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NC AFM 2011

LAKE CONSTANCE

14th International Conferencence on Noncontact Atomic Force Microscopy

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KNMF
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MICRO Facility

Past conferences:

Osaka, Japan (1998)
Pontresina, Switzerland (1999)
Hamburg, Germany (2000)
Kyoto, Japan (2001)
Montreal, Canada (2002)
Dingle, Ireland (2003)
Seattle, USA (2004)
Bad Essen, Germany (2005)
Kobe, Japan (2006)
Antalya, Turkey (2007)
Madrid, Spain (2008)
New Haven, USA (2009)
Kanazawa, Japan (2010)

Forthcoming conference:

Prague, Czech Republic (2012)

Design by: M. Langer

You like the Design? You like to have your own? Mail me: **Markus.Langer@unibas.ch**

WELCOME

Non-Contact Atomic Force Microscopy (nc-AFM) has fulfilled the long-standing goal of true atomic resolution imaging and spectroscopy as well as nanoscale manipulation on all kind of surfaces. As an offspring of the atomic force microscope (AFM) invented by Binnig, Quate and Gerber in 1986 we now celebrate the 25th anniversary of all AFM techniques. Today this technique is widely spread in the scientific community especially in physics, nanosciences and biology and enables the detailed analysis of material properties like structure, elasticity, friction, and force fields down to the atomic and molecular scale.

The nc-AFM 2011 continues a series of international conferences dedicated to research at the frontiers of science and technology of nc-AFM and spectroscopy. The conference covers experimental, theoretical, and instrumental contributions on frequency modulation and other dynamic and static operation modes with particular emphasis on high resolution imaging and force spectroscopy for a broad range of applications in nanosciences. Former conferences where held in Kanazawa, Japan (2010); New Haven, USA (2009); Madrid, Spain (2008); Antalya, Turkey (2007); Kobe, Japan (2006); Bad Essen, Germany (2005); Seattle, USA (2004); Dingle, Ireland (2003); Montreal, Canada (2002); Kyoto, Japan (2001); Hamburg, Germany (2000); Pontresina, Switzerland (1999); and Osaka, Japan (1998).

We welcome you to the 2011 conference which takes place in Lindau at Lake Constance located in the beautfull tri-border region between Germany, Austria, and Switzerland. The historic city of Lindau can be easily reached by train from international airports like Zurich, Munich and Frankfurt. This and the impressive landscape of Lake Constance makes it the perfect spot for our annual meeting. Following the tradition of the previous nc-AFM conferences the nc-AFM 2011 is accompanied by a satellite symposium dedicated to Quantitative Nanoscale AFM Measurements in Life Science which was organized with the help of Prof. Georg E. Fantner (Institute of Bioengineering, EPFL Lausanne, Switzerland).

We hope that you will enjoy the conference with us and have a wonderful time in Lindau at Lake Constance

Hendrik Hölscher, Thilo Glatzel, Ernst Meyer

CONTENTS

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COMMITTEES

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4 GENERAL INFORMATION

Registration:

The registration desk is open during all conference times. Onsite registration is possible.

Tourist and Hotel Information:

A tourist and hotel information desk is located at the conference site on Sunday and Monday. It will be provided by the local tourist organization ProLindau.

Welcome BBQ:

The Welcome BBQ takes place in the Inselhalle at the conference site, and is sponsored in part by Omicron Nanotechnology GmbH.

Conference Hall:

Eating and smoking are not allowed in the Conference Hall. Power supply sockets will be available.

Oral Presentation:

The time for contributed talks is 20 min including 5 min discussions. Projectors are available in the conference room. Backup laptops are provided to ensure a seamless talk session. Please, provide a backup pdf file of your talk on a USB stick.

Poster Presentation:

Poster sessions will be held during the conference. The poster boards are 153 cm height and 90 cm wide. Pins will be provided at the poster boards. Authors are requested to stand at their posters during the scheduled poster session.

Conference Dinner:

The conference dinner will be in following to a visit of the famous Zeppelin museum in Friedrichshafen on Wednesday evening. We will travel to Friedrichshafen with the fairy „Königin Katharina“ (Queen Katharina).

WiFi Access:

WiFi access is available in the Inselhalle. Login information is provided at the registration desk.

5 LOCAL MAPS

Herausgeber und Copyright
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Local map of Lindau

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EXHIBITORS

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Schweiz
www.zhinst.com

Symposium: Quantitative Nanoscale AFM Measurements in Life Science

Due to its unique capability to measure non-conductive materials with nanometer resolution, the atomic force microscope has early on been an attractive tool for nanoscale investigations in biology. Over the last 20 years, AFM has been established in many life science related fields such as biophysics, molecular and cellular biology, biomaterials and pharmaceutics.

While originating from a common ancestor, instruments and techniques used for AFM in life science have become markedly different from those used in UHV and low temperatures, and two distinct AFM communities have emerged. In recent years however, the influence of methods developed for UHV and low temperature AFM are getting adopted in AFM for life science. Frequency modulated AFM and small amplitude AM-AFM have shown tremendous promise for achieving atomic resolution in aqueous environments. In addition, AFM measurements in life science have transitioned from mere imaging to quantitatively measure properties of biological samples at the nanoscale. Multifrequency AFM, single molecule force spectroscopy and nanoscale mechanical property measurements have become reliable tools.

The purpose of the symposium “Quantitative Nanoscale AFM Measurements in Life Science” is to highlight how concepts from non-contact AFM can be applied to life science AFM, and to further the exchange between these two fields. Topics will range from high-resolution imaging of solid liquid interfaces, measurement of dynamic molecular interactions and molecular recognition to the use of AFM for cellular biology.

Scientific sessions start on Sunday, Sep 18th, 2011 at 2:30 pm and overlap with the nc-AFM 2011 conference on Monday Sep 19th. In order to give a broad overview of the field, the symposium consists of 9 regular contributed talks and invited review talks by:

Francesco Stellacci (EPFL)
Ricardo Garcia (IMM, Madrid)
Ozgur Sahin (Harvard)
Thomas Gutsmann (FZ-Borstel, Univ. Lübeck)
Johannes Preiner (JKU, Linz)

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TOPICS

- Novel Instrumentation and techniques in AFM
- Atomic resolution imaging on insulating substrates, semiconductors, and metals
- Atomic resolution imaging on molecular systems
- High-resolution imaging of clusters, biomolecules, and biological systems
- Atomic- and molecular-scale manipulation
- Combined force and tunneling spectroscopy
- High-resolution imaging and spectroscopy in liquid environments
- Theoretical analysis of contrast mechanisms; forces & tunnelling phenomena
- Measuring tip-sample interaction potentials and mapping 2D and 3D force fields
- Small amplitude and lateral force measurements using dynamic methods
- Mechanisms for damping and energy dissipation
- Measuring nanoscale charges, work function, and magnetic properties
- Simulation of images and virtual SPM systems
- Tapping mode versus non-contact mode imaging

nc-AFM 2011
scientific program

	Sunday September 18	Monday September 19	Tuesday September 20	Wednesday September 21	Thursday September 22
08:30		Registration	Registration	Registration	Registration
09:00		O. Sahin (invited)	M. Baykara	F. Mohn	A. Kühnle
09:20			G. Langewisch	M. Corso	R. Pawlak
09:40		H. Onishi	T. Arai	T. Leoni	M. Kittelmann
10:00		H. Asakawa	S. Kawai	C. Chiutu	C. Loppacher
10:20		A. Berquand	A. Baratoff	C. Lotze	P. Rahe
10:40		Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:20		Th. Gutsmann (invited)	L. Nony	L. Kantorovich	F.J. Giessibl
11:40			Y. Miyahara	T. Trevethan	A.J. Weymouth
12:00		D. Vobornik	M. Tsukada	F. Federici Canova	L. Gross
12:20		B. Reischl	P. Milde	S. Jarvis	T. Hofmann
12:40		J. Preiner (invited)	M. Ito	Lunch *70 min.*	I. Swart
13:00	Registration	Lunch *90 min.*	Lunch *90 min.*	A. Schwarz E. Vedmedenko	Best Poster Award IOP Award Closing Remarks
14:30	F. Stellacci (invited)	Opening Remarks	M. Setvin	M. Huefner	Guided City Tour
14:50		Ch. Gerber (invited)	Z. Majzik		
15:10	J.P. Cleveland		Y. Naitoh		
15:30	S. Ido	K. Suzuki	A. Sweetman	Excursion (15:30-18:30)	
15:50	Coffee Break	Coffee Break	Coffee Break		
16:30	R. Garcia (invited)	C. Barth	Y. Sugawara		
16:50		J. Bamidele	N. Hauptmann		
17:10	K. Kaisei	L. Lichtenstein	Y. Hosokawa		
17:30	A. Cerreta	J. V. Lauritsen	C. A. Wright		
17:50		H. Pieper	M. Kisiel		
18:30-20:30		Poster Session I	Poster Session II		
	18:00-21:00 Welcome Barbecue			18:30-22:00 Conference Dinner	

⬛ Symposium
🟥 Liquids
🟦 Oxides & Insulators
🟦 Spectroscopy
🟪 KPFM
🟩 Semiconductors

Techniques 🟪
Molecules I 🟦
Theory 🟩
Magnetics 🟩
Molecules II 🟪
High-k Oscillators 🟧

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ORAL PRESENTATIONS

Sunday 18. September

Symposiums talk

SESSION I

chair: G. Fantner

14:30 Probing of complex Solid-liquid Interfaces with AM-AFM
Francesco Stellacci and Kislon Voitchovsky

15:10 Atomic point-defect resolution in liquids with amplitude modulation AFM
Jason P. Cleveland, Mario B. Viani, Deron A. Walters, and Roger Proksch

15:30 Molecular-scale Investigations of Monoclonal Antibodies in Liquids by FM-AFM
Shinichiro Ido, Hirokazu Kimiya, Kei Kobayashi, Kazumi Matsushige, and Hirofumi Yamada

15:50 Coffee Break

chair: F. Stellacci

SESSION II

16:30 Advances in bimodal AFM imaging of molecules in liquid
E.T. Herruzo, C. Dietz, J.R. Lozano, D. Martinez-Martin, J. Gomez-Herrero, H. Asakawa, T. Fukuma, and R. García

17:10 Applications of three-dimensional force mapping method to imaging of biological samples with large structures in liquids
Kiyohiro Kaisei, Kei Kobayashi, Noriaki Oyabu, Masahiro Ohta, Ryohei Kokawa, Yoshiki Hirata, and Hirofumi Yamada

17:30 Force spectroscopy on DNA and amyloid fibrils by means of FM-AFM
Andrea Cerreta, Dusan Vobornik, Giovanni Di Santo, Susana Tobenas, Jozef Adamcik, and Giovanni Dietler

Welcome BBQ (18:00 -21:00)

19. September Monday

Symposiums talk

SESSION III

chair: J. Preiner

09:00	Microsecond-Timescale Biomolecular Interactions Probed by Dynamic AFM **Ozgur Sahin**
09:40	Hydration to Hydrophilic Monolayers Visualized by FM-AFM Takumi Hiasa, Kenjiro Kimura, and **Hiroshi Onishi**
10:00	Visualizing Molecular Arrangements at the Surface of Cylindrical Protein Structures by FM-AFM in Liquid **Hitoshi Asakawa**, Yukitoshi Katagiri, Koji Ikegami, Mitsutoshi Setou, and Takeshi Fukuma
10:20	Investigation of Mechanical Properties of Living Cells by Combined Optical Microscopy and Atomic Force Microscopy **Alexandre Berquand**, Andreas Holloschi, Hella-Monika Kuhn, Mathias Hafner, and Petra Kioshis
10:40	Coffee Break

chair: O. Sahin

SESSION IV

11:20	How can atomic force microscopy help to understand bacterial infections? **Thomas Gutsmann**
12:00	Challenges of non-contact AFM biological samples studies **Dusan Vobornik**, Andrea Cerreta, and Giovanni Dietler
12:20	Simulating non-contact AFM imaging of calcite in water **Bernhard Reischl** and Adam S. Foster
12:40	Imaging of Molecular Recognition at the Nano-Scale **Johannes Preiner** and Peter Hinterdorfer
13:00	Lunch

Monday 19. September

Opening Remarks (14:30 -14:50)

Liquids

chair: F. Giessibl

14:50	SPM Technologies past, present ,future Christoph Gerber
15:30	Molecular-scale charge distribution at an interface between liquid and surfactant assembly investigated by three-dimensional force mapping Kazuhiro Suzuki, Noriaki Oyabu, Kei Kobayashi, Kazumi Matsushige, and Hirofumi Yamada
15:50	Coffee Break

Oxides & Insulators

chair: M. Reichling

16:30	Two-dimensional growth of nanoclusters and molecules on Suzuki surfaces B. Hoff, M. Gingras, A. Gulans, T. Hynninen, R. Peresutti, C. R. Henry, A. S. Foster, and C. Barth
16:50	NC-AFM Tip & Surface Species Identification on Oxidized Cu(110) J. Bamidele, Y. Kinoshita, R. Turanský, T. Satoh, S. H. Lee, Y. Naitoh, Y. J. Li, M. Kageshima, Y. Sugawara, I. Štich, and L. Kantorovich
17:10	Resolving the Atomic Structure of Amorphous Silica Leonid Lichtenstein, Steffanie Stuckenholz, Christin Büchner, Markus Heyde, and Hans-Joachim Freund
17:30	NC-AFM experiments and atomistic simulations of the surface structure and defects on the MgAl$_2$O$_4$ (100) surface Morten K. Rasmussen, Filippo F. Canova, Kristoffer Meinander, Flemming Besenbacher, Adam S. Foster, and Jeppe V. Lauritsen
17:50	Step structures on CeO$_2$(111) identified by NC-AFM and KPFM Hans Hermann Pieper, Clemens Barth, and Michael Reichling

Poster Session I (18:30 - 20:30)

chair: S. Solares

20. September Tuesday

Spectroscopy

chair: P. Grütter

09:00	Atom-Specific Interaction Quantification and Identification by 3D-SPM **Mehmet Baykara**, Harry Mönig, Milica Todorović, Todd C. Schwendemann, Ruben Perez, Eric I. Altman, and Udo D. Schwarz
09:20	Conservative and Dissipative Tip-Molecule Interactions: Force Spectroscopy Investigations on an Organic Adsorbate **Gernot Langewisch**, Daniel-Alexander Braun, Jens Falter, Harald Fuchs, Andre Schirmeisen, Wojciech Kaminski, and Ruben Perez
09:40	NC-AFM and Force spectroscopy applied to H terminated Si(111)7x7 **Toyoko Arai**, Tatsuya Ikeshima, Yuqi Zhang, and Masahiko Tomitori
10:00	Quantitative static and dynamic force spectroscopy of atomic-scale forces and energy dissipation **Shigeki Kawai**, Filippo Federici Canova, Thilo Glatzel, Adam S. Foster, and Ernst Meyer
10:20	An atomic contact studied by small amplitude dynamic force microscopy Shigeki Kawai, Thilo Glatzel, Sascha Koch, **Alexis Baratoff**, and Ernst Meyer
10:40	Coffee Break

KPFM

chair: H. Onishi

11:20	Polarization effects and charge state characterization in nc-AFM Franck Bocquet, **Laurent Nony**, and Christian Loppacher
11:40	Detection of charge state of individual gold nanoparticles with single-electron resolution **Yoichi Miyahara**, Antoine Roy-Gobeil, Lynda Cockins, and Peter Grütter
12:00	Effect of Orbital Hybridization on Kelvin Probe Force Microscopy Images **Masaru Tsukada**, A. Masago, and M. Shimizu
12:20	Surprise-surprise: local work function variations on clean Au(111) **Peter Milde**, Ulrich Zerweck-Trogisch, Denny Köhler, and Lukas M. Eng
12:40	High-resolution surface potential mapping on single-walled carbon nanotubes using frequency-modulation high-frequency electrostatic force microscopy **Masanao Ito**, Kei Kobayashi, Yuji Miyato, Kazumi Matsushige, and Hirofumi Yamada
13:00	Lunch

Tuesday 20. September

Semiconductors

chair: U.D. Schwarz

14:30 Atomic and chemical resolution of heterogenous In-Sn chains on Si(100)-(2x1) studied by nc-AFM and DFT

Martin Setvín, Pingo Mutombo, Zsolt Majzik, Martin Ondráček, Pavel Sobotík, Vladimír Cháb, and Pavel Jelínek

14:50 Molecular recognition of single molecules adsorbed on the Si(111)-(7x7) surface by means of nc-AFM

Zsolt Majzik, Wojciech Kaminski, Benedict Drevniok, Alastair B. McLean, Vladimír Cháb, and Pavel Jelínek

15:10 Visualization of atomic scale elasticity on Ge(001) surface with multifrequency FM-AFM

Yoshitaka Naitoh, Yan Jun Li, and Yasuhiro Sugawara

15:30 Dopants & Defects on Si(100): Imaging & manipulation by qPlus NC-AFM

Adam Sweetman, Sam Jarvis, Rosanna Danza, and Philip Moriarty

15:50 Coffee Break

Techniques

chair: R. Pérez

16:30 Tip-induced heating of Co atoms on Cu(110)-O surface with low-temperature AFM

Yasuhiro Sugawara, Yukinori Kinoshita, Yoshitaka Naitoh, and Yan Jun Li

16:50 Force and conductance of contacts to a C60 molecule

Nadine Hauptmann, Leo Gross, Fabian Mohn, Gerhard Meyer, Thomas Frederiksen, and Richard Berndt

17:10 Measurement of tip-sample interaction forces under infrared irradiation toward high-spatial-resolution infrared spectroscopy using FM-AFM

Yoshihiro Hosokawa, Kei Kobayashi, Hirofumi Yamada, and Kazumi Matsushige

17:30 Mapping Electron Clouds with Force Microscopy

C. Alan Wright and Santiago Solares

17:50 Topography and KPFM measurements of NaCl islands grown on copper surface by means of nc-AFM in pendulum geometry

Marcin Kisiel, M. Langer, U. Gysin, S. Rast, Th. Glatzel, and E. Meyer

Poster Session II (18:30 - 20:30)

chair: P. Jelínek

21. September Wednesday

Molecules I

chair: A. Schwarz

09:00 Reversible bond formation in a metal-molecule complex

Fabian Mohn, Jascha Repp, Leo Gross, Gerhard Meyer, Matthew S. Dyer, and Mats Persson

09:20 Exploring short range interactions between two neutral molecules

Martina Corso, Christian Lotze, and José Ignacio Pascual

09:40 Measuring the charge state of a single redox molecule with nc-AFM

Thomas Leoni, Hermann Walch, Olivier Guillermet, Véronique Langlais, Andrew Scheurman, Jacques Bonvoisin, and Sébastien Gauthier

10:00 Sub-molecular resolution imaging and orientational control of on tip C_{60}

Cristina Chiutu, Lakin Andrew, Stannard Andrew, Sweetman Adam, Jarvis Samuel Dunn Janette, and Moriarty Philip

10:20 Dynamic Force Spectroscopy at a Single Molecule Junction

Christian Lotze, Martina Corso, Gunnar Schulze, Katharina J. Franke, and Jose Ignacio Pascual

10:40 Coffee Break

Theory

chair: A. Foster

11:20 Measuring individual up and down tip forces in Dynamic AFM

Lev Kantorovich, Adam Sweetman, and Philip Moriarty

11:40 Chemical identification of surface ions on polar surfaces using metallic tips and adsorbed molecule

Thomas Trevethan, Gilberto Teobaldi, Knud Lammle, Matt Watkins, Alexander Schwarz, and Alexander Shluger

12:00 NC-AFM energy dissipation mechanisms

Filippo Federici Canova, Shigeki Kawai, Thilo Glatzel, Adam S. Foster, and Ernst Meyer

12:20 What role does orbital overlap play in atomic manipulation?

Sam Jarvis, Adam Sweetman, Lev Kantorovich, and Philip Moriarty

12:40 Lunch

Wednesday 21. September

Magnetics

chair: E. Meyer

13:50 Properties of Magnetic Tips for Magnetic Exchange Force Microscopy and Spectroscopy

Rene Schmidt, **Alexander Schwarz**, and Roland Wiesendanger

14:10 Atomic Scale Magnetic Dissipation from Spin-Dependent Adhesion Hysteresis

Elena Y. Vedmedenko, Q. Zhu, U. Kaiser, A. Schwarz, and R. Wiesendanger

14:30 Single vortex manipulation in superconducting $NdFeAsO_{1-x}F_x$

Magdalena Huefner, Jeehoon Kim, Matt Tillman, Paul Canfield, and Jennifer Hoffman

Excursion & Conference Dinner (15:30)

15:30 Departure of the Königin Katharina from Lindau Harbour

16:40 Arrival in Friedrichshafen

17:00 Guided tours through the Zeppelin museum

18:45 **Conference Dinner**

21:30 Departure of the Königin Katharina from Friedrichshafen

22:45 Arrival in Lindau

22. September Thursday

Molecules II

chair: A. Shluger

09:00 Exploiting transient non-equilibrium structures for the formation of complex molecular islands on insulating surfaces

Martin Körner, Felix Loske, Mario Einax, Michael Reichling, Philipp Maass, and **Angelika Kühnle**

09:20 Mechanical switching of single porphyrins investigated with a tuning fork sensor

Rémy Pawlak, Sweetlana Fremy, Shigeki Kawai, Thilo Glatzel, Hongjuan Fang, Leslie-Anne Fendt, François Diederich, and Ernst Meyer

09:40 Phase transition of a molecular film: Following the rearrangement of a transient molecular structure on calcite (10$\bar{1}$4)

Markus Kittelmann, Philipp Rahe, Christopher Hauke, Markus Nimmrich, and Angelika Kühnle

10:00 Extended 2-dimensional growth of hexahydroxy triphenylene on KCl

Laurent Nony, Franck Bocquet, Stefan Mannsfeld, Vincent Oison, Franck Para, Louis Porte, and **Christian Loppacher**

10:20 Adsorption and structure formation of organic molecules on CaCO$_3$(10$\bar{1}$4) – Impact for molecular self-assembly on insulating substrates

Philipp Rahe, Markus Nimmrich, Jens Schütte, Markus Kittelmann, and Angelika Kühnle

10:40 Coffee Break

High-k Oscillators

chair: S. Morita

11:20 A comparison of quartz force sensors for scanning probe microscopy based on tuning forks and length extensional resonators

Franz J. Giessibl, Toyoaki Eguchi, Florian Pielmeier, Toshu An, and Yukio Hasegawa

11:40 Probing Local States with the Phantom Force

Alfred J. Weymouth, Thorsten Wutscher, and Franz J. Giessibl

12:00 Combined NC-AFM and STM investigations of individual molecules adsorbed on ultrathin insulating films using functionalized tips

Leo Gross, Fabian Mohn, Nikolaj Moll, and Gerhard Meyer

12:20 Atomic Force Maps on Epitaxial Graphene

Thomas Hofmann and Franz J. Giessibl

12:40 Quantitative atomic force microscopy with CO terminated tips

Z. Sun, M. P. Boneschanscher, **I. Swart**, D. Vanmaekelbergh, and P. Liljeroth

Awards and Closing Remarks (13:00 - 13:40)

Guided City Tour (14:30 - 15:30)

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POSTER SESSION I

19. September POSTER SESSION I

chair: S. Solares

Insulators

P.I-01
Atom-resolved NC-AFM studies of polar surfaces of insulating metal oxides
Morten K. Rasmussen, Thomas N. Jensen, Kristoffer Meinander, Fillipo F. Canova, Adam S. Foster, R. Wahl, G. Kresse, F. Besenbacher, and **Jeppe V. Lauritsen**

P.I-02
Investigation of $TiO_2(110)$ by AFM/STM with the Tungsten-Coated Tip
Lili Kou, Takeshi Kamijo, Yoshitaka Naitoh, Yan Jun Li, and Yasuhiro Sugawara

P.I-03
AFM/STM Simultaneous measurement on Cu(110)-O with metal-coated cantilever
Zong-Min Ma, Yoshitaka Naitoh, Yan-Jun Li, and Yasuhiro Sugawara

P.I-04
The charge state of steps on cleaved CaF_2 studied by NC-AFM and KPFM
Hans Hermann Pieper, Clemens Barth, and Michael Reichling

P.I-05
Classification for the NC-AFM contrast formation on $CaCO_3(10\bar{1}4)$
Philipp Rahe, Jens Schütte, Michael Reichling, Masayuki Abe, Yoshiaki Sugimoto, and Angelika Kühnle

P.I-06
Scanning Probe Microscopy on Organic Layer Compound Crystals
G. Fessler, M. Schulzendorf, S. Kawai, T. Glatzel, S.-X. Liu, S. Decurtins, and E. Meyer

P.I-07
Changes in Morphology and Electronic Structure of MgO on Mo(001)
Stefanie Stuckenholz, Leonid Lichtenstein, Christin Büchner, Markus Heyde, and Hans-Joachim Freund

P.I-08
Stable Contrast Mode on $TiO_2(110)$ Surface Using AFM with Tungsten-coated Tips
Yan Jun Li, Yoshihiro Tsukuda, Yoshitaka Naitoh, and Yasuhiro Sugawara

KPFM

P.I-09
Growth and work function studies of NaCl thin films on silver
Gregory Cabailh, Claude R. Henry, and **Clemens Barth**

P.I-10
Scanning Kelvin Probe Microscopy for C_{60}/TiOPc Molecular Interfaces
Kristen Burson, Yinying Wei, William G. Cullen, and Janice E. Reutt-Robey

P.I-11
Scanning Kelvin Probe Microscopy of Graphene-Supporting Substrates
Kristen Burson, Alexandra Curti,n Shaffique Adam, Michael S. Fuhrer, and **William G. Cullen**

P.I-12
A NC-AFM and KPFM study of a triphenylene derivative on KBr(001)
Antoine Hinaut, Florian Chaumeton, Sonia Bataillé, André Gourdon, David Martrou, and Sébastien Gauthier

P.I-13
Kelvin probe force microscopy on single and bilayer graphene
Christian Held, Thomas Seyller, and Roland Bennewitz

POSTER SESSION I 19. September

KPFM

chair: S. Solares

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P.I-15	The influence of the cantilever capacitance on the accuracy of surface potential measurements in Kelvin probe force microscopy Franciszek Krok, Kristof Szot, Jerzy Konior, Piotr Piatkowski, and Marek Szymonski
P.I-16	CNT-probes in NC-AFM: Tip broadening and KPFM signature Kristoffer Meinander, Thomas N. Jensen, Søren B. Simonsen, Stig Helveg, and Jeppe V. Lauritsen
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P.I-18	Dynamic Force Spectroscopy of Electrostatic Interactions in Aqueous Salt Solutions of Variable Concentration and Valency Daniel Ebeling, Dirk van den Ende, and Frieder Mugele
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P.I-21	High-resolution AFM by tracking the resonance frequency of ultrasmall cantilevers Carl Leung, Jake Stinson, Christian Markovich, and Bart Hoogenboom
P.I-22	High-resolution Imaging on Ionic Liquid/Solid Interfaces using Frequency Modulation Atomic Force Microscopy Takashi Ichii, Motohiko Fujimura, Masahiro Negami, Kuniaki Murase, and Hiroyuki Sugimura
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P.I-28 Adhesion Analysis of Gecko-Inspired Hierarchical Adhesives Using Atomic Force Microscopy

Michael Röhrig, Michael Thiel, Farid Oulhadj, Fabian Pfannes, Matthias Worgull, and Hendrik Hölscher

P.I-29 FM-AFM analysis of dye-adsorbed TiO_2 surfaces in pure water

Tetsuya Yoshi, Le Tran Uyen Tu, Akira Sasahara, and **Masahiko Tomitori**

P.I-30 High Resolution Imaging in Liquid Using an Improved Frequency Modulation Atomic Force Microscope

Katsuyuki Suzuki, Shin-ichi Kitamura, Shulochi Tanaka, Kei Kobayashi, and Hirofumi Yamada

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Shushi Suzuki, Yasuhiro Ohta, Takashi Kurimoto, Susumu Kuwabata, and Tsukasa Torimoto

P.I-32 Quantitative study of local electric double layer force by FM-AFM in aqueous solutions

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P.I-33 Interfaces between solids and ionic liquids investigated by AM-AFM

Kislon Voitchovsky and Francesco Stellacci

P.I-34 FM-AFM phase analysing on the demixed $Ag_xNa_{1-x}Br$ system

Bo Zhang, Friedrich Güthoff, and Götz Eckold

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P.I-35 Suppression of electronic friction on Nb-films below the critical temperature

Marcin Kisiel, Enrico Gnecco, Urs Gysin, Simon Rast, Laurent Marot, and Ernst Meyer

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Arne Köhler, René Schmidt, Alexander Schwarz, and Roland Wiesendanger

P.I-37 Quantifying magnetic moments in magnetic force microscopy (MFM) tips

Denny Köhler, Peter Milde, Ulrich Zerweck-Trogisch, and Lukas M. Eng

P.I-38 Molecular dynamics of Co-Salen on NiO(001) at submonolayer coverages

Josef Grenz, **Kai Ruschmeier**, Alexander Schwarz, and Roland Wiesendanger

P.I-39 qPlus Magnetic Force Microscopy in Frequency-Modulation Mode with milli-Hertz Resolution

Maximilian Schneiderbauer and Franz J. Giessibl

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P.I-41	Self-assembly of Tetrathiafulvalene-Fused Dipyridophenazine (TTF-dppz) analyzed by tuning fork based AFM/STM **Sweetlana Fremy**, Rémy Pawlak, Shigeki Kawai, Thomas Jung, Shi-Xia Liu , Silvio Decurtins, Ernst Meyer, and Thilo Glatzel
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P.I-43	Influence of chirality on molecular structure formation: Helicene molecules on calcite (10$\bar{1}$4) **Christopher Hauke**, Philipp Rahe, Markus Nimmrich, Jens Schütte, Markus Kittelmann, Irena G. Stara, Ivo Starý, Jirí Rybácek, and Angelika Kühnle
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P.I-49	NC-AFM observation of Si(111)7x7 terminated with hydrogen Toyoko Arai, **Tatsuya Ikeshima**, and Masahiko Tomitori
P.I-50	Junction formation of Cu_3BiS_3 investigated by Kelvin probe force microscopy and surface photovoltage F. Mesa, R. Baier, Th. Dittrich, **S. Sadewasser**, and M.Ch. Lux-Steiner
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Rapid reconstruction of frequency shift vs. distance curves by multiple lock-in detection

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Force Field Spectroscopy of Graphene on Ru(0001)

Sascha Koch, Sarah Barja, Enrico Gnecco, Shigeki Kawai, Ernst Meyer, and Thilo Glatzel

P.I-56

Coupling of conservative and dissipative forces in frequency modulation atomic force microscopy – a source of apparent damping

Aleksander Labuda, Yoichi Miyahara, Lynda Cockins, and Peter H. Grütter

Post-Deadline

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Variable temperature liquid AFM reveal change in coverage of water on mica

Hideki Kawakatsu, Shuhei Nishida, Dai Kobayashi, Miao-Miao Wang, and K. Ohashi

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Design of a Low-Temperature Ultra-High Vacuum Non-Contact Atomic Force Microscope

N. Nicoara, B. de la Torre, M. M. Ugeda, J. Gómez-Herrero, O. Custance, and J. M. Gómez- Rodríguez

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Force and Current Spectroscopy with Atomically Defined Tips

William Paul, Jean-Benoît Lalanne, David Oliver, Yoichi Miyahara, and Peter Grütter

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How do you calculate chemical interactions from $\Delta f(z)$?

Andrew Stannard and Adam Sweetman

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Interaction-free measurement with tunnelling microscope

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A low temperature AFM tailored for lowest-noise qPlus operation

Matthias Emmrich and Franz J. Giessibl

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Sébastien Gauthier

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Combined SIMS-SPM instrument for high sensitivity and high resolution elemental 3D analysis

Urs Gysin, Yves Fleming, Tom Wirtz, Urs Wegmann, Thilo Glatzel, Ernst Meyer, and Urs Maier

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The NanoWizard® 3 – The Most Flexible, High Resolution AFM With True Optical Integration

Heiko Haschke, Torsten Jaehnke, Elmar Hartmann, and Gerd Behme

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Combined TEM and NC-AFM study of Al2O3-supported Pt nanoparticles

S. B. Simonsen, S. Helveg, I. Chorkendorff, S. Dahl M. Skoglundh K. Meinander, T. N. Jensen, and J. V. Lauritsen

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Force Control and Bandwidth: Enabling Faster AFM imaging in Survey, Screening and Dynamics Applications

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All digital PLL-based control system for high-frequency AFM cantilevers

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Quantification of noise in NC-AFM systems for UHV applications
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Mathias Neu, Andreas Pöllmann, Florian Albrecht, and Jascha Repp

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NanoXAS - Combining Scanning Probe and X-Ray Microscopy for Nanoanalytics
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Reflection from diffraction grating etched onto the backside surface of AFM cantilever increases the force sensitivity
Sergey Sekatskii, Mounir Mensi, Andrey Mikhailov, and Giovanni Dietler

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Trimodal Tapping-Mode Atomic Force Microscopy
Gaurav Chawla and Santiago Solares

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Silicon AFM probes for dynamic AFM with sub-nanometre amplitudes
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Dennis van Vörden, Manfred Lange, Christian Notthof, and Rolf Möller

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Henning von Allwörden, Kai Ruschmeier, Alexander Schwarz, and Roland Wiesendanger

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Sapphire-based multi-environment AFM tips
Daniel Wastl, Alfred J. Weymouth, Kilian Knot, Elisabeth Wutscher, and Franz J. Giessibl

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Open Source SPM Software GXSM and very a affordable DSP MK2-A810
Percy Zahl

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P.II-28 Split quartz tuning fork sensor for enhanced sensitivity force detection

M. Labardi and M. Lucchesi

P.II-29 Hybrid AFM, STM, and Near-Field Microwave Microscopy

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P.II-30 Ultra-sensitive bias dependence of force-distance curve and hysteresis measured on single Pb adatom on Pb(111)

Hanqing Mao, Na Li, Xi Chen, and Qikun Xue

P.II-31 MgO on Ag(100): A simultaneous STM/AFM study

Florian Pielmeier, Susanne Baumann, Chris P. Lutz, Andreas Heinrich, and Franz J. Giessibl

P.II-32 Development of nc-AFM/STM using a tuning fork quartz force sensor

Toyoko Arai, Tatsuya Sakuishi, Hiroaki Ooe, and Masahiko Tomitori

P.II-33 Small-amplitude FM-AFM using a Si cantilever with very high stiffness

Masahiro Haze, Yoshitaka Naitoh, Yan Jun Li, and Yasuhiro Sugawara

P.II-34 The role of van der Waals versus chemical forces in atom identification

Joachim Welker, Alfred J. Weymouth,Thomas Hofmann, and Franz J. Giessibl

P.II-35 FM-AFM on Epitaxial Graphene in Air with the qPlus Sensor

Elisabeth Wutscher, Daniel Wastl, and Franz J. Giessibl

P.II-36 Exploring the Scale of a Tunnel Current Induced Phantom Force

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P.II-37 Huge & Complex Dissipation Signals from Small & Simple NC-AFM Scans

J. Bamidele, H. Nomura, S. Jarvis, Y. J. Li, Y. Naitoh, M. Kageshima, Y. Sugawara, and L. Kantorovich

P.II-38 A numerical FM-AFM for image calculations of adsorbed molecules

Fabien Castanié, Laurent Nony, Sébastien Gauthier, and Xavier Bouju

P.II-39 Modelling NC-AFM Resolution on Corrugated Surfaces

Kristen Burson, Mahito Yamamoto, and William G. Cullen

P.II-40 Wavelet coherency and phase analysis of cantilever oscillations

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Numerical Analysis of Band Excitation Signals in Atomic Force Microscopy

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Unifying theory of quantitative AFM using piezo excitation in liquids

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Charge Alteration in Si(111)-DAS Surface by Atomic Force Microscopy

Akira Masago and Masaru Tsukada

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Theoretical study of atomic manipulation on metals

Martin Ondráček, Zdeňka Chromcová, Cesar González, and Pavel Jelínek

P.II-47

Theoretical analysis of relation between force and current in the tunnelling regime

Martin Ondráček, Fernando Flores, and Pavel Jelínek

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Multi-Scale Approach to Simulations of Kelvin Probe Force Microscopy

Ali Sadeghi, Alireza Ghasemi, Stefan Goedecker, Alexis Baratoff, Thilo Glatzel, Shigeki Kawai, and Ernst Meyer

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Dependence of the most probable and average bond rupture force on the force loading rate: first order correction to the Bell – Evans model

Sergey K. Sekatski, Fabrizio Benedetti, and Giovanni Dietler

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Development of a KPFM simulator for microscale imaging

Mamoru Shimizu, Akira Masago, Naoki Watanabe, and Masaru Tsukada

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Development of integrated GUI for SPM simulator

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Computational insights into nanotribology: Antimony on HOPG

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Simulation NC-AFM Imaging and Contrast Change on Cu(111) Surface

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DFT analysis of combined 3D NC-AFM and STM imaging of Cu(100)-O

Milica Todorović, Mehmet Z. Baykara, Harry Mönig, Todd C. Schwendemann, Eric I. Altman, Udo D. Schwarz, and Rubén Pérez

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Classical Force Field AFM Simulator

Kazuma Tsutsumi, Mamoru Shimizu, Syuji Shinohara, Akira Masago, Naoki Hashimoto, and Hiroo Azuma

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P.II-56

Molecular dynamics at tip-water-surface junctions

Matthew Watkins and Alexander L. Shluger

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Acquisition of Tip-Sample Dissipation Models through Spectral Inversion

Jeffrey C. Williams and Santiago D. Solares

Post-Deadline

P.II-58

In-situ AFM for catalysis research at high pressures and temperatures

S.B. Roobol, M.E. Cañas-Ventura, C.T. Herbschleb, Q. Liu, V. Navarro, J.W. Bakker, I. Taminiau, W. G. Onderwaater, P. C. van der Tuijn, R. C. T. Koehler, A. Ofitserov, G. J. C. van Baarle and J. W. M. Frenken

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Measurement of atomic-scale potential variations near a LiF step

S. Kawai, F. Federici Canova, Th. Glatzel, A. S. Foster, and E. Meyer

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ORAL ABSTRACTS

Probing of complex Solid-liquid Interfaces with AM-AFM

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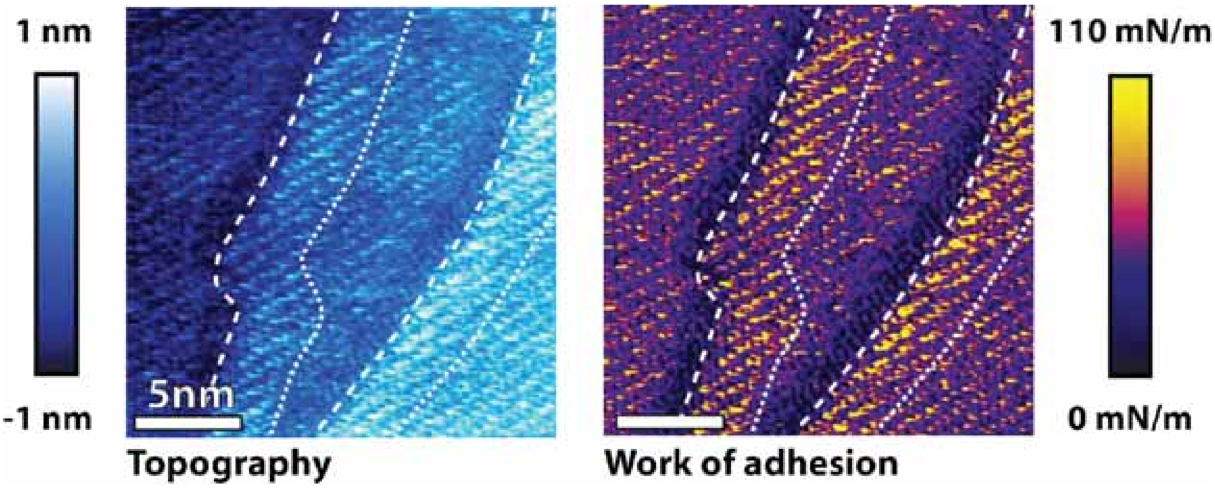
Solid-liquid interfaces (SLIs) occupy a central role in many phenomena from surface electrochemistry to heterogeneous catalysis, wetting, heat transfer, protein functions and self-assembly processes. SLIs are often investigated using diffraction techniques and the interfacial energy quantified with contact-angle measurements. At the molecular level, however, solid-liquid interfaces can be very complex, for example if the surface of the solid is composed of nanoscale domains presenting different structural and chemical properties. This complexity renders any quantification of the SLI particularly challenging with current experimental approaches. Yet it is precisely these minute local variations of the interface that give rise to the most intriguing phenomena: the function of proteins, the toxicity of nanoparticles or the preferential adsorption of a particular molecule.

Here we present investigations carried out with amplitude modulation atomic-force microscopy (AM-AFM) at SLIs exhibiting different levels of complexity from single crystals [1] to 3D mixed self-assembled monolayers forming structure on the surface of gold nanoparticles [2-4]. The results provide subnanometer-level insights into these interfaces, revealing local singularities and defects often with atomic- or molecular-level resolution. We show how the interfacial liquid can be effectively exploited to enhance the imaging resolution and derive quantitative information about the local solid-liquid work of adhesion. The figure below illustrates such a measurement of a wetting anomaly at calcite steps imaged in water.



[1] K. Voitchovsky, J. Kuna, F. Stellacci, et al., Nature Nanotechnology, 5, (6), (2010)
[2] A. Jackson, F. Stellacci, et al., Nature Materials, 3, (5), (2004)
[3] A. Verma, F. Stellacci, et al., Nature Materials, 7, (7), (2008)
[4] J. Kuna, K. Voitchovsky, F. Stellacci et al., Nature Materials, 8, (10), (2009)

Atomic point-defect resolution in liquids with amplitude modulation AFM

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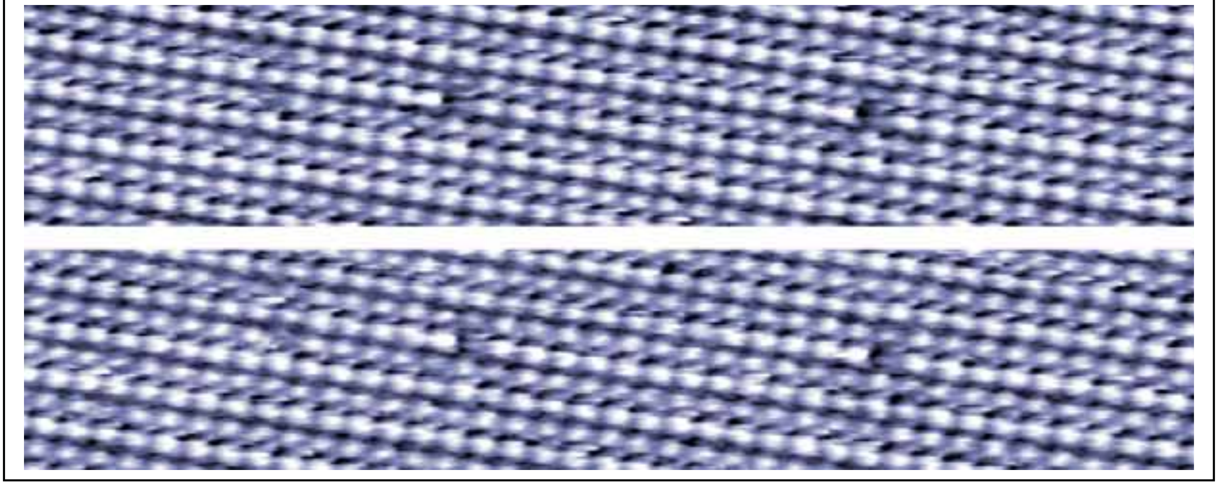
During the last fifteen years, most of the AFM research efforts achieving true atomic resolution have been made in ultra-high vacuum using frequency modulation AFM (FM-AFM). In the past several years, there has been a resurgence of true atomic resolution work in liquids, much of it also done using FM-AFM[1][2].

