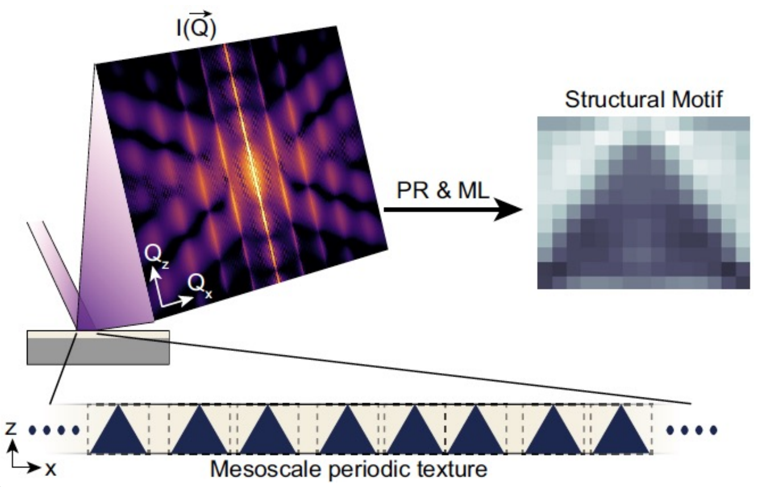
MIP: PARADIM at Cornell University, DMR-2039380
Local User Project - 2023

Imaging Nanotextures in Real Space by Inverting X-Ray Diffraction Data

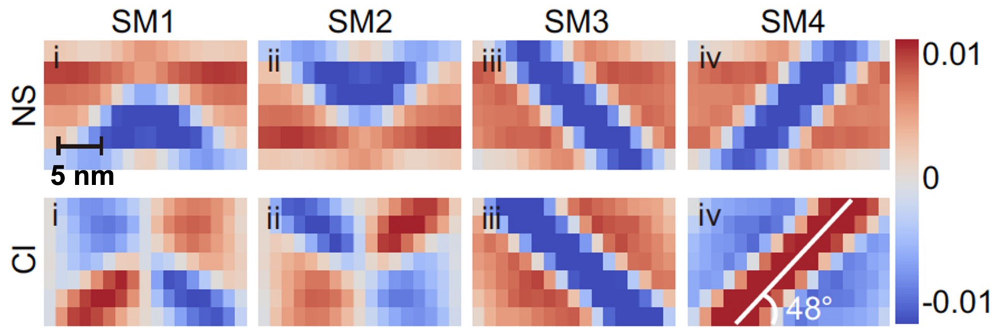
A. Singer, H. Nair, D.G. Schlom, K.M. Shen, L.F. Kourkoutis (Cornell University), V.A. Stoica, L.-Q. Chen (Penn State), J.P. Ruff (CHESS), J.W. Freeland (Advanced Photon Source)

New properties and exotic quantum phenomena can arise due to periodic nanotextures of co-existing materials, including metal-insulator transitions and negative differential capacitance. Here, **users of PARADIM and their collaborators** combine conventional iterative phase retrieval with unsupervised machine learning to extract high-resolution images of nanotextured materials from diffuse diffraction intensities using a conventional, partially coherent synchrotron beam. The method solves a long-standing problem and achieves a direct, model-independent inversion of x-ray diffraction data. Using the technique, a previously unreported nanotexture in a film undergoing a metal-insulator transition (Ca_2RuO_4) is discovered and confirmed by **PARADIM's cryo-STEM capabilities**. The method is relevant to modulated structures in ferroics and topological quantum materials.

Z. Shao, *et al*. [Proc. Natl. Acad. Sci. U.S.A. **120**, e2303312120 (2023)].



Concept: In a reciprocal space map, the mesoscale periodic ordering is evident from satellite peaks around the Bragg reflection. The diffraction intensity shown originates from the schematic periodic textures with triangular motifs, where the dark areas have a constant strain difference compared to the surrounding light area.



X-ray imaging: Nanotextures calculated to be present in a strained Ca_2RuO_4 film measured at 7 K. (A) Measured and (B) reconstructed diffraction pattern. Four characteristic structural motifs (SMs) labelled normal strain (NS) and crystal-plane inclination (CI) are identified.

Electron Microscopy: Cryo-STEM map of the interplanar spacing along [001] of the cross-section of a ~34-nm-thick Ca_2RuO_4 film at ~100 K. The features seen in STEM corroborate the nanotextures calculated from X-ray diffraction data, including the average stripe angle (48°).