O 23: Scanning probe methods II

Time: Monday 17:15–19:15 Location: WIL C307

O 23.1 Mon 17:15 WIL C307

Simulation of a single molecule stretched within an nc-AFM junction — •Christian Wagner, Norman Fournier, Christian Weiss, Ruslan Temirov, and Frank Stefan Tautz — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology

The binding of organic molecules to metal surfaces is extensively studied both in experiment and theory. While techniques such as TDS are valuable tools to determine the binding energy of adsorbed molecules, it does not allow measuring the specific binding properties of individual functional groups or atoms. We approach this question by peeling single PTCDA molecules from a Ag(111) surface using a qPlus sensor. While previous studies already revealed that the molecule can be fully lifted when contacted by a STM tip [1], here, we go one step further and measure the potential energy profile during this pulling process. Due to its complexity, this experiment is very demanding concerning a modeling approach. On the one side, there is the (chemical) interaction between molecule and substrate. On the other side, the measured signal is a frequency shift obtained for an oscillation with a *finite* amplitude. We present a modeling approach that combines less demanding force-field calculations for the description of the molecule, and of its interaction with the substrate, while fully modeling the tip oscillation process. It shows that some of the key features found in the experiment can only be understood in the context of a finite amplitude.

[1] R. Temirov, A. Lassise, F. B. Anders, and F. S. Tautz, *Nanotechnology* **19** 065401 (2008)

O 23.2 Mon 17:30 WIL C307

A strange disturbance in the force — •Jay Weymouth, Thorsten Wutscher, Joachim Welker, Thomas Hofmann, and Franz Giessibl — Universität Regensburg, Regensburg, Germany.

Although atomic contrast with NC-AFM was first reported over fifteen years ago on Silicon [1], several interesting questions remain concerning simultaneous STM and NC-AFM. Arai and Tomitori previously showed that the force signal could be varied with applied bias voltage [2]. Sugimoto and coworkers have recently demonstrated that the distance at which one typically acquires STM data is approximately 4 Å further from the surface than the distance one acquires AFM data [3]. Both sets of experiments were made with a standard cantilever at amplitudes around 200 Å. We have performed similar experiments with smaller amplitudes (<5 Å). A smaller amplitude not only increases the signal to noise ratio, it also simplifies the physical interpretation of the observed frequency shift and makes the measurement more sensitive to short-range forces.

1. Giessibl, F.J., Science, 267, 68 (1995)
2. Arai, M. and Tomitori, M., Phys Rev Lett, 93, 256101 (2004)
3. Sugimoto, Y. et al, Phys Rev B, 81, 245322 (2010)

O 23.3 Mon 17:45 WIL C307

Simultaneous current and force microscopy on epitaxial graphene — •Thomas Hofmann, Markus Duschl, and Franz J. Giessibl — University of Regensburg, Faculty of Experimental and Applied Physics II - Physics, Universitätsstrasse 31, D-93053 Regensburg

Graphite has been investigated extensively with NC-AFM at low temperatures [1]. However, at room temperature atomic resolution could not be achieved. We speculate that the weakly bond layers of the graphite lead to large thermal oscillations normal to the surface. This prevents stable oscillation of the cantilever at room temperature. To circumvent this problem, single layer graphene on SiC [2] is used as sample system. We found that in contrast to the findings on graphite, stable imaging at room temperature and at small tip-sample distances is possible. In this talk we present constant height images which show atomic contrast in both the current and the Δf channel. In the current image both six-fold and three-fold symmetry are observed, attributed to the carbon rings and holes respectively. In both cases the Δf images only show the carbon rings. Consistent with the findings of Hembacher et al. [1], the carbon atoms can only be resolved at tip-sample distances, where the tip atom already feels repulsive forces.

[1] S. Hembacher and F.J. Giessibl and J. Mannhart, and C.F. Quate, Phys. Rev. Lett. 94, 056101 (2005)

[2] P. Lauffer, K. V. Emtsev, R. Graupner, Th. Seyller, and L. Ley, Phys. Rev. B 77, 155426 (2008)

O 23.4 Mon 18:00 WIL C307

Amplitude dependence of long- versus short-range forces on Si(111)7x7 — •Joachim Welker, Thomas Hofmann, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Atomic force microscopy (AFM) senses the forces that act between a tip and a sample. The forces are composed of long- and short range interactions. Sugimoto et al. [1] recently demonstrated chemical identification of atoms by AFM using the short range forces. However, chemical identification was only possible here, because the atoms under investigation all were lying in the top surface layer, such that the long-range van der Waals (vdW) force was the same for all atoms. At step edges, the vdW forces vary strongly and we also expect that corner holes and dimer rows on Si(111) 7x7 lead to a spatial alteration in the vdW forces.

In NC-AFM, the sensitivity to forces of a different decay length can be tuned by the oscillation amplitude of the cantilever. Small amplitudes lead to a lower contribution of van-der-Waals forces to the experimental observable (frequency shift) than larger amplitudes. We performed measurements on Silicon(111)7x7 in constant height mode with oscillation amplitudes from picometer to nanometer range, investigating the contribution of the in-plane local spatial variation, e.g., the corner holes, to the long range van-der-Waals force.