While the FM results have been and continue to be impressive, amplitude modulation (AM, also known as tapping or non-contact) imaging has several advantages. These include a greatly simplified feedback scheme, wherein there is a single feedback loop running rather than the three typically used in FM imaging. Adjusting the gains of the three independent feedback loops has been a barrier to widespread usability of FM. Additionally, dissipation imaging in FM may suffer from crosstalk between the conservative and dissipative channels because of spurious resonances in the cantilever actuation. Since AM imaging is performed at a constant frequency, this crosstalk is substantially reduced.

In this work, we present true atomic resolution images of the cleavage plane of calcite ($CaCO_3$) in water using AM-AFM. We are regularly resolving atomic-scale point defects, both in the form of what appear to be adatoms as well as vacancies (see figure). Additionally, the surface structure we observe is not consistent with the bulk termination of the calcite crystal, suggesting either some surface reconstruction or an ordered hydration layer.

We will discuss several improvements that make this imaging possible including smaller cantilevers, an improved optical detection scheme that allows high SNR measurements of small cantilever amplitudes, and a stable, noise-rejecting microscope design.

[1] T Fukuma, Y Ueda, S Yoshioka, H Asakawa, Phys. Rev. Lett., 104, 016101 (2010)
[2] T Fukuma, MJ Higgins, SP Jarvis. Biophys. J., 92 (10), (2007)



Symp-03

Molecular-scale Investigations of Monoclonal Antibodies in Liquids by FM-AFM

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Recent progress in high-resolution frequency modulation atomic force microscopy (FM-AFM) in liquid environments has opened a new way to directly investigate *in vivo* biological processes at a submolecular resolution. We recently succeeded in imaging the fine structures of a double-stranded DNA in an aqueous solution by FM-AFM, clearly resolving the individual phosphate groups arranged along the sugar-phosphate backbones[1]. In this study, high-resolution imaging of monoclonal antibodies in liquids was conducted toward the molecular-scale analysis of antigen-antibody reactions, which play essential roles in the biological immune system.

We used a low-thermal-drift FM-AFM based on a commercial AFM apparatus (Shimadzu SPM-9600) with home-built low-noise electronics and a controller. Figure 1(a) shows an FM-AFM image of mouse immunoglobulin G (IgG) monoclonal antibodies adsorbed onto a mica surface obtained in a buffer solution containing 50 mM $MgCl_2$. It revealed that the IgG molecules formed into flower-shaped hexameric assemblies making a two-dimensional (2D) crystal. A schematic model of the 2D crystal structure of the monoclonal IgG molecules is shown in Fig. 1(b). It is based on the assumption that the 2D crystal is formed by isologous interactions of Fab (antigen binding) and Fc (crystallizable) fragments. Although previous studies by electron microscopy also reported the 2D crystal formation of the IgG antibodies by depositing them onto an artificial antigenic surface[2], our results demonstrated for the first time that the monoclonal IgG molecules were assembled into the 2D crystals in the electrolyte solution without any antigen molecules.

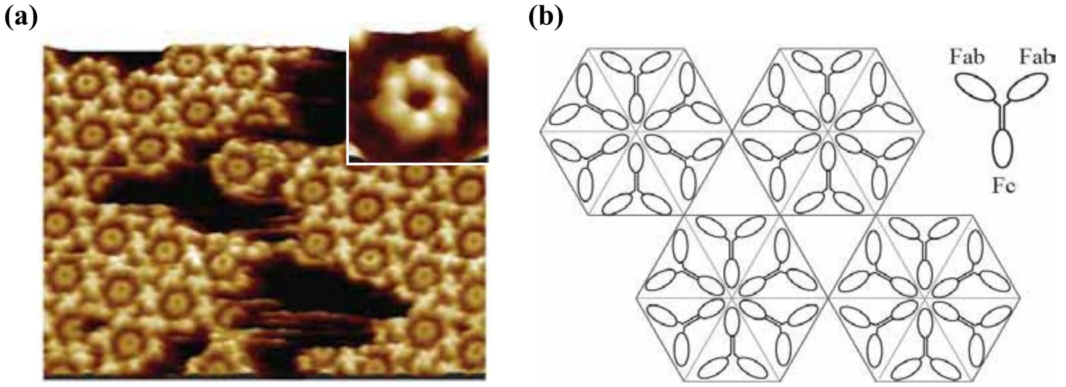

Figure 1(a) FM-AFM image showing 2D crystals of monoclonal antibody (IgG) molecules (50 mM $MgCl_2$, image size: 214 nm × 165 nm). Inset: magnified image of a hexamer of Fc fragments (50 mM $MgCl_2$, image size: 17 nm × 17 nm). **(b)** Schematic model of 2D crystals of IgG molecules.

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[2] E. E. Uzgiris and R. D. Kornberg, *Nature* **301,** 125-129 (1983).

Advances in bimodal AFM imaging of molecules in liquid

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[2] Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid,
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Improving spatial resolution, data acquisition times and material properties imaging are some long established goals in atomic force microscopy (AFM). Currently, the most promising approaches to reach those goals involve the excitation and detection of several frequencies of the tip's oscillation. Usually those frequencies are associated with either the higher harmonics of the oscillation or the eigenmodes of the cantilever. **Bimodal AFM** is an emerging **multifrequency** technique that is characterized by a high signal-to-noise ratio and the versatility to measure simultaneously different forces. The method is also compatible with molecular resolution imaging under the application of **sub-50 pN** peak forces.

Here we will show recent advances in the development of **bimodal force microscopy** for **molecular resolution** imaging **biomolecules in liquid** as well as the three dimensional mapping **of water layers** adsorbed on **proteins**. I will also show some bimodal AFM applications to map simultaneously different interactions such as **mechanical**, **electrical** or **magnetic** interactions. In the presentation I will also discuss the theoretical framework of bimodal AFM operation.

[1] D. Martinez-Martin, E.T. Herruzo, C. Dietz, J. Gomez-Herrero, and R. Garcia, Noninvasive protein structural flexibility mapping by bimodal dynamic force microscopy, *Phys. Rev. Lett.* **106**, 198101 (2011).
[2] C. Dietz, E.T. Herruzo, J.R. Lozano, and R. Garcia, Nanomechanical coupling enables detection and imaging of 5 nm superparamagnetic particles in liquid, *Nanotechnology* **22**, 125708 (2011).
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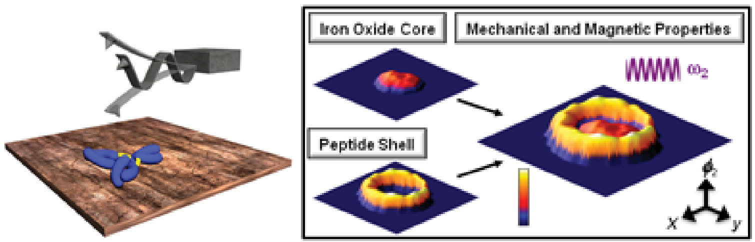

Figure 1. Scheme of bimodal AFM operation (left panel). Imaging the magnetic core of ferritn with sub-5 nm spatial resolution in liquid.

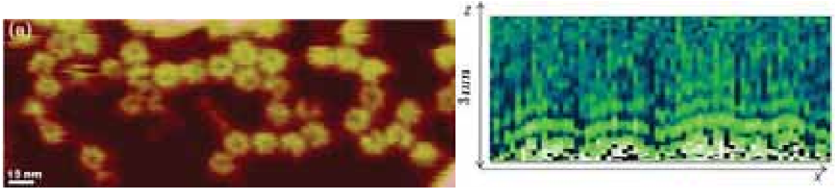

Figure 2. Bimodal AFM imaging of an array of GroEL proteins and the 3D mapping of the water layers on them.

Applications of three-dimensional force mapping method to imaging of biological samples with large structures in liquids

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Frequency modulation atomic force microscopy (FM-AFM) is capable of imaging biological samples with sub-nanometer resolution even in physiological environments. However, for further biological applications imaging of samples with large height variations is required. Three-dimensional (3D) force mapping method is a powerful tool for visualizing hydration structures formed on various solid surfaces such as muscovite mica. High-resolution topographic images can be also obtained by this technique, where the fast tip scanning direction is normal to the surface (Z-scan). Since the major problem in imaging of large structures is an accidental tip collision with large-height side walls of the structures during the horizontal tip scan, the imaging method using the vertical tip scan is extremely useful. In this study we applied the 3D force mapping method to imaging of biological samples with relatively large structures. The Z-scan range in the force mapping method has to be sufficiently expanded according to the thickness of a sample to be investigated.

A low-thermal-drift FM-AFM based on a commercial AFM apparatus (Shimadzu SPM-9600) with a home-built low-noise controller was used for the force mapping measurement. Fibrillar collagens were used in this study. Collagen is the main component of connective tissue in mammals. Although there have been a large number of AFM studies on collagen fibrils, high-resolution FM-AFM imaging of the collagens has not been conducted yet due to their relatively large outer diameters. Collagen fibrils were deposited on a muscovite mica and the force data was acquired in 0.1 M PBS (pH 7.6) with a Si cantilever (PPP-NCH-AuD, Nanosensors). Figure 1 shows an image of a collagen fibril reconstructed from the 3D force mapping data. This image corresponds to a constant frequency shift image in FM-AFM.

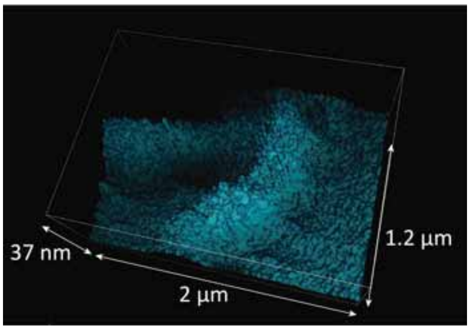

Fig. 1: Collagen fibril reconstructed from the 3D force mapping data.

Force spectroscopy on DNA and amyloid fibrils by means of FM-AFM

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In our research, we perform high resolution imaging and force spectroscopy measurements to study biological samples. Strong interaction of the AFM tip with the sample (as in contact mode AFM) can be invasive for soft samples. The choice of appropriate substrates and the implementation of tapping mode AFM are crucial starting points to obtain any good result in this field of research. We are currently interested in double stranded (ds) DNA and amyloid fibrils, and we perform our measurements by means of FM-AFM. Samples are observed at room and low temperature (RT and LT), in ultra-high vacuum (UHV), and deposited either with Mg^{2+} on mica or on 3-aminopropyltriethoxysilane (APTES) modified mica substrates.

The periodicity and the right-handed chirality of the DNA double helix have been shown by AFM [1,2], but the ultimate sub-molecular resolution is still lacking. Several polymorphisms of DNA have been determined through diffraction measurements on DNA crystals and their structures are well known. We would like to take advantage of AFM to get not only the information about DNA topography, but also the tip-sample interaction forces. The goal would be a better understanding of the mechanisms leading ligands to bind DNA in correspondence of specific DNA sequences, or to explain their minor/major groove binding preference. Other applications could be the DNA sequencing and the study of DNA conformation changes in extreme environments.

Our data shows that with flexible samples such as DNA the substrate flatness is a critical and often limiting factor in obtaining atomic-level resolution. It also must be considered that DNA structure can be influenced by the interaction with the substrate on which molecules are fixed. Our non contact topographic images of DNA in UHV show periodical variations reminiscent of the right handed double helix.

Frequency shift vs. distance curves can be acquired in proximity of the sample surface and converted in force curves [3]. We have measured the reproducibility of the force measurements on different kinds of substrate and along DNA molecules. Force variations along specific directions and force volumes have been acquired. In a statistically significant number of cases, we found a correlation between the force variation and the predicted DNA structure.

Because of its well known and relatively simple structure, DNA is a good proof-of-principle sample demonstrating what can be done on biological samples with non contact AFM. We are presently working on amyloid fibrils, using the same technique and methodology to explain the fibril formation patterns.

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Microsecond-Timescale Biomolecular Interactions Probed by Dynamic AFM

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Biological systems harness mechanical phenomena to serve critical functions at the molecular, cellular, and organismic levels. Beyond the variety in length scales, the mechanical processes are enriched further by the broad range of time scales involved. We have developed AFM based techniques to access forces and displacements on the nanoscale with a temporal resolution around one microsecond. This rapid interface to biological systems allows probing single-molecule interactions with short lifetimes [1], measuring flexibility of proteins that is facilitating conformational changes [2], and visualizing mechanics of live cells with high spatial resolution.

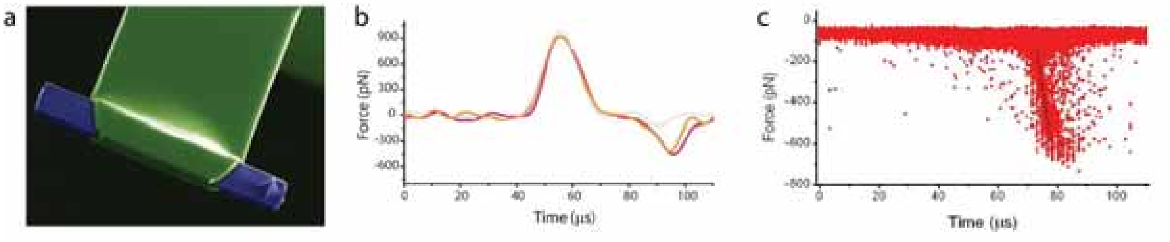

Figure 1. Rapid single-molecule interactions in the tapping mode. (a) Electron microscopy image of a T-shaped cantilever designed for single molecule experiments. (b) Examples of measured tip-sample force waveforms showing unbinding events of biotin and streptavidin using a 7 nm long PEG spacer. A force waveform recorded in the absence of streptavidin is given in light grey. (c) A scatter plot formed by the lowest points of 10^5 force waveforms. The times of unbinding events are determined mainly by the spacer length and vibration amplitude.

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Symp-08

Hydration to Hydrophilic Monolayers Visualized by FM-AFM

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Self-assembled monolayers of mercaptoundecanol (OH-SAM) and mercaptoundecanoic acid (COOH-SAM) were immersed in an aqueous KCl solution and observed with a modified Shimadzu SPM9600 microscope. The shift of resonance frequency (Δf) was determined over the monolayers as a function of the vertical *and* lateral coordinates. We found Δf modulations caused by uneven density distribution of water molecules hydrogen-bonded to the monolayers. Water distribution was enhanced over the topographic grooves of OH-SAM, as opposed to over the protrusions of COOH-SAM. The different distributions are interpreted by the different numbers of oxygen atoms in the two endgroups which accept hydrogen bonds.

Figure (a) shows a Δf distribution cross-sectional to OH-SAM. Positive (negative) Δf is shown to be bright (dark). In the bottom of the distribution, protrusions and grooves of the brightest region periodically appeared along the dark trace. The trace represents the topography of OH-SAM and the protrusions are individual OH endgroups. Δf was modulated from the negative to positive at 0.3-0.4 nm above the SAM surface. Modulated regions periodically appeared in the Δf distribution as dark-to-bright changes marked by the dotted lines. Those modulated regions were always present on the topographic grooves. This suggests that the water density was modulated from low to high in the regions between adjacent OH endgroups. Based on this argument, we propose a possible local structure as illustrated in Fig. (b). Water molecules are hydrogen-bonded to adjacent OH endgroups in a bridge form.

Figure (c) shows a Δf distribution on COOH-SAM. The trace in the bottom represents the topography of COOH-SAM with protrusions assignable to individual endgroups deprotonated in the neutral solution. Double layers of Δf-modulated regions were found in the distribution suggesting extended hydrogen-bond networks. First layer of the modulated regions appeared on the topographic protrusions of the surface. This suggests that water molecules sit on top of the deprotonated endgroups. If a water molecule were a hard sphere having lost its chemical nature, it would surely occupy the hollow site on the groove to kill the vacant volume. This was not the case. Each on-top water molecule is probably hydrogen-bonded to two oxygen atoms of a deprotonated endgroup, as illustrated in Fig. (d).

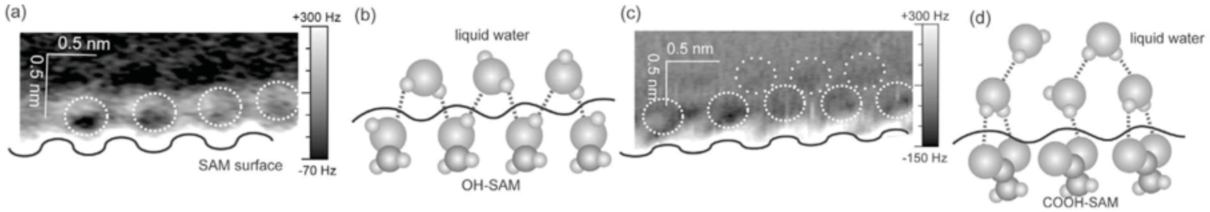

Figure. Two-dimensional Δf distribution over (a) OH-SAM and (c) COOH-SAM immersed in a 50 mM KCl solution. Oscillation amplitude was (a) 0.2 and (b) 0.1 nm. Regions with Δf modulated from the negative to positive are marked by the dotted lines. Possible local structures of water hydrogen-bonded to (c) OH endgroups and (d) deprotonated COOH endgroups are illustrated.

Symp-09

Visualizing Molecular Arrangements at the Surface of Cylindrical Protein Structures by FM-AFM in Liquid

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Liquid-environment frequency modulation atomic force microscopy (FM-AFM) has been used for molecular-scale imaging of various protein structures, including 2D crystals of bacteriorhodopsins, fibrillar structures of amyloid proteins, GroELs fixed on a substrate and sheet-like structures of tubulins. In these examples, proteins at the surface are supported by underlying molecules or a substrate and hence molecular-scale imaging is possible. However, considerable number of protein structures in their native state cannot be imaged in this way. One of the examples is a microtubule having a hollow cylindrical structure where surface molecules (tubulins) are not supported by underlying molecules [Fig. 1(a)]. Although AFM imaging of microtubules have been performed by fixing them on a substrate as shown in Fig. 1(b), detailed molecular arrangements at their surface have not been visualized. This is not necessarily due to the insufficient AFM resolution but due to the large fluctuation of surface molecules that are not directly supported by a substrate. To overcome this limitation, it is critically important to establish a methodology for molecular-scale imaging of biological systems having a hollow structure such as tubes and spheres.

In this study, we perform FM-AFM imaging of microtubules fixed on a substrate in various ways and aim at establishing a model sample that can be imaged with molecular resolution. Our experiments reveal that such a sample can be prepared by increasing the interaction between a microtubule and a substrate using a chemically-modified mica substrate. Although the strong interaction causes deformation of the cylinder structure [Fig. 1(c)], it greatly suppresses the fluctuation of the surface molecules and allows to visualize the molecular arrangement at the surface with unprecedented resolution [Fig. 1(d)]. For example, the repeating units corresponding to αβ-tubulin heterodimers are visualized in real space for the first time [arrows in Fig. 1(d)]. The same methodology should be applicable to other protein structures having a cylindrical or a spherical hollow structure.

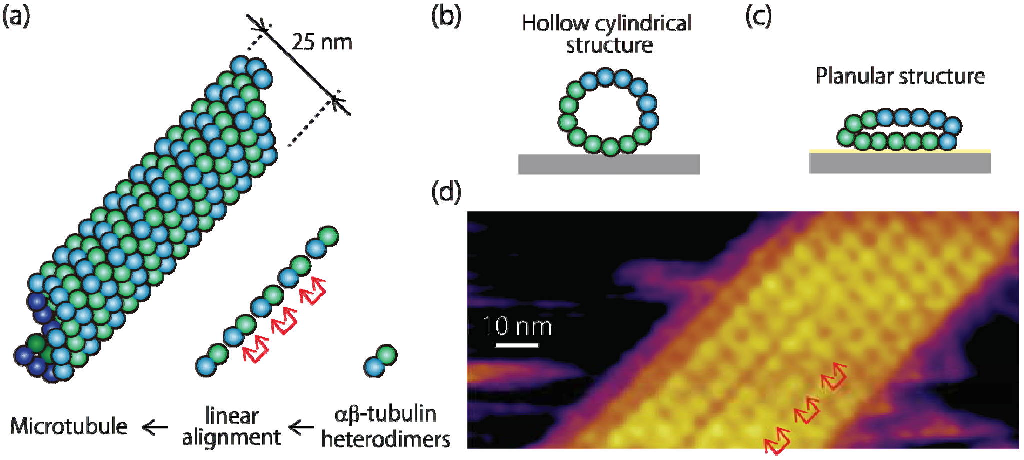

Fig. 1 (a) Structural model of microtubule. (b) and (c) Cross-sectional views of deposited microtubule. (d) FM-AFM image of microtubule with planular structure in liquid.

INVESTIGATION OF MECHANICAL PROPERTIES OF LIVING CELLS BY COMBINED OPTICAL MICROSCOPY AND ATOMIC FORCE MICROSCOPY

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The invasive power of cancer cells is often related to their intrinsic mechanical properties. Atomic Force Microscopy (AFM) has proved itself to be the technique of choice to investigate living cells properties in situ and provide mechanical information in response to various external stimuli. Derivative of tapping mode, the phase signal reflects the energy dissipated between the tip and the sample during each tap on the surface but is a contribution of several factors. Force spectroscopy allows stiffness mapping but suffers from a lack of resolution and a lack of control of the nominal force applied on the sample.

More recently, the combination of most of commercial AFMs with inverted optical microscopy (IOM) techniques, especially epifluorescence, confocal and TIRF, enables easy and straightforward navigation to the location of interest and also displaying both AFM and optical information simultaneously. Moreover, the development of new AFM systems allows the user to gently control the force applied on the sample.

In the first part of this presentation was investigated the effect of two cytoskeleton-disrupting agents, Nocodazole and Latrunculin, on different types of living cells on cell mechanical properties. Actin and tubulin networks were fluorescently labeled. We clearly demonstrate that the drugs induce a specific change in elasticity, which can be correlated to a change in fluorescence signal.

In a second part, we aimed at studying the differences in elasticity between wt glioblastoma cells and cells transfected with different plasmids (including tumor suppressive factors). A clear difference in mechanical properties was observed, which can be directly correlated to a difference in invasive properties.

This type of results may see AFM-IOM combination emerge as a potential diagnosis tool in cancer research.

How can atomic force microscopy help to understand bacterial infections?

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To investigate membrane-based processes being important in inflammation and infectious diseases on the molecular level we use a number of complementary biological and biophysical approaches, in particular atomic force microscopy. The philosophy is on the one hand to reduce the complexity of biological membranes by reconstitution systems allowing to investigate the function of individual molecules as well as of assemblies of molecules and on the other hand to be as close to the biological system as possible to mimic the biologically relevant situation. A prerequisite for our research is the understanding of the structure and function of bacterial membranes and the activity of virulence factors released thereof. Our investigations include the cellular level, i.e. mammalian cells and bacteria, as well as reconstitution systems for biological membranes, i.e. monolayers, liposomes, planar lipid bilayers and solid-supported membranes. These membranes are imaged by atomic force microscopy and by using force spectroscopy binding properties are investigated.

One focus is the membrane interaction of natural and synthetic antimicrobial peptides and proteins (AMP). Bacterial glycolipids function as structural elements and as targets for peptides/proteins of the host´s immune system, in particular of the epithelial defence, and for antibiotics. We investigate the membrane activity of AMPs, mechanisms of resistance of bacterial strains, and synergistic effects of AMPs as well as of classical antibiotics by AFM. We aim at generating new therapeutic peptide-based agents, which are antimicrobial, not cytotoxic, and have the potency to neutralize bacterial virulence factors.

During damage or killing of bacteria virulence factors, such as lipopolysaccharide and lipoproteins, may be released into the circulation and activate immune cells. We investigate the organization and dynamics of the membrane-associated signal transduction mechanisms of human immune cell activation by these bacterial virulence factors. The molecular structures of these play an important role in particular in their AMP-mediated neutralization.

Bacterial adhesion proteins, such as FimH, are important for bacteria to adhere to various surfaces. These interactions depend on the load rate and can only be investigated on the single molecule level by AFM.

Challenges of non-contact AFM biological samples studies

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AFM is a widely used tool in biophysics. Fundamental biological molecules have been studied with AFM such as proteins, DNA, and lipids. However, when applied to biological systems, the resolution of AFM remains relatively limited and is far from atomic resolutions achievable on some non-biological systems. Recent studies have shown that it is possible to obtain atom-resolved images of Pentacene molecules [1] and on the top of single-walled carbon nanotubes [2] at low temperature with dynamic mode AFM. Inspired by these results we set out to verify if non-contact AFM (NC-AFM) can be applied in a similar manner to biological molecules and thus shed new light on some of modern biophysics problems. We decided to focus primarily on DNA and amyloids as they are very resilient biological molecules thought to remain stable over a range of temperatures and pressures. This makes them reasonably good and somewhat rare biological samples well suited for experiments involving techniques such as NC-AFM, where vacuum and low temperature may be essential requirements for successful work. We have a home-built NC-AFM setup that uses commercial cantilevers, is placed in UHV, and that can be cooled to liquid nitrogen or liquid helium temperatures. Since the structure of DNA is relatively simple and well known it appears to be a good proof-of-principle molecule to test the actual capabilities of NC-AFM on bio-molecules. Amyloids are more challenging and interesting as they encompass a variety of different molecular assemblies for many of which mechanisms of formation are still unknown. We are hoping that NC-AFM imaging and force spectroscopy can provide higher resolution structural information that leads to a better understanding of this problem. There are, however, several challenges and open questions concerning the successful implementation of NC-AFM. The first one involves the suitability of NC-AFM and the relevance of the results obtained for real-life processes taking place in physiological environments very different from UHV and low temperature ones required by the technique. Work in UHV on samples that carry surface charge or are zwitter-ionic also poses a challenge, as does the question of eventual hydration of such samples. We will discuss practical issues concerning the way to deal with spatial drifts during measurements that take relatively long time (tens of minutes or more). Finally a discussion of what the optimum way to probe these samples is will be raised, where a comparison of constant height frequency shift images, force maps, and frequency shift feedback images will be made.

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Simulating non-contact AFM imaging of calcite in water

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As a first step towards understanding AFM imaging of complex biosystems in water, we study calcite as a model system. The calcite surface has been studied extensively because of its important role in biomineralization, industrial applications, and as substrate for biomolecule growth and manipulation. Although recent atomically resolved non-contact AFM images of calcite in water [1] resemble those obtained in UHV [2], the imaging mechanism in liquid is more complicated [3], due to the presence of hydration layers around the tip and surface. Displacing these confined water molecules leads to significant entropic contributions to the force on the AFM tip.

In this work, we use molecular dynamics simulations with empirical interaction potentials to study the AFM imaging mechanism of calcite in water. We present two different methods of computing force-distance curves. First, in a quasi-static tip approach, the tip is fixed at a certain position above the surface and the force is obtained from a time average. Second, we use umbrella sampling to calculate the free energy of the system as a continuous function of the tip-surface distance. The force on the tip is then obtained by deriving this free energy profile. In our simulations, the AFM tip apex is modelled as a nanocluster composed either of silica or calcite (see fig. 1), to re-create an oxidized silicon tip, or a tip covered in calcite after initial surface contact. In a final step, the force-distance curves are used to compute AFM images that can be compared to the experimental results.

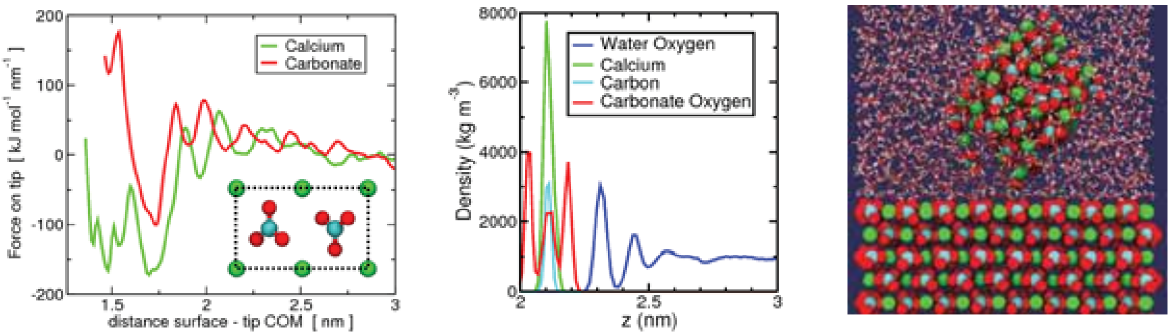

Figure 1: Calcite tip. Force-distance curves over calcium and carbonate groups (left), hydration layers at the calcite-water interface (middle), and snapshot of the simulation (right).

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Imaging of Molecular Recognition at the Nano-Scale

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Atomic force microscopy has developed into an important tool for investigation of biological processes on the molecular and sub-molecular level. In this talk I will focus on two powerful techniques, simultaneous topography and recognition imaging (TREC) and High Speed (HS)- AFM. TREC allows for the investigation of receptor distributions on natural biological surfaces under physiological conditions. Based AFM in combination with a cantilever tip carrying a ligand molecule, it enables to sense topography and recognition of receptor molecules simultaneously with nanometer accuracy . Here, we discuss optimized handling conditions and guide through physical properties of the cantilever-tip-sample ensemble , which is essential for the interpretation of the experimental data gained from this technique. In contrast to conventional AFM methods TREC is based on a more sophisticated feedback loop, which enables to discriminate topographical contributions from recognition events in the AFM cantilever motion. The features of this feedback loop were investigated through a detailed analysis of topography and recognition data obtained on a model protein system. Single avidin molecules immobilized on a mica substrate were imaged with an AFM tip functionalized with a biotinylated IgG. A simple procedure for adjusting the optimal amplitude for TREC imaging is described by exploiting the sharp localization of the TREC signal within a small range of oscillation amplitudes. This procedure can also be used for proving the specificity of the detected receptor-ligand interactions. For understanding and eliminating topographical crosstalk in the recognition images we developed a simple theoretical model, which nicely explains its origin and its dependence on the excitation frequency. Recent developments on tapping mode AFM, conducted in the lab of T. Ando and co-workers (reviewed in) have led to an AFM capable of recording images of 100x100 pixel^2 within 20 ms at sub-nanometer resolution in aqueous solutions. Since the function of proteins is determined by their structure and is generated when changing it dynamically on the time scale of a few tens of milliseconds, this instrument enables for the real-time observation of proteins and other biological specimen ‘at work’. In the second part of this talk I will show applications of this new HS-AFM performed in our lab in Linz. Particularly I will focus on the dynamics of antibodies upon their attachment to various antigenic surfaces, dynamics of 2-dimensional protein-lattices, 2-dimensional protein-diffusion on supported lipid bilayers, and RNA-release from human rhino viruses.

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SPM Technologies past, present ,future

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Nature is the best example of a system functioning on the nanometer scale, where the involved materials, energy consumption and data handling are optimized. Opening the doors to the Nanoworld the emergence of the Scanning Tunneling Microscope 30 years ago in 1981 and the Atomic Force Microscope 25 years ago in 1986 led to a shift of paradigm in the understanding and perception of matter at its most fundamental level. The capability to investigate surfaces with unprecedented atomic resolution in a three-dimensional fashion introduced a wealth of related techniques using probes with local interaction and has been adapted for various environments, such as vacuum, fluidics, ambient, high and low temperatures, magnetic fields etc. In particular AFM , first designed as an instrument to image non- conductive surfaces on the atomic level has surpassed its predecessor in many ways in its wide range of applications. (A reflection)
Concepts in taking AFM technology beyond imaging have already stimulated a number of applications in biology .In recent years we have taken AFM Technology way beyond imaging exploring new frontiers in bio analyses and diagnostics using biochemical cantilever array technology providing a platform applicable in upcoming fields such as system and synthetic biology , bioengineering etc. with far-reaching implications to evaluate treatment response efficacy in personalized and preventive medicine .

Mo-01

Molecular-scale charge distribution at an interface between liquid and surfactant assembly investigated by three-dimensional force mapping

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An electric double layer appears on a charged surface in an electrolyte solution. The surface interaction force in the solution is expressed as the sum of the electrostatic force due to the double layer $F_{\rm DL}$ and the van der Waals force $F_{\rm vdW}$, which is referred to as DLVO (Derjaguin, Landau, Verwey and Overbeek) force $F_{\rm DLVO}$, *i.e.*,

$$F_{\rm DLVO} = F_{\rm DL} + F_{\rm vdW} = C[2\sigma_S\sigma_T \exp(-d/\lambda_D) + (\sigma_S{}^2 + \sigma_T{}^2)\exp(-2d/\lambda_D)] + F_{\rm vdW}$$

where C, σ_S, σ_T, λ_D and d are constant, a surface charge density of sample, a surface charge density of tip, double layer thickness (Debye length) and probe-to-surface distance, respectively. Both σ_S and λ_D are obtained from the DLVO force measurement, which has been mainly performed using a surface force apparatus or a colloidal probe AFM. We recently succeeded in molecular-scale hydration measurement on a mica surface by three-dimensional (3D) force mapping method based on FM-AFM[1]. In this study, we applied the 3D force mapping method to the molecular-scale investigations of the DLVO force on a self-assembled structure of surfactant molecules, SDS (sodium dodecyl sulfate), at a solid-liquid interface.

Figure 1 shows a 3D representation of the frequency shift spatial map obtained near the interface between SDS-aqueous solution and a graphite surface. Hemicylindrical assembled structures of the SDS molecules are clearly visualized. A two-dimensional force distribution across the hemicylinders is shown in Fig. 2(a), where a broken line is a surface of the hemicylinders. We successfully obtained the molecular-scale distributions of both surface charge density and Debye length on the hemicylindrical molecular assembly, as shown in Figs 2 (b) and (c), by fitting the force map data to the DLVO theory.

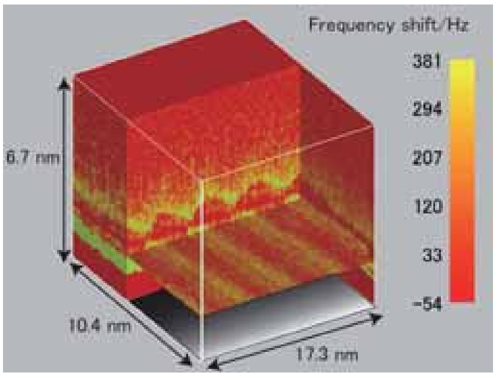

Figure 1: 3D representation of the frequency shift spatial map at the interface between SDS aqueous solution and a graphite surface.

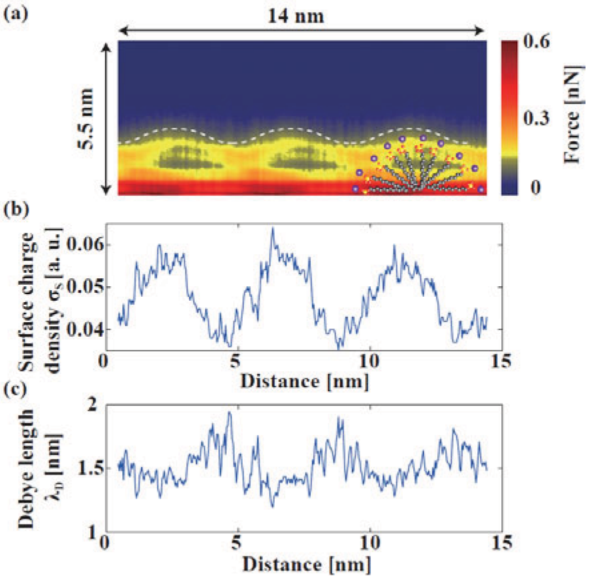

Figure 2: (a) 2D force distribution at the SDS aqueous solution-graphite interface. (b) Surface charge density distribution. (c) Debye length distribution.

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Mo-02

Two-dimensional growth of nanoclusters and molecules on Suzuki surfaces

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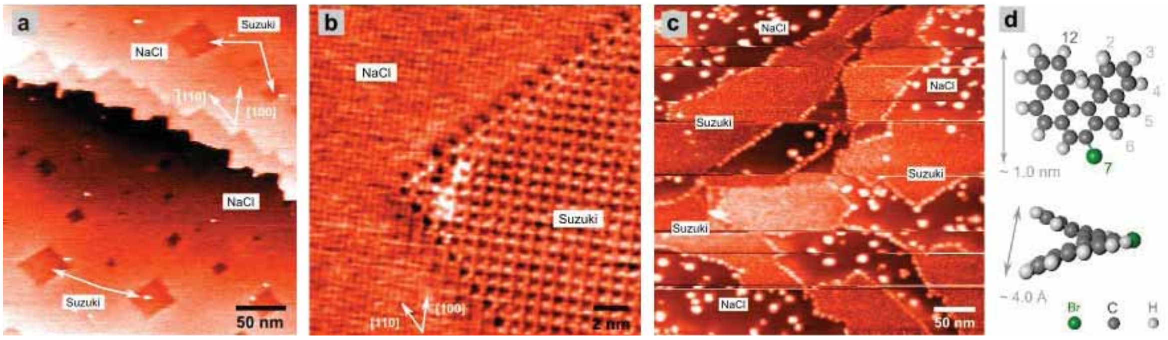
Patterned surfaces are used for confining the growth of molecules and clusters into nanostructured surface regions, which finds nowadays many applications in nanotechnology. In this contribution it is shown that the nanopatterned surface of Cd doped NaCl crystals [1] (*Suzuki surface*) can be used to confine the growth of palladium clusters and functionalized brominated pentahelicene molecules [2] into the Suzuki regions of the surface. It is shown that especially the combination of noncontact AFM (nc-AFM) and Kelvin probe force microscopy (KPFM) in ultra-high vacuum (UHV) greatly helps in the characterization of the structure and morphology but also the electrostatics of the considered surfaces [3].
The growth of palladium onto the Suzuki surface results into nanometre sized clusters, which form two-dimensional cluster arrays inside the Suzuki regions. The clusters exhibit a high cluster density, are uniform in size, and due to the specific Suzuki structure the clusters are polarized or charged. Brominated pentahelicene molecules perfectly decorate the Suzuki regions and form two-dimensional islands whereas no molecules can be found inside the pure NaCl regions. The molecules are in a flat configuration, which finds strong support from first principle calculations. Due to the specific adsorption of the molecules, the surface dipole of the Suzuki regions is modified by the molecules. It is shown that changing the functional group of the helicene molecules leads to different adsorption characteristics, self-assembly phenomena and different surface dipoles [4].



(a) The Suzuki surface is composed by regions of pure NaCl and regions, which contain the impurities and vacancies (Suzuki regions). (b) The interface NaCl-Suzuki is well-defined at the atomic scale. (c) Pd clusters can be found almost only in Suzuki regions. (d) Structure of the functionalized helicene molecules used for the experiments.

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NC-AFM Tip & Surface Species Identification on Oxidized Cu(110)

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Our research has shown, both theoretically and experimentally, that when imaging the oxidized Cu(110) surface with an NC-AFM tip, it is possible to both distinguish and identify the surface atomic species and to characterize the tip apex.

From experimental results it has been suggested that, when performing NC-AFM imaging on Cu(110)/O surfaces with what is believed to be a copper terminated tip, only copper atoms are imaged and likewise with oxygen terminated tips imaging only oxygen atoms, whereas silicon terminated tips image both. Due to the arrangement of the copper atoms on the surfaces being markedly different from that of the oxygen atoms (Fig. 1), it is possible to distinguish and identify both surface copper atoms from surface oxygen atoms as well as copper terminated tips from oxygen terminated tips. Most excitingly, it is possible to manipulate the ‘super Cu’ atoms (cf Fig. 1, right) with atomic precision.

Interestingly, our theoretical results indicate that two tips do in fact only image either one surface species or the other due to the relative strengths of the chemical bonds forming. Note that this system is unique in a sense that there’s a clear-cut difference between the two tip terminations when imaging; this allows for theory, when modelling atomic manipulation, to narrow down the possible tip models to just two and hence perform simulations knowing that the correct tip model was used.

So we discuss here both the nature of tip-surface forces for both copper and oxygen terminated tips above Cu(110)/O copper and oxygen surface sites and the nature of the transitions that occur during manipulation. In all instances the DFT method is implemented with the VASP code, using a plane wave basis set and the GGA Perdew-Burke-Ernzerhof (PBE).

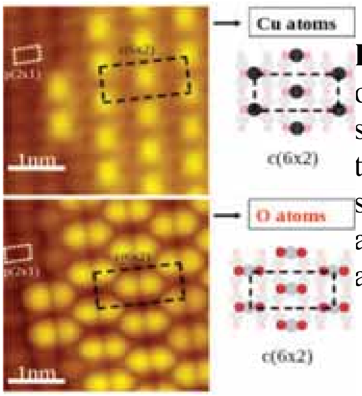
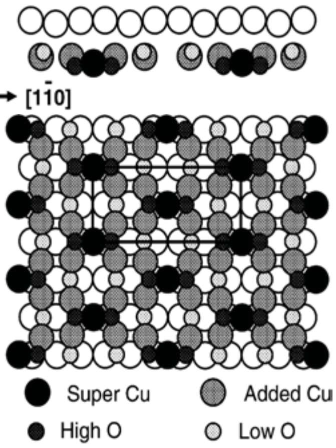


Fig. 1 - left: Two NC-AFM images of the same region of Cu(110)/O surface by two different tip terminations (Cu & O) with schematic on the left. [1]. **Right**: Plan and side view of the c(6x2) atomic arrangement based on [2,3].



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Mo-04

Resolving the Atomic Structure of Amorphous Silica

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The atomic-scale structure of amorphous solids is one of the key unsolved problems in physics [1]. Amorphous silica is important for many technological applications. An ultrathin silica film serves as a model system for catalysis [2]. In this study, we investigated a double layer film of amorphous silica on Ru(0001).

To study the atomic structure, we simultaneously applied frequency modulated dynamic force microscopy (FM-DFM) and scanning tunnelling microscopy (STM) using a tuning fork sensor. All experiments were performed at low temperature in ultra-high vacuum.

In 1932, Zachariasen postulated the structure of vitreous silica [3] consisting of a polygon network of corner sharing SiO_4-tetrahedra. We observe the same network on the thin silica film. Figures (a) and (b) represent one constant height measurement; (a) is a map of the tunnelling current (I_T) and (b) is a map of the frequency shift (Δf), which were both acquired synchronously. Both signals are completely disentangled thanks to a separate I_T-wire attached to the tuning fork tip. Fig. (c) presents a three dimensional frequency shift plot, $\Delta f(x,z)$, along a line. Evaluating such 3D-spectroscopy data can provide information on the image contrast mechanism [4].

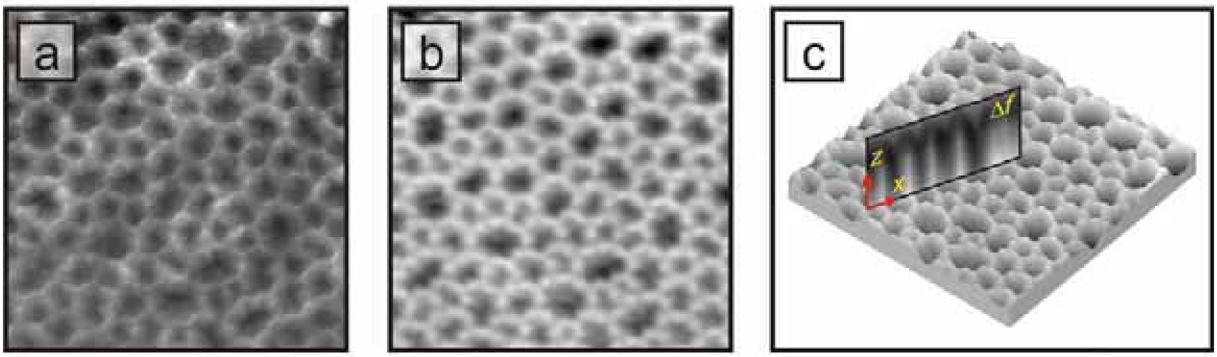

Fig.: (a and b) Constant height image, scan range 5×5 nm², bias voltage 100 mV. (a) Map of the tunnelling current. (b) Map of the frequency shift. (c) 3D-spectroscopy $\Delta f(x,z)$ along a line.

