




Seminar

Machine Learning in Electron Microscopy: From Feature Finding to Discovery and Control

 Tuesday October 6, 2020	Dr Sergei V. Kalinin Sergei Kalinin is a corporate fellow at the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory, USA.
 11.00am	
 ZOOM – PASSCODE: 123456 https://monash.zoom.us/j/6prDluHdOCI-j8knoMKNnbAMXgBnOF	

Abstract

Machine learning (ML) has emerged as a powerful tool for the data and image analysis and enabling component of the autonomous systems in areas ranging from biological and medical imaging to self-driving cars. This rapid growth in ML applications poses the question as to which of these methods can be applied in electron microscopy, and perhaps more importantly, what insight into physics and chemistry of real materials can they yield. In this presentation, I will give a brief overview of recent developments in ML analysis of mesoscopic and atomically resolved images and spectroscopy in electron and scanning probe microscopy, including the deep convolutional neural networks and symmetry-invariant autoencoders. The applications ranging from feature extraction to information compression and elucidation of relevant order parameters to inversion of imaging data to reconstruct structural models have been demonstrated. However, the fundamental limitation of the vast majority of machine learning methods is their correlative nature, leading to extreme susceptibility to confounding factors and observational biases. I will introduce approaches for supervised and semi-supervised analysis of the STEM structural data that can be implemented both as a part of the microscope operation and post-acquisitions workflows. These include atom and building block finding and determination of local symmetries from the structural and spectral data. I will further illustrate several intriguing opportunities in exploring structure-property relationships from STEM-EELS datasets. These approaches are now being extended into the Bayesian domain, that allow to take into consideration the prior knowledge the system and evaluate the changes in understanding of the behaviors given new experimental data. is discussed. All the codes presented during the talk will be available through the GitHub repositories. In particular, it allows to systematically address question such what resolution and information limits are required for observation of certain physical phenomena.

Ultimately, we seek to answer the questions such as whether electronic instability due to the average Fermi level guides the development of the local atomic structure, or frozen atomic disorder drives the emergence of the local structural distortions, whether the nucleation spot of phase transition can be predicted based on observations before the transition, and what is the driving forces controlling the emergence of unique functionalities of morphotropic materials and ferroelectric relaxors. The unique aspect of Bayesian methods is their potential to quantify uncertainty, and harnessing this for automated experimentation

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The Presenter

Sergei Kalinin is a corporate fellow at the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory. He received his MS degree from Moscow State University in 1998 and Ph.D. from the University of Pennsylvania (with Dawn Bonnelli) in 2002. His research presently focuses on the atomic fabrication via electron beams, applications of big data and artificial intelligence methods in atomically resolved imaging by scanning transmission electron microscopy and scanning probes for physics discovery, as well as mesoscopic studies of electrochemical, ferroelectric, and transport phenomena via scanning probe microscopy.

Sergei has co-authored >650 publications, with a total citation of >33,000 and an h-index of >91. He is a fellow of MRS, APS, IoP, IEEE, Foresight Institute, and AVS; a recipient of the Blavatnik Award for Physical Sciences (2018), RMS medal for Scanning Probe Microscopy (2015), Presidential Early Career Award for Scientists and Engineers (PECASE) (2009); Burton medal of Microscopy Society of America (2010); 4 R&D100 Awards (2008, 2010, 2016, and 2018); and a number of other distinctions.

Convener

Professor Joanne Etheridge
Director, Monash Centre for Electron Microscopy