AI/ML/Autonomous Experimentation for Thin Films Processing
Room 317 - Session AIML1-ThA
AI/ML in Materials Characterization

Moderators: Mr. Lucas Kuehnel, University of Missouri, **Dr. Andreas Werbrouck**, Ghent University, Belgium

2:15pm **AIML1-ThA-1 Combining Optimization and Agentic Control in Automated Scanning Probe Microscopy**, ***Boris Slautin,*** *Sheryl Sanchez, Jordan Marshall, Mahshid Ahmadi, Sergei Kalinin,* The University of Tennessee **INVITED**

Closed-loop optimization is increasingly used in automated microscopy for tasks ranging from experimental parameter tuning to mapping unknown structure–property relationships. The core idea is to guide the experiment by selecting the next most informative measurement location or parameter set while accounting for uncertainty, noise, and limited experimental budget. However, when the objective, decision space, and constraints must be defined in advance, the automation remains largely local to a specific task. This becomes limiting for hierarchical or evolving experiments that require coordinated measurement selection, quality control, parameter adjustment, mode switching, and refinement of the experimental question.

The emergence of agentic AI provides a complementary route for automated microscopy. Many experiments are not a single optimization loop, but a set of coupled steps involving data acquisition, image analysis, quality control, parameter adjustment, and physical interpretation. Closed-loop methods are powerful for well-defined local optimization or exploration tasks, but the connection between these steps often still requires expert judgment. Agentic systems can help provide this connecting layer by supporting experiment-level orchestration, propagating information between local loops, incorporating physical context, and dynamically planning the next experimental step. In this sense, agentic control should not replace classical optimization, but rather coordinate optimization modules, data-analysis routines, physical constraints, and microscope-control actions within a broader automated experiment.

In this work, we develop an agentic system for automated scanning probe microscopy (SPM), demonstrated on ferroelectrics using piezoresponse force microscopy as the example. The agent provides global orchestration of the experiment by connecting microscope control with image and spectroscopy analysis, incorporating physical context, and making higher-level decisions about the experimental trajectory. Classical optimization are integrated as local modules for tasks that can be formulated quantitatively, such as tuning measurement parameters or selecting informative measurement locations.

We deploy this approach in a real experimental setting, where the agent coordinates microscope actions, analysis routines, and local optimization loops during PFM measurements. Although demonstrated for ferroelectric PFM, the same architecture can be extended to broader automated experimental problems, including thin-film processing, synthesis–characterization loops, and structure–property mapping.

2:45pm **AIML1-ThA-3 Multi-Agent System for Optical Microscopy of 2D Materials Characterization**, ***Haozhe "Harry" Wang,*** Duke University

Optical microscopy remains an indispensable tool for the rapid characterization of two-dimensional materials, yet conventional workflows depend heavily on trained operators to navigate samples, identify regions of interest, and interpret complex image features — creating a persistent bottleneck in experimental throughput. Here, we present a multi-agent system built on foundation models that fully automates the optical microscopy pipeline for 2D material characterization, from stage navigation to image acquisition to quantitative analysis.

Our architecture decomposes the microscopy workflow into specialized, cooperating agents: a navigation agent that performs intelligent search over the substrate, a perception agent that segments and classifies material features in real time, and an analysis agent that extracts quantitative descriptors such as layer number, domain morphology, and spatial coverage. These agents communicate through a structured orchestration layer, enabling adaptive decision-making — for example, dynamically adjusting scan density in response to local material heterogeneity or prioritizing high-value regions for higher-magnification imaging. Built on the ATOMIC (Autonomous Technology for Optical Microscopy and Intelligent Classification) framework, the system leverages large vision models to achieve zero-shot generalization across material systems and substrate types without task-specific fine-tuning.

We demonstrate the system on chemical vapor deposition-grown 2D semiconductors, where it achieves classification accuracy exceeding 99% while autonomously generating statistically representative maps of growth outcomes across centimeter-scale substrates. By eliminating manual intervention and enabling continuous, unsupervised operation, the multi-agent architecture transforms optical microscopy from a serial, operator-dependent technique into a scalable, intelligent characterization platform — laying the groundwork for closed-loop integration with upstream synthesis and downstream property measurements in autonomous materials laboratories.