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Mo-05

NC-AFM experiments and atomistic simulations of the surface structure and defects on the $MgAl_2O_4$ (100) surface

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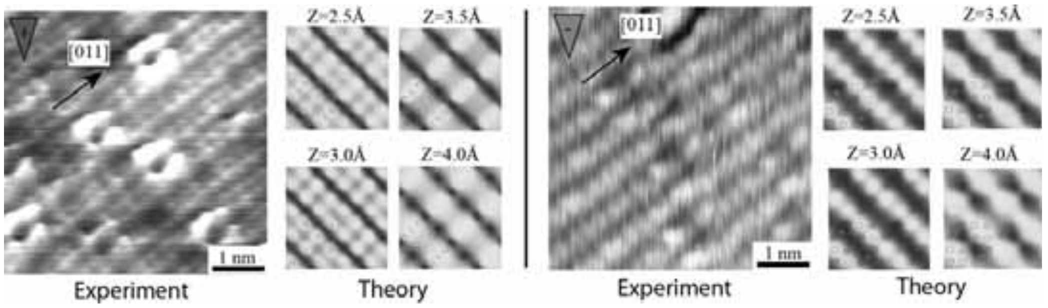
Magnesium aluminate ($MgAl_2O_4$) is a ternary metal oxide with the prototypical *spinel* structure, and it is an important material in many applications as a refractory ceramic, catalyst support or fuel cell membrane. Its crystal structure defines a larger group of so-called spinal minerals which adopt the general formula $A^{2+}B_2^{3+}O_4^{2-}$. However, previous experimental studies have not been able to provide insight on the atomic structure of the surface of $MgAl_2O_4$. Very recently, it was possible in interplay between NC-AFM and surface x-ray diffraction (SXRD) experiment together with density functional theory calculations and NC-AFM simulations to reveal the first atomistic model of the surface structure and the prevalent defect types on this metal oxide [1]. The key insight was provided by NC-AFM, which gave complementary atom-resolved images recorded with positive or negative tip polarizations revealing the structure of the sublattices defined by the surface O atoms and Al or Mg atoms respectively (see Figure). Here we present further NC-AFM experiment and DFT-based simulations of $MgAl_2O_4(100)$ in order to investigate fundamental details of the NC-AFM image contrast formation of the $MgAl_2O_4(100)$ surface structures and the defects that may exist on this surface. Specifically, by analyzing calculated force distance curves, and comparing with experiment we address the importance of the imaging distance and the atomistic nature of the tip termination. Based on detailed force-distance calculations we show that it is possible to discriminate between Al^{3+}, Mg^{2+} species in so-called antisites defects and cation vacancies located in the surface due to their different force interactions with a charged tip. Furthermore, the simulations allow us to address the NC-AFM signatures associated with hydrogen, which is expected to be present as OH (hydroxyl) groups on the $MgAl_2O_4$ surface even under very good UHV conditions.



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Mo-06

Step structures on $CeO_2(111)$ identified by NC-AFM and KPFM

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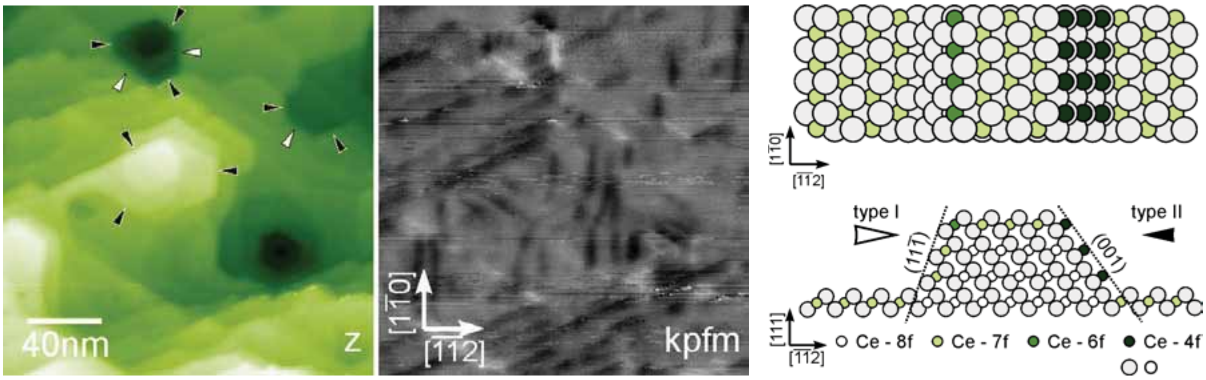
The morphology and charge state of step edges on the $CeO_2(111)$ surface is investigated by non-contact atomic force microscopy (NC-AFM) and Kelvin probe force microscopy (KPFM). The surface is prepared by cycles of sputtering and annealing at 1200 K to produce a terraced surface with equilibrium step structures. Step edges are preferably aligned with <110> directions, resulting in hexagons as the dominating motif of surface morphology. As illustrated in the sketch below, any mesa (or pit) on the surface is terminated by alternating ledges of type I and type II that result from the fluorite crystal structure of ceria. Although, NC-AFM imaging reveals the direction, straightness and perfection of the steps down to the atomic level [1], it is most difficult to identify details of the atomic structure of the step sides. Based on additional evidence from KPFM studies, we propose a model for type II steps where oxygen is released from the (001) facet while cerium remains what effectively results in a surface reduction. To maintain overall charge neutrality, it is assumed that electrons localise at Ce^{3+} ions that occupy low coordinated sites on the step sides [2]. This results in a polarity of the step edges that is predicted to have a finite value for all type I steps while it should increase with step size for type II steps. This proposition is corroborated by our KPFM studies yielding a strong positive charge for type II steps with a height of more than one triple-layer but only slightly negatively charged type I steps. Models for the distribution of charges in the vicinity of the step edges and the origin of the KPFM signals are discussed.



Left panels: NC-AFM and KPFM images of a $CeO_2(111)$ surface. The contrast from dark to bright represents low to high in topography and positive to negative potential for the KPFM signal. Right panels: Models for type I and type II steps on the fluorite (111) surface.

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Atom-Specific Interaction Quantification and Identification by 3D-SPM

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Entire scientific disciplines such as mechanics and chemistry are governed by the interactions between atoms and molecules. On surfaces, forces extending into the vacuum direct the behavior of many scientifically and technologically important phenomena such as corrosion, adhesion, thin film growth, nanotribology, and surface catalysis. To advance our knowledge of the fundamentals governing these topics, it is desirable to simultaneously map electron densities and quantify force interactions between the surface of interest and a probe with atomic resolution. For example, in the case of a catalytically active surface, this would allow studying the role and effectiveness of surface defects such as vacancies, steps, kinks, impurities, and domain boundaries as active sites. An ability to discriminate between different chemical species on the sample surface would offer further insight.

Using the oxygen-reconstructed copper (100) surface as a model system, we demonstrate that much of this information can be derived from combining three-dimensional atomic force microscopy (3D-AFM) [1,2] with simultaneous scanning tunneling microscopy. Thereby, we make use of the fact that the three-dimensional scanning probe microscopy (3D-SPM) variant resulting from this combination provides complementary information in the various interaction channels recorded. The surface oxide layer of copper (100) features defects and a distinct structure of the Cu and O sublattices that is ideally suited for such model investigations. 3D-SPM data sets enable site-specific quantification of force interactions and tunneling currents, with drastically different types of contrast in simultaneously recorded data channels. To further validate the experimental results, DFT total-energy calculations and Non-equilibrium Green's Function (NEGF) methods for electronic transport have been used to determine the force interaction and the tunneling current [3-5] for a large set of tip models. The analysis of our experimental results allows for the identification of atomic species and defects on the sample surface through the comparison of simultaneously recorded force and current data, as well as the study of defect-induced stress fields and their influence on local chemical reactivity and topographical deformation.

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Tu-02

Conservative and Dissipative Tip-Molecule Interactions: Force Spectroscopy Investigations on an Organic Adsorbate

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Non-contact atomic force microscopy is an ideal tool to study structural and mechanical properties of organic layers on solid substrates, which are for instance of high relevance for nanoelectronic applications. However, the image contrast mechanisms in high resolution surface scans and also the processes leading to energy dissipation on organic layers are still under discussion. In previous work [1], we successfully used force field spectroscopy to analyze conservative tip-sample interactions leading to submolecular features in nc AFM topography images of 3,4,9,10-perylenetetra-carboxylic-dianhydride (PTCDA) on Cu(111) [2]. Here, we present force field spectroscopy investigations of PTCDA adsorbed on Ag(111) where we studied not only conservative but also dissipative interactions. From these measurements, we extracted force and dissipation spectroscopy curves that can be assigned to different areas within the molecules. Based on the results, we are able to identify systematic differences in the tip-sample interactions between end groups and the center of the molecules (see figure). The results are interpreted based on ab-initio simulations of the PTCDA/Ag system, giving new insight into the molecular dissipation mechanisms.

In addition to the experiments described above, which were performed at room temperature, we present first results of 3D force field spectroscopy investigations of the same sample system obtained with a new low temperature AFM.

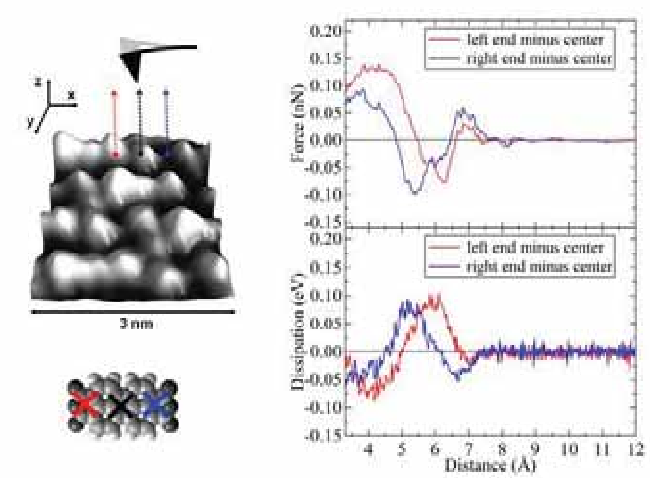

Figure 1: Site-specific tip-sample force and dissipation on PTCDA

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Tu-03

NC-AFM and Force spectroscopy applied to H terminated Si(111)7x7

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Force spectroscopic techniques developed on nc-AFM can be powerful to clarify electronic structures with atomic resolution. The atomic scale change in force between a tip and a sample is dominated by the chemical interaction between a sample surface atom and a tip apex atom. It is, however, still difficult to apply them to various samples, because the force depends on experimental parameters including the tip-sample separation and bias voltage to be optimized and the electronic states of a tip seriously. To elucidate the techniques, chemical modifications of surface atoms that changes the electronic states is of great interest as tests; hydrogen termination of silicon is one of them, which makes the dangling bonds at surfaces unreactive with no significant atomic configuration. In this study we examine a Si(111)7x7 terminated with atomic hydrogen using nc-AFM and force spectroscopic techniques.

A Si(111)7x7 surface was terminated with atomic hydrogen using an H_2 gas cracker with a W filament. Figure 1(a) and (b) show an nc-AFM image under a constant frequency shift (Δf) and a current image of it, simultaneously observed. Three adatoms in a faulted half, one corner and two center adatoms in region A, are depicted brighter than three adatoms in region B. The atoms in region B have larger current than those in region A; this is attributed to the closer tip-sample separation in region B than in region A in the mode of constant Δf. Consequently, the electric conductance in region B is probably of the same order of magnitude in comparison of that in region A. On the other hand, adatoms in region C of the faulted half are depicted darker in the nc-AFM image, and lower current than those in region A and B. According to ref. 1, the adatoms in region A and B are not terminated with H, but the rest atom in region A are terminated with H, while the adatoms in region C are terminated with H. Although the adatoms in region D have almost no current, depicted darker in the nc-AFM image, partly the current passes over slightly protruded positions different from the adatom sites. In region D adatoms are missing and partly the rest atom layer are observed as the underneath layer of adatoms. Based on the above atomic feature on this surface, we will discuss results of the force spectroscopy to reveal the electronic and chemical properties.

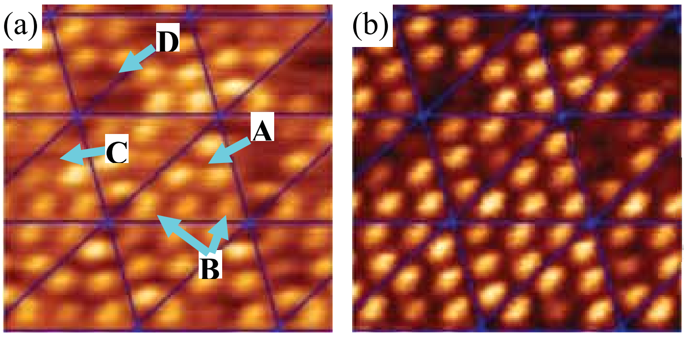
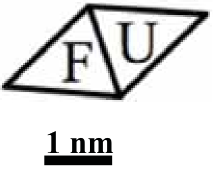


Fig. 1 (a) nc-AFM image of Si(111)7x7-H at a frequency shift of -46 Hz and sample bias of -600 mV., (b) current image obtained simultaneously with (a).



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Tu-04

Quantitative static and dynamic force spectroscopy of atomic-scale forces and energy dissipation

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Dynamic force microscopy has proven to be an invaluable technique for studying and manipulating nanoscale processes at surfaces[1]. In order to gain a more detailed insight into the tip-sample interaction forces and the resultant dissipation, it would be very beneficial to make observations over a single oscillation cycle. However, due to the narrow measurement bandwidth, a measurement of individual force curve upon tip approach-retract is impossible.

Here, we investigate the dissipative interaction in dynamic force spectroscopy as a stochastic tip and/or sample deformation process with a systematic distance dependent measurement of the *quasi-static* tip-sample interaction force at a certain atomic site on NaCl(001) at room temperature[2]. In order to measure the stochastic tip-sample interaction, 21 approach-retraction sweeps with different initial tip-sample distances were repeated 100 times [Fig. 1(a)]. Infrequently observed large and wide hysteresis loops are attributed to the formation and rupture of atomic chains during tip retraction, leading to a large magnitude of energy dissipation. This stochastic interaction is hidden in the averaged approach and retract force curves [Fig. 1(b)]. Frequency shift and energy dissipation for 21 different initial tip-sample distances were calculated by numerical integrations. The computed frequency shift via the measured quasi-static force curves was in good agreement to that measured by dynamic force spectroscopy at the same atomic site with the same tip. Furthermore, the dynamic force curve was extracted via the computed frequency shift [Fig. 1(c)]. We found that the dynamic force differs significantly from the static force because of the hysteresis loop.

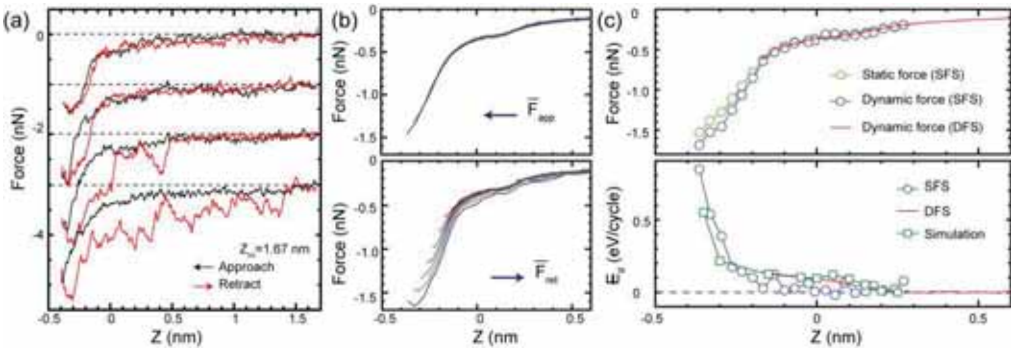

Figure 1: (a) a series of the quasi-static force curves measured at a same atomic site. (b) Averaged distance dependence of force upon approach and retract. (c) Measured static force and extracted dynamic force curves and energy dissipation.

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Tu-05

An atomic contact studied by small amplitude dynamic force microscopy

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Contacts with a NaCl(001) surface were studied in ultra-high vacuum by dynamic force microscopy and spectroscopy at room temperature. The tip-sample separation was controlled by keeping a constant *positive frequency shift* Δf of the second flexural resonance mode of a commercial non-contact silicon cantilever [1]. In contrast to similar measurements with $\Delta f < 0$ and tip oscillation amplitudes $A > 400$ pm [1-2], the contact is not broken, owing to the chosen setpoint. While scanning near $\Delta f = 0$ using an ultra-small oscillation amplitude $A < 50$ pm, the short-range interaction force on the tip apex varies between weak attraction and repulsion. An atomic-scale contact can thus be maintained close to thermal equilibrium and continuously translated, as previously demonstrated with a soft cantilever in quasi-static friction force microscopy (FFM), albeit only slightly before jump-off [3]. The average force on the contact can be continuously tuned by varying Δf on the branch with negative slope with respect to the tip-sample distance.

Compared to non-contact operation (arrows II in fig. 1b), model calculations assuming a 64-ion NaCl tip apex (neglecting relaxation) suggest an improved topographic contrast with reduced noise in this special mode (arrows III in fig. 1c) The measured two-dimensional frequency shift map is consistent with recorded images, while extracted normal and lateral force components suggest growing atomic displacements in both directions with increased Δf. Stick-slip motion, arising from elastic deformations and instabilities along the fast scan direction, is first observed near steps (fig. 2), as recently demonstrated in FFM [4]. The occurrence of slips strongly depends on the variable controlling the topography, however. Discrete contact rearrangements occur only at intervals of seconds and are preferentially triggered upon crossing steps, as established in pioneering non-contact investigations [5]. The contact nevertheless typically returns to a particular stable configuration. At higher frequency shifts, such rearrangements become more frequent and irreversible.

Fig. 1: Computed variations of force and topography contrast at representative Δf setpoints (f = 980 kHz, k_{eff} = 1500 N/m, R_{tip} = 10nm)

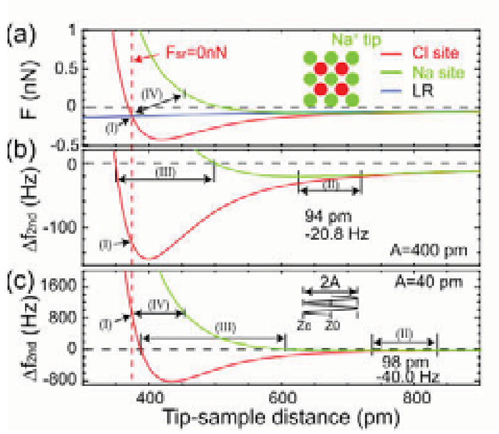
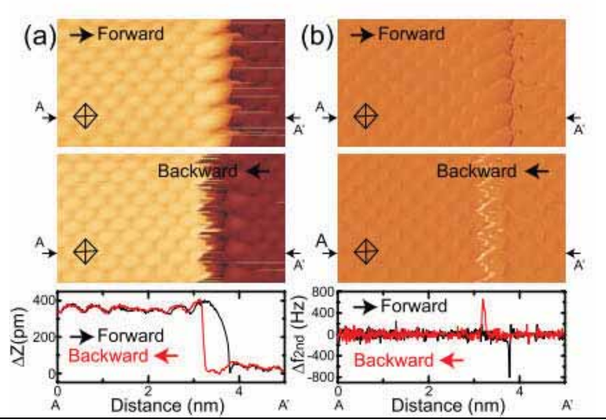


Fig. 2: Topography and Δf error signal recorded across a monatomic step together with profiles revealing slips (f= 978365 Hz, k_{eff} = 1418 N/m, Δf = 0, A = 50 pm)



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Tu-06

Polarization effects and charge state characterization in nc-AFM

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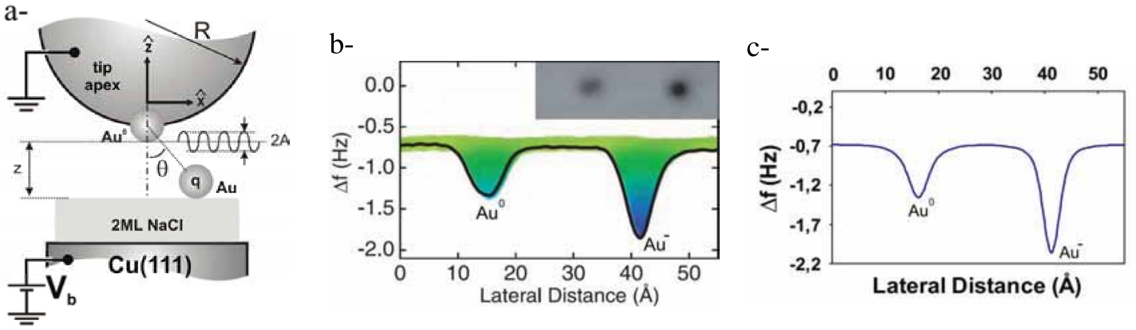
The aim of this work is to discuss the influence of short-range electrostatic forces, so-called dipolar forces, between the tip of an atomic force microscope (AFM) and a surface carrying charged adatoms [1]. Dipolar forces are of microscopic character and have their origin in the polarizability of the foremost atoms on tip and surface. In most experiments performed by noncontact AFM, other forces such as binding forces dominate the interaction. However, in the experiments presented by Gross *et al.* [2], where the charge state of individual gold atoms adsorbed on a thin dielectric layer was determined, binding forces are negligible as the tip-sample distance is relatively large. We have developed a model which mimics the experimental tip-sample geometry of the aforementioned experiments (cf. fig.a below). The model includes van der Waals and long-range electrostatic interactions, as well as the short-range electrostatic interaction based on the self-consistent description of electronic polarization effects on neutral and charged adatoms. The model is based on the calculation of the electrostatic energy of the tip-sample geometry. Our calculations of noncontact AFM imaging as well as of bias spectroscopic curves are in good agreement with the experimental ones presented by Gross *et al.* (cf. figs.b and c below). It is demonstrated that the short-range dipolar force is mainly responsible for the contrast observed in topography imaging above charged species. However, it is the long-range capacitive force which is responsible for the detection of the charge state in bias spectroscopy. The influence of these dipolar forces has recently been confirmed experimentally and theoretically [3], with conclusions that qualitatively match our owns. Implications of our findings on future experiments which aim to detect single charges by means of Kelvin probe force microscopy will be discussed.



a- Geometry of the tip/adatom/thin layer/counter-electrode used in the model. b- Experimental cross section (Δf signal) reported by Gross *et al.* on top of single Au^0 and Au^- adatoms. c- Calculated cross section derived from the model on top of a single Au^0 and on a Au^- adatom. The model fits well to the experimental results.

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Detection of charge state of individual gold nanoparticles with single-electron resolution

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A high force sensitivity of frequency modulation atomic force microscopy (FM-AFM) has enabled the detection of the charge state of individual atoms and quantum dots with single-electron charge resolution by detecting electrostatic force [1,2]. We have shown that a charge detection with FM-AFM can be used as a versatile spectroscopic tool for investigating electronic structure of individual nanometer scale entities such as quantum dots [2-4].

We report the imaging and spectroscopy of the charge state of individual gold colloidal nanoparticles (Au NP) attached onto 1,16-hexadecanedithiol (C16S2) self-assembled monolayer (SAM) formed on a gold substrate (Fig. 1(a)). In this system, the charge state of an Au NP can be changed by the single-electron tunneling through C16S2 SAM which serves as a tunnel barrier. By controlling the tip-substrate bias voltage or the position of the tip, we can control and detect the electric charge stored in individual Au NPs.

Figure 1(b) and (c) show a set of frequency shift and dissipation images simultaneously taken at 4.5 K with a constant-height scan above a few Au NPs with a mean diameter of 5 nm. Both images show a set of concentric rings around each Au NP. Each of the concentric rings corresponds to a change in electric charge in the Au NP by a single electron charge. Furthermore, by performing a voltage spectroscopy of frequency shift and dissipation signals, we can obtain the charging energy, discrete energy spectrum as well as tunneling rate, quantitatively.

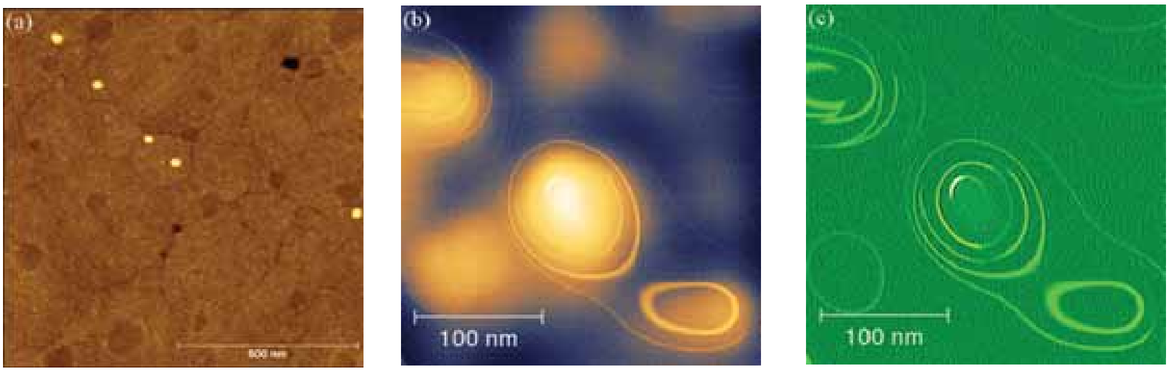

Figure 1: (a) AFM topography image of 5 nm Au NPs on C16S2 SAM on Au substrate taken in air with amplitude modulation mode. (b) and (c) Frequency shift and dissipation images taken at 4.5 K at a constant tip height of about 15 nm. Au substrate bias voltage was 5 V.

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[4] L. Cockins, Y. Miyahara, S. D. Bennett et al., (submitted).

Tu-08

Effect of Orbital Hybridization on Kelvin Probe Force Microscopy Images

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Mechanism of atomic scale resolution of KPFM images i.e., the images of local contact potential difference (V_{LCPD}), has been a recent controversial issue and attract much attention because of expected rich information it may provide. We have already demonstrated that though a nano scale resolution is induced by the electrostatic multi-pole interaction between a KPFM tip and a sample surface[1], true atomic resolution cannot be realized for semiconductor and metal surfaces. In the present work, we clarify that real atomic resolution of KPFM is obtained by the chemical interaction, i.e., by the orbital hybridization effect between the tip and the sample.

In this work, we theoretically simulated KPFM images formed by local contact potential difference of Si(001)-c(4x2) surfaces with and without embedded impurities with a novel developed theoretical approach[2]. In these images, there found two kinds of spots: one is atom scale spots located on surface atoms, and the other is a broad spot spread over on top position above the impurity atom site (see Fig.1 below). The atom scale spots vanish when the tip was set on a distance beyond the orbital hybridization range from the sample surface. Though the atom scale spot is induced by the orbital hybridization effect between the tip and the sample, the nano-meter scale spot is induced by the electrostatic multi-pole interaction. We confirmed this fact by the newly developed KPFM simulation method, which is based on the partitioned real space density functional based tight-binding (PR-DFTB) method, augmented with the perturbation treatment of orbital hybridization terms between the tip and the sample surface.

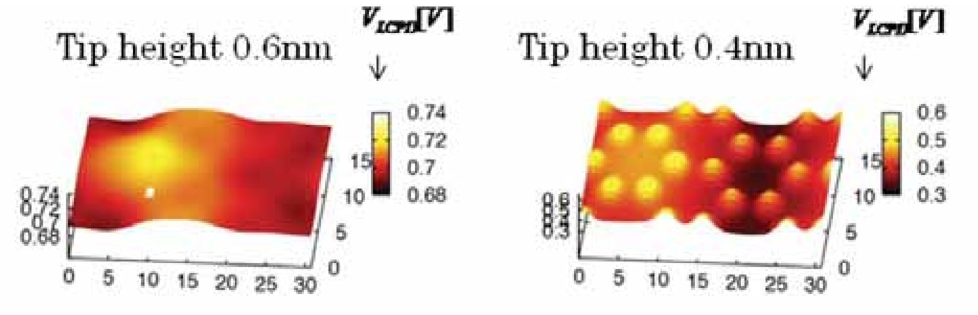

Fig.1 KPFM image of Si(100) c(4x2) surface including an Al impurity atom substituted Si atom in the 4th atomic layer from the top. For the tip height of 0.6nm (left), a large bright spot appears above the impurity, but the top atom cannot be seen. On the other hand for the tip height of 0.4 nm (right), the individual top Si atoms are imaged as bright spots, as well as large bright region centered above the Al site. The length scale is Å.

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[2]A. Masago, M.Tsukada, and M. Shimizu, submitted to Appl. Phys. Lett.

Surprise-surprise: local work function variations on clean Au(111)

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In classical electrodynamics, metal surfaces are perfect equipotential planes. Nevertheless, lateral work function variations due to the surface reconstruction of Au(111) have been reported from scanning tunnelling spectroscopy [1]. Also, speculations were raised whether or not the electric stray field induced by the surface reconstruction can explain the contrast reversal reported for constant frequency shift non-contact atomic force microscopy imaging on Au(111) [2].

Here, we report on the local work function variations on pristine Au(111) surfaces due to the Au(111)–(22×√3) reconstruction, as studied with frequency modulation Kelvin probe force microscopy [3]. We show that indeed a work function variation of ≈ 50 meV is found with the same long scale periodicity Δ as the herringbone pattern [see also figure 1(a/b)]. Moreover, we also report on a novel type of surface morphology [see figure 2(a)] most probably induced by reconstruction networks [4]. Together with this new type of surface pattern a work function change of 330 meV emerges as is depicted in figure 2(b).

The observed lateral work function variations indicate extremely high electric fields in the vicinity of the crystal surface, which are clue for the self assembling process of organic molecules, the formation of inorganic aggregates, and catalytic processes.

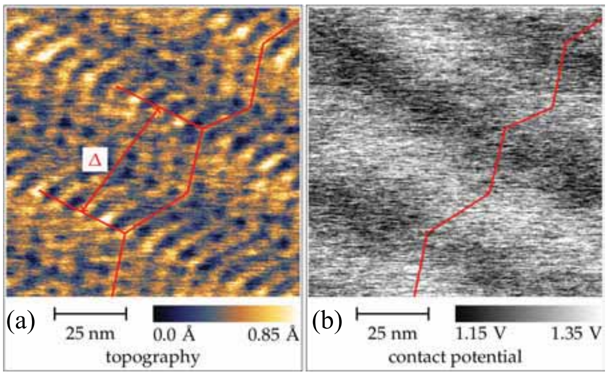

Figure 1: (a) topography and (b) corresponding contact potential of the Au(111)–(22×√3) herringbone reconstruction. The contact potential varies about ≈ 50 meV with the same long scale periodicity Δ as the reconstruction pattern.

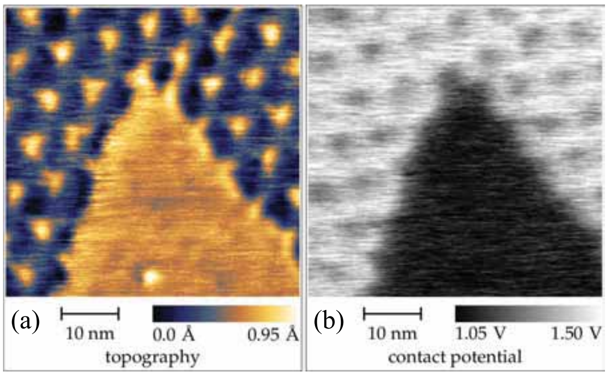

Figure 2: (a) topography and (b) corresponding contact potential of the novel type of Au(111) surface morphology. The contact potential difference between bright and dark areas amounts to 330 meV.

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[4] M. Hohage et al.: Surf. Sc., 337:249, (1995)

Tu-10

High-resolution surface potential mapping on single-walled carbon nanotubes using frequency-modulation high-frequency electrostatic force microscopy

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Carbon nanotube field effect transistors (CN-FETs) are one of the most promising candidates for future nanoelectronic devices because of the superior transport properties of carbon nanotubes (CNTs). Kelvin-probe force microscopy (KFM) is a powerful tool to investigate surface potential (SP) distribution on the gate channel of the CN-FET. However, since the width of the CNT, single-walled CNT (SWNT) in this study, is usually smaller than the tip radius, the measured SP is affected by that of the peripheral area of the SWNT, which hinders quantitative SP measurements. In particular, the trapped charges on the insulating surface around the CNT significantly affect the SP measurement[1]. Here we propose a novel method that is capable of measuring the SP distribution on the CNT less affected by the background electrostatic force, by combining frequency-modulation (FM) KFM and high-frequency electrostatic force microscopy (HF-EFM)[2].

Figure 1(a) shows an FM-AFM image of an SWNT bridging the two Pd electrodes fabricated on a silicon dioxide surface. The upper electrode in Fig. 1(a) and Si substrate was electrically grounded while 1.2 V bias was applied to the lower electrode. Figure 1(b) shows an FM-KFM image acquired simultaneously with Fig. 1(a). A high SP contrast is observed around the SWNT and the lower electrode, which is actually affected by the background electrostatic force. For FM-HF-EFM, we applied two high-frequency modulation voltages with slightly different frequencies (f_1 = 5 MHz, $f_2 = f_1 + f_b$, f_b = 700 Hz) to the lower electrode. Figure 1(c) shows an FM-HF-EFM image showing the magnitude of the frequency modulation of the cantilever resonance frequency at f_b. The contrast of the FM-HF-EFM image corresponds to the magnitude of the HF voltages along the conductive regions. Since the distribution of the background charges was not modulated by the high-frequency voltages, the sharp voltage drop at an SWNT defect was clearly observed, as indicated in the figure.

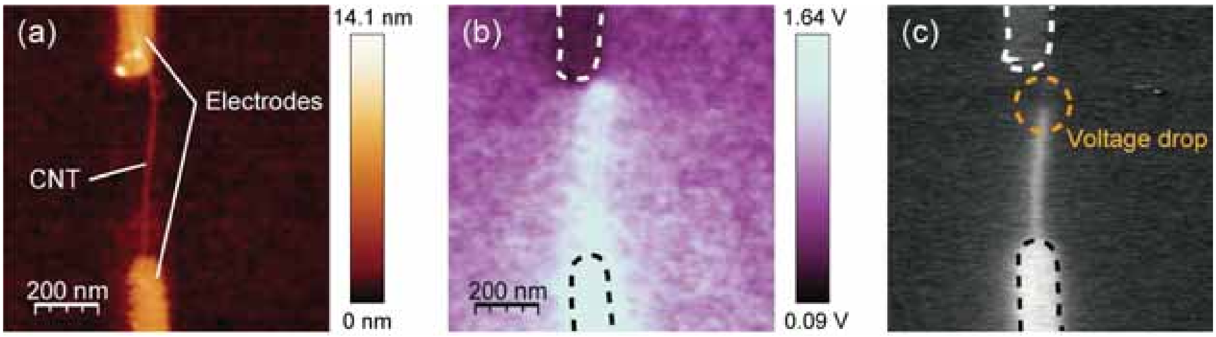

Figure 1: FM-AFM image (a), FM-KFM image (b), and FM-HF-EFM image (c) of an SWNT connecting two Pd electrodes (upper electrode: grounded, lower electrode: 1.2 V).

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Atomic and chemical resolution of heterogeneous In-Sn chains on Si(100)-(2x1) studied by nc-AFM and DFT

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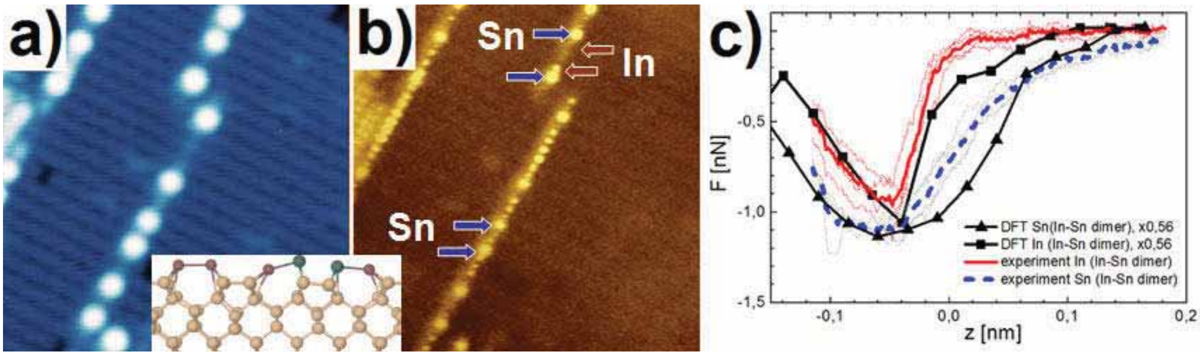
Groups III and IV metals have ability to form 1D atomic chains on Si(100)-2x1 surface [1]. While the chains composed of a single atomic type show a semiconductive character, it is expected that mixing the atoms could result in interesting electronic properties [2]. We investigated bimetallic In-Sn atomic chains consisting of mixed individual hetero (Sn-In) and homo (In-In, Sn-Sn) dimers. Despite of the relatively simple atomic structure of these chains, achieving the true chemical and atomic resolution is a difficult task. Namely, the electron density of the dimers is localized over both atoms, which makes STM difficult to get a single-atom resolution within dimers (fig. a).

We performed FM-AFM measurements at RT using q-Plus sensor. The measurements provide resolution of single atoms in the dimers (fig. b). In addition, we measured force-site spectra (F-z) above single atoms in the chains. The measured curves are compared to DFT calculations. Possibility of discriminating the single chemical species is discussed and the results are compared to previous work [3].



a) STM image of In-Sn chains on Si(100)-(2x1) surface. V_S = -2V. Inset shows atomic structure of the chains (side view).
b) nc-AFM constant height image of the same area.
c) Force curves measured above the positions marked in b). The data are compared to DFT calculaltions

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[2] L. Magaud, A. Pasturel, and J.-Y. Veuillen, Phys. Rev. B 65 (2002), 245306
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Molecular recognition of single molecules adsorbed on the Si(111)-(7x7) surface by means of nc-AFM

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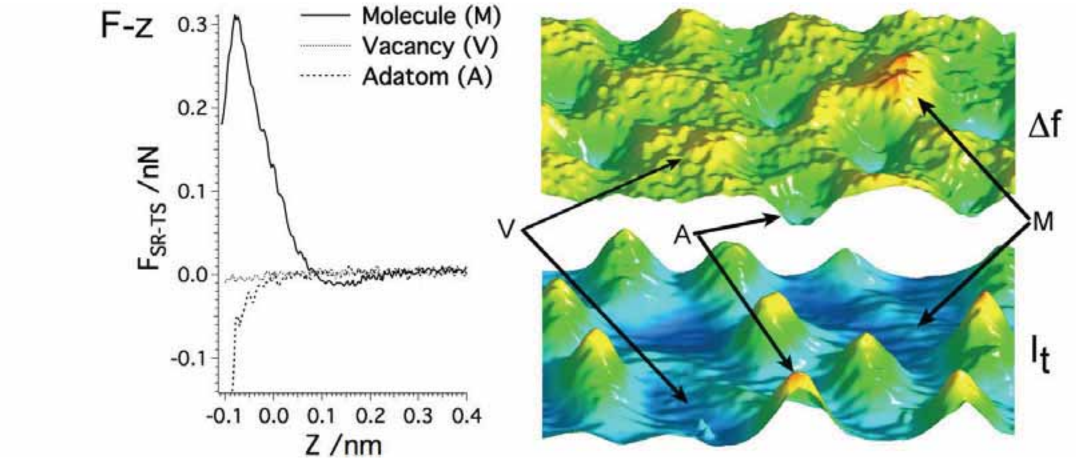
The adsorption of alkenes and aromatic molecules on semiconductor surfaces has been subject of intense study for a long time. On Si(111)-7x7 surface reconstruction, many alkenes and aromatic molecules attached to the surface via a [4+2]-like cycloaddition reaction in which the molecule bridges a Si rest atom and a nearest neighbor adatom. Unfortunately, the formation of C-Si bonds shifts the Si adatom electronic state out of the energy range accessible to STM. This shift produces the characteristic signature of small molecule attachment, a depression similar to the signature of a missing adatom or vacancy. This effect makes difficult to distinguish between Si vacancies and molecular adsorption places using STM (see Fig. I_t). In contrast with STM, AFM has already achieved high-resolution images of individual molecules on surfaces [2, 3].



Here we present a combined experimental and theoretical study of the adsorption of ethylene and benzene on the Si(111)-(7x7). Using force site spectroscopy and DFT simulation, we show that it is possible to clearly discriminate between absorbed molecules and Si vacancies using NC-AFM. This is illustrated in the figure, where a constant height scan of an ethylene molecule adsorbed on 7x7 is present.

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[3] L. Gross et al., Nature Chemistry 2 (2010) 821

Visualization of atomic scale elasticity on Ge(001) surface with multifrequency FM-AFM

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Ge(001) surface, which is very similar to Si(001) surface [1], shows buckled dimer structure and several reconstructed phases. In addition, different interatomic bonding state and surface stress are distributed on the surface at the atomic scale since the dimerization of surface atoms favors compressive lattice strain. However, elastic information at the atomic scale has never been detected experimentally. In this study, we investigated surface elasticity distribution at the atomic scale on Ge(001) surface by the multifrequency FM-AFM method, which is a nice tool for probing such elasticity [2].

AFM experiments were performed in our homemade UHV atomic force microscope operating at room temperature. A tungsten coated Si cantilever was used as the force sensor [2], which was oscillated at the first and second flexural mode (f_1=152.475 kHz and f_2=944.270 kHz). The topography of Ge(001) surface was obtained from feedback signal maintaining a constant frequency shift of the 1st component (Δf_1). Based on theoretical considerations, the surface elasticity is related to the frequency shift of the second component (Δf_2) signal.

Figures 1(a) and (b) are simultaneously obtained topography and Δf_2 mapping of Ge(001) surface at room temperature using the multifrequency method. In the topography the Ge(001) surface shows up with symmetric dimer structure (p(2x1) phase) indicating the flipping dimer state. On the other hand, the Δf_2 mapping has a faint contrast difference between adjacent dimer atoms showing the c(4x2) phase. Line profile analysis reveals that its contrast difference corresponds to 2Hz. This result is originated from surface elasticity difference between the adjacent dimers. We will discuss surface elasticity and physical phenomena on this state.

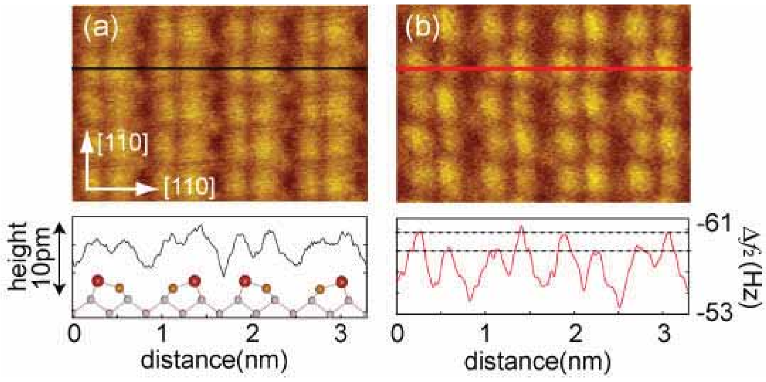

Figure 1: Simultaneously obtained (a) topography and (b) Δf_2 mapping of Ge(001) surface maintaining the 1st mode frequency shift constant at Δf_1= -29 Hz with oscillation amplitudes of A_1=7 nm, A_2=90 pm. Bottom profiles were taken from structural equivalent lines indicated in the upper images.

