Quantitative High-Resolution TEM/STEM and Diffraction

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A modified Bloch-wave approach for dynamical scattering to limited order for structurally complex specimens

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Transmission electron micrographs are often complicated by dynamical diffraction, requiring image simulation using an algorithm like multislice or Bloch-wave. In the Bloch wave formulation, simulating all scattering orders in a single scattering matrix requires performing a matrix exponential, which can be computationally intensive, especially for structurally complex specimens – those with large unit cells and many allowed beam directions (e.g. proteins) [1]. In this work, we explore an approximation to the Bloch-wave algorithm designed to account for dynamical scattering to limited order in each scattering matrix. The matrix exponential is approximated to include only kinematical and first-order dynamical scattering [2], neglecting higher-order scattering. Higher-order scattering is included for thick specimens by computing one approximate matrix exponential for a thin sub-slice, and then propagating the wave function by repeated multiplication of this transfer matrix with the wave function. Figure 1 shows this, and compares it to a single-matrix limited-order approach. In addition, if the full specimen is thin enough (or consists of mostly light atoms, such as organic crystals) then only one column of the matrix is necessary, providing a useful simplification for image simulation of structurally complex specimens. The incident beam can also be tilted as exactly as in the Bloch wave formalism, and both bright- and dark-field images can be calculated. The approximation compares favorably to exact calculations [3] under some conditions. Using silicon as a benchmark, the exit-wave amplitudes and phases are very close to those generated from full (all-order) Bloch-wave calculations using matrix exponentials with zero absorption (Figure 2). When basic electron absorption is included, the approximated exit-wave phases compare favorably to the full calculation, but the approximated exit-wave amplitudes have systematic discrepancies stemming from beam attenuation. In summary, we explored a modified Bloch wave algorithm designed to calculate dynamical scattering to limited order i.e. only kinematical and first-order dynamical scattering, which requires sectioning thick specimens into stacks of thin slices. The resulting approximate exit wave amplitudes and phases were shown to be in good agreement with a full all-order Bloch-wave calculation, except for electron beam attenuation.

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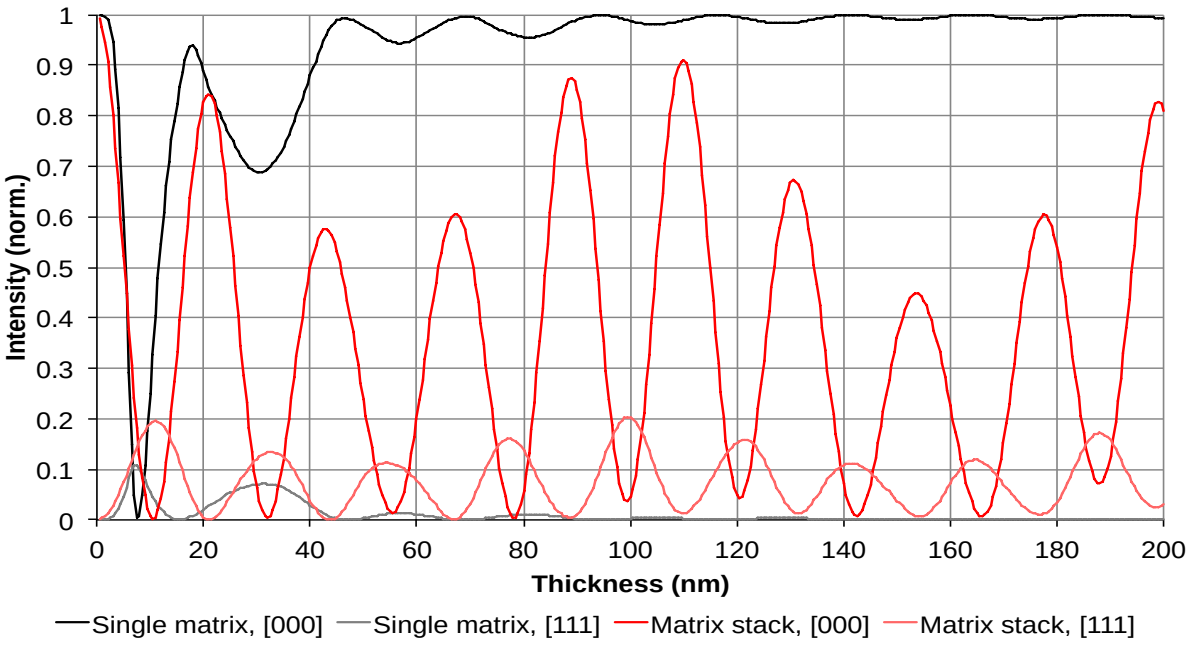

