Bringing AI from Data to Action: Automated Experiment and Atomic Fabrication in Electron Microscopy

Sergei V. Kalinin*

University of Tennessee, Knoxville
**E-mail: sergei2@utk.edu*

The last note left by Richard Feynman stated "*What I cannot create, I do not understand*." Building solid state quantum computers, creating nanorobots, precision medicine based on protein sequencing, and designing new classes of biological molecules and catalysts alike requires the capability to manipulate and assemble matter atom by atom, probe the resulting structures, and connecting them to macroscopic world. In this presentation, I will discuss recent progress in automated experiment in electron microscopy, ranging from feature and physics discovery via active learning to direct atomic fabrication. As a motivation for the development of ML-enabled electron microscopy, I will illustrate several examples of electron beam atomic fabrication that my colleagues and I have explored over the last decade. These include directed atomic motion and artificial molecule assembly in graphene, non-twisting Moire reconstructions in phosphosulfides, 3D nanofabrication and atomic motion in Si, plasmonic patterning in nanoparticles, and defect line and pore patterning in MXenes and dichalcogenides. However, harnessing the power of electron beam for direct control of matter on the intrinsic timescales of microscope operation that are well below human reaction times requires seamless ML control of the instrument. I introduce the concept of the policy- and reward-driven experimental workflow planning and discuss how these workflows can be implemented via domain-specific hyper languages. The applications of classical deep learning methods in streaming image analysis are strongly affected by the out of distribution drift effects, and the approaches to minimize though are discussed. The real-time image analysis allows spectroscopic experiments at the predefined features of interest and atomic manipulation and modification with preset policies. I will further illustrate ML methods for autonomous discovery, where the microstructural elements maximizing physical response of interest are discovered. Jointly, the ML-based optimization and control allows transforming electron microscopy to a powerful physics discovery and atomic fabrication tool, building the window for ML agents to act on the atomic scale and bringing Feynman vision closer to reality.

Sergei Kalinin is a Weston Fulton chair professor at the University of Tennessee, Knoxville. In 2022 – 2023, he has been a principal scientist at Amazon special projects (moon shot factory). Before then, he spent 20 years at Oak Ridge National Laboratory where he was corporate fellow and group leader at the Center for Nanophase Materials Sciences. He received his MS degree from Moscow State University in 1998 and Ph.D. from the University of Pennsylvania (with Dawn Bonnell) in 2002. His research focuses on the applications of machine learning and artificial intelligence methods in materials synthesis, discovery, and optimization, automated experiment and autonomous imaging and characterization workflows in scanning transmission electron microscopy and scanning probes for applications including physics discovery, atomic fabrication, as well as mesoscopic studies of electrochemical, ferroelectric, and transport phenomena via scanning probe microscopy. When at ORNL, he led several major programs integrating the ML and physical sciences and instrumentation, including the Institute for Functional Imaging of Materials (IFIM 2014-2019), the first program in DOE

integrating ML and physical sciences, and the microscopy effort in INTERSECT program that realized first ML-controlled scanning probe and electron microscopes. At UTK MSE, he participated in building one of the first efforts in the country on ML-driven materials exploration. At UTK, his team has now realized fully AI-controlled SPM and STEM systems and co-orchestration workflows between multiple characterization tools for scientific discovery. He has also taught multiple courses on the ML for materials science and microscopy including Bayesian optimization methods. Sergei has co-authored >650 publications, with a total citation of ~58,000 and an h-index of ~116. He is a fellow of NAI, Academia Europaea, AAAS, RSC, AAIA, MRS, APS, IoP, IEEE, Foresight Institute, and AVS; a recipient of the Adler Lectureship (APS 2025), Duncumb Award (MSA 2024), Medard Welch Award (AVS 2023), Orton Lectureship (ACerS 2023), Feynmann Prize of Foresight Institute (2022), 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); 5 R&D100 Awards (2008, 2010, 2016, 2018, and 2023); and a number of other distinctions. As part of his professional services, he organized many professional conferences and workshops at MRS, APS and AVS; for 15 years organized workshop series on PFM, and served/s on multiple Editorial Boards including NPJ Comp. Mat., J. Appl. Phys, and Appl. Phys Lett.