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Dopants & Defects on Si(100): Imaging & manipulation by qPlus NC-AFM

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The Si(100) surface has been well studied by numerous surface science techniques, and its atomic structure has been resolved by both STM and NC-AFM. Importantly, it is known that defects on the surface affect both the local electronic [1] and mechanical [2] properties.

By using a qPlus NC-AFM operating at low temperature we have investigated both native and dopant related defects. Intriguingly, we have observed that dopant related ad-atom complexes [3] are occasionally manipulated during imaging at high setpoint in the absence of tunnelling electrons, raising the possibility of atomically precise manipulation of dopants and ad-atom complexes on semiconducting surfaces by purely mechanical means. We also present low bias simultaneous df/tunnel current imaging of defects, highlighting the differences in chemical reactivity and electronic structure as probed by the same tip. We also present imaging of a defect type observed on both p-and n-doped samples that does not appear to correspond to any of the commonly observed native (dimer vacancy), dopant, or adsorbate (e.g. C-type) defects.

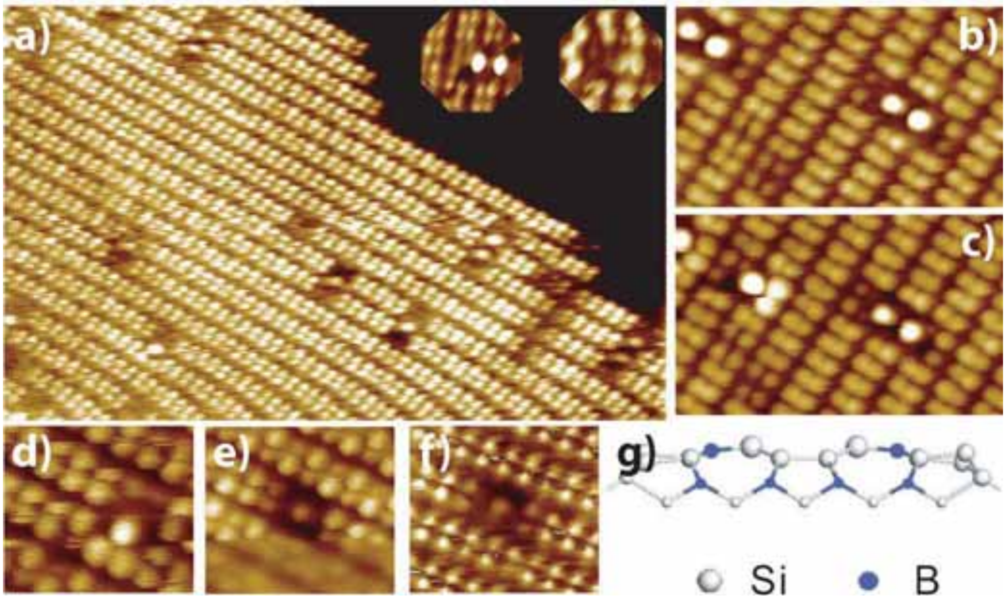

Figure 1: (**a**) Large scale, high setpoint NC-AFM image showing numerous defects (inset: NC-AFM (left) and tunnel current (right) of B double ad-dimer defect). (**b**) before & (**c**) after manipulation of double B defect (see left of image) (**d**) single B-ad-dimer defect. (**e**) & (**f**) defect of unidentified structure on p and n type silicon. (**g**) Ball and stick model of double B ad-dimer defect.

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[3] Z.Liu et al. Phys. Rev. B 77, 035322 (2008)

Tip-induced heating of Co atoms on Cu(110)-O surface with low-temperature AFM

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Manipulation of single atoms and molecules is an innovative experimental technique of nanoscience. Atom manipulation by atomic force microscopy (AFM) has opened up the possibility of assemble and probe nanostructures even at insulating surface [1]. Atom manipulation with an AFM is particularly promising, because it allows the direct measurement of the driving forces involved in manipulation.

In this study, we investigate the dynamics of a single copper (Cu) or cobalt (Co) atom during lateral manipulation on Cu(110)-O surface. Experiments were performed by using noncontact atomic force microscopy (NC-AFM) at 78 K. Lateral manipulation for a single Cu or Co atom was performed by using the pulling mode. After the lateral manipulation for the Cu atom, the Cu atom was unpertubated at the present imaging parameters and resided on a binding site on the surface. On the other hand, after the lateral manipulation for the Co atom, as shown in Fig. 1, the Co atom became unstable at the present imaging parameters, and hopping of the Co atom between the adjacent binding sites was induced. We for the first time observed the atom hopping. No bias voltage was applied between the tip and the surface, so that the hopping of Co atom is not due to excitation by inelastic electron tunneling [2]. We investigated the life time of the hopping of Co atom. The hopping seems to be due the tip-induced heating of the Co atom.

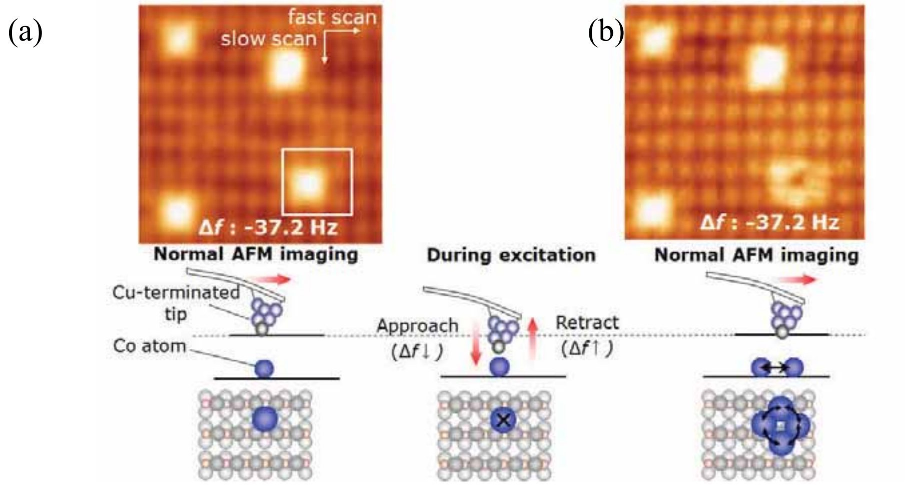

Fig. 1 AFM images of Co atom on Cu(110)-O surface (a) before and (b) after lateral atom manipulation. After the atom manipulation, Co atom became unstable due to tip-induced heating.

[1] M. Terns *et al.*, Science, 319, 1066 (2008).
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Tu-16

Force and conductance of contacts to a C_{60} molecule

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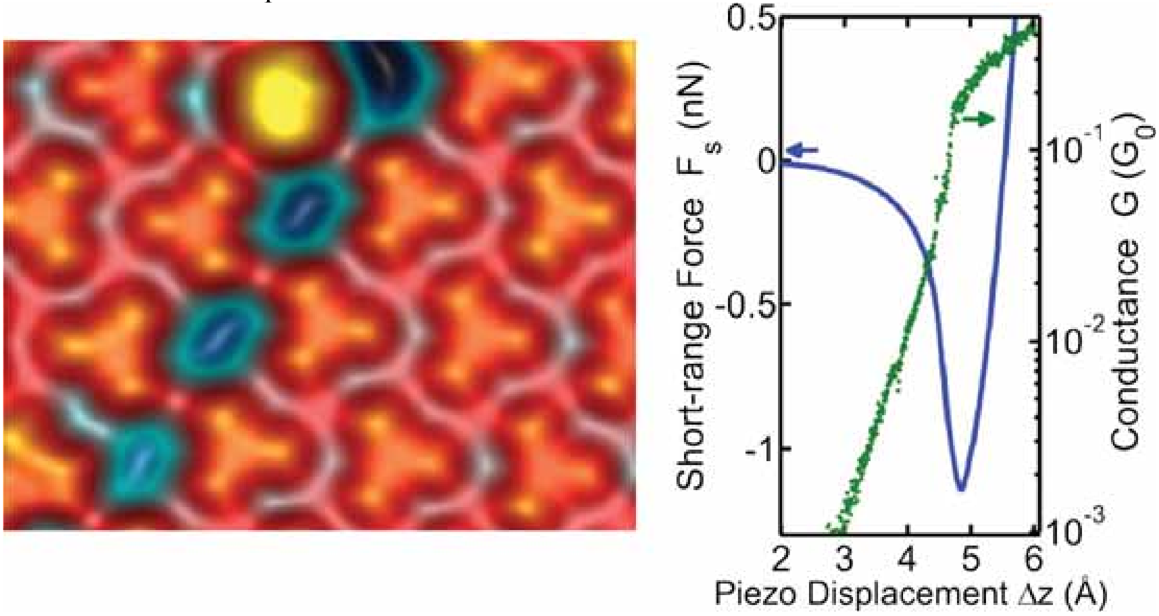
Electron transport through single molecule contacts is the basis of designing molecular electronics. To understand the geometry of the junction that underlies its transport properties, the forces arising during conductance measurements in such contacts are important. Simultaneous measurements of force and conductance have been addressed before in single-atom contacts [1,2] and on a Si(7x7) surface [3]. Using a robust molecule (like C_{60}) for the tunneling tip [4] is promising to obtain a well-defined contact electrode.

We present the first low-temperature force and conductance data from controlled Cu-C_{60} and C_{60}-C_{60} contacts with submolecular resolution. The contact conductances reported in prior work are shown to correspond to the junction being under maximal tensile stress.

In order to estimate relaxations we fit the calculated conductance for a rigid system to the experimental data considering an effective spring constant for the molecular junction. The results indicate that most of the deformation in a Cu-C_{60} contact may be ascribed to relaxations of the Cu tip.



Left: Pseudo-three dimensional illuminated constant-current STM image of a C_{60} island on Cu(111); Right: Short-range force and conductance in a Cu-C_{60} contact.

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Measurement of tip-sample interaction forces under infrared irradiation toward high-spatial-resolution infrared spectroscopy using FM-AFM

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Infrared (IR) spectroscopy is a superior analytical technique which is capable of identifying functional groups having characteristic vibration frequencies. However, the spatial resolution in the conventional IR spectroscopy is on the order of micrometers because of the diffraction limit. We are developing high-spatial-resolution infrared spectroscopy using frequency modulation AFM (FM-AFM), which is capable of detecting tip-sample interaction forces with a very high sensitivity. Recently, we succeeded in detecting frequency modulation of the cantilever resonance frequency when the cantilever was brought in the proximity of a polydimethylsiloxane (PDMS) film irradiated with an IR beam using a free electron laser at Forschungszentrum Dresden-Rossendorf, Germany[1]. In this presentation, we show the measurement results of the tip-sample interaction forces of FM-AFM on polymer thin films under IR irradiation using a quantum cascade laser (QCL) toward high-spatial-resolution infrared spectroscopy using FM-AFM.

We spin-coated PDMS on a highly-oriented pyrolytic graphite (HOPG) surface, as shown in Fig. 1(a). While the distance between the AFM tip and the sample surface was regulated utilizing the second resonance frequency (420 kHz), we irradiated an IR beam from QCL (1050 cm^{-1}) whose intensity was modulated at a frequency close to the first resonance frequency (67 kHz). Figure 1 (b) shows an FM-AFM topographic image, and Fig.1 (c) and (d) show the magnitude of the cantilever oscillation induced by the IR irradiation at 69 kHz and 65 kHz, respectively. In Figs. 1(c) and 1(d), we found that the the magnitude of the cantilever oscillation was different on PDMS and HOPG, and that the contrast was dependent on the modulation frequency.

[1]Y. Hosokawa et al. 18th International Colloquium on Scanning Probe Microscopy, (2010)

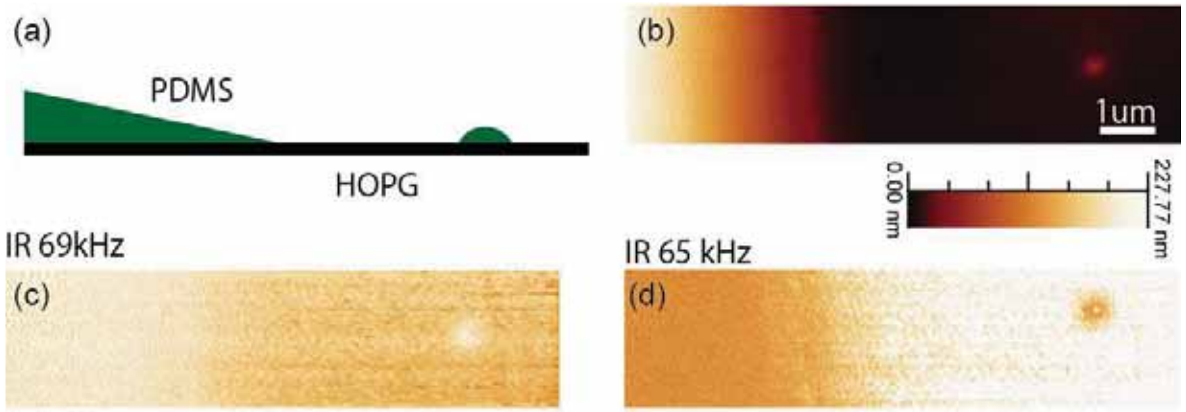

Figure 1: (a) Illustration of PDMS film on HOPG. (b) Topographic image of PDMS film on HOPG. (c) and (d) show the magnitude of the cantilever oscillation induced by irradiation of IR laser beam modulated at 69 kHz and 65 kHz, respectively.

Tu-18

Mapping Electron Clouds with Force Microscopy

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NC-AFM can routinely achieve atomic resolution in ultra-high vacuum (UHV), but as with any imaging technique, one wishes to push the achievable resolution to its limit. In 2004, Hembacher et al. reported simultaneous STM/AFM experimental images for a tungsten tip imaging a graphite surface [1]. The tip was attached to a qPlus sensor [2], and imaging was done in UHV at 4K. Remarkably, the image created by the higher harmonics of the cantilever trajectory revealed features within the diameter of a single W atom, which the authors interpreted as bonding lobes of increased charge density at the tip's apex atom. Although this interpretation has been controversial, an *in-depth* theoretical study of the experiment has yet to be produced. We use density functional theory (DFT) to investigate the ability of force microscopy to map an individual atom's electron density via higher harmonic imaging. We focus on the experimental image of Ref. [1] that exhibits four-fold symmetry (Figure 1), which is attributed to the bonding lobes of a W(001) tip apex cluster. As a precursor to the multiscale modeling needed to study the complete imaging experiment – which would necessarily include the effects of the cantilever dynamics and subsequent filtering of the tip trajectory – we use the fundamental theory of Dürig [3] to calculate the harmonic amplitudes from the simulated tip-sample force curves. In spite of the reduction of variables achieved through this approach, there exist unique challenges inherent to the simulation of higher harmonic imaging that are not present in the typical simulation of frequency shift images. Nevertheless, we find that four lobes of increased electron density are indeed present at the apex atom of a W(001) tip model and that simulated higher harmonics images are capable of producing subatomic features similar to those observed experimentally. However, we have not yet established a quantitative connection between the images and the tip apex electron density.

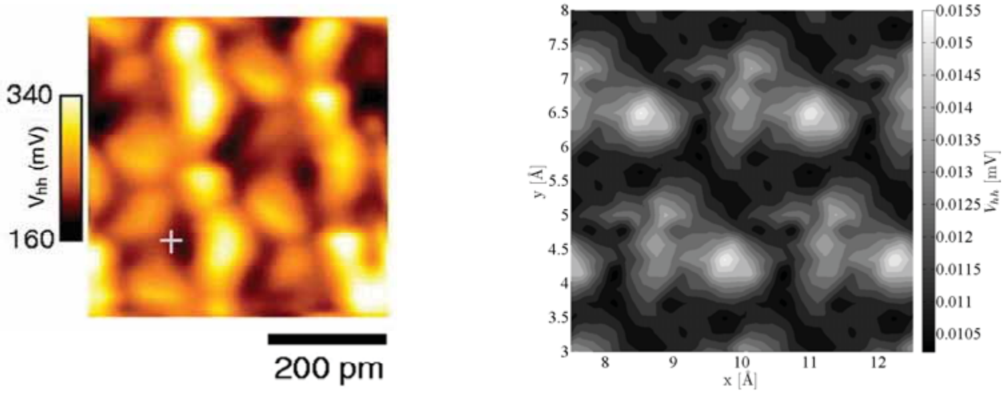

Figure 1 – Experimental (left) and simulated (right) higher harmonics (V_{hh}) images of a W tip imaging a graphite surface, each exhibiting four-fold symmetry within a W atom diameter.

[1] S. Hembacher, F.J. Giessibl, J. Mannhart, Science, 305, (5682), (2004)
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[3] U. Dürig, New Journal of Physics, 2, (2000)

Topography and KPFM measurements of NaCl islands grown on copper surface by means of nc-AFM in pendulum geometry

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Ultra sensitive cantilevers oriented perpendicularly to the sample surface (so called pendulum geometry) can be successfully used to study energy dissipation mechanism [1, 2]. In many cases it is also necessary to characterise the topography of the surface. However, the topography measurement is limited owing to fundamental reasons. The amplitude of the soft cantilever limits the spatial resolution. Moreover, calculation showed that in pendulum geometry AFM the cantilever tip is influenced by two types of forces – the axial force and the lateral force gradient. This is also confirmed experimentally. The voltage dependence of the frequency shift shows parabolic behaviour. While approaching the tip to the surface the parabolas change the slope due to change of the force interaction. Both force components contribute to the cantilever frequency shift signal causing the frequency modulated – AFM (fm-AFM) difficult.

In this contribution we present a method to overcome this obstacle. Our experiment showed that proper design of the tip shape leads to increased sensitivity of the cantilever to the normal force component and thus makes the FM-AFM possible. The topography measurement of 1ML NaCl islands grown on Cu(100) surface simultaneously with frequency modulated - Kelvin Probe Force Microscopy (FM-KPFM) were done. Owing to small stiffness (~mN/m) the cantilever motion is very sensitive to electrostatic forces and thus very small modulation voltage (~mV) can be used in FM-KPFM in pendulum mode. At the same time the amplitude modulated – KPFM is not possible due to high quality factor of the cantilever. The measurements of cantilever frequency shift and energy dissipation on metal (Cu) and insulator (NaCl) are also presented. The results showed increase of energy dissipation on metal when compared to insulator.

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[2] M. Kisiel, E. Gnecco, U. Gysin, L.Marot, E. Meyer, Nature Materials, 10, 199-122, (2011)

Reversible bond formation in a metal-molecule complex

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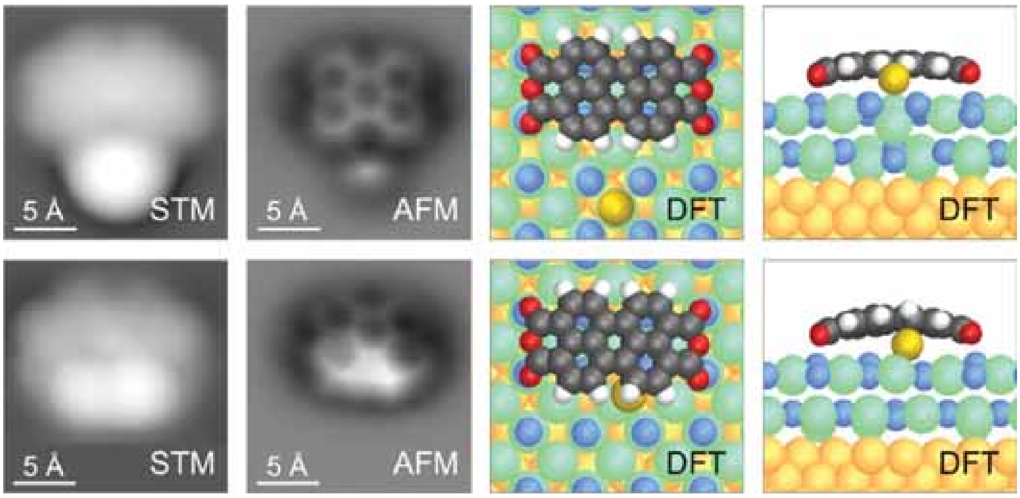
We report on the formation of a metal-molecule complex that can be used as a molecular switch [1]. Using a cryogenic combined scanning tunneling and atomic force microscope, a covalent bond could be formed reversibly between a gold atom and a perylene-3,4,9,10-tetracarboxylic dianhydride molecule supported by a thin insulating NaCl film on Cu(111). The switching between the bonded and the nonbonded state of the complex was found to be accompanied by a considerable change in the tunneling current and could be reliably controlled by locally applying voltage pulses of according polarity. Atomic-resolution molecular imaging by noncontact AFM [2] was employed to determine the structure of the complex before and after switching. Our experimental results were corroborated by extensive density functional theory calculations. A new mechanism of bond formation, which involves different charge states of the metal-molecule complex, was identified as the reason for the enhanced reliability compared to bond activation by inelastic electron tunneling.
Our results demonstrate the high degree of insight into both the atomic and the electronic structure of a molecular complex that can be gained by combining AFM and STM imaging and spectroscopy.



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[2] Gross et al., Science **325**, 1110 (2009)

Exploring short range interactions between two neutral molecules

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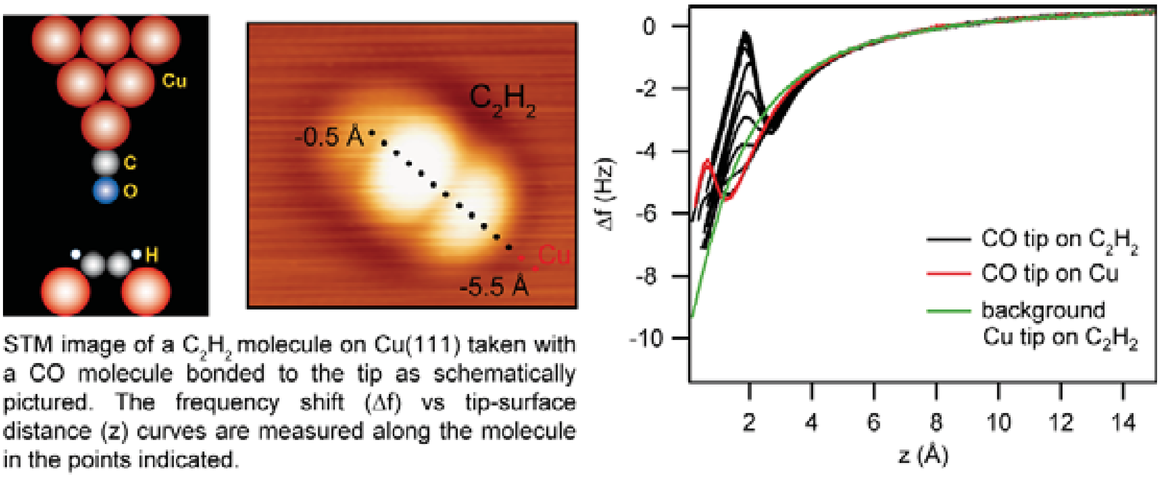
Typically forces between neutral molecules are weak and extend significantly over large distances. But what happens when two neutral molecules weakly interacting are approached so close that chemical forces may build up?
Here we explore the interaction energy landscape when a carbon monoxide (CO) molecule is brought in the proximity to an acetylene (C_2H_2) molecule adsorbed on a Cu(111) surface. For this purpose we use a STM/NC-AFM based on a *qPlus* sensor design operated in frequency modulation mode, at 5K and in UHV. By means of tunneling electrons we transfer a CO from the Cu surface to the STM tip [1] and approach it to close proximity of an acetylene molecule. We record the frequency shift as a function of the tip-surface distance probing in this way, site specific interactions between the two molecules and between the CO and the Cu atoms on the surface. By removing the contribution of long range interactions we are able to access forces appearing exclusively in a short range regime. In this case, we find that the two molecules show attractive interactions up to distances where chemical bonds are typically formed, with maximum interaction energy of ~40 meV. We interpret this as the formation of a weak chemical bond from the overlapping of C_2H_2 π states with lone pair electrons of the oxygen in the CO molecule. At closer distances the interaction potential is repulsive. The repulsive force gradient is not homogeneous though, at distances too small it decreases, presumably due to the bending of the CO at the tip [2]. Also within the C_2H_2 molecule the force is not uniform; the stronger variation occurs at the hydrogen positions where a peculiar dissipation fingerprint is additionally measured.



STM image of a C_2H_2 molecule on Cu(111) taken with a CO molecule bonded to the tip as schematically pictured. The frequency shift (Δf) vs tip-surface distance (z) curves are measured along the molecule in the points indicated.

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We-03

Measuring the charge state of a single redox molecule with nc-AFM

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We use a nc-AFM equipped with a qPlus tuning fork to perform charge transfer and acquire frequency shift spectroscopy on a single redox molecule deposited on a thin NaCl film. When a voltage pulse is applied on the metal organic complex bis-dibenzoylmethanato-copper, a charge is transferred to the molecule. This electron capture is accompanied by a conformational change from a square planar (sp) to tetrahedral (td) geometry (fig 1.a). This switch is reversible by applying a voltage pulse of opposite sign (fig 1.a). For each of these two states, we perform Δf(V) spectroscopy in order to characterize the electrostatic force between the molecule and the tip. Resulting spectra are parabola indicating that the only forces exerted are Van der Waals force and electrostatic force. Following a recent work [1], these parabola are precisely fitted to extract the maxima V*, the so called local contact potential difference, which shifts when a charged object is present (fig 1.b). Due to the difference heights of the square-planar and the tetrahedral conformational state, we perform a complete set of measurements for different tip heights (fig1.c). We show that the behavior of the square planar molecule does not deviate significantly from the NaCl. On the other hand for the tetrahedral species a clear shift on V* is observed. According to [1] and [2], these shifts are attributed to the presence of a supplementary negative charge on the tetrahedral.

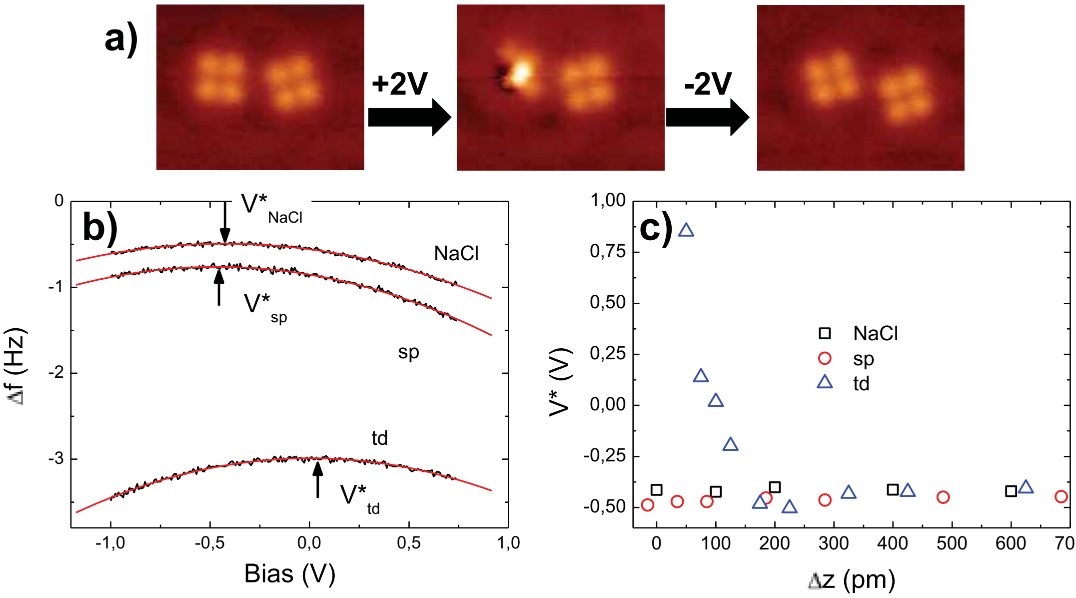

Figure 1: a) STM image of the reversible switch of $Cu(dbm)_2$ from a neutral square planar state (sp) to a charged tetrahedral specie (td). b) Frequency shift spectroscopy above NaCl, sp and td at Δz = +100pm from the regulation point. c) V*(Δz) showing the presence of negative charge for the td species.

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[2] F. Bocquet, L. Nony, and C. Loppacher, Phys. Rev. B 83, 035411 (2011).
[3] T. Leoni et al., Phys. Rev. Lett 106, 216103 (2011)

Sub-molecular resolution imaging and orientational control of on-tip C_{60}

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Sub-molecular resolution imaging is now commonplace in scanning tunnelling microscopy. The fullerene family of molecules has been particularly important in this regard and a number of groups have reported the observation of intramolecular features arising from the orbital structure of, for example, C_{60} adsorbed on metal and semiconductor surfaces [1]. The elegant experiments of Gross *et al.* [2] showed that imaging of molecular structure with resolution significantly higher than that achievable in conventional STM is possible using qPlus atomic force microscopy. Prior to this, Giessibl's group had pioneered "sub-atomic" resolution imaging [3], where spatially localized surface orbitals are used to image tip structure.

We show that it is possible to exploit the relatively narrow spatial extent of dangling bond orbitals on the Si (111)-(7x7) surface to image the orbital structure of a C_{60} molecule adsorbed on a tip. After the transfer of a single C_{60} molecule from the (7x7) surface to the tip, subsequent dynamic STM measurements yielded images where the silicon adatoms each show structure (see Fig. 1), arising from the charge density distribution of the transferred C_{60} molecule. The size and the shape of the molecular orbitals vary with the adsorption and rotation angle of the C_{60} on the tip. Experimental data are in good agreement with predictions made by Hückel molecular orbital theory calculations.

In addition, qPlus AFM imaging reveals high resolution of intramolecular structure (Fig. 1). We have also measured the force between the on-tip adsorbed C_{60} molecule and silicon surface using qPlus AFM frequency shift-vs-tip displacement spectroscopy.

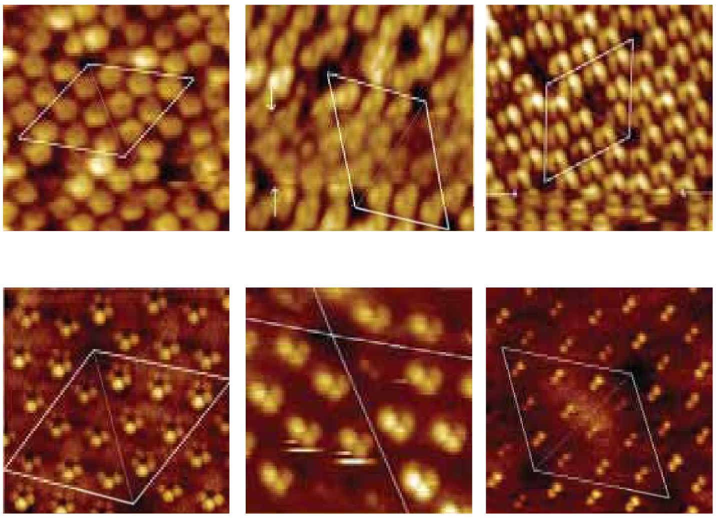

Fig. 1: Dynamic STM (top row) and qPlus AFM (bottow row) images of Si (111)-(7x7) with a C_{60} functionalized tip. The differences in adatom sub-structure clearly arise from variations in the orientation of the C_{60} molecule. (Note, in particular, the five-fold symmetric structure - arising from a "pentagon-down" orientation of the on-tip C_{60} - seen in the image in the lower left corner). Using lateral manipulation of C_{60} molecules adsorbed on the surface, the molecule at the end of the tip can be rotated. Spontaneous changes are also observed during scanning (and are marked by arrows in the dynamic STM images in the top row).

[1] P. Moriarty, *Surf. Sci. Rep.,* **65**, 175 (2010)
[2] L. Gross *et al.*, *Science*, **325**, 1110 (2009)
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We-05

Dynamic Force Spectroscopy at a Single Molecule Junction

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Recent Developments in Atomic Force Microscopy made it possible to probe not only electronic properties of single molecules and atoms on conducting surfaces but also acquiring information about forces in the pN regime simultaneously. Determination of the charged state of single metal atoms [1] or resolving the chemical structure of a molecule [2] are just some of the possibilities, opening new dimensions of scanning probe spectroscopy.

In our experiments we create molecular nanocontacts to get insight into the correlation between conductance and molecular conformation. The process of contacting and pulling a molecular junction has been investigated previously under different conditions. For instance Gaub et. al [3] observed non-linear force-distance curves while unfolding comparatively big proteins. This behavior they assign to deformations of the molecule. In contrast, metal junctions behave elastically like harmonic springs following hooks law with no significant difference between single- and many-atomic contacts [4].

We utilize a tuning fork based LT STM/AFM with the qPlus design operated at 5K to perform single molecule force spectroscopy and conductance measurement simultaneously. With our STM tip we contact a functionalized polyphenyl molecule in one side and lift it up from the surface, while the other side remains attached to the substrate [5]. During lift up we observe sawtooth like features in the df spectra, representing alternative stages of elastic deformations and plastic rearrangements of the junction. In the elastic stages, the force gradient (stiffness) changes with pulling distance, in opposition with results on atomic contacts [4]. We assign this to (elastic) intramolecular structural changes occurring during the stretching of the molecular junction. Furthermore we present force field calculations to simulate the lift up process and support our findings.

[1] Leo Gross, et al., Science 324, 1428 (2009)
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[3] M. Rief, M. Gautel, F. Oesterhelt, J. M. Fernandez, H. E. Gaub, Science 276, 1109 (1997)
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Measuring individual up and down tip forces in Dynamic AFM

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Measuring the frequency shift as a function of the tip height in Dynamic (Non-Contact) Atomic Force Microscopy (D-AFM) allows obtaining the average tip force over the whole oscillation cycle (force spectroscopy). It is known that measuring the dissipation signal involves the difference of the tip down and up forces, so that one may think that doing this would help in determining the tip up and down forces separately in spectroscopy experiments. We explain here that although formally a solution exists for the difference of forces to be restored from the dependence of the excitation signal on the tip height, the dissipation information cannot help in practice to obtain both forces because of the specific nature of the hysteresis phenomenon widely believed to be responsible for the dissipation effects in the D-AFM.

Theoretical calculations based on a one-loop hysteresis model show however that it is still possible to *measure* experimentally separate down and up tip forces in specially designed spectroscopy experiments performed at low temperature and sufficiently low oscillation amplitude. This means that, at least in principle, the whole hysteresis curve can be directly measured and then compared with theoretical calculations. This method will be introduced and its main ideas explained. Then we will discuss the theoretical proposal in the context of qPlus AFM measurements above an adatom of the Si(111)-(7x7) surface.

Chemical identification of surface ions on polar surfaces using metallic tips and adsorbed molecules

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We demonstrate that well characterized Cr tips can provide atomic resolution on the bulk NaCl (001) surface with dynamic atomic force microscopy in the non-contact regime at relatively large tip-sample separations [1]. At large distances of closest approach, above 5 Å, the surface chemical structure can be resolved yet tip-surface instabilities are absent. We have performed realistic density functional theory (DFT) calculations employing metallic tip models which demonstrate that chemical identification is unambiguous, because the tip-surface interaction is always largest above the Cl anions in the surface. This is due to the fact that the metallic tip generates a permanent dipole with the positive end facing the surface due to the the Smoluchowski effect [2]. This effect is caused by the incomplete screening of the positive ion cores in the asperity by conduction electrons, and is universal to all metals. Therefore, for metallic tips qualitative interpretation of contrast patterns on ionic surfaces can be made independently of the tip material and apex structure based only on the positions and charges of surface ions.

The position of adsorbed organic molecules and the atomic structure of the surface are resolved simultaneously, which enables the determination of the exact adsorption site, and along with DFT calculations of the molecular adsorption, the identity of surface ions imaged as bright is independently verified. By combining information on the closest approach tip-sample separation at which the molecules are manipulated with DFT calculations of the tip-molecule and surface-molecule interaction, we are also able to independently verify the absolute tip-surface separation in experimental force-distance curves.

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[2] R. Smoluchowski, Phys. Rev. 60, 661 (1941)

NC-AFM energy dissipation mechanisms

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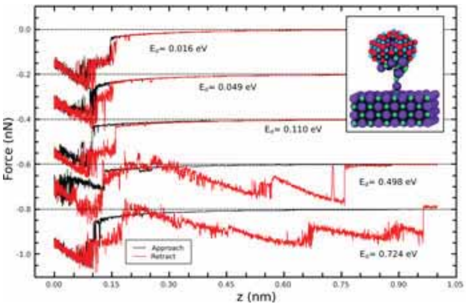
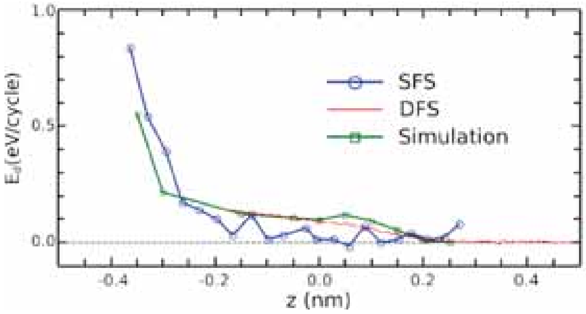
NC-AFM is an invaluable tool when probing surfaces, providing atomic resolution topography and detailed 3D force maps. As the tip scans the surface, the feedback gain signal associated to the energy dissipated in the oscillation cycles is also recorded, and this often differs from conventional topography images, showing different contrast patterns, periodicity and tip-surface distance dependence. Although many different surfaces have been studied with atomic resolution, a routine interpretation of these measurement has yet to be found, since the atomic processes at the surface responsible for energy dissipation are not well understood and the influence of the tip is not clear. In order to understand better the role of the tip in measured dissipation, we carried out extensive atomistic calculations using a wide variety of different tip materials and structures, and a simple NaCl (100) surface. After studying simple processes with quasi-static calculations [1], testing several tip geometries and materials [2], we are now investigating the atomic-scale dissipative processes using GPU accelerated finite temperature molecular dynamics (MD) simulations, and comparing directly to static force spectroscopy (SFS) and dynamic force spectroscopy (DFS) experiments. Ideal NaCl tips are too stable and do not give dissipation although in presence of defects at the apex, the system shows reversible reconstructions involving the tip and the surface, giving an average dissipation up to 0.02 eV/cycle, smaller than experimentally seen. MgO tips are even more stable but the oxygen's charge at the apex makes the surface unstable leading to formation of atomic chain and, consequently, irreversible surface alteration, which is again in contrast with the experiment, showing no decoration and stable operation. Finally we focused our efforts on simulating the experiment from the very beginning, where an oxidized tip indents the surface adsorbing a NaCl nanocluster at the apex. The average dissipation we calculate with this tip is in a quantitative agreement with DFS data and the distance dependence is also reproduced. We found that dissipation comes from stochastic formation of atomic chains of different lengths.





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[2] F. Federici Canova and A.S. Foster, Nanotechnology 22, 045702, (2011)

What role does orbital overlap play in atomic manipulation?

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Atomic manipulation at the single atom level with NC-AFM is now becoming routine, allowing extraordinary experiments to be realised on surfaces previously inaccessible by STM, or in systems where NC-AFM greatly assists single atom precision [e.g. 1, 2]. However, due to the complex interaction between the scanning probe apex and surface atoms, atomic manipulation with NC-AFM remains fraught with difficulties and experimental unknowns.

Recently [3] we demonstrated atomic resolution manipulation of dimers on the Si(100) surface via chemical force alone. In this work we present density functional theory (DFT) simulations which show that the ability to successfully flip dimers depends on the precise orientation of the dangling bond(s) of the atom(s) at the tip apex with respect to those of the surface atoms. We demonstrate, using simulated tip apices and a variety of lateral positions during simulated force spectroscopy, the extent to which orbital overlap affects the strength of the interaction between a Si tip and the Si(100) surface and, thus, modifies the outcome of attempts to flip a dimer. A test system for atom deposition/extraction on/from Si(100) is also considered, where we establish tip apex structures which either deposit or remove a bonded atom at the surface. Our results provide key insights into the 'orbital engineering' which is required to perform particular atomic manipulation tasks in covalently bound systems.

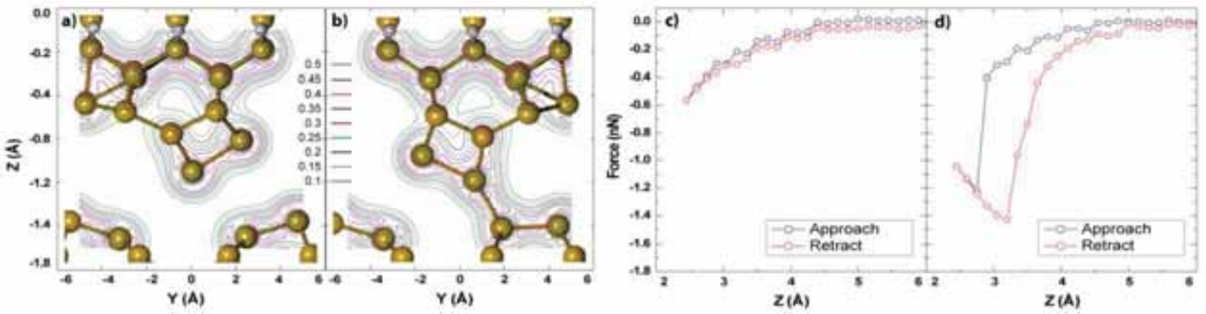

Figure 1: Variation in electron density between tip and surface during flipping of a Si(100) dimer with calculated F-z curves. The tip apex atom is laterally shifted 2.5Å away from the Si(100) dimer. Changing the orientation of the tip's free bond, such that it is (a), (c) misaligned, or (b), (d) aligned with the surface dimer axis, affects the interaction and therefore the outcome of attempted manipulation.

[1] M. Ternes *et al*. Science, **319**, 1066. (2008).
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[3] A. Sweetman *et al*. PRL, **106**, 136101, (2011).

We-10

Properties of Magnetic Tips for Magnetic Exchange Force Microscopy and Spectroscopy

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Recently, we demonstrated the feasibility of Magnetic Exchange Force Microscopy (MExFM) [1,2] and Spectroscopy (MExFS) [3] with atomic resolution. As for all scanning probe techniques, the tip plays a crucial role in the data acquisition process on the atomic scale. In this presentation different routes to prepare and characterize atomically sharp and magnetically sensitive tips *in situ* are discussed.

To perform MExFM or MExFS experiments, standard silicon cantilevers are coated with magnetic material. It turns out that usually these coated tips are neither atomically sharp nor magnetically sensitive at the beginning. Therefore, it is necessary to sharpen the tip and to make it magnetically sensitive by inducing strong chemical and magnetic tip-sample interactions to alter the tip apex. Indenting the tip into the surface or scanning at close distances across step edges eventually produces in most cases the desired tip. However, such tips sometimes exhibit an increased dissipation signal, which can be interpreted in terms of adhesion hysteresis. While such *dissipative* tips are sufficient for simple imaging, a correct quantitative evaluation of spectroscopy data requires stable *non-dissipative* tips. It will be shown how stable and unstable tips can be distinguished from each other, by evaluating the dissipation signal (see Fig.1).

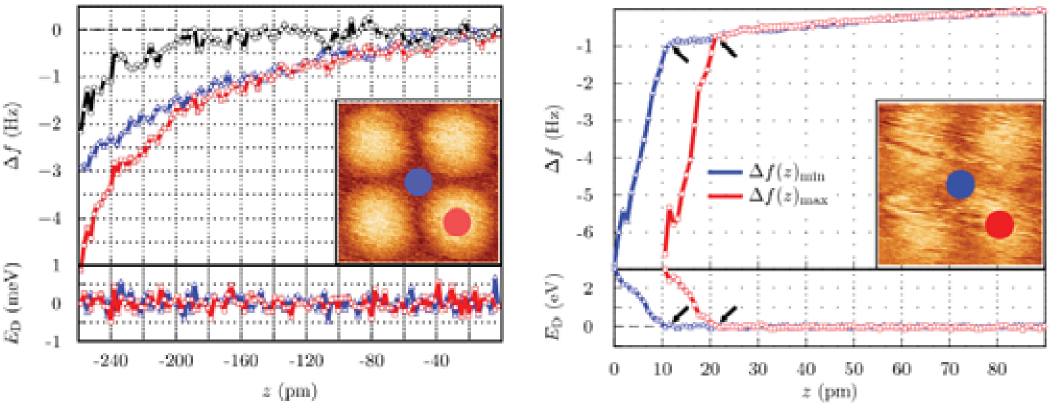

Fig.1: Non-dissipative (left) and dissipative tip (right). Only in the former case extraction of the magnetic exchange interaction is possible via subtraction of spectroscopy curves recorded on sites with opposite spin marked by a blue and a red dot (black curve). Note that the dissipative tip on the right also exhibits more noise in imaging mode (cf. insets).

