## Nanoscale Science and Technology Division
## Room 304 - Session NS+AP+BI+SS-WeM

## Frontiers in Scanning Probe Microscopy Including Machine Learning

**Moderators: Wonhee Ko**, University of Tennessee, Knoxville, **Adina Luican-Mayer**, University of Ottawa, Canada

8:40am **NS+AP+BI+SS-WeM-3 Decay Rate Spectroscopy for a Direct Probe of Josephson and Andreev Currents on the Atomic Scale**, ***Wonhee Ko,*** University of Tennessee, Knoxville*; J. Lado,* Aalto University, Finland*; E. Dumitrescu, P. Maksymovych,* Oak Ridge National Laboratory

The tunneling current in superconducting tunnel junctions involves several mechanisms in addition to the normal-electron tunneling, such as Josephson tunneling and Andreev reflection. Identification of the tunneling mechanisms as a function of external parameters, such as barrier height, bias voltage, temperature, and so on, is the key to elucidating the characteristics of the superconductors, such as paring symmetry and topology. Here, we present a method to identify distinct tunneling modes based on the decay rate of tunneling current measured by scanning tunneling microscopy (STM) [1,2]. Precise control of the tip-sample distance in picometer resolution allows us to quantify the decay rate as a function of bias $V$ and tip height $z$, with which we identified the crossover of tunneling modes between single-charge quasiparticle tunneling, (multiple) Andreev reflection, and Josephson tunneling. The method was both applied to S-I-S [1] and S-I-N [2] junctions, to unambiguously identify Josephson and Andreev currents. Moreover, mapping decay rates in the atomic resolution with STM revealed the intrinsic modulation of Andreev reflection and Josephson current. The result shows that the decay rate spectroscopy will be crucial for addressing the superconducting characteristics of the materials and their applicability for Josephson-junction devices.

This research was performed at the Center for Nanophase Materials Sciences which is a DOE Office of Science User Facility.

[1] W. Ko, E. Dumitrescu, and P. Maksymovych, *Phys. Rev. Res.***3** 033248 (2021)

[2] W. Ko, J. L. Lado, and P. Maksymovych, *Nano Lett.***22** 4042 (2022)

9:00am **NS+AP+BI+SS-WeM-4 Machine Learning-Driven Automated Scanning Probe Microscopy: Application to Ferroelectric Materials**, ***Yongtao Liu****, K. Kelley, R. Vasudevan,* Oak Ridge National Laboratory, USA*; H. Funakubo,* Tokyo Institute of Technology, Japan*; S. Kalinin,* University of Tennessee Knoxville*; M. Ziatdinov,* Oak Ridge National Laboratory, USA

Scanning probe microscopy (SPM) has become a mainstay of many scientific fields including materials science, condensed matter physics, and so on. Machine learning (ML) and artificial intelligence (AI) have been applied to determine the physical mechanisms involved in phenomena encoded within microscopy data, enabling ML/AI to rapidly become an indispensable part of physics research. However, the real-time connection between ML and microscopy—which enables automated and autonomous experiments for microscopy imaging and spectroscopy measurements—still lags. Until now, the search for interesting functionalities in microscopy experiments has been guided by auxiliary information from microscopy to identify potential objects of interest based on human intuition; the exploration and verification of physical mechanisms depend on human-based decision making, i.e., operators determine the parameters for subsequent experiments according to the previous experiment. Here, we developed ML-driven automated experiment (AE) scanning probe microscopy (SPM) workflow to learn the functionality and mechanism in materials in an automatic manner. We demonstrate the application of deep kernel learning and hypothesis learning based workflows by investigating ferroelectric materials, including studies of domain wall dynamics, domain switching mechanism, the conductivity of topological defects, and relationship between domain structure and local properties. Using these approaches, we observe larger hysteresis opening near 180° domain walls due to the larger polarization mobility in the vicinity of the 180° walls in a $PbTiO_3$ sample and find that the domain switching in a $BaTiO_3$ thin film is determined by the kinetics of the domain wall motion, etc. We implemented these approaches in SPM for ferroelectric materials investigation, however, the workflows are universal and can apply to a broad range of imaging and spectroscopy methods, e.g., electron microscopy, optical microscopy, and chemical imaging.

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9:20am **NS+AP+BI+SS-WeM-5 AVS Dorothy M. and Earl S. Hoffman Scholarship Talk: Direct Imaging of Light-Matter Interaction of 0-dimensional Excitonic Emitters using Tip-enhanced Scanning Probe Technique**, ***Kiyoung Jo***[1]*, E. Marino, J. Lynch, Z. Jiang, N. Gogotsi,* University of Pennsylvania*; P. Schuck,* Columbia University*; N. Borys,* Montana State University*; C. Murray, D. Jariwala,* University of Pennsylvania

Strong light-matter interactions of 0-dimensional emitters on plasmonic Au substrate were explored using both contact and tapping mode tip-enhanced scanning probe micro-spectroscopy. The plasmonic tip engaged with contact mode couples with the excitonic dipole in CdSe-CdS nanoplatelets, leading to strong exciton-plasmon coupling. Unlike the contact mode, the directional propagation of surface plasmon polariton from the excitonic emission of the nanoplatelets on Au as wave-like fringe patterns was probed by taking advantage of the tapping mode. Since tapping mode operates a few nanometers away from the surface, the near-field photoluminescence with in-plane wavevectors can be collected, leading to form fringe patterns propagating from the quantum plate. Extensive optical simulations proved that the fringes are the result of standing wave formed between the tip and the nanoplatelets. The effect of excitonic dipole orientation and dielectric layers on the fringe patterns were investigated by the simulation which matched with experimental results. The fringe patterns were also observed in WSe2 nano-bubbles, and the CdSe/CdS nanoplatelet in SiO2/Si substrate which means the phenomenon is universal in 0-dimensional emitters and various substrates. We envision that the discovery excels in understanding in-plane near-field light signal transduction from 0-dimensional emitters toward nano and quantum photonics.

