OpenSPM 2024 Conference EPFL (Lausanne)

Monday April 22nd (Zoom https://epfl.zoom.us/j/61640229991)

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9:45-10:15 Sample Preparation and Environment Control for AFM: a missing opportunity - *Chanmin Su*

10:15-10:45 Hacking Optical Storage Drives for SPM development: Opportunities and challenges - *Edwin Hwu*

10:45-11:15 Coffee break

11:15-11:45 Improvement of the temporal resolution of high-speed AFM - *Noriyuki Kodera (in Zoom)*

11:45-12:15 Instrumentational Aspects of AFM under Vacuum and UHV Conditions - *Hans J. Hug*

12:15-14:00 Lunch

14:00-16:30 Discussion on the development of open science hardware

Visit Lavaux Vineyard Terraces and dinner at Le Deck restaurant in Chexbres

Tuesday April 23rd (Zoom https://epfl.zoom.us/j/66038982870)

9:00-9:30 Open software and hardware tools for advanced SPM scanning regimes – *Petr Klapetek*

9:30-10:00 Navigating the OpenSPM project: key challenges and needs in open software development – *Marcos Penedo*

10:00-10:30 Enhancing SPM Performance Through Modular Software Design and Data-Driven Control – *Navid Asmari*

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11:00-11:30 Integration of the Scanning Probe Microscope with the High Performance Computing: reward-driven workflow implementation - *Richard (Yu) Liu (in Zoom)*

11:30-12:00 Autonomous Microscopy: From Learning Physics and Structure-Property Relationships to Materials Discovery - *Sergei V. Kalinin (in Zoom)*

12:00-14:00 Lunch

14:00-16:30 Discussion on the development of open science software

Visit Lausanne center and dinner in Crêperie la Chandeleur

Wednesday April 24th (Zoom https://epfl.zoom.us/j/62112962166)

9:00-9:30 TopoStats - driving a community effort for shared, improved, modern computational infrastructure in AFM – *Alice Pyne*

9:30-10:00 Quantitative Electrical Properties of nanostructured materials from DC to GHz frequencies – *Georg Gramse*

10:00-10:30 Academic and industrial perspectives on SPM hardware development – *Jonathan Adams*

10:30-11:00 Coffee break

11:00-11:30 Advancing SPM probe microfabrication through open science – *Nahid Hosseini*

11:30-12:00 Open hardware collaboration between Weizmann SPM unit and LBNI lab at EPFL - *Irit Rosenhek-Goldian*

12:00-14:00 Lunch

Monday April 22nd: 9:15-9:45

Difficulties in Developing Hardware, Software and Firmware for In-Liquid High-Speed Frequency Modulation AFM

Takeshi Fukuma

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I have been engaged in the development of home-built frequency modulation AFM (FM-AFM) system in the past twenty years. Here, I would like to introduce the difficulties that I faced during this development and discuss possible solutions for them.

1. Analog vs. Digital Controllers

I personally like an analog one as its ultimate noise performance and speed is often better than the digital one. However, it is only when I do experiments and developments by myself. As a professor, I prefer to use a digital one as it is much easier to duplicate and difficult to break.

2. FPGA (Firmware) Development

Currently, I think the combination of LabVIEW and NI FPGA board seems to be the best option. However, in the long-term view, it is risky for all the community to rely on the products of one company. This is already evident from the recent price increase of LabVIEW and discontinuing of the high-speed AD/DA modules. Thus, we should seek for another option for open-source development.

3. Software Development

The main challenge is human resource development. For one thing, not all students have enough aptitude for the software development. For another, relatively high learning load is required to do practical development. Finally, important or difficult development does not necessarily results in a big academic achievement. As a best practice, now I have been trying to arrange a relatively low-load and impactful application subject combined with a software development subject.

4. Hardware Development

This requires very high educational load. AFM system consists of electronic, mechanical and optical parts. For the development of each component, a well-experienced engineer should give a hands-on-style training. In addition, the brush-up of ideas often requires insights only available by hands-on-style lab work. For a professor, this is very difficult to manage. Ideal solution may be to hire a well-experienced technician and prepare good educational resources such as manuals and movies. Sharing of such resources may help to lead the development of this community.