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Atomic Scale Magnetic Dissipation from Spin-Dependent Adhesion Hysteresis

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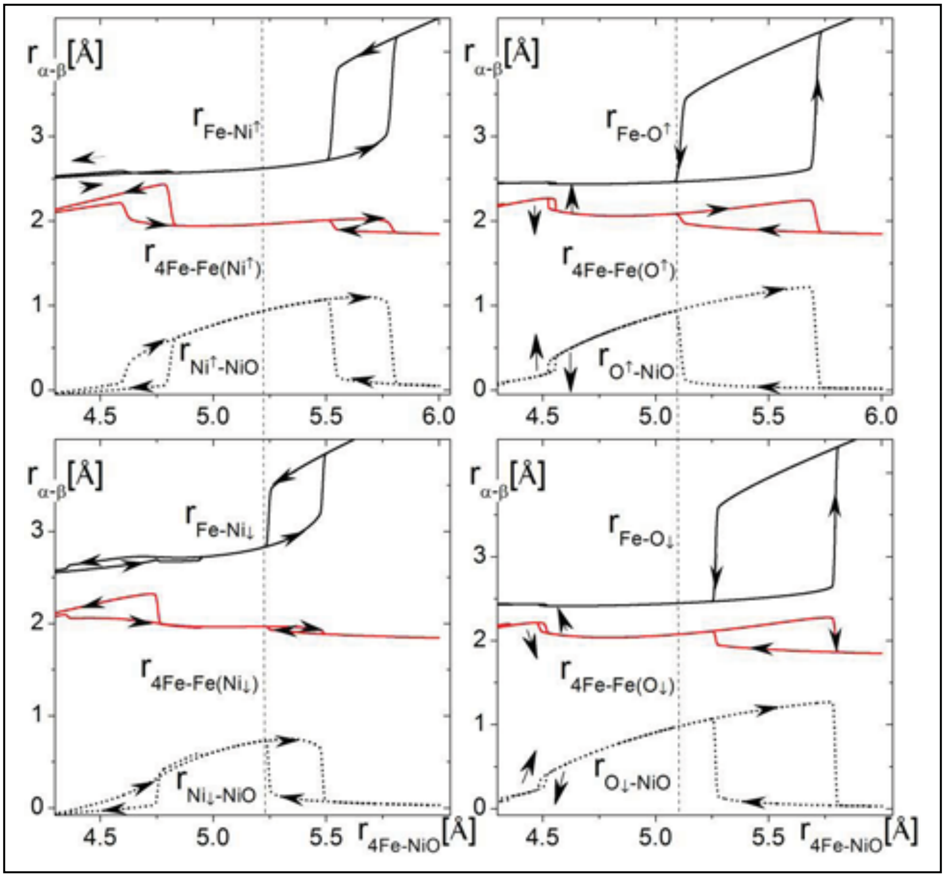
The experimental observation of atomic scale magnetic dissipation obtained by magnetic exchange force microscopy [1] on NiO(001) with an Fe-coated tip is reported. The origin of dissipation signal has been investigated using Monte-Carlo energy minimization technique and compared with experimental results. The calculations predict that the Caldeira-Leggett-type dissipation proposed previously [2] is a special case of the general phenomenon of adhesive hysteresis. According to our calculations the adhesion hysteresis is distance as well as spin dependent and should be measurable not only above magnetic Ni but also on paramagnetic O atoms as demonstrated in figure below. The energy released during binding or the unbinding process may be then dissipated via spin flips or phonons. Considering the simplicity of our theoretical model, the calculated energy dissipation agrees surprisingly well with the measured energy dissipation.



Calculated equilibrium distances between tip and surface atoms. Approach and retrace curves exhibit site, distance and spin dependent hysteresis.

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[2] F. Pellegrini, G. E. Santoro, E. Tosatti, Phys. Rev. Lett. 105, (146103), (2010)

Single vortex manipulation in superconducting $NdFeAsO_{1-x}F_x$

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The motion of magnetic vortices in superconductors leads to undesired dissipation and places severe limits on the critical current J_c in superconducting devices. Vortex pinning challenges, stemming in part from large electronic anisotropy, have severely hampered attempts to incorporate cuprate high T_c superconductors into technology.

The 2008 discovery of high-T_c superconductivity in iron-based materials brought new hope for deciphering general mechanisms of high-T_c superconductivity, as well as for bringing superconductivity into mainstream technological applications. The Fe-based superconductors are more isotropic than the older cuprates. Furthermore, transport experiments on the Fe-based high-T_c superconductors have suggested a strong native pinning mechanism, of yet-unknown origin. Understanding and improving the pinning of quantized magnetic vortices remains an important engineering challenge.

We use a homebuilt low temperature scanning force microscope, shown in Fig. 1, to image and manipulate vortices in single crystal $NdFeAsO_{1-x}F_x$. We can deliberately drag a single vortex to a predetermined position as shown in Fig. 2. Our results help to shed some light on the questions of anisotropy and pinning mechanisms in iron pnictides.

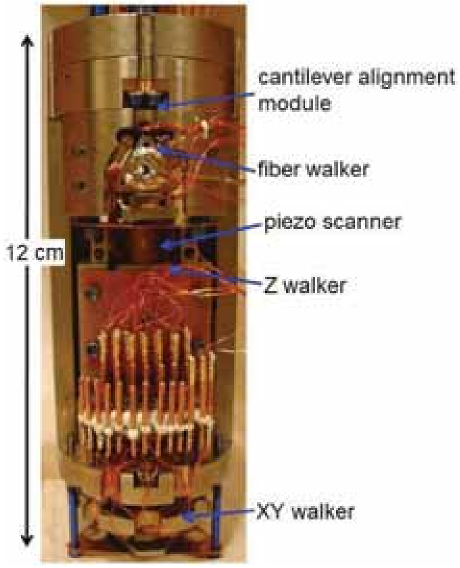

FIG. 1: Photograph of the force microscope head. The microscope is equipped with several piezo walkers, which allow for positioning in xyz direction. The cantilever position is detected via laser interferometry. The microscope is housed on a cryostat which can be operated at temperatures from 2 to 360K. The dewar is equipped with a 5T magnet.

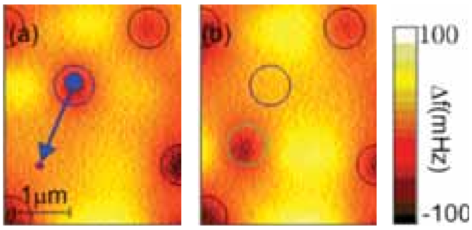

FIG 2: Images of vortex manipulation. (a) Vortices in $NdFeAsO_{1-x}F_x$, imaged with large tip-sample separation (small tip-sample interaction). Subsequently, the vortex marked with the blue circle was deliberately dragged along the blue arrow. (b) Same field of view, after manipulation. The colorscale shows the cantilever frequency shift Δf, which is proportional to the gradient of the force.

Th-01

Exploiting transient non-equilibrium structures for the formation of complex molecular islands on insulating surfaces

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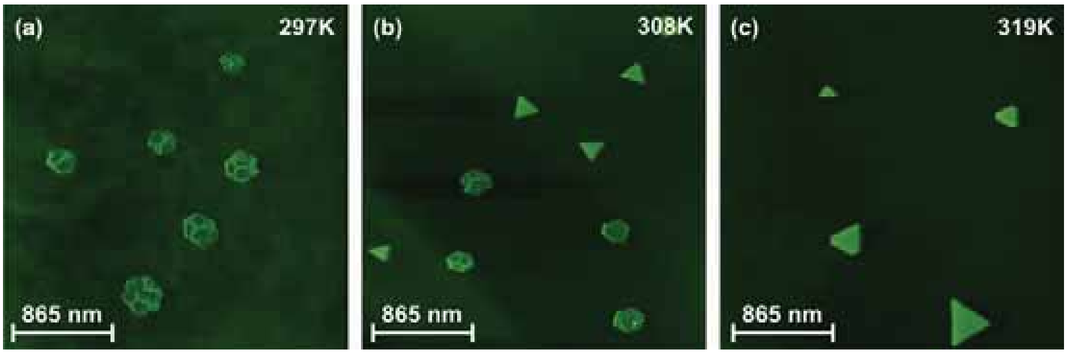
Deposition of fullerenes on the $CaF_2(111)$ surface yields peculiar island morphologies that exhibit close similarities to previous findings for (100) surfaces of other ionic crystals [1,2]. By means of non-contact atomic force microscopy we find a smooth transition from branched hexagonal islands to compact, triangular islands upon increasing the temperature. By developing a kinetic growth model we unravel the microscopic mechanisms of the structure formation [3]. Based on this model, the formation of both islands types can be understood.

Compared to molecular self-assembly on metal substrates, the island morphologies are qualitatively different. The key to understand the characteristic morphology of molecular islands on an insulating substrate is the process of facilitated dewetting. In particular, while a weak molecule-substrate interaction is a prerequisite for dewetting, we unravel that the island shapes are governed by the second-layer occupation rather than by the incommensurability between the structures of molecular islands and the substrate.

Finally, we point out that the complex hexagonal islands originate from a transition of simple non-equilibrium structures that transform into stable islands with complicated morphology by dewetting. This work demonstrates that transient non-equilibrium structures might be deliberately employed for the formation of complex, functional structures on insulating substrates.



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[3] M. Körner et al., Phys. Rev. Lett. in press (2011)

Mechanical switching of single porphyrins investigated with a tuning fork sensor

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Knowledge about the forces needed to lift up, pull or push a nano-object is as primordial as the development of efficient manipulation techniques for future functional devices. Recently, advances in non contact atomic force microscopy (nc-AFM) have demonstrated the detection of “the force needed to move an atom” **[1]** or inner structure of molecules **[2-3]**. Tuning fork based nc-AFM **[4]** is perfectly suited for the detailed investigation of molecules and their elastic properties at the nano-scale.

In this contribution, we show a combined low temperature STM/nc-AFM study of porphyrin equipped with two dicyanophenyl and two *tert*-butylphenyl side groups (Fig. a) **[5]** adsorbed on Cu(111). After adsorption, a “saddle” conformation is observed by STM **[6-8]**. Systematic 3D-spectroscopic force measurements performed above single molecules proved this conformation and revealed local elastic properties of this molecule. We demonstrate that a tip/molecule link can be created allowing controlled manipulations (Fig. b).

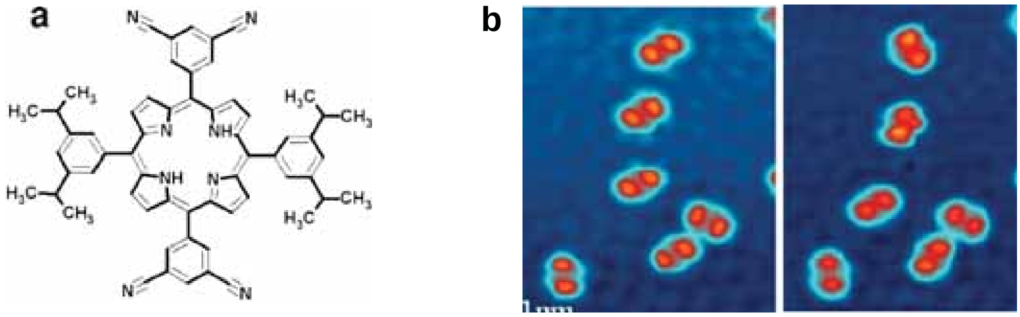

Figure a) *H_2-porphyrin equipped with* with two *meso*-(3,5-dicyanophenyl) and two *meso*-(3,5-di-*tert*-butylphenyl) rings.
Figure b) *STM images showing porphyrin molecules before and after successive manipulations. The molecule adopts after adsorption a “saddle conformation”, (10x14) nm^2 I = 25 pA, V = + 66 mV .*

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[4] F. J. Giessibl, S. Hembacher, H. Bielefeldt and J. Mannhart, Science 289**,** 422, (2000)
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Th-03

Phase transition of a molecular film: Following the rearrangement of a transient molecular structure on calcite $(10\bar{1}4)$

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Molecular self-assembly on surfaces has attracted great attention as a very promising strategy for fabrication of future molecular electronic devices. Consequently, molecular self-assembly has been studied extensively using scanning tunneling microscopy, revealing detailed insights into the processes governing molecular structure formation on metallic surfaces [1]. Future application in electronic devices will, however, require electronic decoupling from the supporting substrate surface, thus, electrically insulating rather than metallic surfaces will be mandatory.

Due to the comparably weak molecule-substrate interaction on insulating surfaces, a process referred to as molecular dewetting has frequently been observed, which is different from the classical growth modes as an initially formed wetting layer transforms into the thermodynamically stable phase though the dewetting process. [2-3].

Here, we present the structural transition of 2,5-dihydroxy benzoic acid on the natural cleavage plane of calcite, studied in ultra-high vacuum by non-contact atomic force microscopy (NC-AFM). Upon deposition at room temperature, 2,5-dihydroxy benzoic acid forms a highly ordered molecular structure. This structure constitutes a transient layer that rearranges into a stable island phase. We have followed this phase transition by NC-AFM over a time period of more than 17 hours, revealing details of the kinetics of the structural rearrangement.

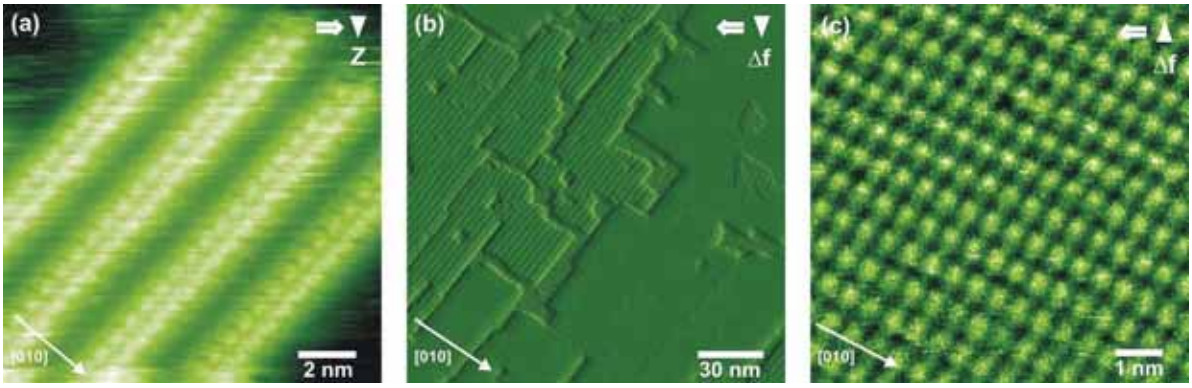

Figure 1: 2,5-dihydroxy benzoic acid molecules on the $(10\bar{1}4)$ cleavage plane of calcite.
(a) Transient structure, (b) overview with both arrangements, (c) stable molecular film.

[1] J. V. Barth Annu. Rev. Phys. Chem. 58, 375 (2007)
[2] S. Burke et al. J. Phys.: Condens. Matter 21, 423101 (2009)
[3] M. Körner et al. Phys. Rev. Lett, in press (2011)

Extended 2-dimensional growth of hexahydroxy triphenylene on KCl

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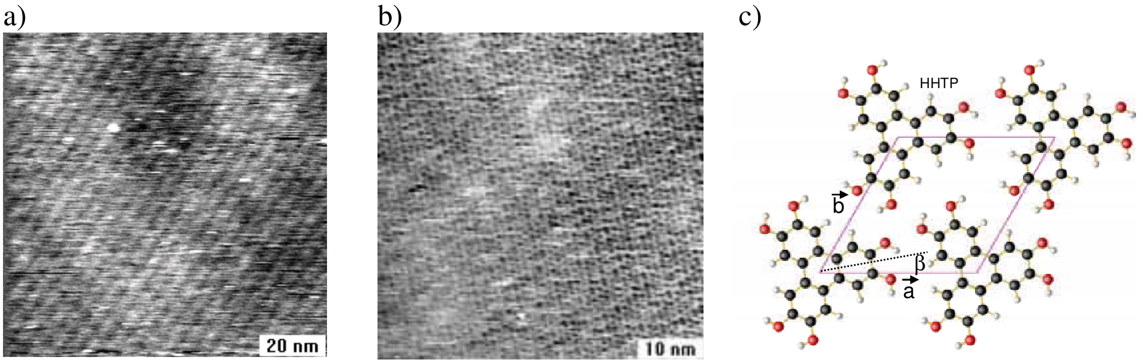
The formation of ultrathin organic layers on insulating substrates is a challenging task since in most cases dewetting takes place (Volmer-Weber growth). In order to facilitate the growth of ultrathin layers, one can either rely on strong molecule-substrate interactions to induce flat-lying molecules by employing metallic or reactive substrates, or strengthen the molecule-molecule interaction by means of directional H-bonds as shown in our recent work, for example [1]. In the present work we report on the formation of an extended 2-dimensional layer (Stranski-Krastanov growth) of 2,3,6,7,10,11-hexahydroxy triphenylene (HHTP) on a KCl single crystal. The first monolayer extends over the whole substrate, is almost defect free, shows a hexagonal ordering (lattice constant 11.7±0.3Å) and forms a “Moiré pattern” with lines that are separated by approximately 48Å (fig. b).

In order to explain why this organic layer shows a 2-dimensional growth with the observed “Moiré pattern”, we compare our experimental data with both, DFT calculations of the freestanding film (SIESTA, fig. c) [2], and large scale energy calculations by means of “Powergrid” [3]. A comparison between our experimental data and the theoretical calculations allows us to draw conclusions about the driving forces and the energies involved in the adsorption process of HHTP on KCl, and to determine the origin of the observed “Moiré contrast”.



Figs. a) and b): nc-AFM topography of the first monolayer HHTP on KCl showing the “Moiré” pattern as well as the hexagonal ordering of the molecules respectively. c) depicts the equilibrium structure of the freestanding film obtained from DFT calculations. a=b=11.6Å, β=17.3°

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[2] P. Ordejón, E. Artacho and J.M. Soler, *Phys. Rev. B,* **53**, R10441 (1996)
J.M. Soler *et al., J. Phys.: Condens. Matter,* **14**, 2745 (2002)
[3] S.C.B. Mannsfeld and T. Fritz, Physical Review B **71**, 235405 (2005)

Th-05

Adsorption and structure formation of organic molecules on $CaCO_3(10\bar{1}4)$ – Impact for molecular self-assembly on insulating substrates

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Bottom-up fabrication of molecular devices, beginning at the single-molecule level, provides utmost control of structure and functionality. Exploiting molecular self-assembly on surfaces bears the potential for fabricating molecular devices with unique versatility and cost-effective production. Consequently, molecular self-assembly has been studied extensively using scanning tunneling microscopy on metallic and semi-conducting surfaces, resulting in well-controlled structure formation with two-, one-, or quasi zero-dimensionality [1,2]. For many applications, however, insulating rather than conducting surfaces are mandatory in order to reduce electronic coupling to the substrate surface. So far, employing molecular self-assembly on insulating surfaces has been hampered by high molecular mobility and dewetting processes, frequently leading to clustering and bulk structure formation at step edges [3,4].

Here, we present a non-contact atomic force microscopy (NC-AFM) study of molecular self-assembly on the $(10\bar{1}4)$ cleavage plane of calcite $CaCO_3$. The deposition of different classes of organic molecules results in a rich variety of ordered, substrate-templated patterns at room temperature. Most importantly, dewetting processes are only rarely observed on this surface.

Our findings demonstrate advantages of using $CaCO_3(10\bar{1}4)$ over other insulating surfaces when studying molecular adsorption. Reasons for this accomplishment will be discussed and they will be related and adapted to other insulating surfaces.

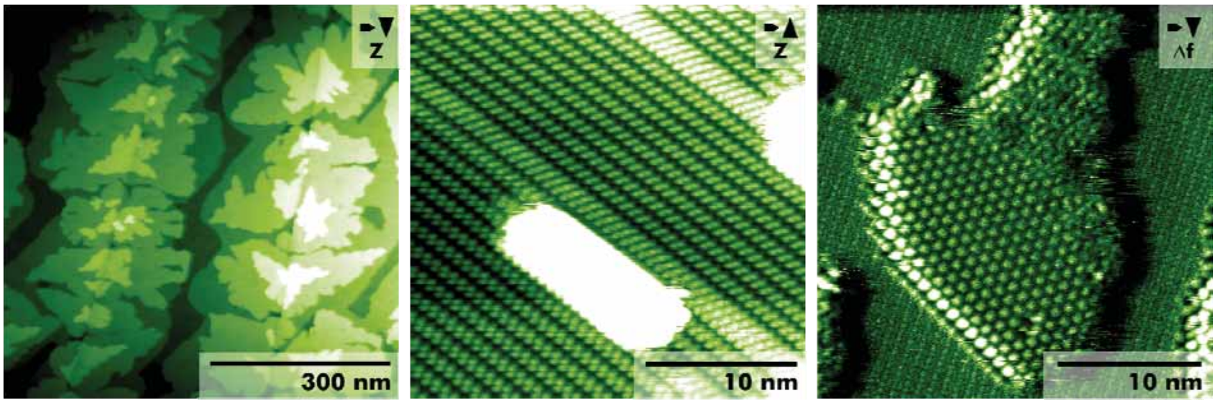

Figure 1: Self-assembly of different organic molecules on $CaCO_3(10\bar{1}4)$ surfaces studied by NC-AFM. (a) C_{60} fullerene, (b) terephthalic acid, (c) trimesic acid.

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[4] S. A. Burke et al., J Phys: Cond Mat 21, 423101 (2009)

A comparison of quartz force sensors for scanning probe microscopy based on tuning forks and length extensional resonators

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[2]NAKAJIMA Project, ERATO, JST, 3-2-1 Sakato, Takatsu-ku, Kawasaki 213-0012, Japan
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The force sensor is key to the performance of atomic force microscopy (AFM). Nowadays, most AFMs use micro-machined force sensors made from silicon, but piezoelectric quartz sensors are applied at an increasing rate, mainly in vacuum. These self sensing force sensors allow a relatively easy upgrade of a scanning tunneling microscope to a combined scanning tunneling/atomic force microscope. Two fundamentally different types of quartz sensors have achieved atomic resolution: the needle sensor that is based on a length extensional resonator and the “qPlus sensor” that is based on a tuning fork. Here, we calculate and measure the noise characteristics of these sensors. We find four noise sources: deflection detector noise, thermal noise, oscillator noise and thermal frequency drift noise. The first three noise sources are inversely proportional to amplitude. Thermal drift noise is independent of the amplitude, proportional to the spring constant of the sensor and roughly proportional to $1/f_{\mathrm{mod}}$. Finally, we suggest how the signal-to-noise ratio of the sensors can be further improved and briefly discuss the challenges of mounting tips.

[1] Franz J. Giessibl, Toyoaki Eguchi, Florian Pielmeier, Toshu An, Yukio Hasegawa
http://arxiv.org/abs/1104.2987

Probing Local States with the Phantom Force

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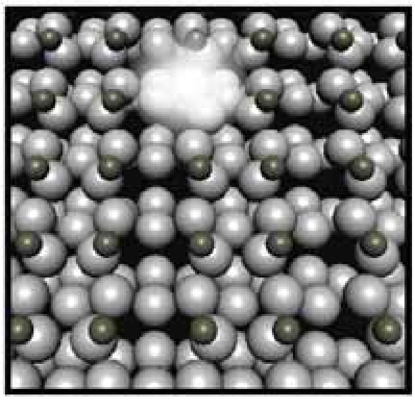
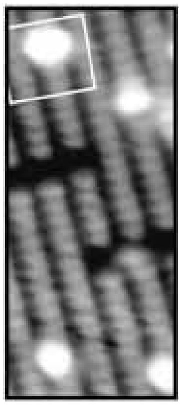
We have recently reported upon an apparently repulsive force when performing simultaneous AFM and STM above a semiconductor [1]. We described this phantom force in terms of the voltage drop near the tip-sample junction due to the tunneling current, and thus as a decrease in the attractive electrostatic force. In our simple model, the effect is highly localized (~1Å) and should therefore be able to probe local charging effects in heterogeneous samples.

One of the most common defects on a H-saturated Si surface is a missing H-atom, resulting in an unsaturated Si dangling bond. It has been previously shown that these dangling bonds on highly-doped Si(100) can be used as quantum dots to explore the physics of interacting quantum dots, even at room temperature [2]. Their localized nature makes this surface ideal for exploring the charge carrier dynamics we are able to probe with the phantom force. We report upon the local phantom force we are able to observe on this surface, and how it relates to our model.



When one H atom is missing above a Si adatom on the hydrogenated Si(100) surface, a localized electronic state is created (shown as a white cloud, left). This state can be easily observed in STM data (right, with a white box corresponding to the area shown in the left figure) and has a distinct Phantom Force signature observable with simultaneous AFM/STM.



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Combined NC-AFM and STM investigations of individual molecules adsorbed on ultrathin insulating films using functionalized tips

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The contrast mechanisms of noncontact atomic force microscopy (NC-AFM) and scanning tunnelling microscopy (STM) using functionalized tips are discussed for the case of individual organic molecules.

Using atomic manipulation, the tip of an AFM or STM can be functionalized in a controlled manner. As a result the contrast can be increased, and even more important the interpretation of images benefits from the knowledge of the chemical composition of the tip apex [1]. On the one hand, by using NC-AFM with CO terminated tips, atomic resolution has been demonstrated and the contrast mechanism was assigned to the Pauli repulsion [2,3]. On the other hand, by using STM and by decoupling the molecules from the metallic substrate by an ultrathin insulating film, the molecular frontier orbitals, i.e. the highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO), could be mapped and the resolution could be increased by tips functionalized with organic molecules [4]. Thus, combining AFM and STM, complementary information could be obtained (see Fig. 1).

We will present results measured with metal and CO terminated tips on pentacene and naphthalocyanine molecules adsorbed on bilayer NaCl grown on Cu(111) using a tuning fork STM/AFM system at 5 K.

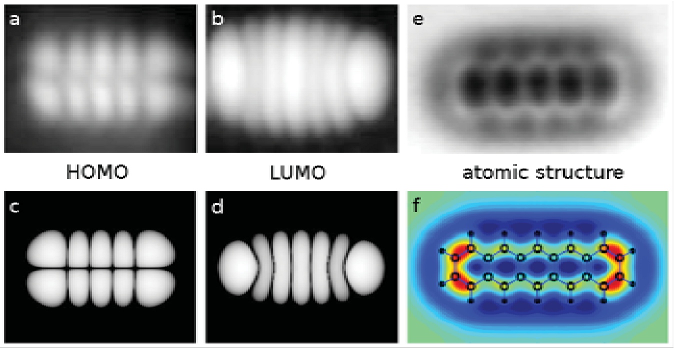

Figure 1: Pentacene on bilayer NaCl on Cu(111). (a), (b) Molecular orbital images obtained by STM using a pentacene terminated tip compared to (c), (d) calculated contours of constant orbital probability distribution [4]. (e) NC-AFM image using a CO terminated tip [2] compared to (f) DFT calculations [3].

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Th-09

Atomic Force Maps on Epitaxial Graphene

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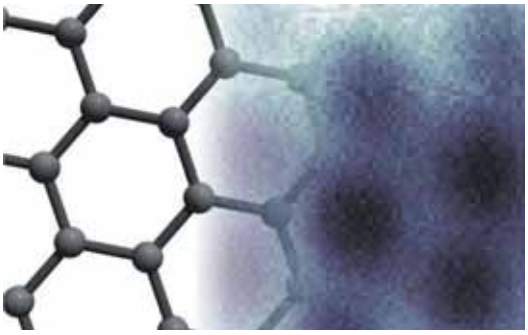
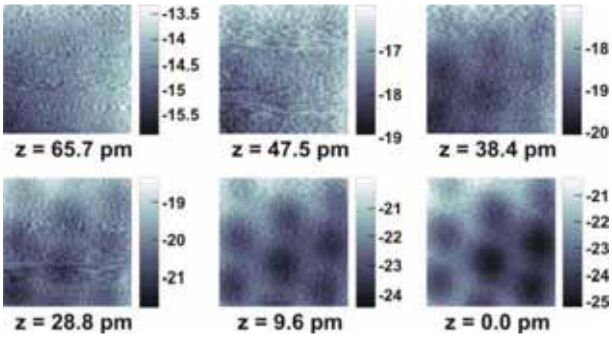
Graphite and carbon nanostructures have been studied intensively with the atomic force microscope [1, 2, 3, 4] and basically two image patterns are reported. Results obtained in non-contact topographic mode [1] usually show spots of larger apparent height arranged in a hexagonal lattice. These sites are referred to as the hollow site of the lattice [2]. In a constant height measurement [3] and in images obtained with a higher flexural mode of the cantilever [4], hexagons which represent the honeycomb lattice are observed. In a recent theoretical study [5] the influence of the reactivity of the tip cluster on the observed image pattern is discussed. For metal tips the calculations predict that atomic contrast can be obtained due to attractive short-range forces.

We performed measurements on epitaxial graphene grown on SiC [6] at both room and low temperature and with two different tip materials (tungsten and beryllium). The presented Δf maps show the evolution of atomic contrast with decreasing tip-sample distance. All images, recorded with different tip materials and at different temperatures, resolve the honeycomb lattice representing the carbon-carbon bonds. Additionally, the carbon rings always appear less attractive (less negative Δf) than the background which is consistent with results obtained on pentacene [7]. Therefore, we claim that atomic contrast on graphene is only obtained due to short-range repulsive forces and attractive forces only lead to a background.





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Quantitative atomic force microscopy with CO terminated tips

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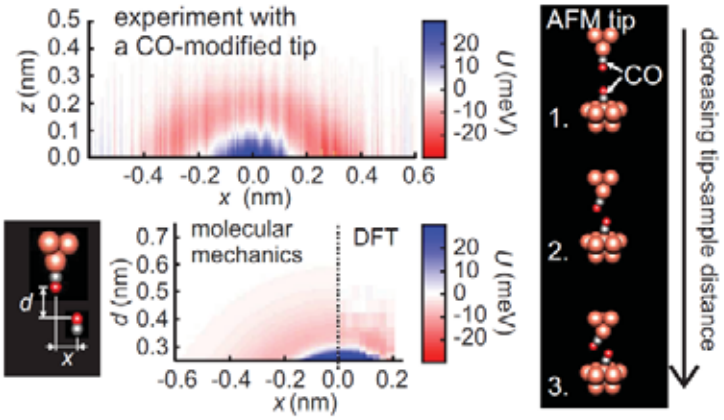
Non-contact atomic force microscopy (nc-AFM) has recently progressed tremendously in achieving atomic resolution imaging through the use of small oscillation amplitudes and well-defined modification of the tip apex. In particular, it has been shown that picking up simple inorganic molecules (such as CO) by the AFM tip leads to a well-defined tip apex and enhanced image resolution [1]. This has allowed, for example, atomic resolution imaging of individual organic molecules [1, 2].

Here, we use the same approach to experimentally study the three-dimensional intermolecular interaction potential between two molecules and focus on the implications of using molecule-modified AFM tips for microscopy and force spectroscopy experiments [3]. The measured interaction energy between two CO molecules (one adsorbed at the AFM tip and the other on the Cu(111) substrate) closely follows the calculated interaction energy between two isolated CO molecules (Figure, left). However, at close tip-sample distances, chemical repulsion between the CO molecules can cause atomic reconfiguration (Figure, right), which limits the achievable resolution both in imaging and force spectroscopy. These effects are expected to be general and occur in all nc-AFM experiments employing molecule-terminated tips.



Left: Measured (top) and calculated (bottom) interaction energy between two CO molecules. Right: Increasing repulsive interaction causes reconfiguration of the CO molecules at small tip - sample distances.

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POSTER SESSION I ABSTRACTS

Atom-resolved NC-AFM studies of polar surfaces of insulating metal oxides

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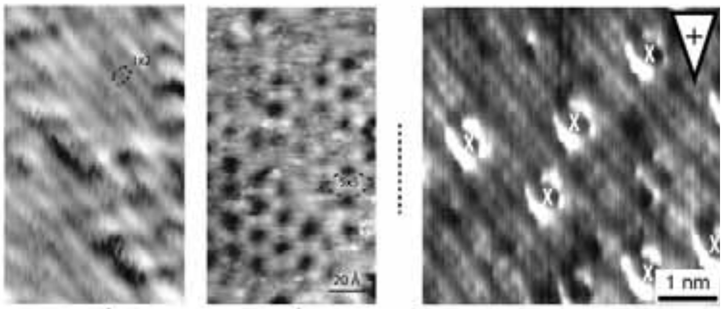
Polar metal oxide surfaces formed by crystal truncation are unstable due to a diverging surface dipole, and the surface must therefore be compensated by adopting a modified or reconstructed surface [1]. For insulating metal oxides, the field remains very poorly explored experimentally, but with atom-resolved NC-AFM it is possible to provide new atomic-scale understanding. Here I will demonstrate how NC-AFM has been successfully applied in the determination of the atomic-scale structure of two pronounced polar surfaces, namely the O-terminated ZnO(000) and $MgAl_2O_4(100)$. NC-AFM imaging of O-terminated ZnO(000) reveals that the surface at room temperature adopts a (1×2) striped surface attributed to a regular structure of OH groups on the ZnO(000) lattice. Calculations show that this structure reflects 0.5ML of adsorbed H which fully compensates the polarity. At elevated temperatures, above 300°C, H begins to desorb, and to uphold a non-polar configuration the ZnO undergoes a reconstruction reflected by a (5×5) structure and, at higher temperatures, a (2×2) surface reconstruction composed of patches with alternating wurtize and an unusual zinc-blende ZnO stacking. The findings are supported by NEXAFS spectroscopy and DFT calculations, and interestingly show that the stabilization mechanism for ZnO(000) is in distinct contrast to the morphology-driven stabilization previously observed to be predominant on the opposite Zn(0001) surface [2]. In the case of polar $MgAl_2O_4(100)$, complementary tip-dependent NC-AFM images could be obtained with both negatively (O-terminated) or positively (Mg-terminated) charged tips, which revealed the structure of the surface cation and oxygen lattices, respectively. The surface is in this case shown to be O and Al terminated. NC-AFM images, however, also reveal a distinct atomic defect type shown to be so-called Mg-Al antisites formed by an interchange of surface Al and Mg in the subsurface. Surprisingly, the antisite formation is calculated to be very favorable, and the antisites therefore contribute to an overall stabilization of the otherwise polar $MgAl_2O_4(100)$ surface [3].



ZnO(000$\bar{1}$) (RT) ZnO(000$\bar{1}$) (450°C) $MgAl_2O_4(100)$ (RT)

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Investigation of TiO_2 (110) by AFM/STM with the Tungsten-Coated Tip

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Rutile(110) is the most stable crystal face and has been extensively studied during the past decades. AFM images of the TiO_2 (110)-(1×1) surface were classified into several modes, because in the scanning process the silicon tip apex was spontaneously attached with positive, negative, neutral and other atoms on the surfaces[1-3], which bring much confuse on interpreting the images.

In this study, we performed the simultaneous AFM and STM experiments to clarify the electric polarity of tip termination. Furthermore we performed force-spectroscopy and current-spectroscopy to make clear of the distance dependence of force and local density state.

In the experiment, the tungsten coated tip was chosen for avoiding the influence of silicon tip apex change on the imaging modes. The TiO_2 (110) surface was prepared by repeated cycles of sputtering and cleaning and it was observed at the constant height mode. The measurement procedures are as follows: first, the contact potential difference was compensated by applying the bias voltage to reduce the electronic force, next the thermal drift was compensated by atom tracking, then the force and current spectroscopy was performed on different atom sites.

When the tip approached the surface gradually, the AFM images pattern were almost same, while the STM images pattern changed a lot, that is in the AFM image, the bridging oxygen atom in the frequency shift image was always bright, in contrast, in STM image except the titanium atom was always bright, the deficiencies both the hydroxyls and the oxygen vacancies disappeared gradually. The unchanged oxygen and titanium atoms verified the unchanged tip termination. The surface atom force/current spectroscopy proved the distance dependence of force/current image variation.

So the simultaneously operated AFM and STM with the tungsten coated tip can overcome the limitations of AFM or STM, it can detect uniform atom contrast and is especially useful for the transition metal oxides.

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AFM/STM Simultaneous measurement on Cu (110)-O with metal-coated cantilever

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Atom/molecular manipulation is an innovative technique in nanotechnology. Recently, manipulating single atoms and molecular using NC-AFM has attracted many groups because it can detect the driving force involved in manipulation directly.

In previous experiments, we have succeed in imaging and manipulating atoms on Cu(110)-O surface. Adsorption super copper can be observed as bright spots by the Cu-terminated tip apex, while oxygen atoms can be observed as protrusion by the O-terminated tip apex. In the case of Cu-terminated tip, the super Cu atom on the surface was pulled by attractive force at a lateral tip position; in contrast, in the case of O-terminated tip, the super Cu atom was pushed by repulsive force over the top of the Cu atom. However, we doubted about the tip apex species of the Si cantilever, and these results were also different from that of the STM experiments [1].

In this experiment, in order to explain this inconsistence, we investigated the tip apex species dependence of atomic resolution of the Cu(110)-O surface by simultaneous measurement of STM and NC-AFM at 75K. W-coated Si cantilever was used to keep the tip apex stable and to realize simultaneous measurement. In detail, by controlling the frequency shift as the feedback, first, we could control tip apex species of the cantilever, second, atomic resolution of Cu(110)-O surface was observed by tip apex soft touching the sample surface, after that we switched off the feedback and constant height method was performed, frequency shift images and averaged tunneling current images was observed simultaneously using the same tip apex. The tip-surface separation, bias dependence of frequency shift and tunneling current were recorded, and oxygen and Cu atoms of the Cu(110)-O surface were separately recognized by frequency shift and tunneling current images. Relationship between the force and the tunneling current was also investigated according to the experiment results.

In summary, simultaneous measurement of tunneling current can give a comprehensive answer to identify atom species on the Cu(110)-O surface with W-coated Si tip which can be used to fully understand the experiments difference obtained by STM or NC-AFM.

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The charge state of steps on cleaved CaF_2 studied by NC-AFM and KPFM

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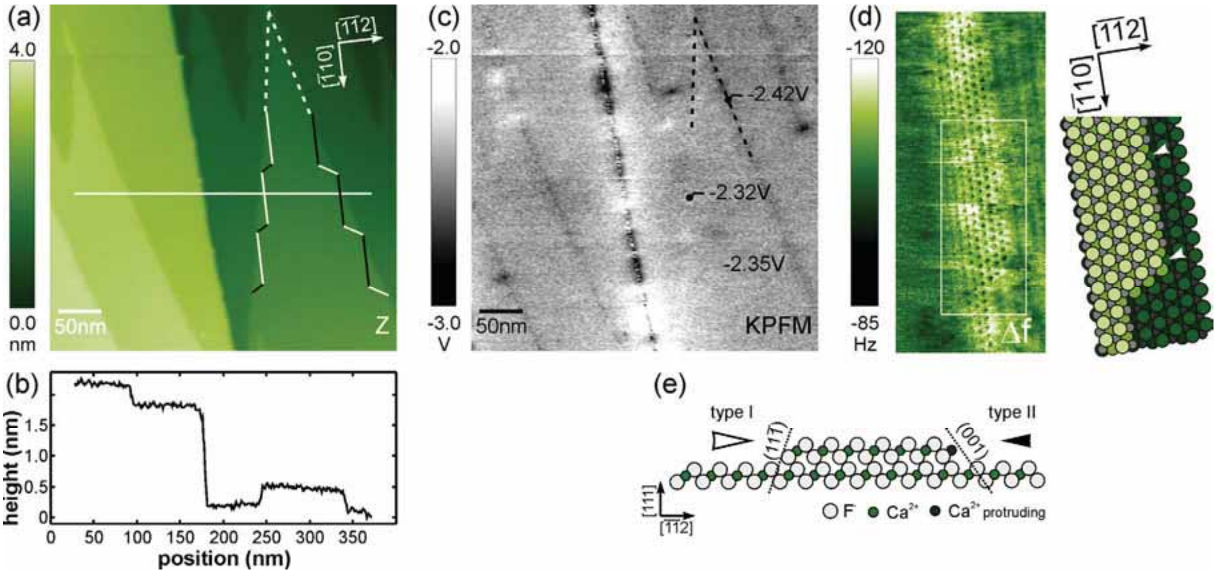
Step edges and kinks that are non-equilibrium structures on a cleaved $CaF_2(111)$ surface are investigated by non-contact atomic force microscopy (NC-AFM) and Kelvin probe force microscopy (KPFM). NC-AFM permits imaging insulating surfaces with atomic resolution [1] whereas KPFM images the distribution of surface charges and dipoles on insulating surfaces [2]. Step edges generally form acute angles with each other but do not have uniform directions. High resolution NC-AFM imaging yields, however, that they are composed of sections following the <110> directions and, thus, exhibit alternating type I and type II steps. The surface potential determined by KPFM at ledges having a high amount of type I step edges exhibits a slightly enhanced potential while the potential of type II ledges is reduced by 70 mV with respect to the potential of the stoichiometric terrace. This points to an overall positive net charge present at ledges. We propose that the positive charge stems from low coordinated Ca^{2+} ions present at type II ledges and confirm this by atomically resolved NC-AFM images revealing the Ca^{2+} ion sub-lattice with *repulsive-mode* imaging contrast [3].



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P.I-05

Classification for the NC-AFM contrast formation on $CaCO_3(10\bar{1}4)$

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Calcium carbonate ($CaCO_3$) is one of the most abundant simple salts in nature. It is found in the shells of mollusks such as slugs or sea shells. Together with an organic phase, it forms materials with both, outstanding material properties and amazing elegancy. Consequently, these biominerals have attracted much attention during the last decades, with the goal to understand and mimic the formation processes [1].
The $(10\bar{1}4)$ surface of calcite is the most stable cleavage plane and has been studied by means of low-energy electron diffraction, X-ray photoelectron spectroscopy and atomic force microscopy [2,3]. A detailed understanding of the fundamental $(10\bar{1}4)$ surface properties is of great importance in the context of molecular adsorption.

Two surface characteristics, namely row-pairing and the (2×1) reconstruction, have often been observed and are subject to controversial discussions. Using NC-AFM, we recently presented distance-dependent data clearly revealing the (2×1) reconstruction [3]. However, these and other surface characteristics manifest themselves in a large variety of contrast patterns, depending on the tip condition and the tip-surface distance.
In this study, we present a large number of different contrast patterns observed in NC-AFM imaging of $CaCO_3(10\bar{1}4)$ surfaces. A systematic classification scheme is introduced and relations to surface characteristics are discussed. The distance dependence for some of these contrasts are analysed using high-resolution NC AFM data acquired in the 3D AFM mode at room-temperature, using our newly developed atom-tracking system [4].

