APS Scientific Computation Seminar Series

Speaker: Siddharth Maddali, Assistant Scientist
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Title: New characterization methods for crystalline materials at fourth-generation coherent light sources

Date: Monday, March 28, 2022

Time: 1:00 p.m. (Central Time)

Location: **Join ZoomGov Meeting**
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Hosts: Mathew Cherukara and Nicholas Schwarz

Abstract: Fourth-generation synchrotron light sources like the APS-U present several novel capabilities for materials characterization when coupled with new inversion methods. In this talk I will present new prospects in lens-less and lens-based imaging of crystalline materials, that will exploit the bulk penetrative capabilities of high-brilliance coherent x-rays of the APS-U. In particular:
(i) a new high-fidelity, multi-reflection Bragg coherent diffraction imaging (BCDI) algorithm tailored to crystals/polycrystal grains with significantly more dislocation content than current phase retrieval capabilities permit to reconstruct. The new differentiable forward model uses Fourier-based methods to explicitly maintain fidelity to high-frequency features like lattice discontinuities in modeling the eventual measured signal. I will demonstrate the vast improvement in reconstruction quality over present-day concurrent reconstruction methods.
(ii) the potential to observe irreversible processes in structural materials with coherence-enhanced dark-field x-ray microscopy (DFXM), through evolving signatures of structural defects in out-of-focus measurements of an x-ray lens. I will show with simulations how this modality could reveal structural features in crystalline bulks that may not be evident in a conventional lens-generated image, without the need for image reconstruction. This capability stands to fill a critical gap in the size of crystals that can currently be spatially resolved with synchrotron imaging methods.

Biography: Siddharth Maddali is a staff scientist in the Synchrotron Studies of Materials group in the Materials Science Division at ANL. He received his PhD in physics from Carnegie Mellon University in 2016 and has done post-doctoral research at ANL and the National Energy Technology Laboratory, where he worked on machine learning for materials discovery. He specializes in computational methods for multi-scale materials imaging using incoherent and coherent synchrotron x-rays. He has developed algorithms tailored to future imaging applications at next-generation light sources.