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Multislice Electron Scattering Simulations for Angstrom-scale Magnetic Measurements with 4D-STEM

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Understanding how spins interact at the atomic scale is key for miniaturization of real, scalable devices. Lorentz transmission electron microscopy (LTEM) [1], holography [2-3], and differential phase contrast (DPC) imaging [4-5] have been standard imaging techniques local arrangement of spins, e.g. magnetic domains and topological structures such as skyrmions [6]. These techniques have been limited to spatial resolutions of a couple of nanometers [6-8]. While new methods such as 4D-STEM might enable magnetic measurements with angstrom-scale probes, extracting magnetic signals has been challenging because the electron scattering from the atomic potential is roughly 1000-fold stronger than scattering from the local magnetic moment at the angstrom-scale [4, 8].

A key part of developing new magnetic imaging techniques is the ability to conduct quantitative electron scattering simulations. We add magnetism to conventional multislice simulations [9] in order to create a quantum mechanical model for electron scattering in magnetic materials. This model takes as an input density functional theory simulations of the magnetization as well as the atomic potentials for a given crystal. We then propagate the wavefunction through the crystal in slices, treating the electron scattering from both the atomic potential and the magnetization as strong phase objects [10]. At this step of the simulation, we take the wavefunction after scattering through each slice of the crystal and add a magnetic phase to it. Using this model, we tested acquisition parameters to determine the ideal convergence angle and combination of sample thickness to maximize the magnetic signal. We find that the strongest magnetic signals are obtained when the probe size is matched to the size of the features to be probed. We also tested data analysis methods to extract the local magnetic moment. We found that, while in simulations with only magnetic fields, measurements of the center of mass could readily track the deflection of the electron beam [4] and be converted to a magnetic field, more sophisticated approaches are needed to isolate the magnetization from electron scattering due to the atomic potentials, particularly when dynamical scattering occurs [13].

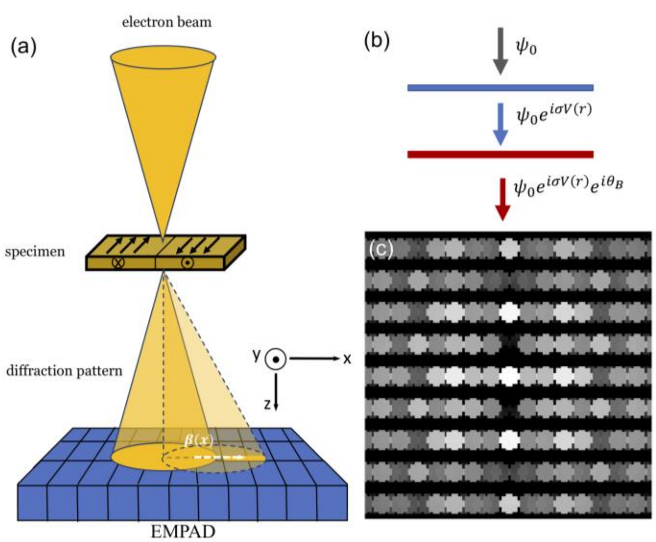

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Figure 1. Figure 1. (a) Schematic of magnetic imaging with 4D STEM with the electron microscope pixel array detector (EMPAD). (b) Electron scattering simulation with magnetism is performed when a magnetic phase is added to the wave function after atomic scattering. (c) We capture the full CBED pattern at every scan position to reconstruct the deflection of the electron induced by the magnetic moment, from which we can reconstruct the local magnetic field.

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