WORKSHOP #8

SPM User Community Meetup: "Hands-on Open" Source SPM Software Virtual "Hack a Day" Learning Session and Future Outlook on Artificial Intelligence Driven Autonomous SPM

Percy Zahl (CFN) and Thorsten Wagner (Johannes Kepler University Linz, Austria)

This workshop aims to bring the SPM user community together to share latest developments and capabilities for remote or autonomous control of instruments and analysis of data.

The field of "Scanning Probe Microscopy (SPM)" is continuing to grow into diverse facets of scientific data acquisition. "Home built" or specialized microscope instruments require the control of various types of (nano) positioning mechanisms in combination with line by line imaging. In this meeting we would like to showcase capabilities of existing facilities, and particularly look forward towards new demands and opportunities in the field.
We plan on engaging participants to present their particular application and problems and provide an opportunity to meet the developers of existing facilities (in particular the developers of open source GXSM project *) in a dedicated "hack-a-day" like session — having virtually hands on microscope operation demonstrations.

Wednesday, May 25, 2022

Start Time (ET)	Title	Speaker (Affiliation)
8:00 a.m.	Opening and Introduction to the GXSM project – deployed and developed at the CFN LT-STM/HR-AFM facility	Percy Zahl, CFN
8:20 – 8:50 a.m.	Automated HR-AFM to facilitate molecular discovery and research for complex mixtures	Yunlong Zhang ExxonMobil Research and Engineering
8:50 – 9:10 a.m.	On-surface synthesis of atomically precise graphene nanoribbons	Alexander Sinitskii University of Nebraska @ Lincoln
9:10 – 9:30 a.m.	Finding needles in haystacks – defects in catalysis, quantum computing and optoelectronics	Peter Grutters McGill University
9:30 – 9:50 a.m.	Scanning-Probe-Microscopy @ Deutsches Museum: From science communication to basic research and back	Markus Lackinger
9:55 – 10:00 a.m.	BREAK	
10:00 – 12:00 p.m.	WORKSHOP HACK-A-DAY SESSION DAY ONE	Moderators: P. Zahl, T. Wagner – everyone is invited to actively participate and engage.

11:00 – 11:05 a.m.	BREAK	

Thursday, May 26, 2022

Start Time (ET)	Title	Speaker (Affiliation)
8:00 a.m.	Session opening and GXSM Packaging and Support	Thorsten, Wagner Johannes Kepler University Linz
08:20 – 8:40 a.m.	Unlocking magnetic flavors and switching in single molecule adsorbate systems: A combined STM- STS- HR-AFM analysis	Oliver Monti, University of Arizona
08:40 – 9:00 a.m.	Studying the Carrier Dynamics in Nanomaterials by Scanning Photocurrent Microscope	Mingxing Li, CFN
09:00 – 9:20 a.m.	Application of GXSM to analysis of the spectro-microscopic datasets	Jurek Sadowski, Center for Functional Nanomaterials
09:20 – 9:40 a.m.	Implementation of Gnome X Scanning Microscopy for Time-resolved Characterization of Inorganic Oxides	Bugrahan Guner, École de technologie supérieure, University of Quebec, Montreal, Quebec, Canada
09:40 – 9:55 a.m.	Local Mapping of Thermoelectric Properties of 2D Structures via Scanning Thermal Gate Microscopy	Pascal Gering University of CLouvain, Belgium
9:55 – 10:00 a.m.	BREAK	
10:00 – 11:45 a.m.	WORKSHOP HACK-A-DAY SESSION DAY TWO	Moderators: P. Zahl, T. Wagner – everyone is invited to actively participate and engage.
11:45 – 12:00 p.m.	Future outlook on AI based fully autonomous and curiosity driven SPM	Steven Arias, University of New Hampshire and Percy Zahl, CFN

Abstracts and detailed Agenda follows on the next pages

Workshop Agenda

DAY 1 — Wednesday, May 25, 2022, from 8 a.m. to 12 p.m. (EST)

08:00-08:20 Opening and Introduction to the GXSM project – deployed and developed at the CFN LT-STM/HR-AFM facility

Percy Zahl, Center for Functional Nanomaterials, BNL

Welcome and a brief introduction to the Open Source SPM Software/Hardware Project "GXSM". A historic review to nearly the roots of SPM software and STM – still surviving at the core design and leading an amazing way into the future. Enabling explorative SPM sciences around the world.

