Spring 2025 Joint Colloquium Materials Department & Materials Research Laboratory

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Advancing Materials Analysis and Discovery: 4D-STEM and Intelligent Data Exploration

Four-dimensional scanning transmission electron microscopy (4D-STEM) revolutionizes materials characterization by capturing millions of spatially-resolved 2D diffraction patterns with near unit-cell spatial resolution. This large dataset enables detailed mapping of crystal symmetry, orientation, strain, and defects over micron-scale areas, allowing statistically robust microstructure analysis. As data quality and acquisition speed improve, advanced methods for analyzing massive 4D-STEM datasets are becoming essential for materials design and discovery. This talk will present our recent approaches for 4D-STEM analysis using digital image processing, dynamic electron diffraction simulations, and machine learning. We will highlight our investigation of nanoscale fluorite-structured ferroelectric thin films, which exhibit multiple metastable phases with random orientations and varying grain sizes. By precisely mapping the spatial distribution and orientation of polymorphs, we provide statistical insights into how various thin film processing conditions influence the microstructure and ferroelectric performance. We will also demonstrate clustering diffraction patterns in 4D-STEM dataset using unsupervised machine learning and Cepstral analysis to quantify strain and microstructure in precipitation-hardened shape memory alloys. These results introduce a novel methodology for exploring the microscopic mechanisms through which nano and microscale phase competition controls materials properties.

Bio: Honggyu Kim is an assistant professor in the Department of Materials Science and Engineering at the University of Florida (UF). He received his Ph.D. in the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign. Before joining the faculty at UF in Fall 2019, he was a postdoctoral researcher at the University of California, Santa Barbara, investigating vacancy characterization and phase evolution in functional oxides. His primary research focuses on the development and application of advanced transmission electron microscopy techniques to establish direct relationships between the structure and properties of materials on the atomic scale. His recent research topics include quantitative imaging of defect and domain structure in ferroelectric thin films, symmetry

determination of quantum materials, and characterization of phase transformation in novel metallic alloys. He is the recipient of a 2024 NSF CAREER award.

Hosted by Susanne Stemmer