O 56: Scanning probe techniques: Method development II

Time: Wednesday 10:30–12:15 Location: HSZ/0401

O 56.1 Wed 10:30 HSZ/0401

Simulation of coupled AFM and constant current STM images — •Marvin Krenz[1,2], Miguel Wiche[1,3], Daniel Ebeling[1,3], and Simone Sanna[1,2] — [1]Center for Materials Research, Justus-Liebig University, Giessen, Germany — [2]Institute of Theoretical Physics, Justus-Liebig University, Giessen, Germany — [3]Institute of Applied Physics, Justus-Liebig University, Giessen, Germany

We present a simulation method for AFM images with a constant current STM feedback loop. In contrast to regular AFM constant height images, those images can picture the features of bulky or corrugated molecules, as shown by experiment [1].

The method is based on the electronic density of the molecules, and thus applicable to virtually any DFT code. We apply this method to two test systems, the 6F-Pentacene molecule at Cu(111) and the iodotriphenylene at Ag(111), at different level of approximation.

Both systems compare well to the experimental images; at the highest level of approximation nearly all features of the experiment are reproduced.

[1] Martin-Jimenez, D.; Ahles, S.; Mollenhauer, D.; Wegner, H. A.; Schirmeisen, A.; Ebeling, D. Physical Review Letters 2019, 122, 196101.

O 56.2 Wed 10:45 HSZ/0401

High spatial resolution of Si(111)-7x7 using LFM with a CO-tip — •Shinjae Nam[1,2], Thomas Holzmann[1], Franz Giessibl[1], and Alfred Weymouth[1] — [1]University of Regensburg, Regensburg, Germany — [2]Center for Quantum Nano Science, Seoul, South Korea

The Si(111) 7x7 reconstructed surface has long served as an iconic benchmark for proving the capabilities of scanning probe microscopes. Since STM first resolved the 7x7 pattern in 1983, advances in frequency-modulation AFM have enabled true atomic resolution and quantitative access to short-range chemical and frictional interactions. In this work, we report unprecedented atomic resolution and quantitative mapping of site-dependent lateral forces on the Si(111) 7x7 surface using a qPlus-based lateral force microscope. The tip is terminated with a CO molecule, and oscillating laterally with an amplitude of 50 pm. Unlike reactive Si tips, the CO tip provides a chemically inert and well-defined probe apex, enabling exceptionally sharp contrast and resolving subtle differences between faulted and unfaulted half-cells. The measured lateral force maps agree quantitatively well with theoretical models. These results establish CO-tip LFM as a powerful technique for probing lateral interactions with single-atom precision.

O 56.3 Wed 11:00 HSZ/0401

Spatially Resolved Mode Analysis of Ultra-Long qPlus Probes for STM/AFM — •Aleksander Bogucki[1,3], Yeon-Ji Kim[1,2], Yewon Kim[1,2], Sarah Yi[1,2], German Orlov[1,3], Lei Fang[1,3], Wonjun Jang[1,3], and Andreas Heinrich[1,2] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea — [3]Ewha Womans University, Seoul 03760, Republic of Korea

Combined scanning tunneling and atomic force microscopy (STM/AFM) based on quartz tuning forks (qPlus) typically relies on short tip lengths (<0.5 mm) for optimal performance. However, restricted sample environments such as liquid cells or setups requiring significant clearance for high-numerical-aperture optical elements demand probe geometries far exceeding standard dimensions. While tips in the 1-3 mm range have been recently explored [1], the dynamics of significantly longer tips are less well characterized.

We present a systematic study of qPlus sensors with ultra-long tips (>8 mm). We correlate electrical response spectra with spatially resolved optical vibrational analysis to map eigenmodes and identify non-vertical components. Supported by FEM simulations, we demonstrate that tip material and geometry can be optimized to tune the spectral response. Finally, we assess the potential of these ultra-long designs for specialized SPM setups.

References: [1] T. Yamada et al., Nanoscale Adv. 5, 840-850 (2023).

O 56.4 Wed 11:15 HSZ/0401

Comparative Analysis of SPM-Based Work Function Measurement Techniques with Application to Work Function Engineering of Superconducting Nb(110) — •Daryoush Nosraty Alamdary, Matthias Bode, and Artem Odobesko — Physikalisches Institut, Lehrstuhl für Experimentelle Physik 2, Julius-Maximilians-Universität Würzburg, Germany

The engineering of the work functions at the interface of complex materials for energy band tuning [1] requires precise and reliable measurement methods, sensitive to atomic monolayer thin films. While there are handful of established methods that allow a precise determination of the work function, scanning probe microscopy-based methods constitute a class of their own since they are based on a local probe. In this work, we present a comparative study of three techniques, i.e., $I(z)$ spectroscopy, field emission resonances, and Kelvin probe force spectroscopy, regarding their complexity and reliability to determine the local work function. For a few well-studied model systems we analyze the respective benefits and challenges. Using the most reliable methods, established by the comparative analysis, we systematically study the coverage-dependent crystal structure and work function of epitaxial Ir films on superconducting Nb(110) [2] and discuss the suitability for work function engineering towards induced superconductivity.

