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Mapping Picometer Scale Periodic Lattice Distortions with Aberration Corrected Scanning Transmission Electron Microscopy

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Tremendous strides have been made in tracking atomic positions using aberration corrected STEM in the last several years, enabling direct measurement of atomic shifts due to local ferroelectric polarization or nanoparticle surface relaxation with picometer precision [1,2]. In charge density wave (CDW) states, charge-lattice coupling leads to concomitant periodic modulations of both the electron density and atomic lattice positions, where the magnitude of periodic lattice distortions (PLDs) are often on the order of picometers. Direct observation of these states via atom tracking in STEM requires, however, addressing the somewhat subtle issue of defining an appropriate reference lattice, which may be further complicated by the presence of local PLD phase variations and multiple interpenetrating modulations.

Here, we directly map the displacement vectors at each atomic site of a transverse PLD field in the manganite oxide (Bi,Sr,Ca)MnO_3 (BSCMO) (Fig. 1). We solve the issue of the reference lattice by leveraging the convenient decoupling of the modulation and its underlying lattice in Fourier space. The transverse, displacive modulations give rise to a particular pattern of satellite peaks about each Bragg peak (Fig. 2a,b). By identifying and damping all satellite peaks associated with a single modulation from the Fourier transform of the original image (Fig. 2c-e), we generate a local reference lattice. Fitting and subtracting corresponding lattice positions from the image pair yields the PLD at each atomic site with ~2 pm precision. Our approach naturally accounts for any image distortions present. Simulated STEM data with known PLD structures confirm that our method accurately reconstructs the PLD structure everywhere except at lattice sites directly adjacent to atomically sharp discontinuities in the PLD field.

CDWs are a common feature in many strongly correlated materials, playing a pivotal role in mediating the colossal magnetoresistance mechanism and competing with high temperature superconductivity. Mounting evidence indicates that their nanoscale spatial inhomogeneity plays a central role in the emergence of exotic phenomena in complex electronic systems quite broadly [3]. Direct observation of their local structure, and particularly their local symmetry and topology, is therefore crucial to understanding these systems. Our PLD mapping approach enables such characterization, exemplified in the PLD dislocation shown in Fig. 2f. Notably, the topological defect shown is present in the PLD field, despite the absence of any defects in the underlying crystal lattice. By combining picometer precision atom tracking with a Fourier approach to generate a reliable reference lattice, we reveal the detailed local structure of PLDs in BSCMO.

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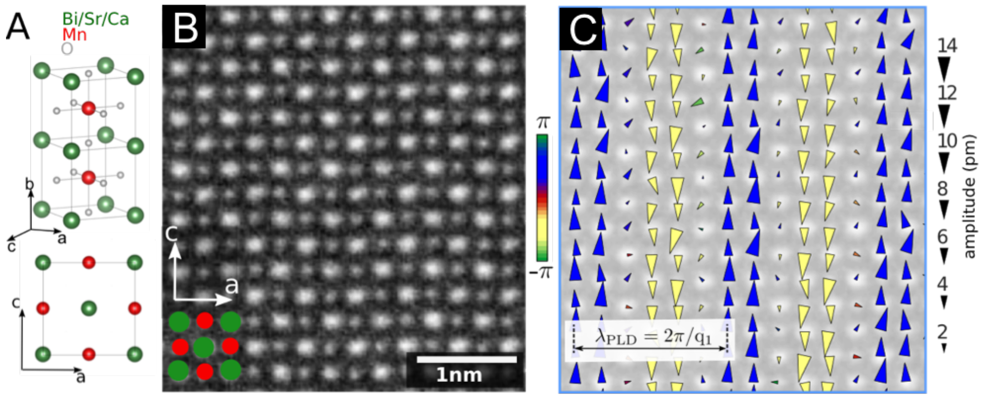

Figure 1. (a) The orthorhombic *Pnma* structure of BSCMO. **(b)** Frame averaged HAADF-STEM image of BSCMO, imaged along the b-axis. **(c)** Quantitative map of the PLD structure in BSCMO. The lattice modulation is transverse, displacive, and has a periodicity of 3 unit cells. The triangles represent the displacement vectors, with the magnitude of the displacement scaling linearly with the triangle area. The colorscale represents each displacements polarization relative to the modulation wavevector.

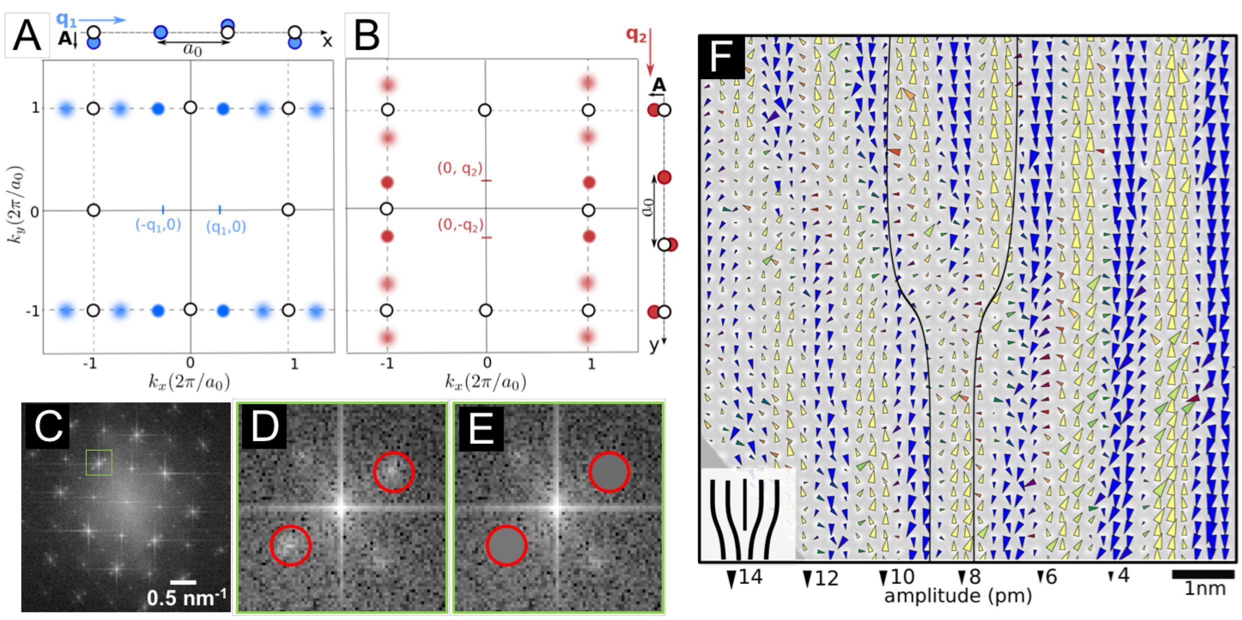

Figure 2. **(a,b)** Schematic of the Fourier space structure of a transverse periodic lattice displacement with wavevectors along the *x* and *y* directions, respectively. **(c)** Fourier transform of a STEM image. Bright peaks are the Bragg peaks, while the four dimmer peaks around each are the satellite peaks of the PLDs. **(d,e)** To generate a reference lattice, satellite peaks corresponding to the modulation of interest are identified, and their intensity is scaled down to the local background level. **(f)** A PLD map, generated by subtracting the positions of identical atomic sites in the original and Fourier damped image. A topological singularity in the PLD field is observed at the center of the image.