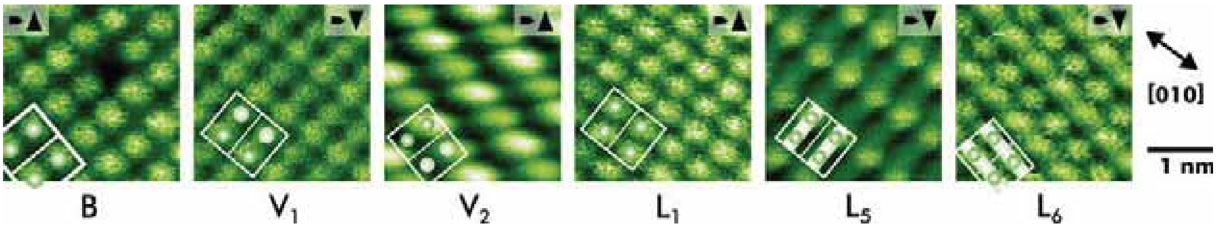

Figure 1: Some of the NC-AFM contrast patterns observed on $CaCO_3(10\bar{1}4)$ surfaces. Labels B to L_6 refer to the introduced classification scheme. All images represent NC-AFM frequency shift (Δf) raw data.

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Scanning Probe Microscopy on Organic Layer Compound Crystals

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The inorganic $[Cu(C_2O_4)_2]^{2-}$ complex forms a polar two dimensional structure stabilized by two surrounding organic layers of benzylammonium [1]. We performed Scanning Probe Microscopy studies in contact and non-contact mode in ultra high vacuum on this organic layer compound crystal surfaces. The measurements revealed the exceptional quality of the benzylammonium crystal surface forming a robust and regular molecular arrangement on several 100 nanometer wide and molecular flat terraces. Single molecular defects in the surface can be imaged in non-contact as well as using the contact mode which gives evidence for extremely small contact areas. The highly ordered arrangement of the benzylammonium molecules virtually sticking out of the surface with two distinct orientations was analyzed with single molecular resolution [2]. High resolution friction maps and non-contact AFM measurements are presented showing the molecular asymmetry. Using multi-modal dynamic spectroscopy techniques we get deeper insights into dynamic processes of the molecules on the surface which helps to understand basic friction processes.

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Changes in Morphology and Electronic Structure of MgO on Mo(001)

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Morphology and electronic structure of oxide surfaces play an important role in surface reactions. In catalysis oxides are often present either as catalyst or as support. An insight into the chemical reactions on the oxide surface can be gained by characterizing the local charge state and morphology of defect sites at the atomic level.

The main tool we use is a dual microscope combining frequency modulation dynamic force microscopy (FM-DFM) with scanning tunneling microscopy (STM). Since our custom-made sensor can be operated in both modes simultaneously, the same site can be characterized by FM-DFM and STM [1]. This provides atomically resolved complementary information about morphology and electronic properties of local surface sites. The setup is operated at low temperature and ultra-high vacuum to ensure stable operation conditions.

Our group already investigated the local charge state of individual point defects on thin MgO films on Ag(001). We were able to characterize the charge state of electron trapping sites, i.e. color centers and of morphological defects such as divacancies [2].

Following the previous studies we want to use our versatile microscope to characterize the change in morphology and electronic structure of the oxide surface with respect to the transition from a thin film to a bulk-system. For this study we use MgO on Mo(001) as a model system for catalysis. By tuning the metal/oxide interactions with increasing film thickness we want to understand fundamental phenomena. In this investigation the potential of FM-DFM, especially in the transition region of the film system, is used to characterize the model system.

We present results from a preliminary growth study of MgO on Mo(001). Here, the thickness transition is investigated with low energy electron diffraction (LEED) as well as FM-DFM.

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P.I-08

Stable Contrast Mode on TiO_2 (110) Surface Using AFM with Tungsten-coated Tips

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In recent years, non-contact atomic force microscopy (NC-AFM) in ultrahigh vacuum (UHV) is widely used in catalyst field due to its ability of imaging insulator surfaces with true atomic resolution. Many NC-AFM experiments have been carried out on TiO_2 (110) surface and different atomic contrasts which are classified into positive, negative, neutral, all-inclusive and hidden modes have been observed [1-4]. These modes are explained by the effects of easy structural relaxations and tip terminations because Si have low binding energy and hence the structure of Si tip apex easily changes [2]. Therefore, it is necessary to avoid the ambiguous imaging modes on TiO_2 (110) surface.

In this presentation, we propose the method to solve the problem of different atomic contrasts by coating the Si tip with mechanically very strong tungsten (W) thin film. In the experiments, the Si tip was coated with W thin film by using Ar ion sputtering. The thickness of the W thin film is about 3-5 nm [5]. This method can be processed in the sample processing chamber, and it is possible to transport it to the AFM chamber without polluting the tip. We find that W-coated tip is stable unlike Si tip, and it can provide the stable atomic contrast without ambiguous on TiO_2 surface (Fig.1 (a)). Here, the image corresponds to “neutral mode”, namely, O rows on TiO_2 (110) appear bright, the Ti rows appear dark, and the OH defects appear brightest in neutral mode on TiO_2 surface.

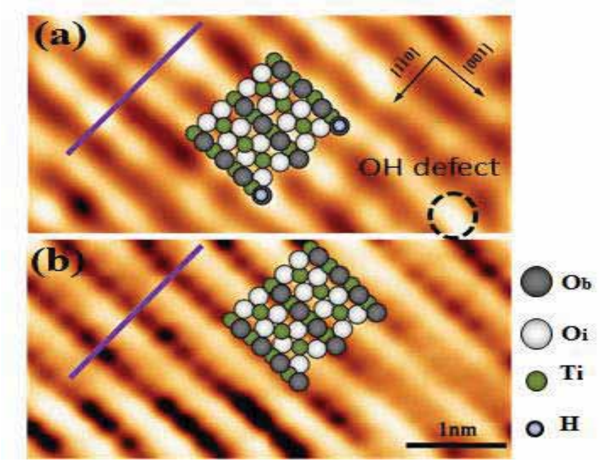

Fig. 1 (a) AFM and (b) tunneling current images on TiO_2 (110).

Our results support that the chemical nature, structure and the foremost atom of the tip apex directly affect the formation of atomic contrast, and W-coated tip can provide chemical resolution at ionic crystal surfaces [6]. Furthermore, we demonstrate that the AFM/STM simultaneous measurement by W-coated tip.

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Growth and work function studies of NaCl thin films on silver

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Sodium chloride thin films on metal surfaces are important thin film systems, which are used to decouple the intrinsic electronic properties of atoms, molecules and clusters from metal surfaces [1,2] as well as reducing the work function of a metal surface [3]. Hence it is crucial to understand the growth at the interface to characterize the physical properties of such systems.

In this work, the morphology of NaCl thin films deposited on Ag(001) surfaces has been characterized in ultrahigh vacuum by noncontact atomic force microscopy (NC-AFM) and Kelvin probe force microscopy (KPFM) as a function of substrate temperature. As previously observed for MgO/Ag(001) [4], NaCl deposition on the Ag sample at 373K leads to a higher density of islands one mono-layer (ML) thick. As the temperature is increased, the density decreases and the islands grow predominantly as multi-layered islands with their average size increasing. Islands of up to 500 nm in size can be grown which stands in strong contrast to the MgO thin film system (max size: 15 nm for 1ML nominal film thickness) [4]. Local work function variations monitored by Kelvin probe force microscopy (KPFM) show that the NaCl islands exhibit a strong dark Kelvin contrast with respect to the Ag substrate as soon as the first ML is formed. This corresponds to the expected reduction of the work function of the silver surface by the NaCl film [3]. A clear tip-sample distance dependency in the Kelvin contrast is observed.

The NaCl film morphology, the surface work function of silver in dependency on the thickness of the NaCl islands but also the distance dependency of the Kelvin voltage will be discussed in the contribution.

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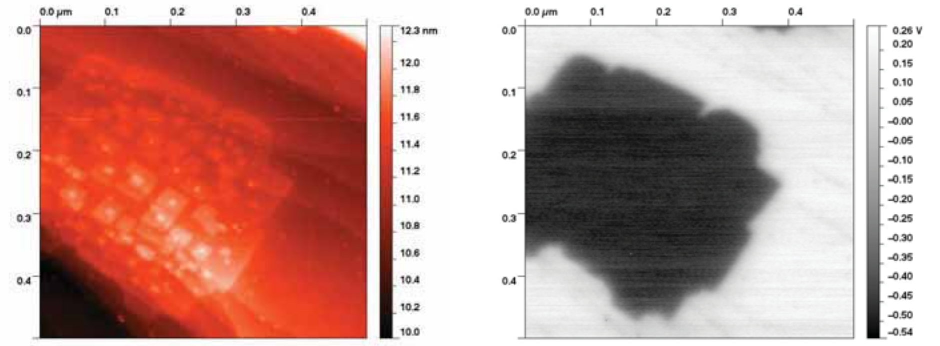

Figure 1. Topography image (left) and corresponding KPFM image (right) of a NaCl thin film deposited on Ag(001). (500 x 500 nm^2).

P.I-10

Scanning Kelvin Probe Microscopy for C_{60}/TiOPc Molecular Interfaces

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One challenge for increasing the efficiency of organic photovoltaics is to understand the barrier to exciton separation that exists at the interface between organic molecules. Small molecule organic donor-acceptor heterojunction systems such as C_{60} and TiOPc present an ideal system for characterizing interface effects due to their facile deposition and ordered self-assembly.[1,2]

We employ UHV AFM (atomic force microscopy) and KPFM (Kelvin probe force microscopy) to obtain simultaneous images of the potential and topographic landscapes at the interface between submonolayer C_{60}, a good electron acceptor, and honeycomb phase TiOPc, an organic with high hole mobility, on Ag(111). This technique allows for high spatial resolution of both the potential and the topography. The statistically averaged work function differences for C_{60} on Ag(111) and C_{60}/TiOPc on Ag(111) are found to be 27 +/- 11 mV and 207 +/- 66 mV, respectively. Additionally, a direct measurement of the step edge dipole is made on Ag(111).

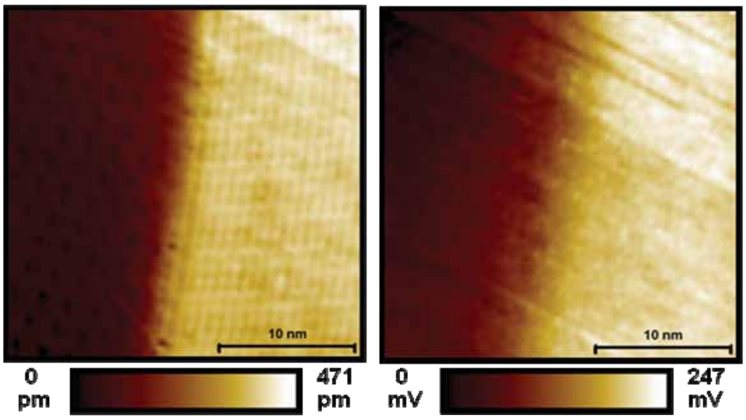

Figure 1: AFM topography (a) and KPFM potential (b) for domains of sub-monolayer C_{60} (right) and sub-monolayer honeycomb phase TiOPc (left) on a Ag(111) surface.

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Scanning Kelvin Probe Microscopy of Graphene-Supporting Substrates

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Many transport properties of graphene on SiO_2 are well-described by Coulomb scattering of charge carriers, if one assumes a (2D) distribution of impurity charges (10^{11} – 10^{12} cm^{-2}) at a distance ~ 1 nm from the graphene [1]. This varying potential from random charges causes the carriers to arrange into a collection of electron and hole "puddles", at lengths ~ 20 nm.

However, a definitive measurement of this charge density has been lacking. Earlier results using a scanning single-electron transistor (SET) [2] were resolution-limited at a length scale ~ 150 nm, and consequently obtained a lower estimate of the potential variation. STM/STS detects the presence of scattering centers below the graphene [3], but does not probe electrostatic potential directly and cannot image the bare (insulating) substrate. Here, we present results of UHV Kelvin-probe microscopy obtained in non-contact mode. We map the surface potential of SiO_2 from few-nm to few-micron length scale, bridging the gap between STM and SET measurements and revealing rms potential variation ~ 100 mV. This is quantified using an analytic model of randomly distributed charges of density n, along with simulation of potentials for random charges with both 2D and 3D distributions. Our results indicate a (2D) charge density ~ 3 x 10^{11} cm^{-2}, providing strong evidence for Coulomb scattering as the dominant influence of electronic transport in SiO_2-supported graphene. In combination with measurements on other substrates, this suggests that measurements of inhomogeneity in substrate surface potential may be *predictive* for electronic mobility in graphene devices.

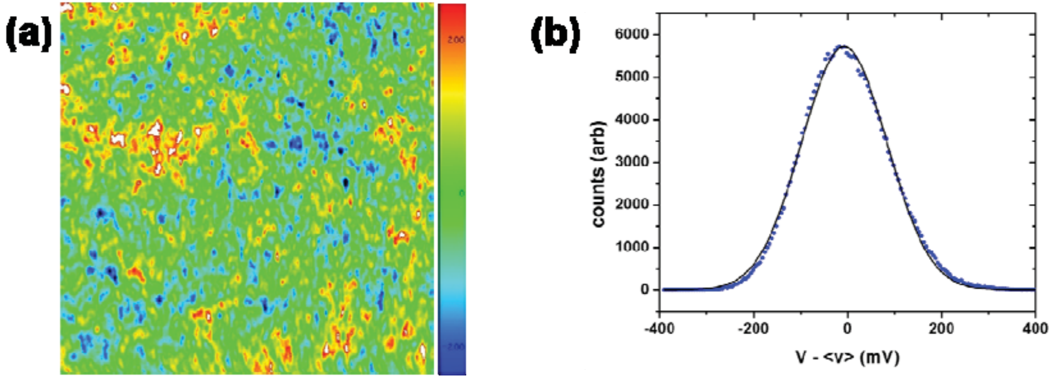

Figure 1: (a) SKPM potential map of SiO_2 surface in UHV, image size 3.128 x 3.128 μm. **(b)** Histogram of surface potential, with standard deviation σ ~ 100 mV.

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*Work supported by UMD NSF-MRSEC under DMR 05-20471 and U.S. ONR MURI.

P.I-12

A NC-AFM and KPFM study of a triphenylene derivative on KBr(001)

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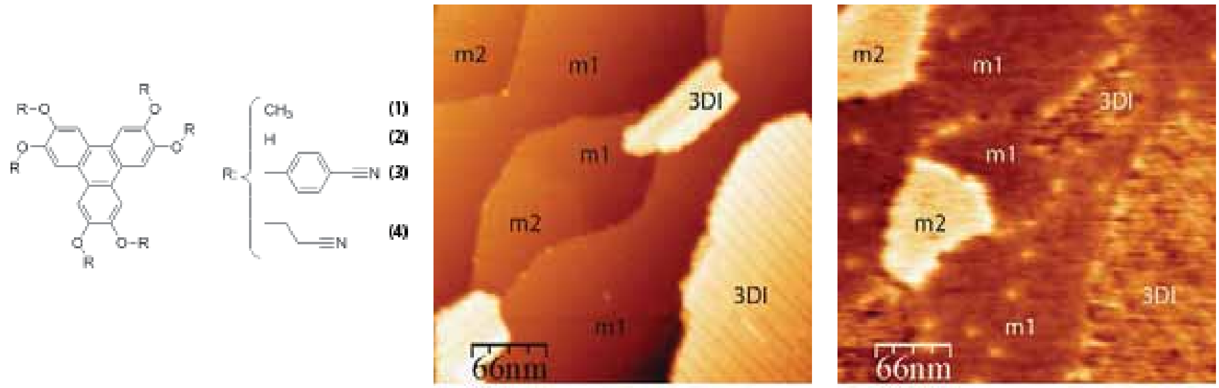
We have started a program aimed at imaging single molecules on the surface of a bulk insulator at room temperature. This task is essential to the goal of connecting a molecule to metallic electrodes in a planar geometry to build a single molecular device [1]. One of the major difficulties in this task is to immobilize the molecules. The diffusion barrier of most molecules on usual insulating surfaces is generally quite low making room temperature diffusion too fast for imaging. In this study KBr(001) was chosen as a substrate for its ease of preparation and the relative facility for atomic resolved imaging. On this ionic substrate, the molecule-surface interaction is usually dominated by electrostatic forces.

Our approach consists in equipping a flat, aromatic triphenylene molecular core with different peripheral polar groups, as shown in fig. 1a. Results on molecule (1) [fig. 1a] are reported in a recent publication [2]. In the following, we present our results for molecule (4) where 6 - oxygen-propyl-nitrile legs are connected to the triphenylene core. It was demonstrated recently that nitrile groups are suitable for adsorption on KBr(001) due to their strong dipolar character [3].

Molecule were deposited on the cleaved (001) face at room temperature. The surface was examined from submonolayer to multilayer coverage and after annealing to increasing temperature from 350K to 420 K. Different structures are observed:

- -isolated molecules or few molecules clusters,
- -two types of monolayer structure that are nearly indistinguishable on the topography but give a strongly different contrast in KPFM (m1 and m2 in fig. 1b and c),
- -nanometer high structured 3D islands (3DI in fig. 1b and c).

The complementary between these topographical and Kelvin data will be used to suggest structural models for these different structures.



(a) (b) (c)

Figure 1

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[2] A. Hinaut et al, accepted to J. Phys. Chem. C. (2011)
[3] B. Such et al, ACS Nano, 4, (3429), (2010)

Kelvin probe force microscopy on single and bilayer graphene

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Layers of graphene are grown on SiC(0001) samples by means of thermal decomposition in Ar [1]. The resulting structure consists of atomically flat terraces of SiC with a width of hundreds of nanometers, covered with single and bilayer patches of graphene. Zero, single and bilayer coverage can be identified by Kelvin force microscopy [2]. The correlation between topography and contact potential will be presented in a novel fashion which allows a direct analysis of the combined surface structure of substrate and graphene film. Contact potential contrasts other than the well-known 135 meV between first and second layer will be discussed with respect to lateral resolution effects.

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[2] T. Filleter et al. , Appl. Phys. Lett., 93, (133117), (2008)

Work function of graphene exfoliated on insulating substrates

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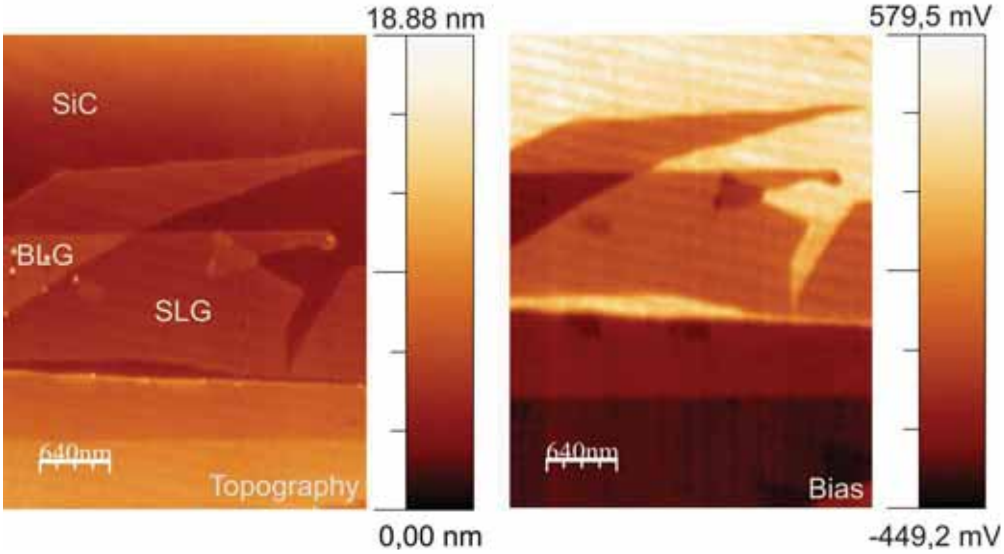
We present atomic force microscopy and scanning Kelvin probe data obtained under ultra-high vacuum conditions from graphene exfoliated on crystalline $SrTiO_3$ and SiC substrates. The contact potential difference for both systems shows a monotonic increase with the number of graphene layers until after several layers a saturation value is reached. By identifying the saturation value with the work function of graphite we determine the work function of single and bilayer graphene to be $\Phi_{SLG} = 4.409 \pm 0.039$ eV and $\Phi_{BLG} = 4.516 \pm 0.035$ eV, respectively on the $SrTiO_3$ substrate [1].
Graphene grown epitaxially on SiC has already been investigated by Filleter et.al. [2]. SLG showed a lower work function compared to the bilayer graphene. This behavior we also find for exfoliated graphene on SiC in our measurements. This is surprising as the interface of the two systems should be completely different. While it is abrupt for exfoliated G/SiC it consists of a carbon rich layer in the case of epitaxial G/SiC.
In agreement with the higher work function of single-layer graphene with respect to free-standing graphene, our measurements indicate an accumulation of charge carriers corresponding to a doping of the exfoliated graphene layer with electrons for both systems.
We investigated the influence of adsorbants on the work function and found that water leads to a significant reduction of the work function.



[1] B. Kleine Bussmann, O. Ochedowksi and M. Schleberger Nanotechnology 22 265703
[2] T. Filleter , K.V. Emtsev , Th. Seyller and R. Bennewitz Appl. Phys. Lett. **93** 133117

The influence of the cantilever capacitance on the accuracy of surface potential measurements in Kelvin probe force microscopy

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We report on studies concerning contribution of the cantilever on the accuracy of surface potential imaging of heterogeneous surfaces in Kelvin probe force microscopy, working in frequency modulation mode (FM-KPFM), performed in ultrahigh vacuum. The system under investigation consisted of a set of electrically isolated Pt nanowires (of 100 nm in width) lithographically deposited on SiO_2/Si substrate. The metallic nanowires were externally biased, with respect to the Si substrate, with dc voltage ($V^{ext.}{}_{dc}$). Then, with the standard FM-KPFM imaging of the $Pt/SiO_2/Si$ system, the spatial distribution of the contact potential difference (V_{CPD}) signal as a function of the dc voltage applied to the Pt nanowires, was measured. A CPD-gradient i.e. ($dV_{CPD}/dV^{ext.}{}_{dc}$) measured at specific surface location allowed to evaluate the effect of parasitic capacitance between the cantilever and the sample on the accuracy of surface potential imaging. For this case, the experimental findings are compared with the predictions of theoretical calculations based on a realistic model for the cantilever-sample geometry.

P.I-16

CNT-probes in NC-AFM: Tip broadening and KPFM signature

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High aspect ratios, outstanding mechanical durability, and almost complete chemical inertness are a few of the unique properties that have compelled researchers to explore the use of carbon nanotubes (CNT) as probes in various atomic force microscopy (AFM) techniques [1]. Unrivaled results in tapping-mode AFM [2] give reason to believe that these CNT-terminated probes could be of use in non-contact atomic force microscopy (NC-AFM) studies of highly reactive metal cluster covered oxide surfaces – samples that often cause unwanted cluster-tip reactions, limiting both the lifetime of the probes and the reproducibility of the measurements, and moreover offer a challenging topography for the physical dimensions of typical Si-probes.

Commercial CNT-probes have been used in NC-AFM measurements of Pt nanoclusters supported on Al_2O_3 surfaces [3], and results have been compared to measurements done with regular Si-tips as well as with transmission electron microscopy (TEM) images, which give accurate values for the lateral dimensions of the supported particles. The distinct characteristics of CNTs result in novel features emerging in the signals from both topography as well as cantilever excitation. Coupled together with Kelvin probe force microscopy (KPFM) results, a detailed interpretation of the interactions between CNT-terminated probes and supported metal clusters is offered. These findings open up possibilities for new KPFM-mediated measuring techniques with CNT-probes, as well as provide unique insight into a dissipative mechanism in NC-AFM.

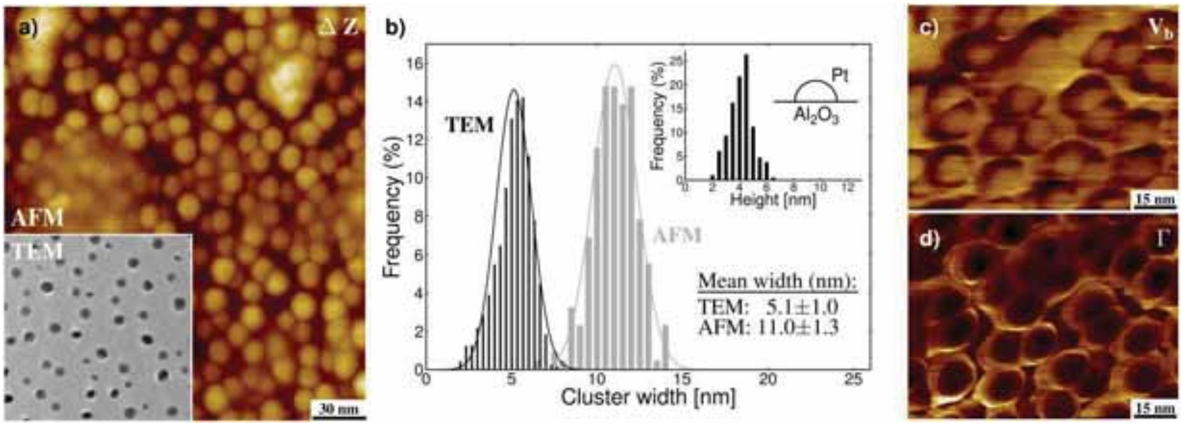

Figure: **a)** NC-AFM topography image of Pt clusters on Al_2O_3 (inset: TEM image), **b)** histograms showing cluster widths from AFM and TEM, **c)** KPFM image, **d)** dissipation image.

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[3] S. B. Simonsen, et al., (2011) submitted for publication.

Nucleation, growth and shape of Au cluster on CeO_2(111)

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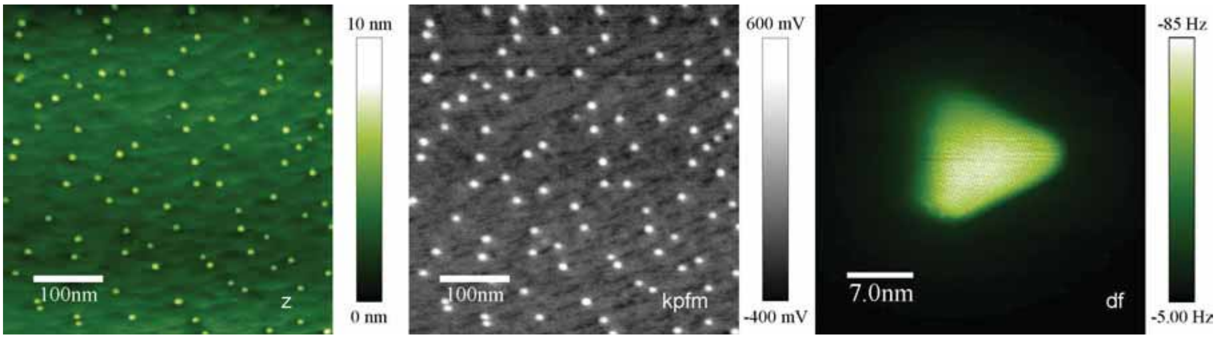
Gold nano-clusters of variable size are deposited on CeO_2(111) by sublimation of Au from a Knudsen cell onto the substrate surface kept at various temperatures during deposition ranging from 300 K to 1050 K. Samples are investigated by non-contact atomic force microscopy (NC-AFM) and Kelvin probe force microscopy (KPFM) performed at room temperature. Measurements of surface topography are complemented by KPFM compensation to determine the true height of the cluster [1]. The cluster size is determined as a function of deposition temperature. For small clusters, the shape and their orientation with respect to the substrate is determined NC-AFM measurements performed in the constant height mode revealing the top facet [2]. Furthermore, we establish a relation between the KPFM contrast and the cluster size and demonstrate charging of individual clusters to an equivalent of a few electrons.



0.7ML Au deposited at sample temperature of 950K.

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P.I-18

Dynamic Force Spectroscopy of Electrostatic Interactions in Aqueous Salt Solutions of Variable Concentration and Valency

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We use frequency modulation dynamic force spectroscopy (FM-DFS) to determine electrostatic interactions between Si tips and Si wafers in aqueous electrolytes of variable composition [1]. We demonstrate that the usage of stiff cantilevers and sharp tips in the dynamic mode allows for a continuous detection of the tip-sample interactions without the mechanical "jump-to-contact" instability and with substantially higher lateral resolution than standard colloidal probe measurements. For four different species of salt (NaCl, KCl, $MgCl_2$, $CaCl_2$) we find repulsive electrostatic forces at the lowest salt concentration (1 mM) that become progressively screened until the interaction is dominated by attractive van der Waals forces at the highest concentration (100 mM) (Fig. 1a). For the divalent cations the cross over from repulsive to attractive forces occurs at lower concentrations than for monovalent cations. Surface charges obtained from comparison with standard Poisson-Boltzmann double layer theory indicate a rather weak dependence of the surface charge on the ion concentration.

The high lateral resolution of our approach is illustrated by 2D force field measurements over patterned surfaces consisting of nanosized gibbsite platelets adsorbed to Si substrates. The gibbsite platelets which have a diameter in the range of 100-200 nm and a thickness of several nm have a non-uniform surface charge distribution (Fig. 1b). This results in local variations in the electrical double layer interactions which are clearly observed in the force fields with a lateral resolution in the nm range.

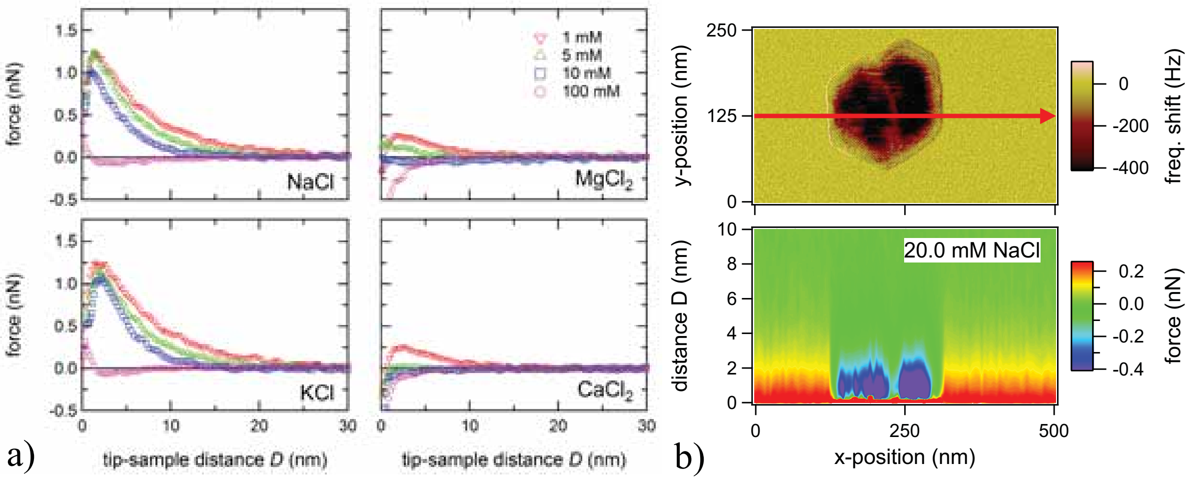

Fig. 1: a) Comparison of tip-sample interaction forces for different ion species and different concentration. b) Frequency shift image (250 x 500 nm^2) and 2D force field measured over gibbsite platelet attached to silicon oxide substrate in 20 mM NaCl solution.

[1] D. Ebeling, D. van den Ende, F. Mugele, Nanotechnology, (accepted)

Cantilever array sensing techniques in life sciences

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Differently to AFM, cantilever sensor technique detects processes taking place on the surface of the beam and thus, uses the cantilever surface as sensor surface. A sensor operated in static mode measures the bending of cantilever due to stress formation generated by asymmetrical adsorption of molecules (i.e. on the upper functionalized cantilever side). Cantilever array platform provides a unique tool for a label-free, time-resolving sensor for applications in fundamental biological research and medical diagnostics. We illustrate this with two examples.

In the first one, we used cantilever array technique to investigate molecular interactions in the nuclear pore complex (NPC), a supramolecular assembly of proteins (nucleoporins) regulating transport across the nuclear envelope in vertebrate. We demonstrate the application of the sensor for a fast characterization of binding between surface-tethered nucleoporins Nup153 and the transport receptor Importin.

The second addresses the analysis of melanoma-specific genetic markers and the direct detection of metastatic melanoma cells in blood using selectively functionalized cantilevers. Metastatic melanoma represents one of the most difficult tumors to treat. Fortunately, the cure rate of early melanoma results in a much better prognosis and, therefore, an accurate early diagnosis of precursor lesions and of primary tumors is of crucial importance. A fast and accurate detection of melanoma specific mutations, capture and analysis of metastatic circulating tumor cells with specific antibodies could help in the treatment and prognosis of this cancer. This eventually could lead to the application of microcantilever arrays in medical diagnostics.

High resolution Kelvin Probe Force Microscopy of single biomolecules

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Electrostatic forces and potentials are key in determining the interactions between biomolecules. We demonstrate the ability of Kelvin Probe Force Microscopy (KPFM) to image surface charges on biological samples in air and at molecular resolution [1,2]. Specifically, we show that high resolution KPFM reveals the electrostatic potential of buffer salts shielding negatively charged DNA molecules assembled on silicon and also on an insulating surface such as mica, which provides access to configurations of DNA that are projections of its structure in solution. In particular, we apply dual-frequency mode to minimise the tip-sample distance at which the Kelvin probe signal is acquired and use the fundamental resonance of the cantilever to determine surface potential and its first overtone to detect the topography. We anticipate that measuring the electrostatic potentials of proteins and DNA by KPFM will be an important step towards the understanding of biomolecular physics on surfaces, especially in the fields of biosensing and bionanoelectronics.

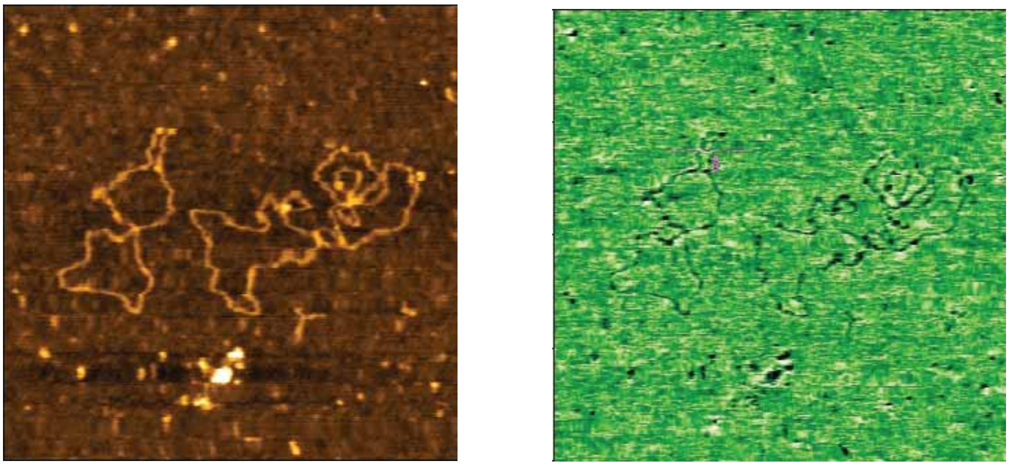

Figure: DNA adsorbed on mica, topography (left) and surface potential (right).

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[2] C. Leung *et al.*, Applied Physics Letters, 97, 203703 (2010).

High-resolution AFM by tracking the resonance frequency of ultrasmall cantilevers

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Ultrasmall cantilevers have been a key element for fast-scanning AFM experiments. They are characterised by their low lateral dimensions (typically few microns), by their high resonance frequencies (MHz), and a relatively low thermal noise threshold which determines the ultimate noise floor for AFM. Thus far, such cantilevers have been operated in intermittent contact (tapping) mode but not in the so-called non-contact modes for imaging biomolecules in liquid. These modes rely on tracking shifts in cantilever resonance frequency [1]. With conventional cantilevers, they have been successfully applied to obtain atomic-resolution images in liquid and are increasingly used for high-resolution imaging of biomolecules.

Here we report on high-resolution imaging experiments on a number of benchmark samples, obtained by tracking MHz resonance frequencies of cantilevers of 3~4 microns width. Overcoming a number of experimental obstacles that have thus far prevented this type of experiments, our experimental set-up uses an interferometric detection scheme [2-4], photothermal cantilever actuation, and a customised version of the Vortis controller from JPK Instruments. It has achieved subnanometre-resolution on mica and on the membrane protein bacteriorhodopsin. In addition, it enables us to measure DNA at higher resolution and at significantly lower forces than intermittent contact mode.

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P.I-22

High-resolution Imaging on Ionic Liquid/Solid Interfaces using Frequency Modulation Atomic Force Microscopy

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Room-temperature molten salts, which are also called “ionic liquids (ILs)”, have superior properties compared to water and organic solvent, such as high ionic conductivity, non-volatility, and non-combustibility. They are expected to be adopted as a new electrolyte in electrochemistry. FM-AFM studies on IL/solid interfaces would provide helpful information for electrochemical reactions using ILs. However, since ILs have high viscosity (typically 100 times higher than that of water), FM-AFM imaging using Si cantilevers is considered to be unstable because of extremely low Q-factor in ILs. Recently, we have developed FM-AFM with quartz tuning fork sensors for the investigations in ILs. The Q-factor in our system was kept more than 100 even in ILs and stable topographic imaging was successfully achieved [1].

In this study, we demonstrated high-resolution imaging on IL/solid interfaces. Figure 1 (a) shows a FM-AFM image obtained on an interface of a cleaved mica surface and 1-ethyl-3-methylimidazolium acetate (EMI-AcO, viscosity: 93 cP). The tip jumped from *Terrace 1* to *Terrace 2* as schematically shown in Fig. 1(b). The height of the jump was 2.0 nm, which are almost equal to the thickness of 3 layers of EMI-AcO ion pairs. Figures 1(c) and (d) show the magnified images of *Area (1)* in *Terrace 1* and *Area (2)* in *Terrace 2,* respectively. Figure 1(c) clearly shows the molecular-scale contrast, which should correspond the arrangement of the ions composing the solvation layers. Defects on the solvation layers were also imaged. The right part of Fig. 1(d) shows a honeycomb-like structure; that is, atomic-resolution imaging of the mica surface was successfully achieved. The left part of Fig. 1(d) shows hexagonally-packed brighter spots. These spots should be the ions arranged on the mica surface. These results indicate that our FM-AFM is capable of visualizing both atomic-scale contrast of solid surfaces and molecular-scale contrast of solvation layers in ILs.

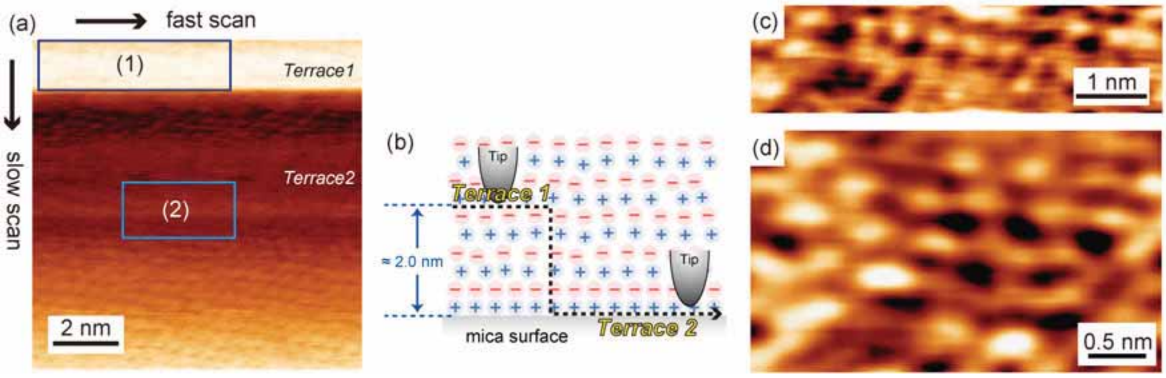

Fig. 1(a) FM-AFM image obtained on a mica/EMI-AcO interface, 10 nm × 10 nm, $\Delta f = +100$ Hz, $A_{\text{p-p}} = 100$ pm. (b) Schematic illustration for explaining the expected tip trajectory. (c) Magnified image of *Area (1)*. (d) Magnified image of *Area (2)*.

[1] M. Fujimura, T. Ichii, K. Murase, H. Sugimura, *Abstract booklet of NC-AFM2010*, P1-3-8

Phase Modulation Atomic Force Microscopy in Ionic Liquids using quartz tuning folk sensors

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Room-temperature molten salts, which are also called “ionic liquids (ILs)”, have superior properties compared to water and organic solvent, such as high ionic conductivity, non-volatility, and non-combustibility. They are expected to be adopted as a new electrolyte in electrochemistry. AFM studies on IL/solid interfaces would provide helpful information for their application and we have developed FM-AFM using quartz tuning folk sensors for investigating IL/solid interfaces [1]. Phase modulation (PM) AFM has several advantages compared to FM-AFM such as high stability and simple experimental setup.

In this study, we demonstrated PM-AFM investigations on IL/solid interfaces. Figure 1 (a) shows a PM-AFM topographic image of a Si(111) substrate covered with a hexadecyl monolayer (HD-SAM) obtained in 1-ethyl-3-methylimidazolium bis[(trifluoromethyl) sulfonyl]amide (EMI-Tf_2N, viscosity: 28 cP). The phase shift was kept 90 degree during imaging and the driving frequency was changed in order to regulate the tip-to-sample distance. The atomic steps originated from the Si substrate were imaged. In addition, a phase shift vs. distance curve clearly showed an oscillation with a period of 0.67 nm as shown in Fig. 1(b), which indicates the presence of multiple solvation layers on the interface. These results suggest that the PM-AFM using quartz tuning folk sensors can be a powerful technique for investigating on IL/solid interfaces.

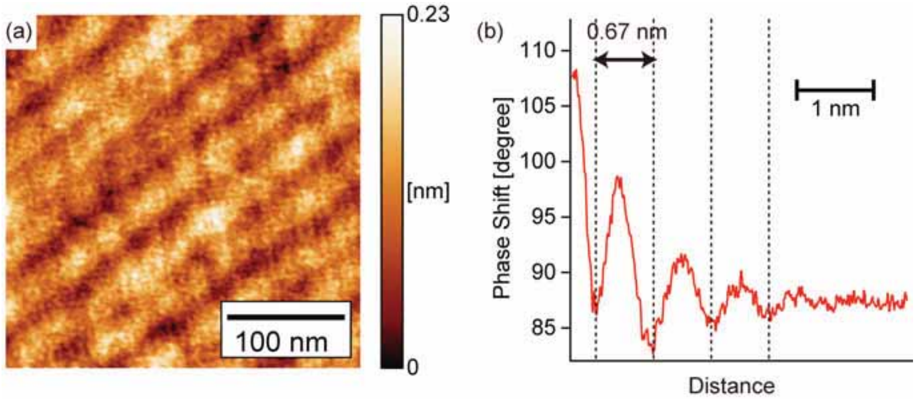

Fig. 1 (a) PM-AFM image of a Si(111) substrate covered with HD-SAM obtained in EMI-Tf_2N, 300 nm × 300 nm, $\Delta f = +50$ Hz, $A_{\text{p-p}} = 1.0$ nm. (b) Phase shift vs. distance curve obtained on a HD-SAM/EMI-Tf_2N interface, $A_{\text{p-p}} = 0.25$ nm.

