O 77: Scanning Probe Techniques: Method Development II

Time: Thursday 10:30–12:45 Location: REC C 213

O 77.1 Thu 10:30 REC C 213

How cold is the junction of a millikelvin scanning tunnelling microscope? — Taner Esat[1,2], Xiaosheng Yang[1,2], Farhad Mustafayev[1,2], Helmut Soltner[3], Stefan Tautz[1,2,4], and •Ruslan Temirov[1,5] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Jülich, Germany — [3]Zentralinstitut für Engineering, Elektronik und Analytik (ZEA-1), Forschungszentrum Jülich, Germany — [4]Experimentalphysik IV A, RWTH Aachen University, Aachen, Germany — [5]University of Cologne, Institute of Physics II, Cologne, Germany

We employ a millikelvin scanning tunnelling microscope (STM) cooled to millikelvin temperatures by an adiabatic demagnetization refrigerator (ADR) to perform scanning tunnelling spectroscopy (STS) on an atomically clean surface of Al(100) in a superconducting state using normal-metal and superconducting STM tips. Varying the ADR temperatures between 30 mK and 1.2 K, we show that the temperature of the STM junction T is decoupled from the temperature of the surrounding environment T_{env}. Simulating the Josephson current with the $P(E)$ theory, we determine that $T_{\mathrm{env}} \approx 1.5$ K, while fitting of the superconducting gap yields the lowest $T \approx 77$ mK.

O 77.2 Thu 10:45 REC C 213

Ultrahigh Vacuum Scanning Tunneling Microscopy with z Resolution of 2 pm at 1.3 K using Combined Pulse Tube and Joule-Thomson Cooling — •Marcus Esser[1], Marc Frömming[1], Marco Pratzer[1], Michael Krzyzowski[2], and Markus Morgenstern[1] — [1]2.Physikalische Institut B, RWTH Aachen University, Aachen, Germany — [2]CryoVac GmbH & Co KG, Troisdorf, Germany

The cooling of scanning tunneling microscopes with liquid helium by bath or flux cryostats suffers from He losses that get increasingly expensive. However, alternative closed cycle systems based on pulse tube refrigerators can induce additional mechanical noise into the tunneling contact due to mechanical vibrations in the μm range and acoustic emissions. We will present an STM system that reaches temperatures of 1.3 K and a z resolution of 2 pm (feedback loop off) with the help of a pulse tube cooler and a Joule-Thomson stage. The challenge is to provide a good thermal coupling as well as an good vibration damping. For this purpose, a new concept with multiple decoupling stages including negative stiffness isolation, detached coaxially guided shields for the different temperature stages and an optimized conical microscope design made out of Shapal Hi M-soft has been realized. Numerical calculations of transfer functions are compared with measurements on test setups using accelerometers as well as the tunneling contact of the STM. Eventual measurements on Au(111) showed atomic resolution and mechanical vibrations below 2 pm. The ongoing work to optimize spectroscopic resolution will be reported.

O 77.3 Thu 11:00 REC C 213

Development of a closed-cycle dilution refrigerator scanning tunneling microscope — •Mate Stark[1], Daria Sostina[2], Wantong Huang[1], Paul Greule[1], Christoph Sürgers[1], Philip Willke[1], and Wolfgang Wernsdorfer[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology, Karlsruhe, Germany

Throughout the last decades, scanning probe techniques, such as scanning tunneling microscopy (STM), have been successfully paving the way to discover and understand physics on the atomic scale. However, recent developments in studying single atoms' electronic and magnetic properties have shown experimental limitations. For instance, the combination of electron spin resonance (ESR) with STM has shown short spin relaxation time T_1 and phase coherence time T_2 on single atoms, among others limited by thermally excited electrons [Willke et al., Sci. Adv. 4(2), 1543 (2018)].

