Quantitative electron microscopy as a tool to determine structure-property relationships at the picoscale?

Electron microscopy is one of the most powerful techniques available to investigate materials at the micro, nano, and even picometer length scales. After nearly 100 years of innovation, capabilities of the instrument continue to advance rapidly. Within the past twenty years, for example, electron microscopy has been revolutionized by the advent of the aberration corrector, new detector technologies, and dramatic improvements to electron sources. At the same time, direct measurements from the images had remained largely qualitative or semi-quantitative. This was particularly true for scanning transmission electron microscopy (STEM) images, where accuracy and precision had been significantly hampered by sample drift and scan distortion which prevented the ability to fully characterize and quantify the atomic structure changes that can ultimately define material properties. Moreover, these instruments require months or even years of practice to drive efficiently and to acquire reproducible atomic scale, quantitative information. As a result, the necessary experience (and often luck) has prevented even experts from being able to capture more than a few dozen datasets in a session on the microscope, thereby limiting statistical significance.

In this talk, I will highlight approaches that we developed to make electron microscopy absolutely quantitative and how we’ve applied those techniques to solve a variety of materials challenges in metals, semiconductors, and functional oxide systems. I will describe the various approaches and demonstrate that the techniques can achieve sub-picometer accuracy and enable real-space crystallographic measurements in STEM. Our investigations of relaxor ferroelectrics will be presented to demonstrate the power of these techniques to understand the physical behavior of materials. I will show, for example, how picometer precise measurements enable the capability to directly observe static atomic displacements within complex oxide solid solutions and to understand how short-range order gives rise to the properties of relaxor ferroelectric materials. We will also reexamine thermal diffuse scattering (TDS) in electron diffraction and show how lattice dynamics throughout the Brillouin zone can be captured. By comparing experiments from Si and SrTiO3 to results from molecular dynamics using state-of-the-art machine learned atomic potentials, we will show that even subtle changes in atomic vibrations due to temperature and anharmonicity are embedded within TDS and ripe for quantification. Looking to the future, I will also discuss our work on applying artificial intelligence to both determine, in real-time, sample thickness/tilt and to automate the scanning transmission electron microscopy workflows, reducing the barrier to capturing statistically significant data.

James LeBeau earned his B.S. in Materials Science & Engineering from Rensselaer Polytechnic Institute in 2006 and his Ph.D. from the University of California Santa Barbara in 2010. After his graduate work, he joined the faculty of the Department of Materials Science and Engineering at North Carolina State University in January 2011. In 2019, he moved his group to the Department of Materials Science & Engineering at MIT. His research focuses on applying and developing (scanning) transmission electron microscopy techniques to quantify the atomic structure and chemistry of materials to inform our understanding of relaxor/ferroelectric, mechanical, optical, and quantum properties. For his research, he has been honored with awards including the Presidential Early Career Award for Scientists and Engineers (PECASE), NSF CAREER award, an AFOSR Young Investigator grant, the Microanalysis Society K.F.J Heinrich award, and the Microscopy Society of America Burton Medal.

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In person only; no Zoom

Questions? Contact allison.macknick@northwestern.edu and megan.ray@northwestern.edu