3:00pm **AIML1-ThA-4 A Reference Architecture for Complex Scientific Chatbots Based on ChASE, an AI Assistant for SIMS**, ***Jordan Barrette,*** *Jerry Hunter, Prateek Maheshwari,* Beamline Incorporated

Secondary Ion Mass Spectrometry analysis planning requires synthesizing multiple knowledge sources: textbook physics governing sputter rate, ion yields, depth resolution, and matrix effects; institutional memory encoded in years of past setups; and analyst judgment about instrument state and sample characteristics. We present ChASE (Chat-bot Augmented for SIMS Expertise), a chatbot-style AI assistant for SIMS laboratories that integrates theoretical, historical, literature, and tribal knowledge into a unified decision-support tool. Rather than treating the underlying language model as an oracle trained to know everything a priori, we instruct it as a research expert—one that synthesizes information from many sources, much as a lab scientist draws on tribal knowledge, reference literature, recent work, and customer expectations.

The presentation outlines the architecture of ChASE, composed of three primary components: technical “skills,” tribal knowledge, and a reference literature corpus. Using this architecture, we demonstrate automated setup guidance that consults and reconciles historical setups, theoretical predictions, laboratory best practices, and published experimental methods. Building on the suggested setup guidance, we demonstrate automated scheduling across the current job queue. The setup-related predictions produced—sputter rate, required depth, estimated tuning overhead—roll up into time estimates that are compared against similar historical runs to produce expected and worst-case total analysis times, giving lab managers a preliminary schedule with built-in margin.

Central to this research-expert approach is the skill framework, which mirrors the way an experienced analyst decomposes a complex problem into prerequisite questions before synthesizing an answer. Skills are applied recursively: complex tasks decompose into collections of prerequisite subtasks that themselves constitute skills. For instance, a “SIMS Setup Predictor” skill leverages “Primary Ion Predictor,” “Mass Resolution Predictor,” and “Depth Resolution Predictor” as constituent skills. Each is a sophisticated model on its own, built on the same reference architecture—hence the recursive nature—supporting prediction models for ion yield, mass interference, and cascade mixing, respectively. We compare the architecture’s response accuracy for complex scientific tasks with a standalone language model and more common adaptation approaches such as pre-training, fine-tuning, prompt engineering, and retrieval-augmented generation. Finally, we discuss strengths and limitations of the approach, within the context of the ultimate goal—an AI framework that can be expanded beyond SIMS.

3:15pm **AIML1-ThA-5 Leveraging Automated Characterization and Machine Learning to Optimize Defects for Quantum Sensing**, ***Dane deQuilettes,*** Princeton University

Spins in solid-state materials, molecules, and other chemical systems have the potential to impact the fields of quantum sensing, communication, simulation, and computing. In particular, color centers in diamond, such as negatively charged nitrogen vacancy (NV^-) and silicon vacancy centers (SiV^-), are emerging as quantum platforms poised for transition to commercial devices. A key enabler stems from the semiconductor-like platform that can be tailored at the time of growth. The large growth parameter space makes it challenging to use intuition to optimize growth conditions for quantum performance. In this work, we use supervised machine learning to train regression models using different synthesis parameters in over 100 quantum diamond samples. We train models to optimize NV^-defects in diamond for high sensitivity magnetometry. Importantly, we utilize a magnetic-field sensitivity figure of merit (FOM) for NV magnetometry and use Bayesian optimization to identify critical growth parameters that lead to a 300% improvement over an average sample and a 55% improvement over the previous champion sample. Furthermore, using Shapley importance rankings, we gain new physical insights into the most impactful growth and post-processing parameters, namely electron irradiation dose, diamond seed depth relative to the plasma, seed miscut angle, and reactor nitrogen concentration. As various quantum devices can have significantly different material requirements, advanced growth techniques such as plasma-enhanced chemical vapor deposition (PE-CVD) can provide the ability to tailor material development specifically for quantum applications.

Author Index

Bold page numbers indicate presenter