08:20-08:50 Automated HR-AFM to facilitate molecular discovery and research for complex mixtures

Yunlong Zhang, Hydrocarbon Science, Corporate Strategic Research, Rm LA262, ExxonMobil Research and Engineering, 1545 Route 22 East, Annandale, NJ, 08801 **– Key-Note Speaker –**

Due to its single molecule sensitivity, high-resolution Atomic Force Microscopy (HR-AFM) has proved to be a valuable and uniquely advantageous tool to study complex mixtures, such as petroleum, biofuels/chemicals, and environmental samples. However, significant challenges remain in order to achieve the full potential of the challenging and time-consuming experiments. Automated HR-AFM, in conjunction with machine learning and artificial intelligence, will be the key to overcoming many bottlenecks today, and crucial for research on solutions for the energy transition and environmental sustainability.

08:50-09:10 On-surface synthesis of atomically precise graphene nanoribbons

Alexander Sinitskii, University of Nebraska – Lincoln, Lincoln, NE

This presentation will overview the experiments on on-surface synthesis of atomically precise graphene nanoribbons (GNRs) performed at the Center for Functional Nanomaterials. GNRs with very diverse chemical structures were synthesized by coupling properly designed molecular precursors on Au(111) substrates and planarization of the resulting polymers via annealing. The atomically precise structure of these GNRs was revealed by noncontact atomic force microscopy and analyzed using the GXSM software.

09:10-09:30 **Finding needles in haystacks – defects in catalysis, quantum computing and optoelectronics**

Peter Grutters (and group), Department of Physics, McGill University – Montréal, QC

Canada H3A 2T8

The Grutter group is interested in understanding how the structure of defects relates to the properties of materials. The challenge is to find and characterize the different type of defects (=needles) in materials (haystacks). Specifically, we are 1) investigating the in-operando catalytical sites for electrochemical conversion of CO2 to fuel on defects on steps on Cu, 2) trying to find individual atomically positioned 'defects' in silicon (aka as dopant atoms) to perform single electron energy level spectroscopy relevant for quantum computing and 3) are investigating the time resolved opto-electronic properties and atomic structure of defects on 2D materials. To improve productivity, we are interested in artificial intelligence driven autonomous SPM to find and characterize these needles in haystacks.

09:30-09:50 **Scanning-Probe-Microscopy @ Deutsches Museum: From science communication to basic research and back**

Markus Lackinger, Deutsches Museum, Museumsinsel 1, 80538 München, Germany and Department of Physics, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany

Scanning-Probe-Microscopy is a landmark of historic nano-science that has never lost its actuality and utility. This is reflected in exhibitions, demonstrations and hands-on lab courses at the Deutsches Museum – one of the world's largest science and technology museums. On the other hand, the Deutsches Museum is also a research museum with own activities in nano- and material-science. In this presentation, we highlight the added value of interrelations and cross-links between basic research and science communication, and why Scanning-Probe-Microscopy is particularly well-suited therefore.

09:55-10:00 Virtual Coffee Break. (Sorry need to get your own coffee)

Please participate in our "GXSM Workshop Hack-a-day Topics" survey ASAP to help us identity most priority items: https://tinyurl.com/2p9f4vsd

Note: topics are subject for on demand change!

10:00-12:00 WORKSHOP HACK-A-DAY SESSION DAY ONE

Moderators: P. Zahl, T. Wagner – everyone is invited to actively participate and engage.

Note: All Hack-a-day session topics are open and anything on request can be given preference!

Topics room A – data analysis methods, basic instrument controls/testing:

Moderators: T. Wagner

General operations, analysis:

- Gxsm installation – demo install from SVN/GIT (Gxsm4), …
- Basic instrument setup, configuration and instrument controls
- The Z-Servo
  - Testing [Bias-loop-back self test]
  - Understanding the Z-Servo and Z-Offset controls – tip engage/retract options
  - Auto approach options
- Data analysis part one: Image review, "display" scaling, objects, palettes, legends, figure export, image math and filter operations
  - Scan/Image "Data Types"
  - Extra dimensions: Layer, Time
  - Open modes: append in time, replace, stitch
  - Scan-Events: user, probe
  - Math Plug-Ins

Topics room B – under the hood and advanced operation techniques:

Moderators: P. Zahl

Advanced experiments and life demos – suggested when familiar with "A":

- Under the hood:
  - DSP RTE4Linux (SPM-SCAN-CONTROL) ← USB dev/module → Gxsm
  - DSP manager/configurations, signals, monitoring, digital patch-rack [MK3]