[1] M. Fujimura, T. Ichii, K. Murase, H. Sugimura, *Abstract booklet of NC-AFM2010*, P1-3-8

P.I-24

Pulse-response measurement of frequency-resolved water dynamics on a hydrophilic surface using a Q-damped AFM cantilever

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Water dynamics on hydrophilic surfaces has aroused much controversy as measurement with atomic force microscopy (AFM) often suggested anomalous time-scales for its response. In order to circumvent frequency selectivity in AFM measurement magnetic control of the cantilever was introduced to suppress its resonances and to exert a well-characterized stimulus onto it. Detail of the experimental setup is described elsewhere [1]. A spherical magnet with a diameter of ca. 7 μm was attached onto the end of a 0.03 N/m silicon nitride cantilever and was driven with a small electromagnet and a wide-band constant current driver [1,2]. A quality-factor (Q-) controller differentiates cantilever's deflection signal from ca. 2 kHz to 50 kHz and feed it back to the regulation signal so that the 1st and 2nd resonances are suppressed. With a square pulse with duration of 10 μs applied to the magnet driver, the cantilever instantaneously deflected toward a mica substrate placed in water by 0.2-0.3 nm and then relaxed. Figure 1 shows cantilever responses at two positions, ca. at 300 nm from the substrate ("mild" interaction) and close to the contact ("strong" interaction). With "strong" interaction the relaxation time of the response seems to be slightly shortened. Fourier-Laplace transform of these responses gives complex compliances of the cantilever-water system. By inverting the compliances to the stiffnesses and taking their difference the complex stiffness, or viscoelasticity, of the confined water can be derived in a frequency-resolved form. Figure 2 shows the real (*K*') and imaginary (*K*'') parts of the obtained complex stiffness. Although the data from 4 to 8 kHz is disturbed by slight residual response of the 1st resonance mode, *K*' seems to retain a positive value in the entire frequency regime, indicating a solidifying character. On the other hand *K*'' does not undergo significant change in the low frequency regime whereas it comes to show increase with the frequency over 10 kHz.

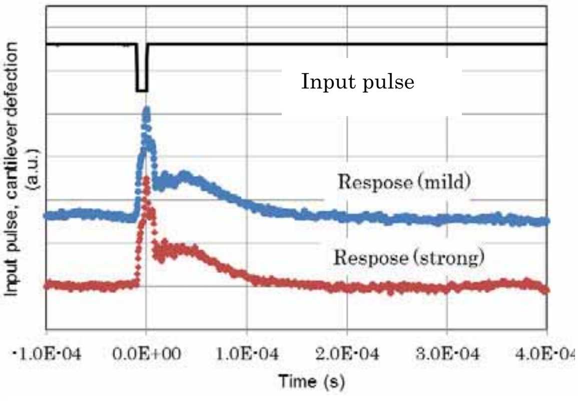

Fig. 1 Responses of a Q-damped cantilever to a pulse signal at two positions.

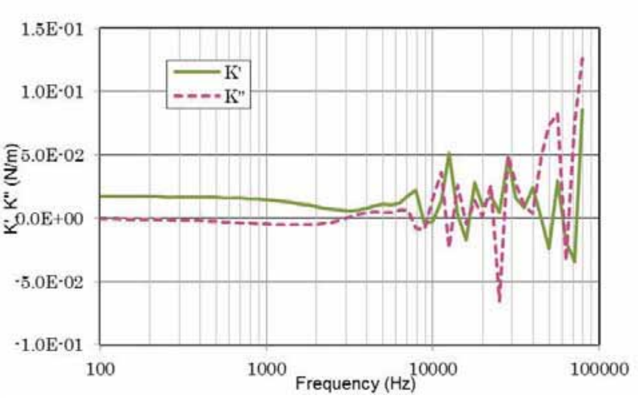

Fig. 2 Real (*K*') and imaginary (*K*'') parts of stiffness of confined water in 100 Hz-100 kHz.

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Subnanometer-scale Imaging of CaF_2(111) Surfaces by FM-AFM in Various Solutions

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Recent progress in FM-AFM enabled us to image surface structures with true atomic resolution even in liquid. Moreover, it has become possible to visualize there-dimensional (3D) distribution of hydration layers at a solid/liquid interface with subnanometer-scale resolution by 3D scanning force microscopy [1]. However, the mechanism of subnanometer-scale imaging by FM-AFM in liquid has not been understood. Hence, it is often difficult to interpret the experimental results. To obtain a further understanding of the imaging mechanism, we have performed subnanometer-scale imaging of CaF_2(111) surfaces by FM-AFM in liquid. CaF_2(111) surfaces have been extensively investigated by FM-AFM in UHV [2]. In addition, the imaging mechanism for the experimental results has been well explained by the theoretical simulations [2]. Recently, theoretical simulations of the imaging mechanism of CaF_2(111) surfaces in water have been reported [3]. Thus, CaF_2(111) surfaces are considered to be an ideal model sample for the investigations on the imaging mechanism of FM-AFM in liquid. In this study, we have investigated the solution conditions that allows to image CaF_2(111) surfaces with subnanometer-scale resolution.

Figure 1(a) shows an FM-AFM image taken in pure water. In this condition, we found that atomic-resolution images can be obtained on the terraces, but only for the first 10 to 20 min after the start of the experiment. This is due to the dissolution of CaF_2 and the generation of $Ca(OH)_2$ as indicated by the arrows in Fig. 1(a). In 200 times supersaturated solution, clear terraces without dissolution and generation of $Ca(OH)_2$ are imaged [Fig. 1(b)] for more than 1 hour and atomic-resolution images were stably obtained on the terrace [Fig. 1(c)]. These results indicate that supersaturated solution makes it possible to image CaF_2(111) surfaces with subnanometer-scale resolution for a long time.

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[2] A.S. Foster, C. Barth, A.L. Shluger, R.M. Nieminen, and M. Reichling, Phys. Rev. B **66**, 235417 (2002).
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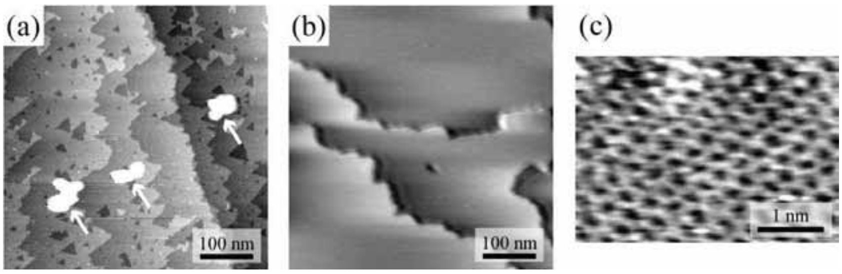

Figure 1. FM-AFM images of a CaF_2(111) surface taken in (a) pure water and (b) 200 times supersaturated solution. (c) Atomic resolution image taken on the terrace in (b).

IP.I-26

FM-AFM study of *n*-Alkane-Adsorbed Graphite Immersed in Liquids

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[3] Department of Chemistry, Kobe University, Kobe, Japan.

Organic polymers provide one major class of materials for wide applications in industry. There is intense demand to characterize liquid-polymer interfaces. In this study, *n*-alkanes including polyethylene, the simplest polymer, were physisorbed on graphite, immersed in water or alkanes, and imaged with a modified FM-AFM (Shimadzu, SPM-9600).
Polyethylene with an averaged molecular weight of 560, which is equivalent to a *n*-alkane of $C_{40}H_{82}$, was dissolved in *p*-xylene at 120° C. A drop of the solution was placed on a cleaved graphite wafer. When the solvent was evaporated, the wafer was immersed in pure water. Figure 1(a) shows a constant Δf topography of the immersed wafer. Physisorbed polyethylene presented stripes epitaxial with the graphite lattice. The distance of neighboring stripes was regulated to be 6 nm by the length of one polyethylene molecule. A zoomed-in topography is presented in Fig. 1(b). A two-dimensional Δf distribution was observed on the white line in image (b) and shown in (c). The protrusions and trenches at the bottom of Δf distribution represent the cross section of the polyethylene stripes. Three, four pairs of dark and bright layers are identified over the stripes, showing an uneven density distribution of the liquid as a function of the vertical distance from the surface. Furthermore, the density distribution of the layered liquid was uneven along the lateral coordinates. The topography of the stripes was projected on the liquid structure. Similar results were obtained with dodecane $C_{12}H_{26}$ and tetradecane $C_{14}H_{30}$, shorter *n*-alkanes. The relationship of surface topography and liquid structure is discussed in the presentation.

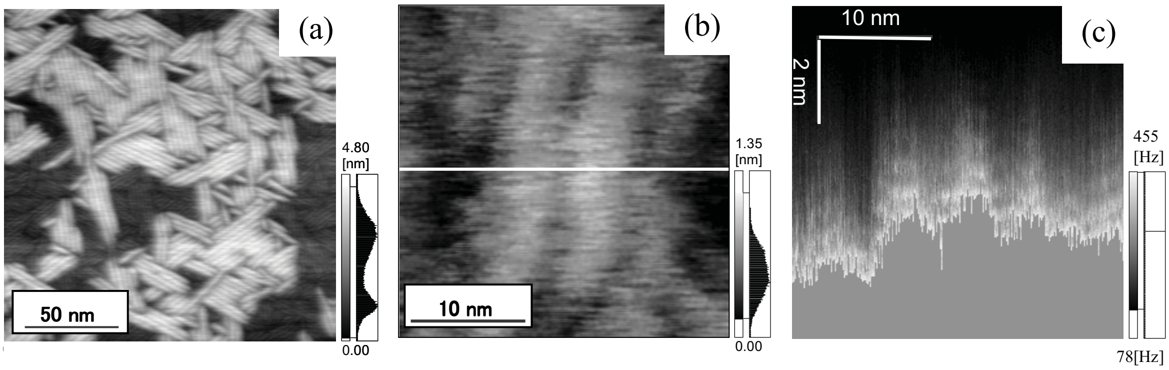

Fig. 1. Polyethylene-adsorbed graphite in water. Constant Δf topography of (a) 350 x 350 nm^2, peak-to-peak amplitude, $A_{p\text{-}p}$ = 0.74 nm, Δf = 10 Hz; and (b) 30 x 30 nm^2, $A_{p\text{-}p}$ = 0.57 nm, Δf = 418 Hz. A two-dimensional Δf distribution of 30 x 8 nm^2 was observed on the line in (b). Positive (negative) Δf is shown to be bright (dark) in (c).

Atomic-Resolution Imaging of Clean Lithium Niobate Surfaces in Aqueous Solution

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Lithium niobate ($LiNbO_3$) is a superior artificial material with intensive use in electro-optical applications. The ferroelectric phase of $LiNbO_3$ exhibits a multitude of unusual optical, piezoelectric, electro-optic, elastic, photoelastic and photorefractive properties [1].
Although $LiNbO_3$ constitutes one of the most thoroughly characterized electro-optic materials, the microscopic understanding of its surfaces is rather poor [2]. The strong spontaneous polarization (0.7 C/m^2) of $LiNbO_3$ Z-cut precludes the experimental investigation of the clean surface by high-resolution FM-AFM under vacuum condition.
Recently, high-resolution FM-AFM imaging under liquid conditions became possible making use of optimized read-out electronics [3,4]. Within liquids, the adsorption of screening charges onto $LiNbO_3$ surfaces enables high-resolution imaging.
In this contribution, we present first atomic-resolution FM-AFM images of different $LiNbO_3$ surfaces taken in liquid environment. Our results clearly show that high-resolution FM-AFM in liquid environment allows for investigating new sample systems that have not been accessible before. The obtained results are compared to density functional theory calculations, which predict different surface terminations after high-temperature annealing, a known method to produce atomically flat surfaces. Interestingly, high-temperature annealing produces step-structures with pronounced directions, not observed before. High-resolution imaging enables identifying these directions, after careful drift-correction procedure.

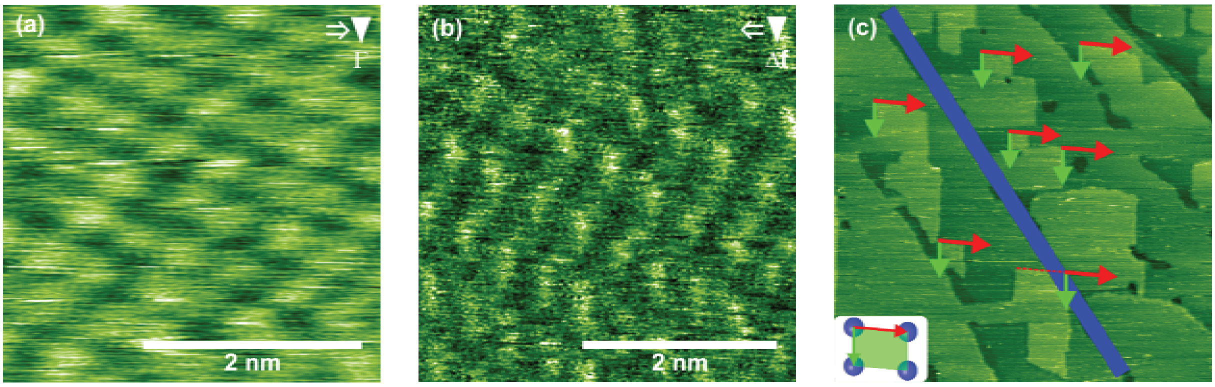

Figure 1: High-resolution images of $LiNbO_3$ Z- (a) and X-cut (b) surfaces in liquid environment. (c) Step structures after high-temperature annealing, extracted surface unit cell (inset).

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P.I-28

Adhesion Analysis of Gecko-Inspired Hierarchical Adhesives Using Atomic Force Microscopy

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Geckos are well-known for their impressive attachment system based on the hierarchical structures on their toes. Due to this famous design, geckos achieve intimate contact with smooth and rough surfaces and stick to walls and ceilings with the help of van der Waals forces. Mimicking the gecko's micro- and nanostructures leads to artificial dry attachment systems. We present two Gecko-inspired hierarchical fibrillar adhesives fabricated by two very different fabrication methods.

The technique of 3D laser lithography [1] allows for the fabrication of arbitrary 3D nanostructures in suitable photoresists and is based on multiphoton polymerization. By using this very flexible method, several gecko-mimicking structures have been fabricated varying in their geometrical parameters. Adhesion analysis based on atomic force microscopy has been used to study how these geometrical parameters affect the adhesion of the hierarchical structures.

Hot pulling [2] is a recently introduced hot embossing [3] process, enabling the cost-effective large-area fabrication of delicate polymer fibrils with highest aspect ratios and diameters in the nanometer range. Threefold hierarchical fibrillar structures have been fabricated by the combination of hot pulling and classical hot embossing. To characterize the adhesive properties of such attachment devices, the structures have been analysed by atomic force microscopy as well.

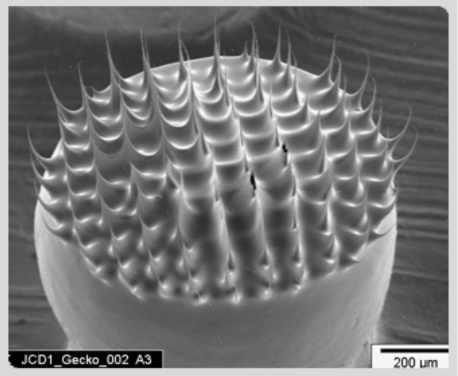

Fig. 1: Hierarchical polycarbonate structures fabricated by hot embossing and subsequent hot pulling.

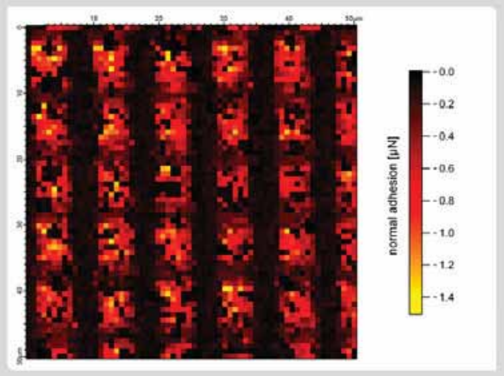

Fig. 2: Adhesion map of a gecko-mimicking attachment device fabricated by 3D laser lithography.

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P.I-29

FM-AFM analysis of dye-adsorbed TiO_2 surfaces in pure water

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Dye-adsorbed titanium dioxide (TiO_2) is a representative photo-anode for dye-sensitized solar cells. The solar cell consists of an electrolyte sandwiched between the photo-anode and a counter cathode. Photoexcited electrons in the dye molecules are extracted to an external circuit through the conduction band of the TiO_2. The geometric and electronic structures of individual N3 molecules affect the electron injection to the TiO_2. The chemical stability of dye molecules in the electrolyte determines the lifetime of the photo-anode. Thus, the nano-structures of the dye-adsorbed TiO_2 surface in an electrolyte are the key to the improvement of the photo-anode performance.

The frequency modulation atomic force microscope (FM-AFM), which provides high-resolution images of surface nano-structures in liquid, is promising for analysis of the dye-adsorbed TiO_2 surface in the electrolyte. We examined a model surface of the photo-anode prepared by Ru(4,4'-dicarboxy-2,2'-bipyridine)$_2$(NCS)$_2$ (N3) and a rutile TiO_2(110) surface using FM-AFM in pure water.

The TiO_2(110) surface was cleaned in ultrahigh vacuum with cycles of Ar^+ sputtering and annealing to show (1×1) structure (Fig. 1). After cooled to room temperature, the TiO_2 wafer was removed from the vacuum chamber and immersed in an acetonitrile solution of the N3. A commercial intermittent contact mode atomic force microscope (5500 AFM/SPM, Agilent Technologies) was operated as an FM-AFM by using a phase locked loop detector (easy PLL plus, Nanosurf AG).

Figure 1(b) shows an FM-AFM image of the TiO_2(110)-(1×1) surface in water [1]. The strings elongated to the [001] direction were assigned to the row of the clusters of H_2O molecules. The corrugation of the image was within 0.2 nm. After immersion in the N3 solution, particles were observed as shown in Fig. 1(c). The particles protruding by 0.7-1.0 nm were assigned to adsorbed N3 molecules. Photostability of the adsorbed N3 molecules under visible and ultraviolet light irradiation will be presented.

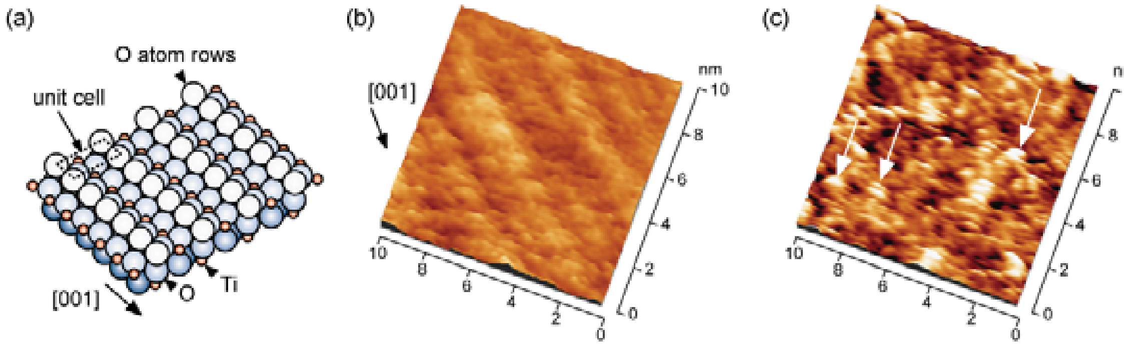

Fig. 1 (a) A ball model of the TiO_2(110)-(1×1) surface. (b) The FM-AFM image of the clean TiO_2(110) surface in pure water. Frequency shift (Δf) : +440 Hz. (c) The FM-AFM image of the TiO_2(110) surface immersed in N3 solution. Δf: +339 Hz.

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High Resolution Imaging in Liquid Using an Improved Frequency Modulation Atomic Force Microscope

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The dynamic mode atomic force microscope (AFM) using the frequency modulation (FM) detection technique has been used for high-resolution imaging in ultra-high vacuum (UHV) owing to a high Q-factor of the cantilever. However, high-resolution imaging in liquid environments by FM-AFM is extremely difficult because of the large decrease in the Q-factor caused by the hydrodynamic damping in liquid. In recent years, several high-resolution observations of mica surfaces and organic molecules including biomolecules have been reported using FM-AFM in liquids [1].

In this study, we improved a commercial AFM (JEOL : JSPM-5200) to a high-resolution AFM for imaging in liquid and succeeded to obtain high-resolution images of a polyethylene crystal surface in a buffer solution. Polyethylene single crystals were obtained by isothermal crystallization at 83 °C from xylene solution. The solution containing the crystals dropped on a cleaved mica. After the solvent was evaporated, the substrate was immersed in a buffer solution (0.1mol/L KCl). Images of the FM detection mode in the buffer solution are shown in Figure1. The typical rhombic single crystal [2] was observed as shown in Fig.1(a). As shown in Fig.1(b), a magnified image showed the roughness with several nanometers on the terrace of the rhombic crystal. Further, in a magnified image, the periodic structure was visualized corresponding to molecular array as shown in Fig.1(c).

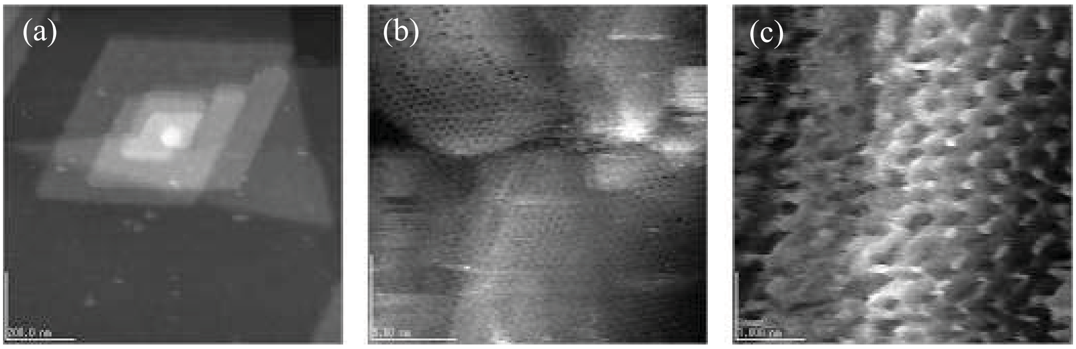

Fig.1 Topographic images of a polyethylene crystal surface taken with the FM detection mode in a buffer solution (0.1mol/L KCl). Scan sizes of (a),(b) and (c) are 1000 x 1000, 20 x 20 and 5 x 5 nm^2 , respectively.

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Effect of Ionic Liquid on Immobilizing Au nanoparticle onto $TiO_2(110)$

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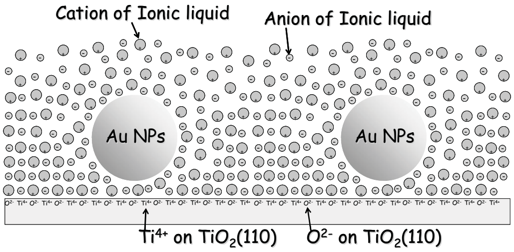

Fig. 1 Schematic drawing of IL/NPs/$TiO_2(110)$

Formation of the ionic liquid (IL) layers formed on mica has recently been investigated experimentally in several AFM studies, indicating that the thickness of the layer was dependent on ILs having a single layer form or a multi-layered form[1,2]. Ordering of ILs through electrostatic interactions on $TiO_2(110)$ was also predicted[3]. Such rigid layer structures may provide high fluid resistance environment for nanoparticle (NP) diffusion adsorbed on a substrate surface, and such ordering of IL may stabilize the NPs on $TiO_2(110)$ in a segregated manner(Fig. 1). Thus, combination of charged surface and molecules has a potential to control the adsorption states of NPs on ionic solid surfaces through the electrostatic interaction.

Here, we studied the immobilization of Au NPs on a $TiO_2(110)$ single crystal surface and examined how the ILs influenced the immobilization by AFM. Three kinds of ILs including 1-butyl-3-methylimidazolium ($[C_4MIm]$) cation-based ILs of tetrafluoroborate ($[BF_4]$), hexafluorophosphate ($[PF_6]$) and bis(trifluoromethylsulfonyl)amide ($[NTf_2]$) were used. Prior to the immobilization by heating at 323 K, Au NPs were synthesized in the ILs by the sputter deposition[4]. The excess amount of ILs was removed by immersing gently in acetonitrile solution for 18 h. AM-AFM observation w as carried out at room temperature in atmosphere.

Figure 2 shows a typical result of the sample surface for $[C_4MIm][NTf_2]$. We considered the immobilization from the view point of electrostatic interactions between IL and IL and between IL and the surface, with assuming that the all the NPs were encapsulated by ILs (Fig. 1). We deduced the influence of these interactions from the increments of NP's diameter and the amount of NPs after the immobilization compared to the ones as-prepared in ILs, and obtained the order as $[C_4MIm][BF_4] \approx [C_4MIm][NTf_2] > [C_4MIm][PF_6]$. Interestingly, the above orders were no match with the conventional physicochemical parameters but Kamlet-Taft solvent descriptors and Lewis basicity. Therefore, the result indicates that the chemical natures might affect the immobilization of NPs on the surface through hydrogen bonding or coordination bonding. The trend does not conflict with the trend in the layer thickness like thin layers of $[C_4MIm][PF_6]$[1] and thick layers of $[C_4MIm][NTf_2]$[2], if the layer provide high fluid resistance for NP diffusion. We suggested that such trend in anions was 'local viscosity' of ILs in the vicinity of surface.

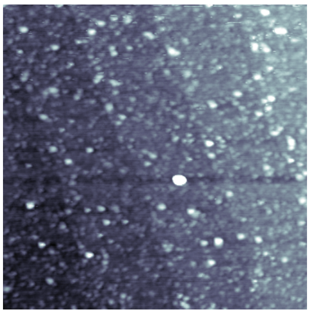

Fig. 2 A typical AFM image of $TiO_2(110)$ surfaces treated with the $[C_4MIm][NTf_2]$.

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Quantitative study of local electric double layer force by FM-AFM in aqueous solutions

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Significant progress has been made in frequency modulation atomic force microscopy (FM-AFM) in liquids, which is capable of imaging with atomic/molecular resolution as well as studying molecular-scale hydration structures. For further applications, especially for biological applications, local charge information of a sample surface has to be investigated because it is directly related to various biological interactions. However, since the charge at a sample surface is dynamically screened by the electric double layer (EDL) in aqueous solution, the electrostatic force acting on the tip of a cantilever does not simply originate from the surface charge. For precise analysis of the surface charge it is required to quantitatively measure the EDL force due to the overlap of EDLs of the probe tip and the sample surface.

For quantitative force measurements in liquids colloidal probes (sQube, CP-NCHSIO) were used, which allows us to define the interaction area. In addition, we adopted a photothermal excitation setup. Figure 1(a) shows frequency shift-distance curves obtained on a muscovite mica surface in KCl aqueous solutions with three different KCl concentrations. The data was taken with a colloidal probe. The result clearly shows that three measured curves with an exponential dependence on the tip-to-sample distances agree well with theoretical-calculation curves (dashed curves). We measured EDL force on a lambda DNA molecule deposited on a poly-L-lysine (PL) coated mica substrate by force mapping technique with a normal cantilever (Nanosensors, PPP-NCHAuD). Figure 1(b) shows frequency shift-distance curves obtained on a DNA molecule, as shown in the inset of Fig. 1(b), in 100 mM KCl aqueous solution. Both measured curves taken on the PL layer and the DNA molecule are well fitted to the calculated curves (dashed curves), reflecting each surface charge polarity. The result indicates that the force mapping technique using FM-AFM is useful for obtaining local charge information.

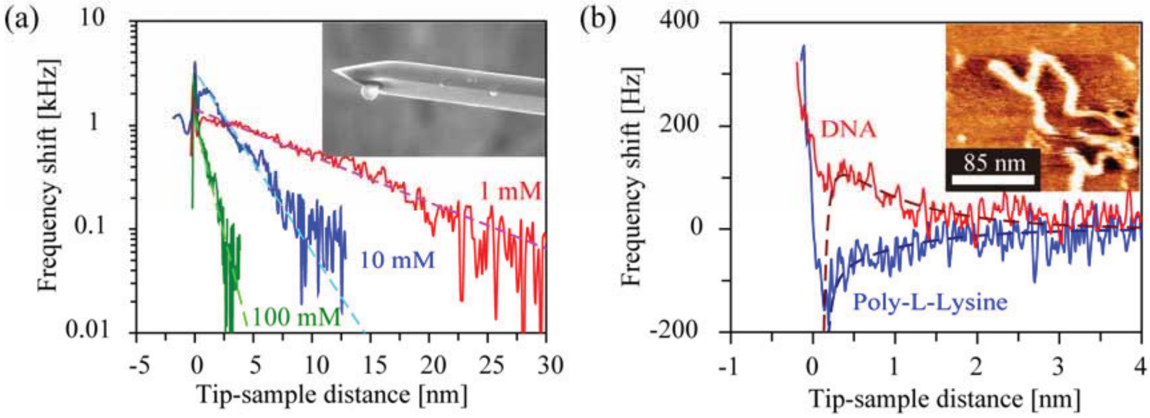

Fig. 1. (a) Frequency shift-distance curves obtained on a muscovite mica surface and (b) those obtained on a lambda DNA molecule on a poly-L-lysine layer in aqueous solutions.

Interfaces between solids and ionic liquids investigated by AM-AFM

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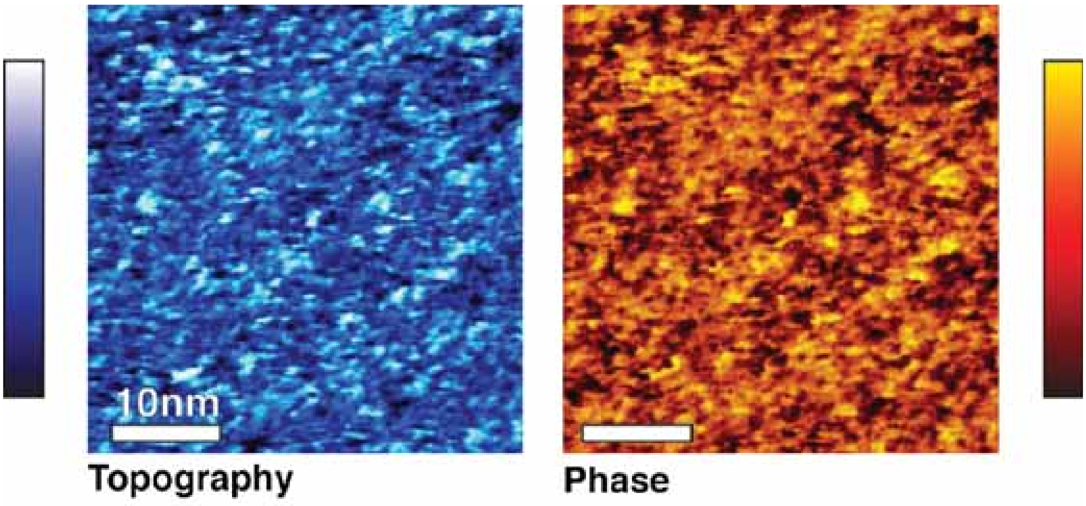
Ionic liquids (ILs) physico-chemical properties can be largely tailored through appropriate choices of cation/anion. This flexibility enables ILs to replace ordinary solvents advantageously in many practical applications such as heterogeneous catalysis, chemical synthesis [1] and photovoltaics [2]. At the molecular level, interfaces formed by ILs with solids are still poorly understood. Recent force spectroscopy measurements have shown that ILs form structured layers of anion-cation pairs at the surface of crystalline solids [3].

Here we apply an approach based on small (<1nm) amplitude-modulation atomic force microscopy [4] to probe the interface formed calcite, mica and *1-Ethyl-3-methylimidazolium Bis(trifluoromethane sulfonyl) imide* ([EMIm]TFSA), an IL routinely employed in photocells. We were able to image the interface with molecular-level resolution over several layers of the IL, while simultaneously deriving information about the adhesion energy between the probed IL layer and the solid [4]. The figure below shows the interface between ([EMIm]TFSA and mica. The IL follows loosely the crystalline orientation of mica with two different layers of the IL visible in the phase (darker and brighter). The z-scale is 0.5nm in topography and 5 degrees in phase.



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P.I-34

FM-AFM phase analysing on the demixed $Ag_xNa_{1-x}Br$ system

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Abstract

Quasi-binary ionic crystals like the $Ag_xNa_{1-x}Br$ system are ideal for the study of decomposition mechanisms. Different from metallic alloy or polymer systems this phase separation is completely limited to the fcc cation sublattice while the halide ions provide an almost rigid frame. The simple phase diagrams with no structural anomalies makes these systems well suited for detailed investigations on the microscopic mechanism.
The kinetic of decomposition of silver-alkali halides mixed crystals was studied in great detail by means of inelastic and small angle neutron scattering experiments [1]. The spinodal decomposition, can be influenced by temperature in the quenching process. This enables us to control the formation of nano-scaled structures of the quasi binary system.
With FM-AFM measurements ($Ag_xNa_{1-x}Br$, $x = 0.23$, 0.35 and 0.6) we aimed at the distinction of the two phases at ambient temperatures [2] due to contrast effects. Therefore we make use of the spectroscopic method, by varying the voltage between tip and surface during the scan process at equidistant positions. In addition of the evaluation of differences in the work function [3], we particularly focused on the behavior of the resonance frequency depending on the applied bias voltage. Even if the tip-sample interaction depends in a complex way on the tip-size, oscillation, amplitude and frequency-shift setpoint for distance control, etc. we were able to separate a contribution that depends on the chemical composition of the surface. This allows us to distinguish between silver and sodium rich phases of the demixed sample.
Furthermore, we have evidence that tip interactions with compensated bias lead to dynamical reorganization of surface structure in this system. During a scan with about 2s time resolution, clusters can appear or disappear. Combined spectroscopic and surface scans show reversible deformations of the surface with a relaxation time in the order of milliseconds.

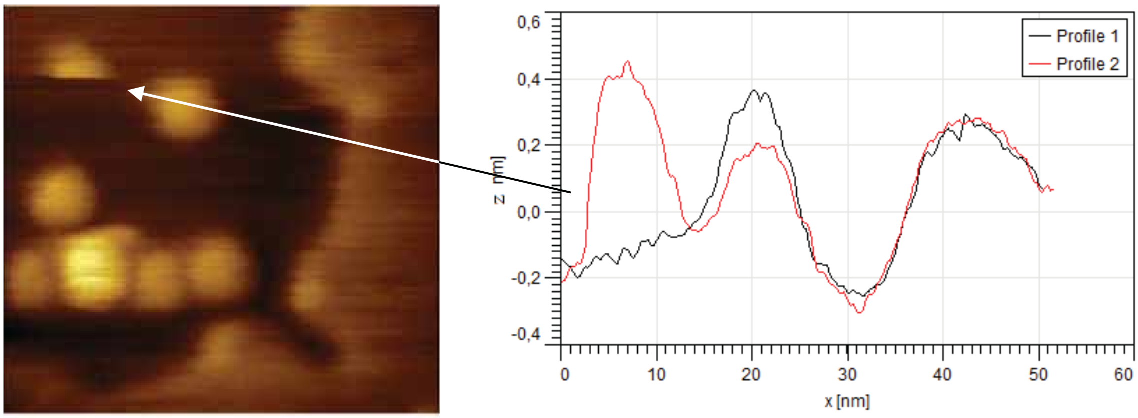

Fig. 1) Scan 90 nm on AgNaBr. Du to tip forces, satelites appear and vanish during one scan line

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Suppression of electronic friction on Nb-films below the critical temperature

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The origins of non-contact friction are investigated by highly sensitive force microscopy in the pendulum geometry. In this mode probe is suspended perpendicularly to the sample and the tip's vibrational motion is parallel to the surface. In the pendulum geometry very soft (k~mN/m) and therefore sensitive cantilevers can be used avoiding snapping into the contact due to high longitudinal stiffness.

The friction forces acting on a sharp probe tip oscillating below 3nm distances from 140nm thick Nb surface have been measured. Measurements reveal a reduction of dissipation in the superconducting state compared to the normal state by a factor 3. Therefore, electronic friction is found to be the dominant dissipation mechanism with power losses of 80ueV/cycle at separations of 0-3nm. Measurement across the critical temperature of Nb film shows that the character of transition is smooth reflecting the increasing normal electron population which are giving rise to the electronic induced friction. A good agreement with the BCS theory has been found in the drop of friction coefficient, as predicted by the theory [1].

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Structural Phases of the first Co layers on W(001)

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The structure of a substrate strongly influences the growth of a chemically different material onto it. Very often the deposited material adopts the crystal structure of the substrate at the interface and only assumes its own crystal structure for a sufficient large film thickness, e.g., the Fe/W(001) system.

We have investigated atomically thin highly strained films of a similar system, i.e., Co on W(001). While the first atomic layer (AL) of Fe on W(001) grows pseudomorphically, interestingly, three phases are found in the first AL of Co on W(001): a pseudomorphic p(1x1) phase, a p(2x1) phase and a (√5x√5)R27° phase. In the second AL, Fe still is mainly pseudomorphic with only a few stress induced line defects. For Co on the other hand, two phases have been observed: a pseudomorphic p(1x1) and a (√2x√2)R45° phase. The origin of the peculiar different behaviour of Fe and Co, respectively, is their different crystal structure with respect to bcc W: Fe is a bcc metal as well, while Co crystallizes in an hcp structure. The variety of observed phases are shown in Fig. 1 for the Co/W(001) system and will be discussed in terms of lattice mismatch, orientation and packing density.

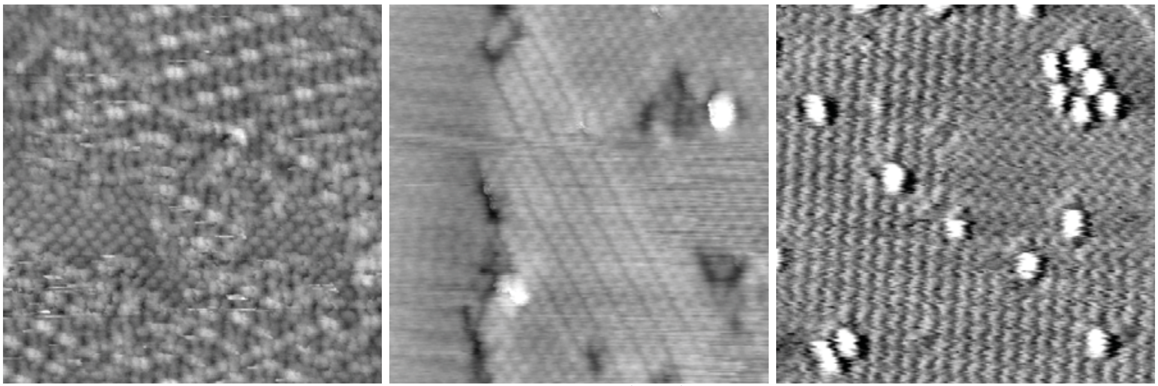

Fig. 1: Left: On the first ML, the high density (√5x√5)R27° phase is imaged together with patches of the p(1x1) phase. Middle: The second ML (left side) exhibits a (√2x√2)R45° pattern in multiple orthogonal domains, while the adjoining first ML (right side) shows the p(2x1)-reconstruction alongside p(1x1) growth. Right: On a fully closed second ML, a patch of p(1x1) growth alongside the (√2x√2)R45° reconstruction. The size of all images is (10nm)².

Quantifying magnetic moments in magnetic force microscopy (MFM) tips

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Measuring quantitative magnetic moments becomes one of the major tasks in nanomagnetic research. Here, we present a novel way to characterize magnetic force microscopy (MFM) tips in homogeneous external magnetic fields which is essential for all measurements and characterization techniques under the influence of such a field. Our methods basis on the deflection of the cantilever caused by the mechanical torque [1] as it is induced by an external magnetic field.

Low temperature measurements of the frequency-shift and the static deflection of the cantilever in a variable external magnetic field are used to access the different vectorial components of the magnetic moment of the tip. This allows to quantify both the magnitude and the orientation of μ. Experimental results are compared with the theoretical behaviour of the magnetic dipole moment of the cantilever as calculated by combining a harmonic oscillator model with the minimization of the magnetic energy.

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Molecular dynamics of Co-Salen on NiO(001) at submonolayer coverages

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The Schiff base complex Co-Salen is a planar molecule with a notable oxygen affinity. Studies of Co-Salen grown on NaCl(001) show bulk-like island growth and step edge decoration already at very low coverages below 1 monolayer (ML) [1]. The island growth indicates a strong intermolecular interaction compared to the molecule-substrate interaction.

In contrast, our present study of Co-Salen on NiO(001) reveals a different behavior. Although the substrate also crystallizes in the rocksalt structure, a layer by layer step-flow growth is observed at coverages larger than 1 ML, indicating a stronger molecule-substrate interaction than on NaCl(001). Peculiarly, at coverages below 1 ML we notice step edge decoration, but hardly any molecules are found on terraces when measuring at room temperature. Instead, our images show spikes, which are not present when measuring on the bare NiO(001) substrate. The number of spikes increases with increasing coverage up to 1 ML. When leaving the tip at one position of the substrate with feedback on, we observe distinct jumps in the z-signal, which are more frequent, if more molecules are deposited onto the surface.

Since the z-heights of the spikes and jumps approximately correspond to the height of a Co-Salen molecule, they most likely stem from mobile molecules, which interact shortly with the tip. A control experiment at low temperatures (T = 8 K) reveals that under these conditions molecules become visible on the terraces (see Fig. 1), because thermally activated motion is inhibited. Our findings regarding the molecular dynamics in the submonolayer regime at room temperature and the transition to the subsequently observed step-flow growth above one ML will be discussed.

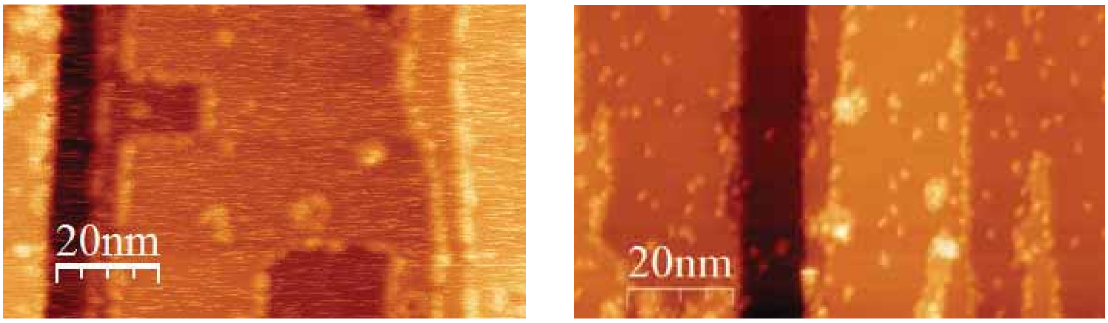

Fig. 1: Measurements of Co-Salen on NiO(001) carried out at room temperature (left) and at T = 8 K (right). Both samples were covered with 0.1 – 0.2 ML Co-Salen at room temperature. Both images exhibit step edge decoration. Excess molecules are mobile at room temperature and hence are only visible as spikes. At 8 K they are immobile and randomly distributed on the terraces.

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qPlus Magnetic Force Microscopy in Frequency-Modulation Mode with milli-Hertz Resolution

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Magnetic force microscopy (MFM) allows to image the domain structure of ferromagnetic samples by probing the dipole forces between a magnetic probe tip and a magnetic sample. The magnetic domain structure of the sample depends on the atomic arrangement of individual electron spins. It is desirable to be able to image both, individual atoms and domain structures, with a single probe. However, the force gradients of the interactions responsible for atomic contrast and those causing domain contrast are 6 orders of magnitude apart - ranging from 100 N/m for atomic interactions down to 0.0001 N/m for magnetic dipole interactions.

Here, we show that this gap can be bridged with a qPlus sensor, with a stiffness of 1800 N/m (optimized for atomic interaction), that is sensitive enough to measure milli-Hertz frequency contrast caused by magnetic dipole-dipole interactions. Thus we have succeeded to establish a sensing technique that performs atomically resolved Scanning Tunneling Microscopy and Atomic Force Microscopy as well as domain resolved MFM with a single probe.