Here, we present the implementation of a compact closed-cycle dilution refrigerator (DR) reaching milli-Kelvin temperatures, which we combine with a commercial STM under ultra-high vacuum (UHV) conditions. This combination enables a fast cool down, shows a low vibrational level, and requires a minimum of everyday maintenance. We demonstrate the functionality of the DR-STM by performing ESR measurements on individual magnetic molecules.

O 77.4 Thu 11:15 REC C 213

Machine learning: radical technique or plus ça change? The case for automated scanning probe microscopy — •Dylan Barker, Adam Sweetman, and Phil Blowey — University of Leeds

Atomic resolution scanning probe microscopy (SPM) provides a critical tool for studying the chemical and electronic structure of surfaces at the single atom scale, however, practically these techniques require a large amount of experimental time to manually prepare the scanning probe tip in-situ, usually via controlled indents into the surface. This apparently simple, but time-consuming process, is potentially an ideal candidate for automation using machine learning and computer vision techniques. Previous attempts to automate the classification of probe tips from topographical images have been made using machine learning methods [1-2], however using prior knowledge of the system in question we find it is also possible to classify the tip state using computationally simple image analysis methods such as Fourier ring correlation and cross-correlation. In this work I will present a comparison between "deterministic" image analysis methods and machine learning approaches for tip state classification. I will also address the known issue of small sample sizes for training ML techniques for SPM image classification, via an automated (scripted) data generation approach.

[1] Rashidi, M & Wolkow, R. A. ACS Nano 12, 5185-5189 (2018).

[2] Gordon, O. et al. Review of Scientific Instruments 90, 103704 (2019).

O 77.5 Thu 11:30 REC C 213

Artificial Intelligence finds the optimal STM manipulation parameters of unknown molecules — •Bernhard Ramsauer[1], Grant J. Simpson[2], Leonhard Grill[2], and Oliver T. Hofmann[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Department of Physical Chemistry, Institute of Chemistry, NAWI Graz, University Graz, Heinrichstraße 28, 8010 Graz, Austria

Scanning probe microscopy gives us the possibility to precisely control the position and orientation of single molecules and unlocks the possibility of nanofabrication of novel structures with enhanced properties. However, interaction processes at the nanoscale are stochastic processes, and because their motion itself is often unintuitive and hard to predict, inducing controlled movements is not trivial at all.

In this study we present how a reinforcement learning algorithm identifies optimal manipulation parameters (i.e., the bias voltage, height, and lateral position of the STM tip relative to the molecule) for any unknown molecule to allow for precise control of its movement.

Leaving all the manipulation parameters open for investigation requires a method to exclude manipulation parameter that pick-up or destroy the molecule. Furthermore, already learned information is used to infer prior knowledge to similar manipulation parameters (e.g.: to infer knowledge at the same bias voltage to adjacent tip positions).

This allows for autonomous control of initially unknown molecules with high sub-nanometer precision that set the basis to construct molecular nanostructures from the bottom up.

O 77.6 Thu 11:45 REC C 213

Field-emission resonances at exceptional large voltages: Consequences for determining work functions — •Anika Schlenhoff[1], Gerassimos C. Kokkorakis[2], and John P. Xanthakis[2] — [1]Institute of Physics, University of Münster, Germany — [2]Electrical and Computer Engineering Department, National Technical University of Athens, Greece

In a scanning tunneling microscopy (STM) setup, a series of unoccupied electronic states evolve in the vacuum gap between the probe tip and the surface. Due to limited bias voltage ranges, so far only a small number (typically 4 - 8) of these so-called field-emission resonances (FERs) have been detected. Here, we report a combined experimental and theoretical study of FERs over an exceptional range of energy and number, typically tens of an eV and over thirty in order n [1]. Unlike commonly assumed, the triangular potential well is not found to be a good approximation for the high-n states. Although the spectroscopy mode assures a constant electric field at the tip apex, this leads only

for the intermediate FERs (approx. $2 < n < 6$) to reside in a linear potential between the tip and the surface. At higher tip-sample distances d and bias voltages $U(d)$, the quantum well is no longer triangular but attains a curvature, which is d-dependent. Each high-n state resides in its own well that can be well-approximated by a polynomial of second order. Hence, the range of U_n to be analyzed in terms of spectroscopic positions needs to be chosen with great care when deducing surface work functions.
[1] A. Schlenhoff *et al.*, Appl. Phys. Lett. **120**, 261601 (2022).