    - Do's and don't – understanding possibilities and limitations
- Scan Data channel/signal management and assignments
- World Map and special purpose scan modes:
    - "RAD" mode (Remap Available Data)
    - "SLS" mode (Sub Line Scan)
    - Tip position control at your fingers – tip marker/point object
- PAC-PLL (MK3 and RedPitaya High Speed Dual-PAC-PLL Controller – a Lock-In Alternative)
- HR-AFM operation
    - "assisted" manual Z-control: Gxsm's "Fuzzy Const Height Mode" >CZ-FUZZY-LOG <
    - Scripted automated mode transitions
- From simple STS to Vector Probing:
    - STS, TS,..., GVP programming multidimensional real time operations
    - Raster Scan / Probing, Data Sources and Graphing

Break/Coffee room C – consider taking a break for coffee and random chatting around 11:00:

An optional place for individuals to retreat/discuss to not disturb A,B.

<u>11:00-11:05</u> Coffee Break for above session

DAY 2 — Thursday, May 26, 2022, from 8 a.m. to 12 p.m. (EST)

08:00-08:20 Session opening and GXSM Packaging and Support

Thorsten Wagner, Johannes Kepler University Linz | JKU · Institute of Experimental Physics

In this presentation a short introduction into the maintenance of the source code (on github.com) and the packaging (as Debian package available via launchpad.net) of the GXSM program and the kernel modules will be given. It will be also briefly discussed how to deploy GXSM on other linux distributions than Ubuntu (and maybe Windows based machines) via flatpack. Finally, it will be discussed how to contribute to the GXSM project actively by submitting patches, new features or extending the documentation.

08:20-08:40 Unlocking magnetic flavors and switching in single molecule adsorbate systems: A combined STM- STS- HR-AFM analysis

Anubhab Chakraborty†, Oliver Monti‡; University of Arizona

† Presenting author, ‡ Corresponding author

The ability to control the magnetic state of molecular adsorbate-on-metal systems has emerged as an important question in the field of information storage and "spintronics". Here, we utilize a sub-monolayer organic semiconductor HATCN/Ag(111) system to demonstrate control over the magnetic state of an adsorbate vis-à-vis the Kondo effect. We use low temperature non-contact High Resolution Atomic Force Microscopy (HR-AFM), Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) to reveal different magnetic states and switching in the same adsorbate without any modulation of temperature or adsorption geometry. Our work opens up avenues for precise control of molecular Kondo switches and tailoring of surface-adsorbate interactions in organic semiconductor interfaces.

08:40-09:00 Studying the Carrier Dynamics in Nanomaterials by Scanning Photocurrent Microscope

Mingxing Li, Center for Functional Nanomaterials, BNL

Carrier and spin dynamics of nanomaterials are very important for their applications like photovoltaics, photodetectors, and spintronics. Here, I will briefly show the charge transfer and energy transfer processes in 2D/0D hybrid system and the chiral effect in 1D nanomaterials by using the home-built scanning photocurrent microscope with GXSM software. It was found that charge transfer in 2D/0D system is suitable for photodetection while the energy transfer in 2D/0D is appropriate for light harvesting. Additionally, the spin properties of charge carriers in 1D nanowires are revealed with a circularly polarized excitation. Our studies provide further understanding of charge and spin properties in nanomaterials for their future applications in photoelectronics.

09:00-09:20 Application of GXSM to analysis of the spectro-microscopic datasets

Jurek Sadowski, Center for Functional Nanomaterials, BNL

Electron spectromicroscopy, and more specifically a combination of x-ray photoemission electron microscopy and low-energy electron microscopy (XPEEM/LEEM) is a powerful tool for investigation of structural, electronic, and chemical properties of surfaces and 2D materials. In this technique, the data is acquired in form of images or stacks of images when one, or more of experimental parameters (ie. electron or x-ray photon energy, temperature, deposition, or gas dosing, etc.) are varied. Subsequently, the structural, electronic, or chemical information can be extracted locally by analyzing the changes in the contrast or brightness (intensity) through the stacks of the acquired images. With the advent of fast, direct-electron detection cameras, with pixel arrays often in the 4K range, this means GB of data and 1000s of images from a single measurement, that need to be quickly and efficiently analyzed. In this talk I will give some examples on how GXSM software can be applied for this task. I will also give a perspective on how the user community could benefit from further development of the GXSM to expand its use in the spectro-microscopy research community.

