

“Role of Phase Domains in Complex Materials”

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Abstract

Phase domains are an important, but subtle, kind of disorder has been discovered in a wide variety of crystalline materials. They are revealed by phase sensitive imaging techniques, such as coherent diffraction methods, which see small regions spatially shifted with respect to each other by fractions of a unit cell, while preserving their angular orientations. The domain walls of such structures have translational lattice offsets and zero rotation angle. We refer to these as phase domains because they appear with different phases in the complex electron density maps whenever Bragg peaks are used with X-ray imaging methods, such as Bragg Coherent Diffraction Imaging (BCDI) and Bragg Ptychography. Phase domains are invisible in ordinary diffraction experiments, except as a broadening of the diffraction peaks, which is not explained by traditional mosaic models. They can be detected in lattice imaging by transmission electron microscopy (TEM) through the Geometric Phase Analysis (GPA) approach. Because of the inherent symmetry of phase domain structures, the inversion of their diffraction patterns to images using phase retrieval methods is particularly challenging. The existence of phase domains appears to be fairly common in complex oxides and is possibly associated with chemical disorder. It may be enhanced in so-called "high entropy" formulations of materials and may also be introduced by mechanical preparation techniques such as ball-milling. The wall structures between such phase domains could be responsible for anomalous physical properties of complex oxides, such as magnetoresistance or ion conduction. In this talk, I will present Bragg Ptychography results on the spin-ordered domains of $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$ nickelate [1] and BCDI results showing phase domains in solid-state electrolyte materials. I will also present results from laser melting of gold thin films where grain boundaries are believed to be responsible for an inhomogeneous distribution of melt nucleation sites [2].

[1] Longlong Wu, et al, Physical Review Letters 127 275301 (2021)

[2] I. K. Robinson et al, IUCrJ 10 656–661 (2023)



My research interest is X-ray diffraction using synchrotron radiation. Starting at Bell Labs, then at the University of Illinois (Urbana), I developed the methods for studying surface structure using X-ray diffraction. These methods, based on crystal truncation rods, have become the definitive technique for the determination of the atomic positions at surfaces and interfaces. I was awarded the Warren Prize in 2000, the Surface Structure Prize in 2011 and the Gregori Aminov Prize in 2015 for this work. To further develop the methodology of X-ray diffraction with SR, I built two beamlines, beamline X16A at the National Synchrotron Light Source (Brookhaven) for surface structure and 34-ID at the Advanced Photon Source (Chicago) for coherent diffraction. Since 2006, based in the London Centre for Nanotechnology, I continued to develop the coherent X-ray diffraction methods at the Diamond Light Source. I was a founding "Diamond Fellow" of the Research Complex at Harwell, then I took a part time position running the X-ray Scattering group at Brookhaven National Laboratory, moving in the direction of studying quantum materials with important properties. The Bragg Coherent Diffraction Imaging method is well adapted to

visualising strains and domains within these materials which are often connected with their transport properties. It also allowed me to explore further the materials in the time domain as they respond to laser excitation. This is achieved using X-ray Free electron Laser Sources, such as SACLA (Japan), LCLS (Stanford), European XFEL (Hamburg) and PAL-XFEL (Pohang, Korea).