[1] Y. Sugimoto, P. Pou, M. Abe, P. Jelinek, R. Perez, S. Morita, and O. Custance, Chemical identification of individual surface atoms by atomic force microscopy Nature, 446, 64 (2007)

O 23.5 Mon 18:15 WIL C307

Ac and dc Conductivity measurements vs. KPFM - a methodical study — •Anne-Dorothea Müller[1], Falk Müller[1], Stefanie Wengel[1], Kin Mun Wong[2], and Yong Lei[2] — [1]Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz, Germany — [2]Institute of Materials Physics & Center for Nanotechnology , University of Münster, 48149 Muenster, Germany

This contribution compares a large variety of electrical analysis methods in AFM, such as KPFM, dynamic EFM, CAFM, conductance microscopy and related spectroscopy. In order to push the limits of lateral resolution and to challenge the tip by means of geometry and electrical behavior at the same time, all investigations are carried out on metal nano-dot arrays on silicon with an almost one by one by one ratio of dot diameter, dot height and dot distance. Differences in achievable local resolution and dependencies on the tip geometry and conductance are explained and carefully discussed with the help of numerical simulations.

O 23.6 Mon 18:30 WIL C307

AFM an Nanodrähten: Oberflächenpotentiale und Dissipation aus abstandsabhängigen Resonanzkurven im intermittent-contact-Modus — •Moid Bhatti, Lars Ungewitter, Ivo Knittel und Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken

Der intermittent-contact ist der am weitesten verbreitete Modus der Rasterkraftmikroskopie, insbesondere, weil er schonend mit Probe und Spitze umgeht. Wir haben abstandsabhängige Resonanzkurven im intermittent-contact-Regime aufgenommen und simuliert. Diese Kurvenscharen enthalten mehr Informationen als eine einzelne Kraft-Abstandskurve und erlaubten es, durch Vergleich mit Simulationen detaillierte Aussagen über das Spitze-Probe-Potential und Dissipation zu machen. Die Ergebnisse werden mit einer Analyse konventioneller Kraft-Abstandskurven verglichen.

Nanodrähte mit einer Federkonstanten um 1N/m und Resonanzfrequenzen von 10MHz bis 1GHz werden bereits als AFM-Spitzen mit hohem Aspektverhältnis verwendet und stellen wegen ihrer Resonanzfrequenzen im MHz-Bereich mögliche 'Nanocantilever' für Rasterkraftmikroskope mit hoher Datenrate dar. Die Wechselwirkung zwischen Nanodraht und AFM-Spitze wird für lithographisch hergestellte Silizum-Nanodrähte [1] (Länge 5000 nm, Durchmesser 150nm) und selbstorganisiert gewachsene Zinnoxid-Nanodrähte [2] (Länge 300nm , Durchmesser 20nm) untersucht.

[1] Shunfeng Li et al; Phys. Status Solidi C 7, 84 (2010). [2] S. Barth

et al.; Nanotechnology 20, 115705 (2009).

O 23.7 Mon 18:45 WIL C307

Measuring forces in a single-molecule transport junction — •Norman Fournier, Christian Wagner, Christian Weiss, Ruslan Temirov, and Stefan Tautz — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich and JARA-Fundamentals of Future Information Technology

Understanding of the charge transport on a single-molecule level is vital for the future success of molecular electronics. At the present, however, this understanding is still hindered by the lack of data obtained under well-controlled experimental conditions. Recently we have shown that a low-temperature scanning tunneling microscope (STM) can be used to perform well-controlled and tunable single-molecule transport studies [1]. The high degree of structural control reached in our experiments allowed theoretical analysis of the junction on ab-initio level [2,3]. In this contribution we take further efforts towards even better experimental control over the molecular transport junction: contacting the molecule with the tip of the low-temperature AFM/STM, based on the q-Plus tuning fork design, we demonstrate that the forces acting in the junction can be measured simultaneously with the transport. The results of such measurements help us to gain further insights in the structure of a single-molecule junction and the process of the mechanical gating.

(1) R Temirov et al. Nanotechnology 2008, 19, 065401 (2) A. Greuling et al. submitted to Phys. Rev. Lett. (3) C. Toher, et al. submitted to Phys. Rev. B

O 23.8 Mon 19:00 WIL C307

Structure of the first water layer on Ru(0001) — •Sabine Maier[1,2], Ingeborg Stass[1], Peter J. Feibelman[3], and Miquel Salmeron[1] — [1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [2]Friedrich-Alexander-Universität Erlangen, Erlangen — [3]Sandia National Laboratories, Albuquerque, NM, USA

The structure and chemistry of water at surfaces and interfaces, though fundamental to many areas of science and technology, is largely unknown. Low temperature scanning tunneling microscopy data in combination with DFT calculations can, however, reveal the molecular structure of monolayer thick water films. By these means, we have found that compact clusters of flat-lying H_2O molecules lie low on Ru(0001), and anchor the adsorbed layer to it. They alternate with clusters of molecules possessing a dangling H-bond, which bind weakly to the metal and, correspondingly, lie higher above the surface. Counter to conventional expectation, the high-lying molecular hexagons are rotated 30° relative to the principal axes of the metal crystal surface. This rotation leads to a bonding structure that significantly deviates from the conventional ice-like water model on hexagonal metals. Above 130K, we observed the formation of mixed water-hydroxyl structures following partial dissociation.