yielding four decoupled Klein-Gordon equations

$$\left[E^2 - 2EV + V^2\right]\Psi = \left[c^2\vec{p}^2 + m_0^2c^4\right]\Psi . \quad (2)$$

An analysis of the Klein-Gordon equation yields that the neglection of the squared potential term V^2 yields the so-called relativistically corrected Schrödinger equation

$$\left[\frac{E^2 - m_0^2c^4}{c^2}\right]\Psi = \left[\frac{\vec{p}^2}{2\gamma m} + V\right]\Psi . \quad (3)$$

This approximated Klein-Gordon equation yields accurate results due to the large total energy E of the electron surmounting the potential at orders of magnitude at all regions of the specimen, except a very small area very close to the atom cores, which plays, however, a negligible role as will be demonstrated. We will support these findings by explicit numerical calculations at all intermediate steps of the derivation presented above. In figure 1a and b the difference between scattering simulations on Gold using the Dirac, Klein-Gordon and approximated Klein-Gordon equations stays within the numerical error.

The solution of the approximated Klein-Gordon equation implies the knowledge of the boundary conditions. A general solution only fullfilling the equation of continuity is feasible and computationally very demanding due to a polynomial eigenvalue problem occurring within the solution [2]. In TEM, however, the backscattered electrons can be neglected, allowing a direct integration of the approximated Klein-Gordon equation with the starting condition of an incoming

wave. The approximation is consequently called forward scattering approximation [3]. We will use standard algorithms like Runge-Kutta for the numerical integration of the equation.

One can further restrict the above-mentioned forward scattering approximation to a small angle approximation [3]. The resulting differential equation, sometimes referred to as paraxial equation, can again be solved numerically. The standard way, however, is to predefine the integration steps by hand, normally determined automatically by the algorithm, as slices containing one atomic layer of the specimen. This method is called Multislice algorithm and commonly applied to simulate elastic scattering [4].

By comparing the numerical forward integration and the multislice algorithm, we are able to estimate the error introduced by the small angle approximation and the predefined step size. The results show, that at scattering angles, typically lying within the first order Laue zone of the specimen, the two methods diverge. Since both the scattering angle and the convergence angle within the electron probes used in convergend beam TEM or scanning TEM reach the values in the first order Laue zone, this has to be considered when performing Multislice calculations for these imaging modes.

We examine these differences in detail for different kinds of specimen, i.e. large and small thicknesses, strong and weak scatterers, etc. and different imaging conditions. In figure 1 beam plots of Au calculated by means of numerical forward scattering and Multislice calculations are depicted. They almost perfectly coincide in the case of the zero beam. On the other hand a beam from the first order Laue zone diverges with increasing thickness.

References:
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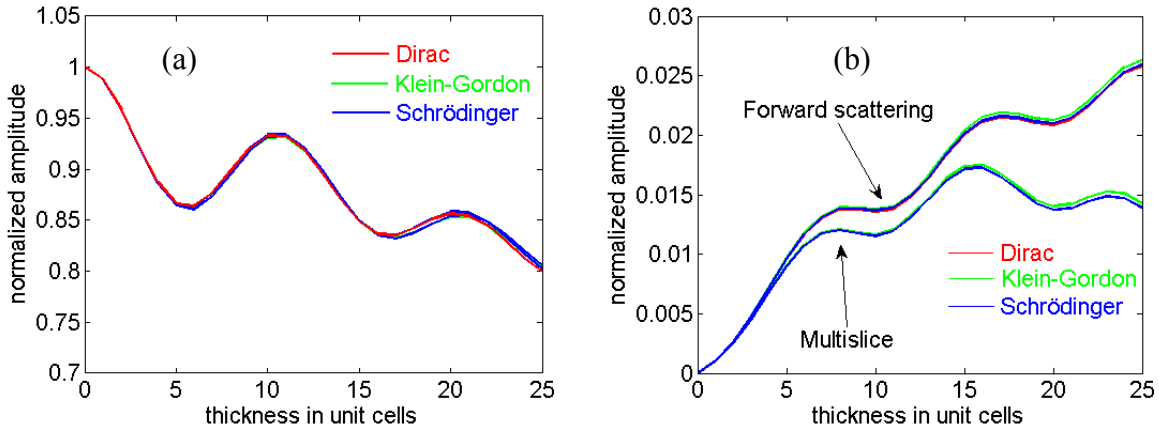

Figure 1: Beamplots of amplitude vs. thickness of the [0 0]-reflection (a) and the [0 28]-reflection (b) of Au simulated at 300 kV acceleration voltage with different types of algorithms