Monday April 22nd: 9:45-10:15

Sample Preparation and Environment Control for AFM: a missing opportunity

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AFM has long been considered as a technology requiring little sample-preparation and effective in mostly ambient environment. This talk will discuss the missing opportunities led by this misconception. Similar to electron beam and optical tools, AFM was aimed to provide the measurements of the intrinsic physical and chemical properties at the nanoscale, enabled by localized tip-sample interactions. Nearly 40 years after inventions of AFM, as dozens of sensing technologies were developed in the 90s and early 2000s, topography is still the only reliable AFM measurements which serves as the golden standards in industrial applications. In fact, most AFM measurements are prone to artifacts introduced by surface contaminations and oxidations. In this talk we will analyze the contributions of these artifacts to AFM measurements, especially electric measurements. We will further discuss solutions to remove these artifacts. In addition, we propose an integrated AFM system with chemically selective masking at the atomic scales. Such masking may take advantage of AFM topographic resolution and enable chemical ID at the near atomic scale. The talk will solicit scientific partnership to explore these less explored or unexplored opportunities.

Monday April 22nd: 10:15-10:45

Hacking Optical Storage Drives for SPM development: Opportunities and challenges

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Scanning probe microscopes (SPMs) have revolutionized our understanding of the nanoscale world, but their high cost and complexity have limited their accessibility. By hacking affordable and readily available optical storage drive components, such as DVD and Blu-ray optical pickup units (OPUs), we can create low-cost, high-performance SPMs that democratize this powerful technology. This approach not only enables the development of affordable, easy-to-use SPMs for a wider audience, including educational settings, but also opens up new possibilities for specialized applications, such as high-throughput skin nanotexture measurements using dermal atomic force microscopes (AFMs).

Our recent work focuses on harnessing the power of Blu-ray OPUs to develop large-range, high-speed AFMs. While this approach presents unique challenges compared to traditional SPM systems, we believe that these can be overcome through a combination of creative repurposing functions inside the Blu-ray OPUs. Besides skin nanotexture recognition, AI-assisted image processing can play a vital role in helping users identify common issues, such as tip artifacts and systematic errors. By embracing the opportunities and addressing the challenges associated with hacking optical storage drives for SPM development, we can expand the SPM user base, foster innovation in specialized applications, and ultimately make these powerful tools more accessible and reliable for researchers and enthusiasts alike.

Improvement of the temporal resolution of high-speed AFM

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High-speed atomic force microscopy (HS-AFM) allowed us to directly visualize the dynamic behaviors of biological molecules in action at nanometer spatial and sub-second temporal resolution. The power of HS-AFM has been demonstrated in the numerous imaging studies on biological molecules [1-3]. For example, from our group, pooling of the translational factors around the ribosomal stalk complex [4], structural dynamics of intrinsically disordered proteins [5], DNA reeling and cleavage reactions by CRISPR-Cas3 [6] were directly captured. However, the vast majority of biological processes have not yet been visualized by HS-AFM due to the limitation of the temporal resolution. In order to apply HS-AFM to a wider range of biological phenomena, further improvements of the temporal resolution of HS-AFM are thus necessary.

In recent years, we have been carrying out research and development to improve the temporal resolution of HS-AFM system. Using a tiny piezo and a new holding method of piezo, the resonant frequency of the Z-scanner was improved from ~0.2 MHz to ~1.1 MHz [7]. We also developed an electrical circuit called "resonance controller (Reso-con)" which can control the resonant frequency and quality factor of a Z-scanner without changing the mechanical part. For the amplitude detection, we invented a differential-based ultrafast amplitude detection method with zero intrinsic latency based on the basic trigonometric theorem [8]. By optimizing the optical parts in the optical beam deflection system of HS-AFM, the lengths of major and minor axis of elliptical laser spot shape became 1.1 μm and 0.76 μm, respectively. The area of leaser spot on a cantilever could be reduced to 10% of that of conventional system, allowing us to use a smaller cantilever with a higher resonant frequency. We then fabricated such smaller cantilevers by processing small cantilevers with a focused ion beam lithography, by which the resonance frequency of the cantilever became ~10 MHz in liquid. These developments combined with the only-trace imaging mode [9] will enable us to perform HS-AFM imaging ~10 times faster than before.