O 77.7 Thu 12:00 REC C 213

Phase compensation for ultrafast dynamic measurements of atomic spins — •Nicolaj Betz[1], Max Hänze[1,2], Gregory McMurtrie[1], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Understanding spin dynamics is vital for a wide range of applications , such as qubit manipulation. However, in many cases, especially for single atoms on surfaces, even stroboscopic measurement techniques, like pump-probe or pulsed electron spin resonance, do not provide enough time resolution to resolve the dynamics of the individual (atomic) spins. Such measurements are generally limited by the attenuation and distortion of the sharp pulses, that inevitably occurs due to imperfections in the instrumental setup. The attenuation in the frequency domain can be measured and compensated for [M. Herve, et al. Appl. Phys. Lett. 107, 093101, 2015]. However, such a compensation only has limited impact on the distortion. Here, we introduce a new technique, that enables the measurement of the phase shift between individual frequencies directly in the tunnel junction of a scanning tunneling microscope (STM). Using these phase shifts it is now possible to fully compensate arbitrary pulses and manipulate atomic spins with picosecond time resolution. Phase information also provides additional insights into stochastic resonance, an effect we recently utilized as an alternative way to measure spin dynamics [M. Hänze, et al. Sci. Adv. 7, 33, 2021], even of multiple spin states.

O 77.8 Thu 12:15 REC C 213

Simultaneous Measurement of Quasiparticle Interference and Decay Length Using Parallel Spectroscopy with the Scanning Tunneling Microscope — •Berk Zengin, Danyang Liu, Aleš Cahlík, Kevin Hauser, and Fabian D. Natterer — University of Zurich, Department of Physics, Winterthurerstrasse 190, 8057 Zurich, Switzerland

Developments in signal processing unlock the possibility to perform significantly faster spectroscopic measurements with a Scanning Tunneling Microscope by utilizing the harmonics created by non-linearities in the current-voltage characteristics. Having the capability to perform spectroscopy on the order of few milliseconds to measure the local density states(LDOS), we can afford to additionally vary the tip sample distance during QPI mapping, providing spatially and energy resolved decay length information. Our work shows how LDOS and decay length mapping can yield valuable insight into the electronic structure and dispersion relation of surface electrons.

O 77.9 Thu 12:30 REC C 213

Unveiling interference of Yu-Shiba-Rusinov states with novel multi-functionalized STM probe — •Artem Odobesko, Felix Friedrich, and Mathias Bode — Physikalisches Institut, Universität Würzburg, 97074, Würzburg, Germany

Scattering of superconducting pairs by magnetic impurities on superconducting surface results into pairs of sharp ingap resonances, known as Yu-Shiba-Rusinov states. By analogue with interference of quasiparticles scattered by defects in normal metals, these excitations form periodic charge density texture around magnetic impurity. Typically, STM is equipped with a superconducting (SC) probe to increase the energy resolution bypassing thermal broadening to detect these states. However, with such STM probe it almost unattainable to observe the spatial oscillatory behavior of YSR wave function due to a very fast spatial attenuation away from the impurity (with decay ~ 1/r). In this work, we attach a CO molecule to a SC-probe to maximize simultaneously both spatial and energy resolution. We examine the LDOS distribution of YSR states around the magnetic Fe dimer on Nb(110). The last leads to hybridization of YSR states, which can be interpreted as symmetric and antisymmetric combinations of YSR excitation of an individual Fe impurity. Using such CO-SC-probe we are able to map both symmetric and antisymmetric oscillatory interference patterns of hybridized YSR states in vicinity of Fe dimer. Compared to measurements made with CO-free probe, we demonstrate an exceptional spatial sensitivity combined with high energy resolution with a new multi-functionalized probe.