Autonomous experiments in the age of computing, machine learning and automation: progress and challenges

Rama Vasudevan
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Machine learning has by now become a widely used tool within materials science, spawning entirely new fields such as materials informatics that seek to accelerate the discovery and optimization of material systems through both experiments and computational studies. Similarly, the increasing use of robotic systems has led to the emergence of autonomous systems ranging from chemical synthesis to personal vehicles, which has spurred the scientific community to investigate these directions for their own tasks. This begs the question, when will mainstay scientific synthesis and characterization tools, such as electron and scanning probe microscopes, start to perform experiment autonomously?

In this talk, I will discuss the history of how machine learning, automation and availability of compute has led to nascent autonomous microscopy platforms at the Center for Nanophase Materials Sciences. I will illustrate the challenges to making autonomous experiments happen, as well as the necessity for data, computation, and abstractions to fully realize the potential these systems can offer for scientific discovery. I will then focus on our work on reinforcement learning as a tool that can be leveraged to facilitate autonomous decision making to optimize material characterization (and material properties) on the fly, on a scanning probe microscope. Finally, some workflow and data infrastructure issues will also be discussed.

This research was conducted at and supported by the Center for Nanophase Materials Sciences, a US DOE Office of Science User Facility.