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Monday April 22nd: 11:45-12:15

Instrumentational Aspects of AFM under Vacuum and UHV Conditions

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Scanning force microscopy (SFM) performed under vacuum or ultra-high vacuum (UHV) conditions enables highest force (gradient) sensitivities, and in the latter case the study of systems with reactive surfaces. The high sensitivities [1] are essential for the mapping tip-sample interactions that produce only very weak force gradients, such as magnetic [2,3,4] and electrostatic forces, the latter of which are investigated in techniques like Kelvin Probe microscopy. To simultaneously map and differentiate the various tip-sample interactions of differing physical natures, it is necessary to employ multi-modal [5] and multifrequency techniques [6].

Here, I will first give an overview on the advantages and challenges of vacuum operation, discussing typical operation modes used, their limits, and highlight a few examples. Then instrumentational aspects will be discussed. First, some instrument design aspects required for positioning, sample exchange and positioning under vacuum conditions while obtaining sub-picometer tip-sample gap stability [7]. Second, the Zurich instruments-based Lock-in PLL system and scan-machine system used for our instruments will be described.

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Tuesday April 23rd: 09:00-09:30

Open software and hardware tools for advanced SPM scanning regimes

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The development of advanced scanning probe microscopy (SPM) scanning regimes imposes novel demands on data acquisition and data processing concepts, which are not always fully (and enough quickly) implemented in the data processing packages. SPM developers and users often need to rely on custom built tools or scripts that might be efficient in the development phase, but can create bottlenecks when the method reaches a wider audience. In this contribution the data handling concepts recently implemented in Gwyddion open-source software will be presented and related to advanced topography measurement regimes. The first example is implemented on high-speed SPM data, where a series of frames was obtained and which should be, due to the number of frames and the relationship between them, be visualised and processed in a different way than is used for standard SPM data. The data handling approach and various tools, e.g. for drift compensation or automated stitching will be presented.

High speed data are often acquired using scan paths that are optimised for minimisation of acceleration and are therefore more complex than traditional raster patterns. This links high-speed microscopy to other types of special topography data concepts: non-raster and adaptive scanning. This approach came originally from another development direction — need for reducing scan time without speeding up the probe motion. The use of adaptive scanning also needs novel visualisation and processing concepts as raster data are no longer available. Ideally, data should be treated and processed as point clouds and rasterization should be used only when necessary. This suits specialised metrology microscopes very well, where position information is available for all the collected data points, typically based on multi-axis interferometric systems. It will be shown that this approach can be extended to high-speed SPMs and that data from such systems can be also processed in Gwyddion.

As an example of an SPM Digital Signal Processor (DSP) natively working with general XYZ data sets, an open hardware module Gwyscope will be presented. Based on a low cost FPGA board and a set of high bit depth AD and DA converters, it can perform of the standard SPM operations. This DSP was designed to work entirely with general data sets and to include various approaches to non-raster scan path generation, including a scan path library and a scripting interface for unsupervised decision making during the scan. The performance and benefits of this approach will be illustrated on a wide range of SPM systems.

Tuesday April 23rd: 09:30-10:00

Navigating the OpenSPM project: key challenges and needs in open software development

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Choosing the programming language for open software in scientific applications is crucial, as it impacts every component of the software suite. Ideally, the language should be widely used, easy to work with, and highly capable. However, these attributes are not always compatible to the desired extent. This challenge extends to other aspect an open software project, such as file storage formats, hardware components, and software architectures. Sometimes, it is necessary to integrate multiple languages to enhance functionality, but this can add complexity, potentially discouraging users, and developers from contributing to the project. Furthermore, the diversity of languages and architectures complicates code sharing among labs worldwide, even within the same field, like scanning probe microscopy. This barrier can hinder collaborative efforts that are vital for improving and refining the software.

Here, I will explore into these issues as part of our ongoing OpenSPM project, which is aimed at developing software for scanning probe microscopes. I will discuss the challenges we encountered and the solutions we implemented. Our project is fully open-source, ensuring that all necessary documentation for building and using the software is freely available to the SPM community. Our setup includes a nano-positioning system and an atomic force microscope (AFM) head, managed by a real-time FPGA controller and a high-voltage amplifier, linked to an AFM base. The software control is handled through a specialized suite developed in the LabView graphical programming environment. Both the controller's designs and the software's code are completely open and accessible. The control electronics, powered by a real-time FPGA (NI-7856R from National Instruments [1]), include interconnect boards that handle signal conditioning—such as filtering, gain, and offset adjustments—and a microscope adapter board for easy customization with various microscope types. This software suite is compatible with a range of SPM techniques, including standard and high-speed AFM [2-6], scanning ion conductance microscopy (SICM) [7], combined AFM/fluorescence or AFM/SEM imaging [8], scanning tunneling microscopy (STM), and scanning near-field optical microscopy (SNOM). This platform is designed to adapt to the varied needs of different SPM applications.

