Tilted multislice approach for quantitative STEM simulation

Xian Li[1], Changlin Zheng[1]
[1]State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai, China

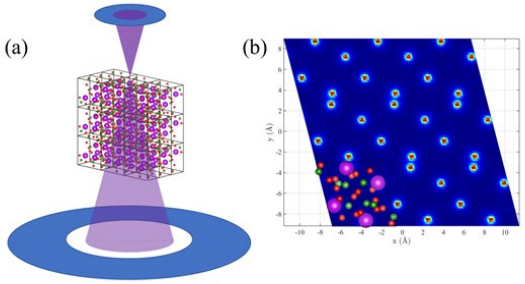
Background incl. aims
Scanning transmission electron microscopy (STEM) is a powerful tool for studying materials down to the atomic scale. Although qualitative STEM imaging offers plentiful information about atom locations and identification, quantitative analysis is becoming increasingly valuable for insights into composition, atom counting and thickness determination [1]. However, due to the strong dynamical scattering in crystals, directly solving the inverse problem from scattered electron intensity in STEM is nearly impossible. As a result, STEM imaging simulation is crucial for quantitative STEM analysis. In this study, we develop a new multislice algorithm that can be applied to nonorthogonal crystal structures, a task generally challenging in conventional multislice simulation [2].

Methods
For nonorthogonal unit cells, such as a triclinic unit cell, we first use an iterative algorithm to find a new unit cell. We aim to make the angles between the three new basis vectors as close to 90° as possible, while the c-axis keeps along the electron beam direction. The nonorthogonal supercell is then divided into a series of tilted slices parallel to the a-b vector plane. The Coloumb potential of the crystal is then projected onto the tilted slices based on a nonorthogonal mesh, and a tilted Fresnel propagation is performed between subsequent slices. The generated STEM image based on nonorthogonal mesh is then re-mapped into conventional format. By using this tilting-slice operation, we can effeiciently model the electron dynamical scattering in nonorthogonal structures.

Results
We implemented the method in our in-house STEM simulation code and performed high angle annular dark field (HAADF) STEM simulations on Gd2B4O9 [0 0 1], as shown in Figure 1.

Conclusion
We develop a tilted multislice approach to simulate focused electron beam propagation in nonorthogonal structures. This effectively extends quantitative STEM analysis to compound materials with more complex structures.

Graphic:



Keywords:

Quantitative STEM, multislice, nonorthogonal crystal

Reference:

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[2] E. J. Kirkland, Advanced Computing in Electron Microscopy, 2nd ed. (Springer, 2012).