Figure 1. Beam intensity for [000] and [111] beam for the limited-order approximation [2] with a single matrix (black/grey) and a stack of 1Å matrices (red/pink) for a Si [110] zone axis at 80keV primary energy. The single-matrix data models only kinematical and first-order dynamical scattering (and hence is unphysical at higher thicknesses). However, the matrix-stack approach models higher-order dynamical scattering by sub-slicing the specimen every 1Å and sequentially multiplying the beam with the resulting limited-order 1Å matrices to propagate the electron beam slice-by-slice.

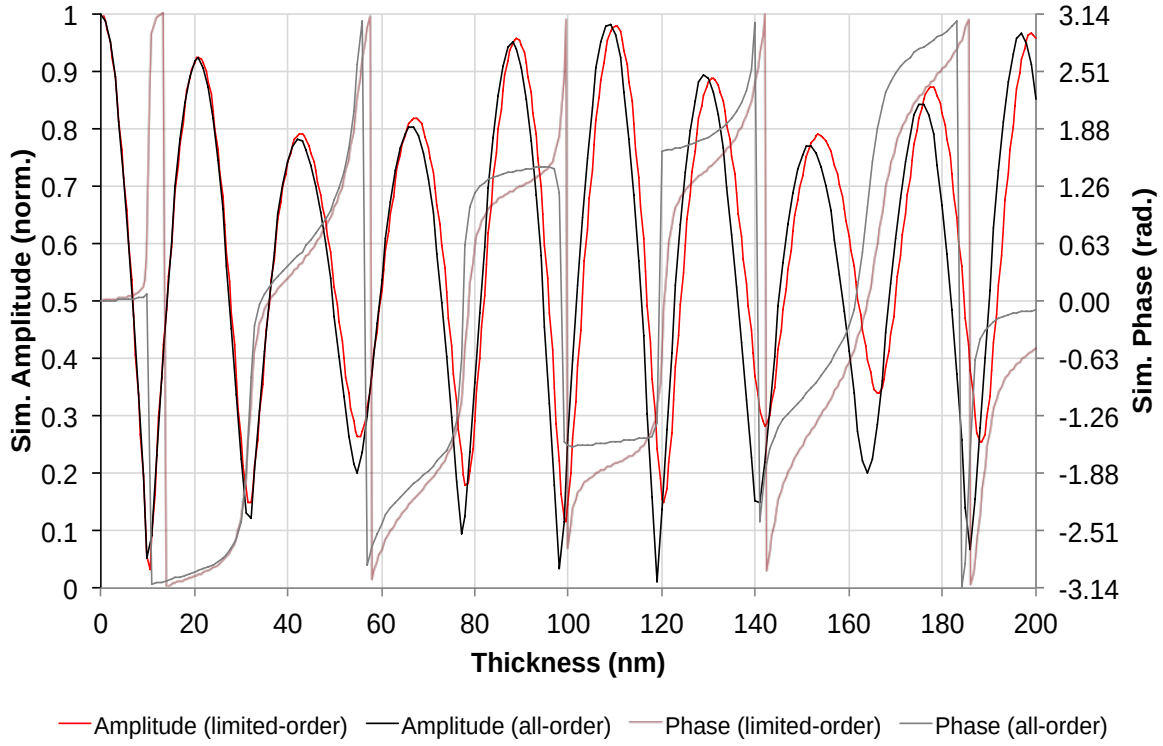

Figure 2. Bloch-wave amplitude (dark) and phase (light) for limited-order approximation (red) and JEMS all-order [3] (black) for a Si [110] zone axis at 80keV primary energy. The limited-order approximation is sliced every 1Å to include the effects of higher-order scattering.