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Tuesday April 23rd: 10:00-10:30

Enhancing SPM Performance Through Modular Software Design and Data-Driven Control

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In the quest for more advanced Scanning Probe Microscopes (SPM), the focus often leans towards hardware improvements. Yet, the software that powers these intricate instruments holds equal potential for innovation. This presentation delves into the transformative power of modular software architecture in elevating SPM performance, highlighting the untapped potential in software design akin to its mechanical and electrical counterparts.

We explore a new approach to software evolution, targeting the SPM's control algorithms. By breaking down the software into smaller, modular components ranging from user interfaces to embedded codes—we simplify the system's complexity. This modularization not only clarifies the relationship between software functions and the physical components they control but also facilitates targeted enhancements in system behavior through precise control adjustments.

Our journey doesn't stop at modularity. We advocate for a data-driven design strategy, where real-world data from the SPM's actuators and sensors guide the optimization of controller parameters. This approach ensures that improvements are grounded in actual system performance, allowing for refined control strategies that directly impact the speed and precision of SPM operations with- out necessitating hardware modifications.

The combination of modular software frameworks with data-driven control de- sign presents a pathway to significant advancements in SPM technology. By fostering a software environment that encourages incremental improvements and adaptability, we can achieve remarkable enhancements in instrument performance. This vision not only proposes a method for pushing the boundaries of what our current technology can achieve but also reinforces the collaborative spirit of the SPM community, emphasizing the importance of shared progress and standards in both software and hardware development.

Tuesday April 23rd: 11:00-11:30

Integration of the Scanning Probe Microscope with the High Performance Computing: reward-driven workflow implementation

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The rapid development of computation power and machine learning algorithms has paved the way for automating scientific discovery with SPM. Conventionally, an SPM must be operated by experienced human operators who will decide what and where to measure next based on the goal of the experiment and the data that has already been collected. Here we present a reward-driven automated experiment (AE) implementation on an Asylum Research Jupiter SPM system integrated with remote high-performance based computer control (ISAACS) at the University of Tennessee, Knoxville.

To automate the SPM operations, we developed an interface enabling Python-based control of the instrument from both local computers and remotely. The communication between the instrument and Python codes is facilitated through a hyper-language interface, designed to mimic human operator actions. It offers instrumental controls as LEGO-style building blocks, based on which users can build automatic workflows for their routine operations. In addition, this interface allows remote control for seamless integration of supercomputers into the workflow. The image and spectroscopy data collected from the instrument can be sent to the supercomputer for advanced analysis in real time.

In the second half of this talk, we will show the reward-driven automated operation of the SPM. To build such workflows, human operators need to first provide a reward function to define the goal of the experiment and guide the operation of the workflow. For example, it can be the quality of the image, switching-on voltage for semiconductor and hysteresis loop area for ferroelectrics, etc. The machine learning algorithm running on the supercomputer computes the reward function based on the acquired image and spectroscopy in the real time. It then determines the next location for the next measurement by learning the hidden correlations within the acquired data. Through the experiment, the algorithm becomes more and more “experienced” at operating the SPM as it acquires more data. In the end of this talk, I will show three examples of reward-driven AE workflows: automatic optimization of scanning conditions for AC tapping mode, optimization of domain writing and reading conditions in the PFM mode and automated exploration of combinatorial libraries.

Tuesday April 23rd: 11:30-12:00

Autonomous Microscopy: From Learning Physics and Structure-Property Relationships to Materials Discovery

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Scanning Probe Microscopy has equipped generation of scientists with the benchtop tools capable of probing structure and functionality of materials on the nanometer and often on atomic scales, in variety of environments ranging from ambient to ultrahigh vacuum and from liquid to in-operando electrochemical cells. Unsurprisingly, SPM now is one of the most popular tools in materials sciences, chemistry, biology, medicine, and multiple other domain areas.