09:20-09:40 Implementation of Gnome X Scanning Microscopy for Time-resolved Characterization of Inorganic Oxides

Bugrahan Guner[1,†] , Mohammad Safikhani-Mahmoudi[1] , Simon Laflamme[1] , and

Omur E. Dagdeviren[1,‡]

1 Department of Mechanical Engineering, École de technologie supérieure, University of Quebec, Montreal, Quebec,

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Time-resolved characterization of metal-oxide semiconductors (i.e., semiconductors consisting of metal and oxygen) and related sample systems (e.g., perovskites) to reveal the dynamics of charge carriers, such as oxygen vacancies and holes have been studied recently [1, 2]. This presentation demonstrates the implementation of Gnome X Scanning Microscopy (GXSM) for the time-resolved, temperature-dependent characterization of inorganic oxides. We will explain the integration of the GXSM controller and software with a traditional non-contact atomic force microscopy-based system, i.e., Veeco EnviroScope. Also, we will discuss the robust automation of GXSM with Python Remote Control Console for time-resolved measurements. Furthermore, we will deliver the integration of the real-time operation of GXSM with MATLAB ® to enable the resonance frequency drift correction with an external phase-locked loop (PLL). We believe that integrating the GXSM with a traditional microscope while utilizing an external PLL and real-time experimental progress monitoring with MATLAB ® may aid in enabling other custom experimental platforms with the GXSM.

1. O.E. Dagdeviren et al., Nano Letters, 2020. 20(10): p. 7530-7535.

2. O.E. Dagdeviren et al., Nano Letters, 2021. 21(19): p. 8348-8354.

Funding information: This work was supported by the Canada Economic Development Fund, Natural Sciences and Engineering Research Council of Canada, and Le Fonds de Recherche du Québec - Nature et Technologies. O.E.D. also gratefully acknowledges funds provided by École de technologie supérieure, University of Quebec.

09:40-09:55 Local Mapping of Thermoelectric Properties of 2D Structures via Scanning Thermal Gate Microscopy

Pascal Gering, University of CLouvain, Belgium

Studying local variations in the Peltier [1] or Seebeck coefficient of materials is important to optimise their thermoelectric properties and to enable applications like single-material thermocouples [2]. Yet most global experiments overlook spatial divergences in the signal and the role of local variation and the internal structure. Here, we developed Scanning Thermal Gate Microscopy (STGM), a non-invasive method to obtain high-resolution 2-dimensional maps of the thermovoltage [3]. We investigate junctions formed between single- and bi-layer graphene, identify the impact of internal strain and reduction of channel width on the local Seebeck. These findings and the newly developed STGM method will help to further understand and improve the thermoelectric properties of 2D devices.

09:55-10:00 Virtual Coffee Break. (Sorry need to get your own coffee)

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– Note: topics are subject for on demand change!

10:00-11:45 WORKSHOP HACK-A-DAY SESSION DAY TWO

Moderators: P. Zahl, T. Wagner – everyone is invited to actively participate and engage.

Note: All Hack-a-day session topics are open and anything on request can be given preference!

Topics room A – data analysis methods, basic instrument motion controls:

Moderators: T. Wagner

General operations, analysis:

- Gxsm installation, basic setup and instrument controls… part 2
- Data analysis part two:
  - Events: Image review with user and probe (STS,...) events, probe data review
  - Multidimensional data slicing and visualization
  - Gxsm's native NetCDF data format: basics, stand alone Python data access
- Coarse motion controls. Wave Form Generator.
- Future hardware pathways: Is it possible: All in one FPGA (RedPitaya ZC20 + custom AD/DA with integrated piezo drive) ? [We will take on this one together and join up at this point "here in room A"]

Topics room B – Gxsm Python remote control/automatization interface:

Moderators: P. Zahl

Advanced experiments and life demos:

- Gxsm remote control and automatization via "embedded" Python
- "Embedded" Python based data analysis/processing
- External Gxsm control and data access via socket/JSON interface provided via embedded Python Socket Server and any external tools. Python, Jupyter, Web, ….

- Join all together in room A: Future hardware pathways

Break/Coffee room C – consider taking a break for coffee and random chatting around 11:00:

An optional place for individuals to retreat/discuss to not disturb A,B.

11:00-11:05 Coffee Break for above session

11:45-12:00 Future outlook on AI based fully autonomous and curiosity driven SPM

Steven Arias, University of New Hampshire and

Percy Zahl, Center for Functional Nanomaterials, BNL

A vision and "GXSM4" road map for the future of SPM: building a generic goal based AI engine based on reinforcement learning, curiosity driven, to explore and navigate a unknown surface "terrain", iteratively optimizing the SPM probe as required, ultimately enabling HR-AFM to autonomously locate and scan many molecules of unknown mixtures/samples for statistical analysis (see Yunlong Zhang, ExxonMobile presentation).

Closing remarks (at end of above's joint presentation)

Percy Zahl, CFN