[1] P. Rüßmann *et al.*, Proximity induced superconductivity in a topological insulator, arXiv:2208.14289 (2022)
[2] P. Beck *et al.*, Structural and superconducting properties of ultrathin Ir films on Nb(110), Phys. Rev. Mater. **6**, 024801 (2022)

O 56.5 Wed 11:30 HSZ/0401

Towards Atomically Precise Fabrication through STM with Flat, Crystalline Probes — •Marc Savoie, Eduardo Barrera Ramirez, Bheeshmon Thanabalasingam, and Marco Taucer — CBN Nanotechnologies Inc, Ottawa, Canada

Scanning Tunneling Microscopy (STM) enables the fabrication of atomically precise structures. Traditionally, STM probes manipulate atoms on the sample surface, but this presents challenges for fabricating covalently bonded structures. The high strength of covalent bonds means that detailed knowledge and control over both the probe and sample sides of the tunneling junction is required to form the desired bond and avoid unwanted changes. We introduce inverted-mode STM, an approach that reverses the roles of probe and sample to enable mechanically controlled chemical reactions for atomically precise fabrication. We have developed flat, crystalline Si(100) STM probes that act as the substrate for atomic manipulations. The flat probe is imaged by tailored, 3D molecules deposited on a surface. By determining the orientation of the molecule, the challenge of knowing the atomic configuration on both sides of the junction is effectively resolved. Treating the two sides of the tunnel junction as reagents whose relative positions can be controlled with sub-angstrom precision, we show that hydrogen atoms can be reproducibly abstracted from a locally flat, crystalline region of the probe apex at zero volts using a novel molecule terminated in an alkynyl radical. Multiple surface-bound reagents can sequentially address the same build site on a probe apex. The approach is expected to apply to abstraction and donation of other elements and moieties.

O 56.6 Wed 11:45 HSZ/0401

Atomically Precise Si Abstraction by Inverted-Mode STM — •Rosemary Cranston, Zehra Ahmed, Eduardo Barrera, Brandon Blue, Adam Bottomley, Christian Imperiale, Alex Inayeh, Mathieu Morin, Marco Taucer, and Bheeshmon Thanabalasingam — CBN Nano Technologies Inc., Ottawa, Canada

Direct 3D manipulation of covalently bonded atoms remains a challenge for atomically precise fabrication. Here, we introduce inverted-mode scanning tunneling microscopy (STM) as a new approach for controlled atomic-scale reactions and demonstrate its application to individual Si atom abstraction. A Si probe chip (SPC) with an atomically clean Si(100)-2x1 crystalline terrace at the apex serves as the probe, while a Si wafer bearing isolated, custom-synthesized, surface-bound molecular tools act as the sample. These molecules function both as imaging agents and as tools for chemical manipulation. As the sample is scanned with the SPC, each protruding molecule provides a mirror image of the probe apex and can immediately participate in surface reactions. For subtractive Si patterning, we employ tripodal molecules featuring an ethynyl iodide moiety. After bias-induced cleavage of the iodine, the resulting radical is aligned with a target Si dimer of the SPC. A controlled approach-retraction process transfers a

Si atom to the molecule, leaving unique Si vacancies at the target site. Imaging with new iodinated molecules elsewhere on the sample surface confirms changes to the SPC lattice, and allows iterative targeting for the next abstraction, thus enabling a new method for atomically precise fabrication, and the manipulation of Si atoms in 3D.

O 56.7 Wed 12:00 HSZ/0401

Graphene Coated Nanoprobes for Local Conductivity Measurements — •Maria Saavedra-Fredes, Valeria del Campo, and Tomas P. Corrales — Universidad Técnica Federico Santa María, Valparaíso, Chile.

Here we explored the fabrication of AFM cantilevers coated with graphene (Gr) with the aim of detecting local electrical currents. The fabrication process begins with the growth of Gr on copper foils via Chemical Vapor Deposition (CVD). Subsequently, the copper substrate is dissolved using a ferric nitrate solution and then replaced with water, leaving a Gr film floating at the water air interface. This film is transferred onto an AFM cantilever using a three-axis hydraulic micromanipulator. Raman spectroscopy and SEM confirm the presence of graphene on our Gr-coated nanoprobes This technique differs from traditional methods because the Gr is collected directly from the air water interface without the use of polymer films in the process (10.3390/cryst7090269). Then, to detect currents using conductive mode AFM (10.1002/adma.201200579) and study the conduction between our Gr-coated nanoprobe and a graphene layer deposited on silicon.