9:40am **NS+AP+BI+SS-WeM-6 Nanoscale Subsurface Depth Sensitivity of Contact Resonance Atomic Force Microscopy on Layered Films**, ***Gheorghe Stan,*** National Institute for Science and Technology (NIST)*; C. Ciobanu,* Colorado School of Mines*; S. King,* Intel Corporation

Probing the mechanical properties is one of the basic inquiries that can reveal the structure and integrity of an isolated material or multicomponent system. At the nanoscale, due to size constrains and defects, mechanical tests become even more relevant as the properties of a part may differ by those of the whole. Over years, contact resonance AFM (CR-AFM) has proved to be a reliable AFM-based technique for nanoscale mechanical property measurements. Mostly operated into the elastic modulus range from few GPa to hundreds of GPa, CR-AFM was used to test different materials and structures at the nanoscale and considered for discerning the mechanical response of subsurface inhomogeneities and buried domains. It remains, however, to directly prove the extent of its quantitative capabilities both in terms of elastic modulus and depth sensitivity. In this work, we develop a quantitative methodology to test the elastic modulus and depth sensitivity of CR-AFM against a set of low-k dielectric bilayer films with the top layer of various thicknesses. We have analyzed the measured contact stiffness as a function of load and film thickness with both a semi-analytical model and three-dimensional finite element analysis. Both analyses confirmed the expected elastic moduli of the layered structures and provided a robust quantitative estimation of the subsurface depth and material sensitivities of CR-AFM. We also developed a correlative measurement-model analysis to assess the convoluted contributions of the structural morphology and mechanical properties to the contact stiffness used by AFM-based subsurface imaging. The results explain the inherent difficulties associated with solving concurrently the material contrast and location of subsurface heterogeneities in nanomechanical subsurface imaging.

11:00am **NS+AP+BI+SS-WeM-10 The Impact of Temperature on Viscoelastic Properties of Nanoscale Domains Within Polymer Composites**, ***Bede Pittenger****, S. Osechinskiy, J. Thornton, S. Loire, T. Mueller,* Bruker Nano Surfaces

The behavior of polymer composites is controlled by the properties of the components as well as the microstructure of the material. Because confinement effects and interphase formation can alter properties of the

[1] **AVS Dorothy M. and Earl S. Hoffman Scholarship Recipient**

microphases, only measurements performed directly on the composite can provide the needed local property distribution. Mechanical properties of polymers are generally temperature (and time) dependent, so a full understanding requires measurements over a range of temperatures and frequencies. Ideally, one would like to observe the mechanical behavior of these microscopic domains while they pass through their glass transitions to appreciate the influence of size effects and confinement on time dependent mechanical properties.

Recently, Atomic Force Microscopy based nano-Dynamic Mechanical Analysis (AFM-nDMA) was introduced. Like bulk DMA, this mode provides spectra of storage and loss modulus across frequency and temperature, allowing construction of master curves through Time Temperature Superposition (TTS). In addition, it allows high resolution measurements localized to the microscopic structures within heterogeneous samples. This presentation will examine the capabilities of this new mode with examples in a wide range of polymers and composites.

11:20am **NS+AP+BI+SS-WeM-11 AFM Force Spectroscopy Combined with Machine-Learning Methods for Identifying Malaria Derived- EV Subpopulations**, ***Irit Rosenhek-Goldian,*** *P. Abou Karam,* Weizmann Institute of Science, Israel*; T. Ziv,* Technion - Israel Institute of Technology, Israel*; H. Ben Ami Pilo, I. Azuri, A. Rivkin, E. Kiper, R. Rotkopf, S. Cohen,* Weizmann Institute of Science, Israel*; A. Torrecilhas,* Federal University of São Paulo, Brazil*; O. Avinoam,* Weizmann Institute of Science, Israel*; A. Rojas,* University of Costa Rica*; M. Morandi, N. Regev-Rudzki,* Weizmann Institute of Science, Israel

The Malaria (*Plasmodium falciparum*) parasite releases extracellular vesicles (EVs) which modulate the mechanical properties of the host red blood celland thus facilitate parasite action. It is understood that EVs are composed of sub-populations with different functions, but little is known of their nature and specialized function. Here, we report the use of Atomic Force Microscopy (AFM) imaging and puncture analysis, combined with state-of-the-art size separation techniques and several biochemical, microscopic and spectroscopic characterization techniques in an attempt to differentiate and characterize the different populations. Specifically, we subjected malaria-derived EVs to size-separation analysis, using Asymmetric Flow Field-Flow Fractionation (AF4). The fractions obtained were characterized by Cryo-transmission electron microscopy (cryo-TEM), and AFM which revealed the presence of two distinct EV subpopulations - small (10-70 nm) and large (30-500 nm). Proteomic analysis revealed that the small EVs were enriched in complement-system proteins and the large EVs with proteasome subunits. In addition, Förster resonance energy transfer (FRET)-based fusion assay showed that small EVs fused to early-endosome liposomes at significantly greater levels than large EVs. Finally, AFM puncture analysis characterized by unsupervised machine-learning verified the presence of two distinct fractions with respect to mechanical behavior which correlate with the EV size groupings. These results shed light on the sophisticated mechanism by which malaria parasites utilize EV subpopulations as a communication tool to target different cellular destinations or host systems.

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