Despite the immense progress in SPM instrumentation over the last 3 decades, the basic principles of SPM imaging remain the same as at the early days of Binnig and Rohrer. Namely, the SPM probe is raster scanned across the surface yielding the image and can be positioned at specified locations for detailed spectroscopic investigations. The latter can be performed on a rectangular grid, giving rise to the hyperspectral imaging modes. These classical modes are easy to implement and yield data that is well amenable to human perception. However, in virtually all applications of SPM the objects and behaviors of interest are concentrated at the small number of locations on the sample surface, necessitating the development of machine learning workflows that can be deployed over the operational microscope to assist and complement human-driven discovery.

In this presentation, I will summarize the needs for the implementation of the ML workflows in SPM, transforming the human-operated tools into autonomous scientists. These include the development of engineering controls available to ML agents, the hyperlanguage that can express the typical human-driven operations, and design of the appropriate reward functions and policies. With these, the SPM field can take advantage of the tremendous body of algorithmic developments in the fields such as Bayesian Optimization, reinforcement learning, and more generally stochastic planning. I will illustrate the development of ML for autonomous discovery, where the microstructural elements maximizing physical response of interest are discovered. Complementarily, I illustrate the development of the autonomous physical discovery in microscopy via the combination of the structured Gaussian process and reinforcement learning, the approach we refer to as hypothesis learning. Here, this approach is used to learn the domain growth laws on a fully autonomous microscope.

Finally, I will discuss the downstream applications of automated microscopy for materials discovery, including exploration of combinatorial libraries derived via compositional spread or pipetting robotics approaches via topographic, electromechanical, and photovoltage detection. In this case, the SPM becomes a crucial tool for closing the materials discovery loop from experiment to characterization and theory feedback.

Wednesday April 24th: 09:00-09:30

TopoStats - driving a community effort for shared, improved, modern computational infrastructure in AFM

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Atomic Force Microscopy (AFM) is unique in its ability to image single molecules in liquid with sub-molecular resolution, without the need for labelling or averaging [1]. However, a lack of community-developed and maintained automated analysis tools in AFM, and the slow integration of machine learning (ML) pipelines is becoming a limiting factor for the development and uptake of AFM as a tool in the (bio)sciences. Gwyddion, an open-source program, is essential to the AFM field. It allows users to process and quantify their data via its GUI interface and batch-process data via its Python2 scripting interface [2].

AFM-specific analysis tools must address issues with raw data before more complex analysis can be performed and are limited by the small datasets available (compared to e.g. Cryo-EM). This issue is exacerbated by closed, manufacturer-specific file types, and a dearth of publicly available data as compared to e.g. the PDB. Finally, there is a high level of variability in the field concerning data handling, cleaning, and processing routines which could be addressed by standardised pipelines or processing metadata being captured.

For community-driven analysis tools to drive progress in AFM, these must be accessible and open to the wider community, and encourage community development and adoption e.g (www.github-com/AFM-SPM). These tools must be well documented, including user guides or READMEs, and where possible developed according to FAIR4RS guidelines [3].

We have developed TopoStats (https://github.com/AFM-SPM/TopoStats [4], a high-throughput, open-source Python package designed to process and analyse large volumes of raw AFM images. We have recently refactored TopoStats to make it easier to use and contribute to, and to support most AFM file formats. TopoStats can read and process raw AFM image files automating file loading, image filtering and cleaning, image segmentation, and feature extraction to produce clean, flattened images and powerful statistical information. TopoStats enables users to standardise analysis over a large range of data and reduces the burden of user oversight including processing of images one at a time for downstream analysis.

We hope that TopoStats can contribute to a community effort to improve the quality and analysis of AFM data published across the field and support the development of robust, open analysis tools for AFM developers and users around the world.

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Wednesday April 24th: 09:30-10:00

Quantitative Electrical Properties of nanostructured materials from DC to GHz frequencies

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The outstanding electrical properties of nanostructured materials are the key for many new applications ranging from quantum computing over 2D-material-based or organic electronics to electrochemical energy storage systems.

The Electrical SPM techniques Scanning Tunneling (STM), Scanning Microwave (SMM) and broadband Electrostatic Force Microscopy (EFM) developed in our lab allow us to visualize their material contrast with nm resolution. With calibration procedures quantitative values of the physically relevant, intrinsic material properties like dielectric permittivity [1], conductivity, carrier concentration and also electrochemical parameters can be extracted.

Based on the specific strength of the developed techniques, the overall focus of my interdisciplinary research is on elucidating local and dynamic electrical processes occurring at nanometric length scales in a quantitative way. We are currently working on integrating these technologies into the open hardware controller platform.

Here, I will give an overview on the scientific results I obtained in various research fields in this still hardly explored domain. In particular, I will cover 3 applications:

1) Semiconductor physics where I show how to pinpoint non-invasively the precise 3D location of buried atomic scale n-type and p-type dopant structures for quantum devices with 1 nm vertical and 10 nm lateral resolution and determine their electrical characteristics by SMM [3] and bb-EFM [4].

2) Local dipole dynamics in protein membranes and its interplay with surface water where I investigated the nanoscale dipole mobility of proteins in a wide frequency range from 3 kHz to 10 GHz. Measurements on bacteriorhodopsin reveal Debye relaxations with time constants being characteristic for the dipole moments of the bR retinal, the a-helices and the entire molecule, respectively [2].

3) High frequency nano-electrochemistry where we did first steps for investigation of fast electrochemical processes of electron transfer through metallo-organic SAMs, showing new potentials for research on catalysis and future battery surfaces [5, 6].

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Wednesday April 24th: 10:00-10:30

Academic and industrial perspectives on SPM hardware development

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The SPM community has a rich history of open and collaborative instrumentation development. I will give some perspectives on this topic gained through experience in SPM instrumentation development in both academic and industrial settings. I will address some of the overlapping and distinctive challenges in both academic and commercial SPM development and discuss some ways that SPM manufacturers can create open systems or provide flexible and accessible ways of enabling the wider SPM development community.

Wednesday April 24th: 11:00-11:30

Advancing SPM probe microfabrication through open science

Nahid Hosseini

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Open science in microfabrication is essential for driving research forward, fostering transparency, and sharing crucial information. Despite the increasing sharing of datasets and analysis routines, the specific details of microfabrication processes often remain undisclosed, posing challenges to reproducibility. Establishing a centralized archive for nano and microfabrication processes holds the potential to mitigate cleanroom failures and improve replicability.

In this presentation, we highlight two examples that underscore the significance of transparency and accessibility in microfabrication. Firstly, during the development of SU8 AFM cantilevers with integrated silicon nitride tips, we encountered hurdles such as internal stress and delamination of SU8 during photolithography steps. Reflecting on this experience, we recognize the value of a shared database containing insights linked to the process run card of the SU8 photoresist. Such a resource could have offered valuable guidance and potentially prevented these issues, emphasizing the importance of collaborative knowledge-sharing platforms in advancing microfabrication techniques.

Similarly, in our work on miniaturized AFM cantilevers, we placed emphasis on openness. By fully disclosing the fabrication process and associated steps, we aim to empower fellow researchers to reproduce our results effortlessly. This commitment to transparency not only encourages collaboration but also drives innovation and progress in SPM technology, specifically in high-speed AFM applications.

Wednesday April 24th: 11:30-12:00

Open hardware collaboration between Weizmann SPM unit and LBNI lab at EPFL

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Our SPM unit at the Weizmann institute of Science (WIS) is a core facility which provides the opportunity to collaborate with many different groups encompassing a variety of disciplines. We are fortunate to have a long-standing collaboration with the Laboratory for Bio- and Nano-Instrumentation (LBNI) at the École Polytechnique Fédérale de Lausanne (EPFL). Our collaboration, to implement the fast scanning AFM, has benefited our lab in two different ways: First, the fast scanning saves valuable measurement time, allowing collection of large amount of images in a short time. This was used to acquire the large amount of images necessary to train a convolutional neural network, which autonomously differentiate between healthy and damaged cytoskeleton images. More significantly, this new capability has opened new scientific directions from fast imaging of soft biological samples under aqueous environment (liposome adsorption process and membranal protein conformation) through utilizing photothermal heating of the AFM probe for nanolithography of organic crystals. In this talk I will describe the process of implementing the system in our lab, its challenges and benefits, and the advantage of this collaboration for testing and implementing methods that open new capabilities and improve our lab performance.