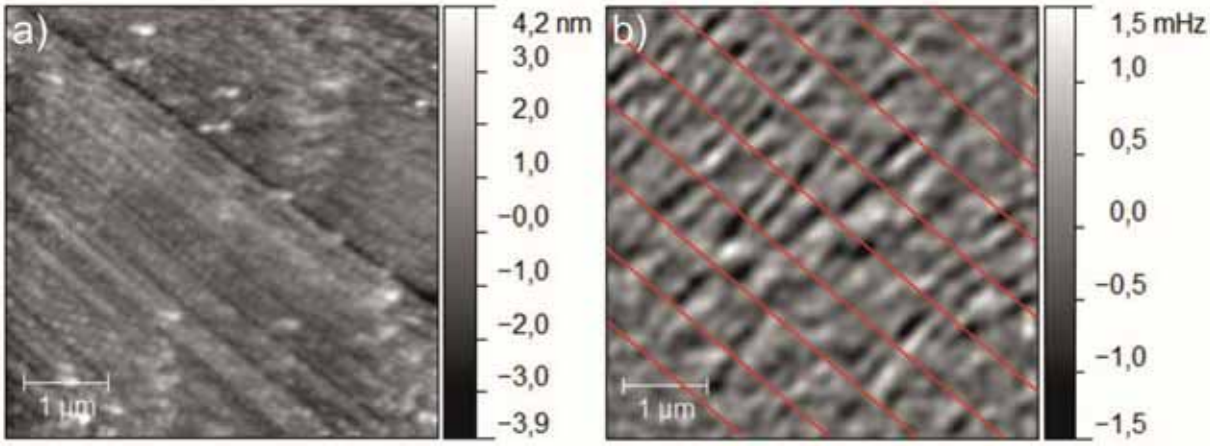

Figure 1: Lift Mode FM-MFM image of a hard disc using a qPlus sensor with an etched iron tip attached to it. Flattened raw data with imaging parameters $f0$ = 31679 Hz; k = 1800 N/m; Q = 1337; A = 100 nm and lift height 50 nm. a) Topography and b) Lift Mode frequency shift (low pass filtered); red lines as a guide for your eyes to the bit-tracks.

P.I-40

Non-contact atomic force microscopy of individual organic molecules

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Recently, Leo Gross et al. achieved atomic resolution on individual organic molecules by means of non-contact atomic force microscopy using oscillation amplitudes in the sub-Ångstrom range and functionalizing the tip. Thereby they resolved the chemical structure of individual pentacene molecules using constant-height frequency modulation imaging [1].

Here, we present data on individual phenacine molecules investigated in a modified commercial (SPS-Createc) low-temperature combined STM/AFM in which we integrated a q-plus sensor [2]. We show high-resolution AFM images using molecule-terminated tips with oscillation amplitudes below one Ångstrom. We were able to resolve the chemical structure of the phenacine molecules adsorbed on a metal substrate and on an ultrathin insulating film. In these images the nitrogen atoms can clearly be distinguished from the C-H groups. We deposited gold atoms onto the sample surface in order to form molecule-gold complexes.

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Self-assembly of Tetrathiafulvalene-Fused Dipyridophenazine (TTF-dppz) analyzed by tuning fork based AFM/STM

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Molecular electronics traces the aim of using molecules as active electronic and optoelectronic components. A main challenge consists in controlling the molecular growth and self-assembly on a surface, which is a higly complex dynamic process with competing binding modes, driven by thermodynamic and kinetic selectivity, the substrate conditions and inter- and intra-molecular interactions.

Here we investigate the self assembly of TTF-dppz (Tetrathiafulvalene-Fused Dipyridophenazine, Fig 1a)) [1] on metal substrates and thin films by combined tuning fork based atomic force and scanning tunneling microscopy at 77K and 5K. The TTF-dppz molecules were additionally functionalized with cyano-groups which yields in a better sticking of the molecules, also on insulating substrates [2].

After deposition on Cu(111), the molecules are assembled in a disordered phase. After post-annealing of the surface at 100°C (Fig. 1b)) a highly ordered self-assembly can be found, consisting of molecular wires, a network with six-fold symmetry, small crystallites and step edge decoration. Most probably the molecules decompose during the post-annealing, involving Cu-adatoms. The fact, that TTF-dppz molecules do not form such ordered structures on a Ag(111)-substrate, strengthens our presumption. Further investigations comprise the study of TTF-dppz on thin films and the adsorption of the two single compounds dppz and TTF.

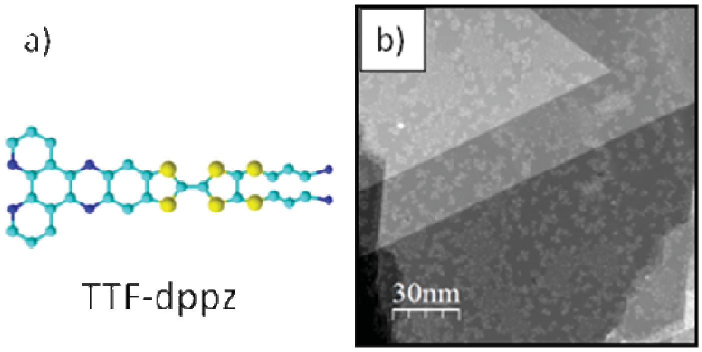

Figure 1: a) Schematic drawing of TTF-dppz. b) Overview of the Cu(111)-surface after post-annealing at 100°C, showing wire- and network areas.

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P.I-42

Systematic measurement of pentacene assembled on Cu(111) by bimodal dynamic force microscopy at room temperature

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Since the first measurement of the PTCDA molecule by dynamic force microscopy (DFM) in 1998 [1], DFM becomes a reliable tool to study the self-assembled molecular system, and so far many measurements have been reported on various systems[2]. Contrary to well-developed scanning tunneling microscopy (STM), DFM can measure mobility of molecules via the dissipation energy channel. However, a mobility of the molecule, especially at room temperature (RT), usually prevents stable small amplitude DFM, which is desirable for higher resolution imaging[3]. We have recently investigated this instability and invented a new method to overcome this instability, namely bimodal DFM[4,5].

Here, we use bimodal DFM to perform a systematic and high-resolution measurement on the complex pentacene self-assembled system.[6] Pentacene on Cu(111) was studied in a wide range of deposition at RT. The morphology and stability of the films were systematically studied via detections of the vertical and lateral tip-sample interactions with sub-molecular-scale resolution. At low coverage, pentacene adsorbs flat on the surface, where two phases of molecular assemblies were observed. At the boundary in between the different phase domains, a large magnitude of the dissipation energy, arising from the high mobility of pentacene, was measured while no significant increase of the dissipation energy is observed at the domain boundary of different orientations in the same phase. By increasing the amount of the deposited molecules, the second layer with the flat molecule tilted with a longitudinal molecular axis was observed in a small area, but most of the molecules moved to a certain site and formed crystallites with bulk structure on top of the first flat layer [Fig. 1(a)]. We found that the work function of the bulk surface was strongly affected by the first flat layer [Fig. 1(b)].

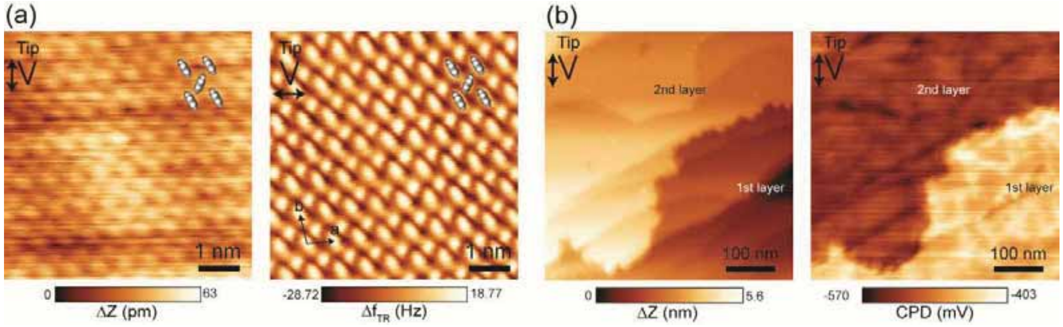

Figure 1(a) Topography and the torsional frequency map on the crystallites of pentacene, measured with bimodal DFM. (b) Topography and contact potential map of the first flat layer and second standing layer.

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P.I-43

Influence of chirality on molecular structure formation: Helicene molecules on calcite $(10\bar{1}4)$

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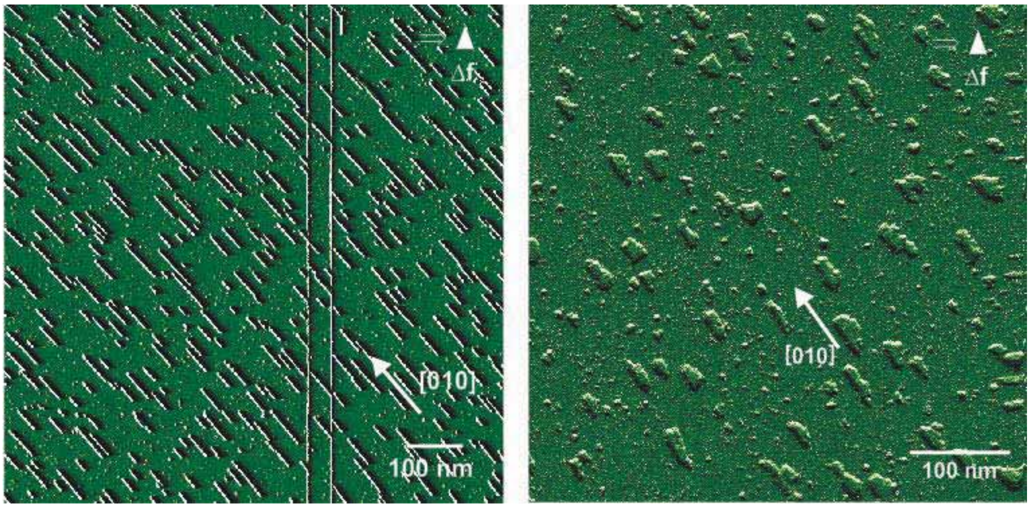
The influence of chirality on molecular self-assembly on surfaces is of great interest within both, fundamental as well as application-oriented fields, including, e.g., chiral recognition and enantioselective catalysis [1]. Ever since Luis Pasteur's famous experiment on the manual separation of a racemic mixture, the separation into homochiral structures such as two-dimensional domains, as well as chiral recognition upon dimer formation have attracted great interest [1,2].

Here, we present a study of heptahelicene-2-carboxylic acid ([7]HCA) on the $(10\bar{1}4)$ cleavage plane of calcite. The molecules were deposited in-situ from a heated glass crucible onto the freshly cleaved calcite surface held at room temperature. Both, deposition and non-contact atomic force microscopy (NC-AFM) imaging was performed under ultra-high vacuum conditions. For the racemic mixture, uni-directional rows consisting of molecular pairs are revealed [3]. However, from the NC-AFM images alone, it remained inconclusive whether these rows constitute heterochiral or homochiral structures. To address this question, we investigate homochiral [7]HCA molecules ((*M*)-[7]HCA and (*P*)-[7]HCA). Upon separate deposition of the enantiomers, islands are formed on the calcite surface in sharp contrast to the rows observed from the racemic mixture. Our results clearly indicate that heterochiral recognition is responsible for the formation of the aforementioned molecular rows.



Frequency shift images taken at room temperature. Deposition of the racemate reveals unidirectional rows [3] (left). Deposition of homochiral molecules results in island growth (right).

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P.I-44

Dynamic force spectroscopy on individual molecules

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In the last decades organic molecules have gained an increasing interest due to the possible use of organic molecules for advanced types of electronic devices [1–3]. A large field of research has emerged, studying the structural and electronic properties of organic molecules on inorganic substrates. There is a large interest in understanding the growth of such molecules on various surfaces.

By evaporating silver onto Si(111)7×7 surface, heterogeneous sample can be prepared showing very different characteristics. In contrast to the bare Si(111)7×7 reconstructed surface, the silver induce surface reconstructions such as the $\sqrt{3}\times\sqrt{3}$. In addition (111) oriented silver islands may also be present. These surface structures can be adjusted by the amount of silver deposited and the temperature during growth and annealing [4]. Organic molecules have been deposited onto these three different surface structures and a direct comparison under the same conditions becomes possible.

In the present study, force-distance spectra of individual PTCDA molecules on different Si(111)7x7-Ag surface reconstructions at 77K are presented. The focus of this work is a comparative study of different types of surfaces using the same tip in order to understand the mechanisme of dissipation in non-contact atomic force microscopy.

The experiments are performed using a homebuilt low-temperature dynamic force microscope with a tuning fork detection [5]. The high spring constant of the tuning fork (8000 N/m) enables very small oscillation amplitudes in the sub-nanometer regime without risk of snap into contact.

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The role of a molecular dipole on the adsorption on an ionic surface

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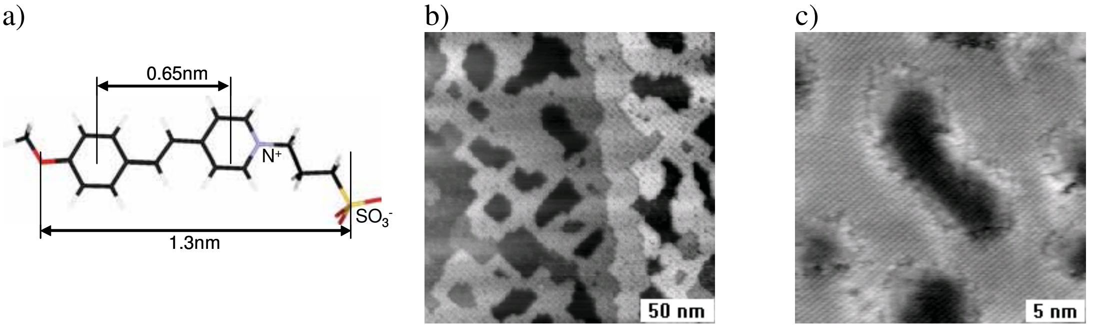
We investigated the adsorption of 4-methoxy-4'-(3-sulfonatopropyl)stilbazolium, (MSPS, (fig. a) [1] on the ionic surface of KCl (001) by means of NC-AFM under ultrahigh vacuum conditions. MSPS is a zwitterionic molecule with a strong electric dipole moment of 16.8D (N^+ and SO_3^-) which was chosen in order to control its adsorption on KCl. The molecule has already been investigated by STM on the surfaces of Si(111)-7x7 [1] and Au(23 23 21) where the molecule adsorbs with the dipolar moment perpendicular to the surface [2]. When deposited onto KCl at room temperature, MSPS diffuses to step edges and defect sites and forms unordered assemblies of molecules. Subsequent annealing induces two different processes: first, at higher coverage, the molecules assemble into well organized quadratic patterns that are perfectly aligned with charged rows on the substrate surface (e.g. (011) directions) and that show also multilayer growth (fig. b). The large scale quadratic pattern is a "Moiré effect" obtained due to the fact that the quadratic molecular pattern coincides every six distances with the substrate lattice constant. Second, at lower coverage and especially on surfaces with a higher density of defects such as electron beam irradiated surfaces with quadratic holes, the molecules reorganize step edges to run along the (011) direction (fig. c). A similar effect was reported by Trevethan et al. [3], however, in our experiments, it is clearly the strong dipolar moment of the molecule which rearranges the surface to create charged steps at which the dipole moment of the molecules can get aligned.

Our results clarify how the molecular dipole moment of zwitterionic molecules can influence both, the reorganization of ionic surface as well as the adsorption on these substrates.



a) molecular structure of MSPS, b) quadratic "Moiré pattern" at larger scale, and, c) reorganization of step edges along the (110) direction on an electron beam irradiated surface with low coverage of molecules, both effects are a result of the annealing process.

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P.I-46

Epitaxial growth of Pentacene thin films on KCl(100)

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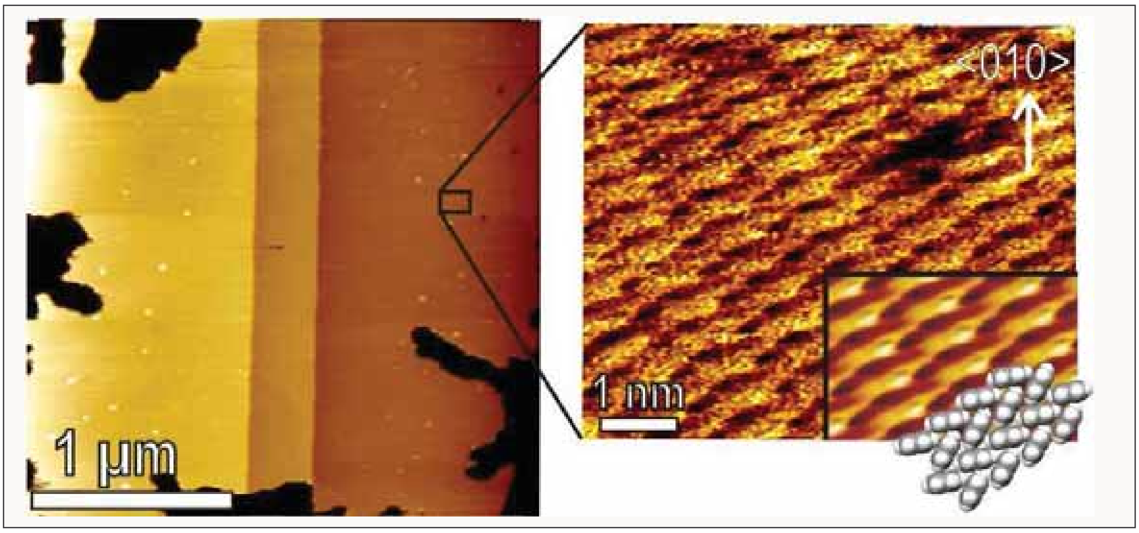
Since the electronic properties of molecular materials are closely related to their structural order a precise control of the molecular packing and crystalline orientation of thin films of the semiconducting organic molecules like pentacene (PEN $C_{22}H_{14}$) is of vital interest for an optimization of organic electronic devices. Of particular interest in this respect is the initial stage of film formation which is largely governed by the interplay of intermolecular and molecule-substrate interactions [1]. One approach to control the molecular film structure is based on substrate mediated growth. In this respect we have investigated by NC-AFM the structural properties of PEN thin films which were epitaxially grown by molecular beam deposition onto KCl(100) [2,3].

On KCl(100) PEN forms islands of a height corresponding to the van der Waals length of a single molecule [2] indicating an upright standing orientation of the molecules with respect to the substrate. This conformation enables islands to overgrow substrate steps which become obvious as steps of the height of KCl step edges on the top of the PEN islands. Having a closer look, images with molecular resolution could be achieved. The right micrograph exhibits several defects while presuming the expected herringbone packing motive of the PEN thin film phase. In agreement with diffraction measurements [3] a correlated average of these molecular resolved image leads to the proposition of a precise arrangement of PEN on KCl(100).



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P.I-47

Structure and energetics of fluorinated C_{60} monolayer on Au(111)

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Understanding of structure and energy level alignment at the interface between the organic molecular film and the metal surface is essential for further advances in organic devices. Structural homogeneity is a key to the achievement of high carrier mobility and the position of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) with respect to the metal Fermi level (E_F) determines the conduction type. One great issue is the limited availability of n-type organic materials. Because fluorination increases the electron affinity of the molecule[1], and thus the LUMO tends to locate closer to E_F than the HOMO, fluorinated molecules are good candidates for the n-type material.

From this perspective, we have studied one of fluorinated fullerene $C_{60}F_{36}$ (3D structure shown in Fig. (a)) deposited on Au(111) using scanning tunnelling microscopy (STM), non-contact atomic force microscopy (NC-AFM), and density functional theory calculations. A well ordered two-dimensional superstructure was successfully formed as shown in STM images (Fig. (b)). We determined the adsorption orientation and the superstructure model based on the calculated LUMO distribution and expected intermolecular CF-π interaction [2]. NC-AFM imaging of various modes as well as spectroscopies are performed. Based on measurements of frequency shift vs. voltage curves obtained on Au(111) and on molecular islands (Fig. (c)), we found an evidence of increase in work function by molecular adsorption. This result agrees with the idea that electrons transfer from Au to molecular film, forming the interfacial dipole. This together with scanning tunnelling spectra, we propose the interfacial energy diagram of $C_{60}F_{36}$/Au system.

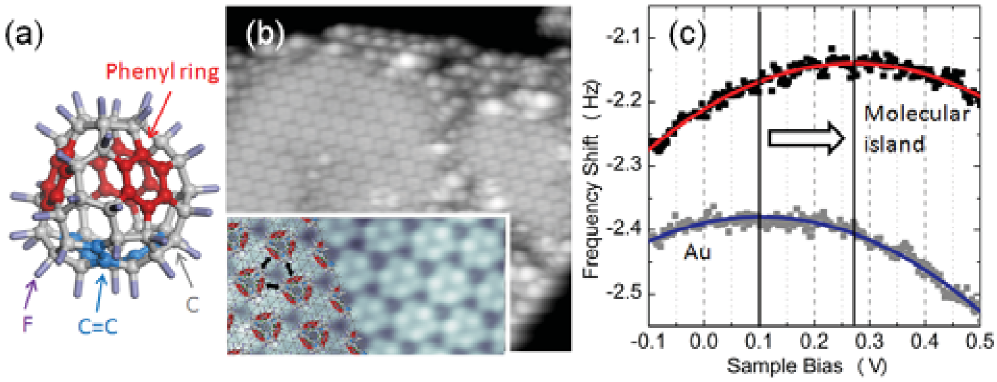

Figure (a) 3D molecular structure of C_3 isomer of $C_{60}F_{36}$. (b) STM images of molecular island. Inset is an enlarged image with its structural model. (c) Comparison of frequency shift vs. voltage curves on Au and molecular island. Data points are fitted using parabolic function.

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P.I-48

Electronic grain boundary properties in Cu(In,Ga)Se_2 -An orientation-dependent Kelvin Probe Force Microscopy study

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Thin film solar cells based on $CuIn_{1-x}Ga_xSe_2$ (CIGSe) absorbers yield the highest conversion efficiency of all thin-film photovoltaic devices. It is believed that benign electronic properties of grain boundaries (GBs) in CIGSe are one reason for this record performance. But in spite of considerable research activities on this phenomenon, the electronic properties of GBs in CIGSe are still discussed controversially. One aspect that is neglected frequently in discussions is the impact of GB symmetry on its electronic properties, as combined information about structural and electronic properties are hard to obtain on a microscopic scale.

In the present contribution, we report on combined measurements of structural and electronic properties of GBs in polycrystalline CIGSe thin films (Fig.1). Electron backscatter diffraction (EBSD) and scanning electron microscopy (SEM) were employed to obtain information about GB-orientation on a microscopic scale, while Kelvin probe force microscopy (KPFM) was applied on the identical locations as EBSD to obtain the corresponding electronic information. By combination of those techniques, it was possible to study electronic properties of GBs in CIGSe in dependence of their symmetry. Our investigations revealed that highly symmetric Σ3 GBs have a higher probability to be uncharged than randomly orientated non-Σ3 GBs. These results can explain the large scattering of electronic GB properties, as widely found by KPFM studies [1-3].

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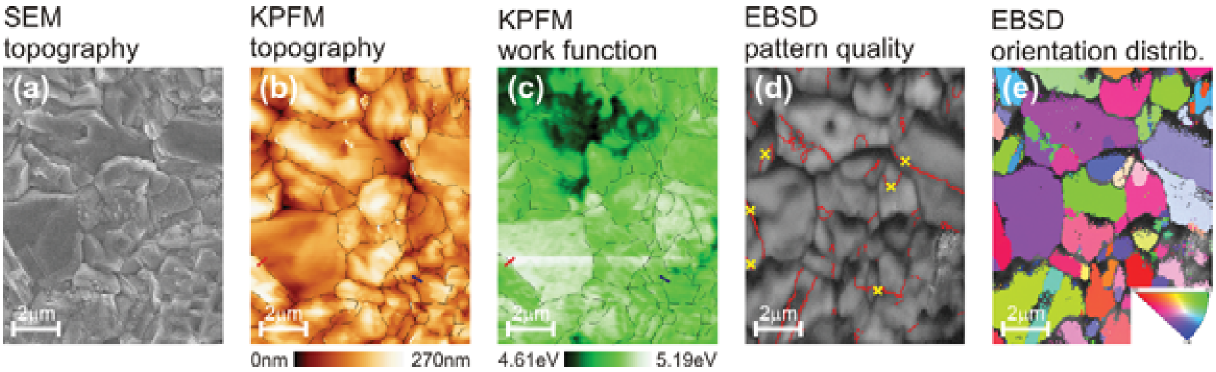

Fig. 1: 9.0μm x 11.3μm images of an identical surface location on a CISe film.
(a) SEM image, (b) KPFM topography image, (c) KPFM work function image, (d) EBSD pattern quality map, (e) EBSD orientation distribution map.

NC-AFM observation of Si(111)7x7 terminated with hydrogen

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Atomic hydrogen adsorption on silicon surfaces has been of great importance in surface science as well as in the process of semiconductor device fabrication in industry. Although various surface analytical methods were applied to the hydrogen terminated silicon, there are still controversial issues. For Si(111)7x7 they are the reactivity of atomic hydrogen to a Si adatom and a rest atom with a dangling bond including back bonds, the surface diffusion of hydrogen, and etching processes of Si atoms, though they have been revealed to some extend; scanning tunneling microscopy (STM) has significantly contributed to infer them. As widely accepted, STM depicts atom-resolved images depending on the local electronic density of states at surfaces. On one hand, nc-AFM can provide the complementary analysis to the STM from a viewpoint of force interaction between a tip and a sample. In this study we report that for the hydrogen terminated Si surfaces with atomic resolution.

We used a home-made UHV nc-AFM with a capability of simultaneous measurement with current and dissipation energy. We cleaned a Si(111) surface by flashing to exhibit the 7x7 reconstruction and terminated it with atomic hydrogen to prepare Si(111)7x7-H using a hand-made H_2 cracker in the nc-AFM UHV chamber; to crack H_2 molecules to be atomic hydrogen, the H_2 gas was admitted to 3×10^{-8} Torr for 10 min at a substrate temperature of 300 °C.

Figure 1(a), (b) and (c) show an nc-AFM image, a current and a dissipation energy of Si(111)7x7-H, respectively, simultaneously obtained with atomic resolution. The atomic contrast changes to various degrees. According to ref. 1 of analysis of Si(111)-H using STM, the atomic contrasts, from the brighter to darker in order, are possibly attributed to Si adatoms adjacent to rest atoms terminated with and without H, and ones with H, respectively. By using the nc-AFM we can compare the change in contrast of current with the change in force interaction to verify the atomistic model proposed on the basis of the STM observation. We will discuss the change in force over each site as well as in the energy dissipation.

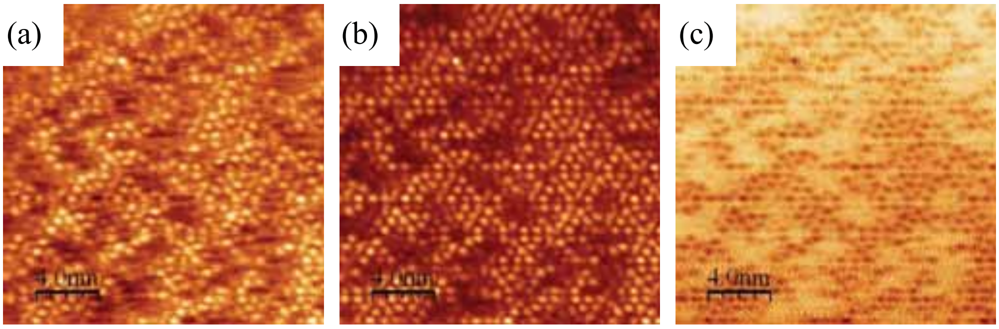

Figure 1 (a) nc-AFM image of Si(111)7x7-H at a frequency shift of -43 Hz and sample bias of -650 mV. (b) current image and (c) dissipation energy simultaneously obtained with (a).

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P.I-50

Junction formation of Cu_3BiS_3 investigated by Kelvin probe force microscopy and surface photovoltage

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The large scale fabrication of current high efficiency $Cu(In,Ga)Se_2$ or CdTe thin film solar cells could evolve into problems regarding the toxicity and limited availability of some constituents, like In, Se, Cd or Te. In the search for alternative absorber materials, Cu_3BiS_3 has been recently demonstrated to have a well suited band gap of ~1.4 eV. Preparation of polycrystalline thin films has been successfully realized using chemical bath deposition and sputtering [1] or coevaporation [2]. For the application in a solar cell device, the formation of the pn-junction is critical, especially considering the polycrystalline structure of the Cu_3BiS_3 thin film.

We present here an investigation of the Cu_3BiS_3 absorber layer and the junction formation with CdS, ZnS and In_2S_3 buffer layers. The surface potential distribution was imaged using Kelvin probe force microscopy (Fig. 1). Grain boundaries in Cu_3BiS_3 play an important role for charge transport and charge separation and their charge state can be influenced by the buffer layer deposition. Surface photovoltage (SPV) measurements at variable excitation wavelength indicate the influence of defect states below the band gap on charge separation (Fig.2) and possible surface defect passivation by the buffer layers [3,4].

Our findings indicate that Cu_3BiS_3 may become an interesting absorber material for thin film solar cells, however, for photovoltaic application the band bending at the charge selective contact should be increased.

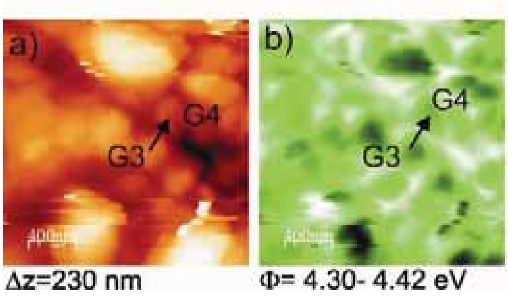

Fig. 1: KPFM measurement on Cu_3BiS_3/CdS.

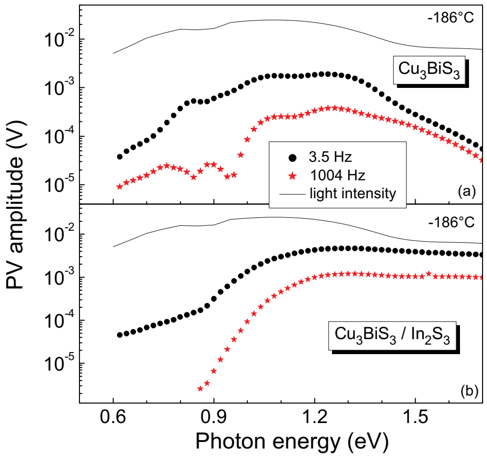

Fig. 2: SPV amplitudes at various modulation frequencies at -186°C for Cu_3BiS_3 and Cu_3BiS_3/In_2S_3.

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[2] F. Mesa and G. Gordillo, J. Phys.: Conf. Ser 167, 012019 (2009).
[3] F. Mesa et al., Appl. Phys. Lett. 96, 082113 (2010).
[4] F. Mesa et al., in preparation (2011).

Passivated Ge(001) surface investigated by tuning-fork NC-AFM at 4K

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The presentation will be focused on the low temperature NC-AFM investigation of a hydrogenated Ge(001) surface. Adsorption of hydrogen leads to change of both electronic and geometric structure of the surface. Reaction of the hydrogen atoms with the dangling bonds present on the clean surface removes buckling of the dimers leading to (2x1) surface structure. At the same time a surface bandgap is opened rendering the surface semiconducting. Recent development of self-sensing non-contact atomic force microscopy (NC-AFM) sensors based on the quartz tuning forks extended applicability of the NC-AFM technique to cryogenic conditions. Thus, the NC-AFM can now fully benefit from methods such as 3D site specific spectroscopy, very difficult at room temperature. We will present that thanks to passivity of the surface it is possible to approach with the NC-AFM probe very close to the surface – entering the regime where the tip apex experiences strong repulsion, and at the same time maintain stable operation of the microscope. As the result, the NC-AFM is able to yield images of much higher resolution compared to STM with individual hydrogen atoms clearly resolved. 3D force spectroscopy reveals complete force field over the surface. Additionally, the surface gives a unique opportunity to study isolated Ge dangling bonds always present, even on the well passivated surface.

P.I-52

Observation of local dipole moments on cleaned Si(111) surface with defects by non-contact scanning nonlinear dielectric microscopy

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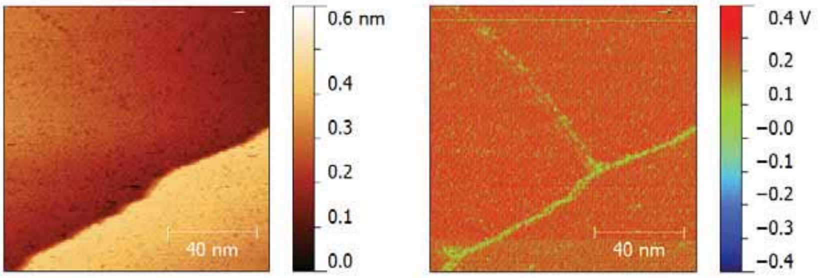
Non-contact scanning nonlinear dielectric microscopy (NC-SNDM) has enabled us to simultaneously image topography and dipole moments of a surface by detecting a local nonlinear dielectric constant [1]. The nonlinear dielectric constant is electrically measured by using a small GHz-range LC oscillator with a metallic sharp tip as a probe, whose frequency is modulated by nonlinear response of the tip-sample capacitance for an ac electric field. The investigation of local dipole moments is important in understanding the local electronic structure of surfaces and interfaces.



(a) topography (b) dipole moments

Figure 1: NC-SNDM images of cleaned Si(111) surface [3]

Our experiment was performed in an UHV chamber with a base pressure of $\sim 5 \times 10^{-11}$ Torr. The sample was n-type Si (111) with a resistivity $< 0.02\,\Omega\,\mathrm{cm}$ and prepared by a standard flashing procedure at ~ 1200°C. A sinusoidal voltage of 1.4 $\mathrm{V_{pp}}$ at frequency of $f = 30\,\mathrm{kHz}$ was applied between the tip and the sample for detecting nonlinear dielectric constants of ε_3 and ε_4 as the fundamental (f) and 2nd higher harmonic $(2f)$ component of the demodulated probe oscillation, respectively. Figure 1 shows topography (Fig. 1(a)) acquired by z-feedback using ε_4 signal and a dipole moment image (Fig. 1(b)) simultaneously obtained from ε_3 signal. The terraces were governed by the dipole moments pointing outward normal to the surface (red colored). The outward dipoles have been considered to originate in the adatoms of the Si(111)-(7×7) surface, as previously reported in Ref. [2]. Each of the adatoms has an outward dipole moment consisting of a positive charged nucleus and three covalent bonds below it. In these regions, the averaged amplitude of ε_3 signal was estimated as ~ 0.25 V. On the other hand, we find much weaker outward dipole moments (green colored), where the averaged ε_3 amplitude is roughly ~ 0.16 V. These dipoles arise, corresponding to the domain boundary and the step in Fig. 1(a). The difference between the two averaged values suggests that additional dangling bonds were created for the adatoms and then canceled a part of the original outward dipole moment at these defects.

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Interpretation of the electrical functionality of Cu(In,Ga)Se_2 grain boundaries based on cross-sectional Kelvin probe force microscopy

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The potential variations at grain boundaries on the surface of the Cu(In,Ga)Se_2 (CIGS) absorber and on the untreated cross section of the solar cell are investigated using Kelvin probe force microscopy (KPFM) in ambient conditions. The results show much smaller work function variations at grain boundaries on the cross section compared to the surface. In addition, the orientations of most grain boundaries are found to be quasi-parallel to the direction of charge carrier transport. Based on these observations, we conclude that the Cu(In,Ga)Se_2 grain structure has only minor influence on the charge carrier collection. This finding may unveil the success of this type of solar cell in terms of high efficiency and provide a guideline for the optimization of solar cells fabricated from other polycrystalline materials.

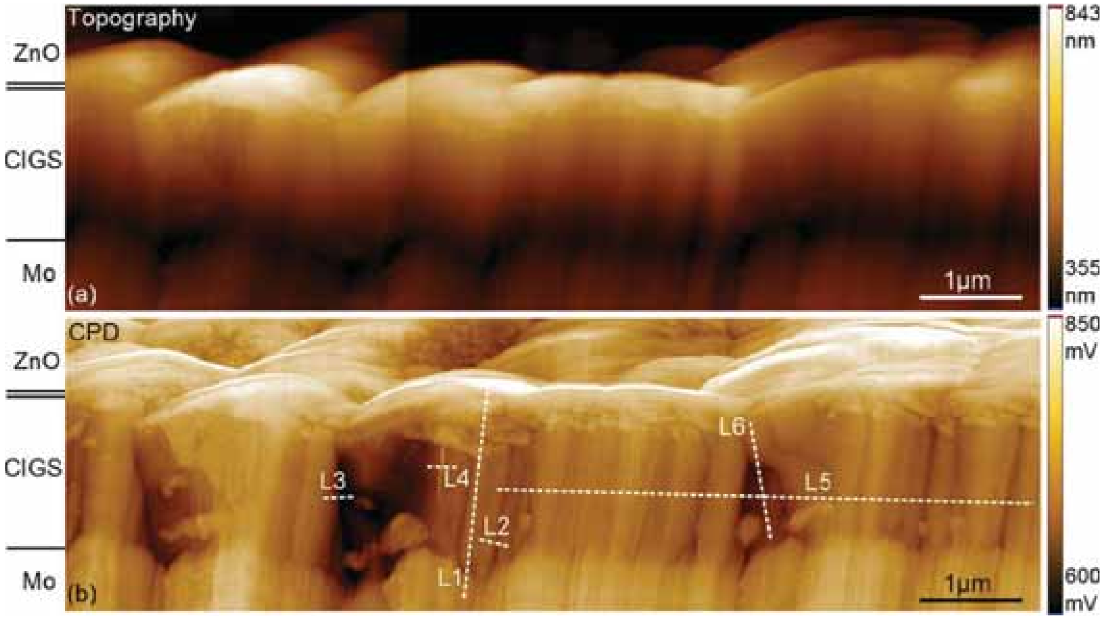

Fig. 1: KPFM measurement results from an untreated cross section of the CIGS solar cell. The topography and CPD images are shown in a) and b), respectively (image size: 2.9 x 9.5 μm^2). Line sections L1 to L6 in b) are analysed further in detail.

Rapid reconstruction of frequency shift vs. distance curves by multiple lock-in detection

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High-resolution three-dimensional dynamic force microscopy (3D-DFS) becomes an important tool to study tip-sample interaction forces. Measurements have been demonstrated mainly at low temperature where the thermal drift is negligibly small[1,2]. By incorporating an atom-tracked tip-positioning for excluding thermal drifts, 3D-DFS measurements recently become possible even at room temperature (RT)[3]. However, in both cases, a measurement usually takes more than 10 hours due to the enormous number of measurement points. Shortening the measurement time is one of the most important objectives, and the specially designed high-speed microscope successfully demonstrated a 3D-DFS measurement in a few minutes in liquid[4]. A general problem in such a time-consuming measurement is that the detection of the frequency shift (Δf) is performed in time-domain although significant signals locate only at a certain separate frequency domain (harmonics).

Here, we present a rapid reconstruction of the 3D-Δf landscape with the selective detection of the harmonic signals of Δf at RT. The second flexural mode of a silicon cantilever is used for the small amplitude operation (100 pm)[5], and df_{2nd} was detected by a digital phase-locked loop demodulator with a bandwidth of 1000 Hz (Zurich Instruments: HF2LI and HF2-PLL option). While scanning surfaces with a low feed-back gain, the Z sample scanner was modulated by 2 nm with a frequency of 45 Hz. The non-linear Z distance dependence of Δf gives rise to higher harmonic signals in Δf. The harmonics were directly detected by twelve digital lock-in amplifiers (Zurich Instruments: HF2LI x 2). The measurement bandwidth of ~1.7 Hz was small enough to separate the harmonics from each other and to obtain atomic resolution. Figure 1 shows a series of the harmonic signal maps of Δf_{2nd}, measured on KBr(001). From the twelve harmonic signals at each pixel, the high-resolution 3D Δf map was successfully reconstructed. The total measurement time amounts to less than 20 min.

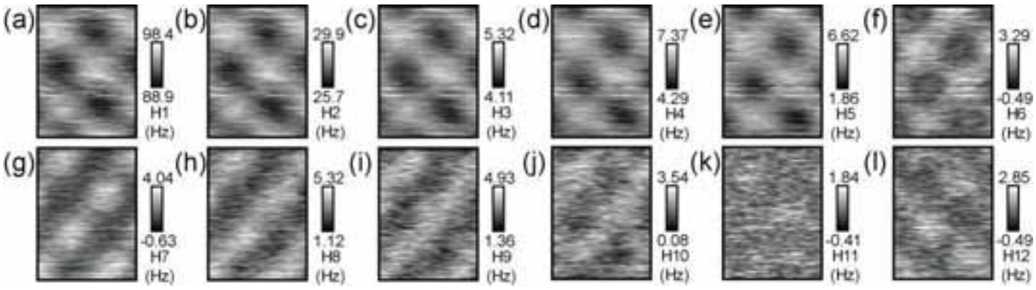

Figure 1: Higher harmonic images of Δf on KBr(001). The shift of the maxima position indicates the tip and sample deformations.

[1] M. Ternes *et al.*, Science **319**, 1066 (2008).
[2] B. J. Albers *et al.*, Nat. Nanotechnol. **4**, 307 (2009).
[2] S. Kawai *et al.*, Phys. Rev. B **83**, 035421 (2011).
[4] T. Fukuma *et al.*, Phys. Rev. Lett. **104**, 016101 (2010).
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Force Field Spectroscopy of Graphene on Ru(0001)

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[2]Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nanociencia), Cantoblanco, 28049 Madrid, Spain
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By high temperature exposure of ethylene gas on Ru(0001) at about 1000°C under UHV conditions a graphene monolayer is formed. A lattice mismatch between the layer and the ruthenium surface causes a superstructure with a periodicity of about 2.5nm [1,2]. The special electronical band structure of graphene as well as its mechanical properties are making it an interesting material for actual and future devices and further fundamental research [3,4].
Here, we are presenting the thoroughgoing investigation of epitaxial grown graphene on Ru(0001) by 2D spectroscopy measurements at room temperature. The periodic surface of its superstructure with different substrate bonded sites are causing site-dependend mechanical and electronical properties [5]. Dynamic Force Spectroscopy as well as Kelvin Probe Force Spectroscopy is done to characterize the nature of this sample system. Additionally, friction measurements by Contact Atomic Force Microscopy are pursued in order to complete the view on this outstanding material.

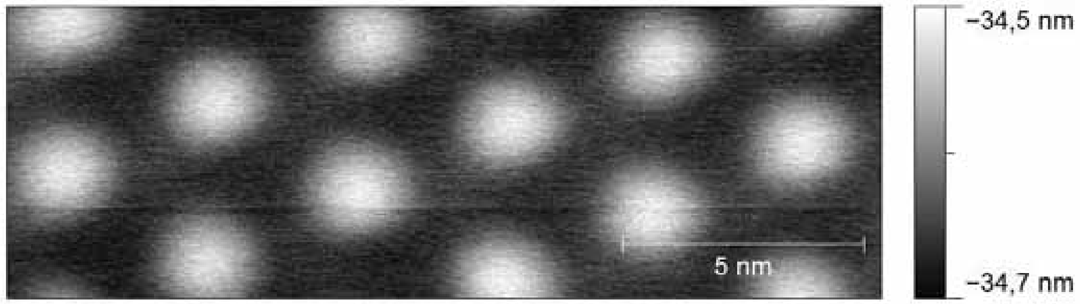

Figure 1: Topographical corrugation of Graphene on Ru(0001) showing the superstructure.
Scan Parameters: df=-8Hz, Amplitude=7nm, V_{DC}=-819mV

[1] A. L. Vázquez de Parga, F. Calleja, B. Borca et al., PRL 100, 056807, (2008)
[2] D. Martoccia, M. Björck, C. Schlepütz et al., NJP 12, 043028, (2010)
[3] M. Katsnelson, Mat.Tod. 10, 1-2, (2007)
[4] K. Novoselov, A. Geim, S. Morozov et al., Science 306, 666, (2004)
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Coupling of conservative and dissipative forces in frequency modulation atomic force microscopy – a source of apparent damping

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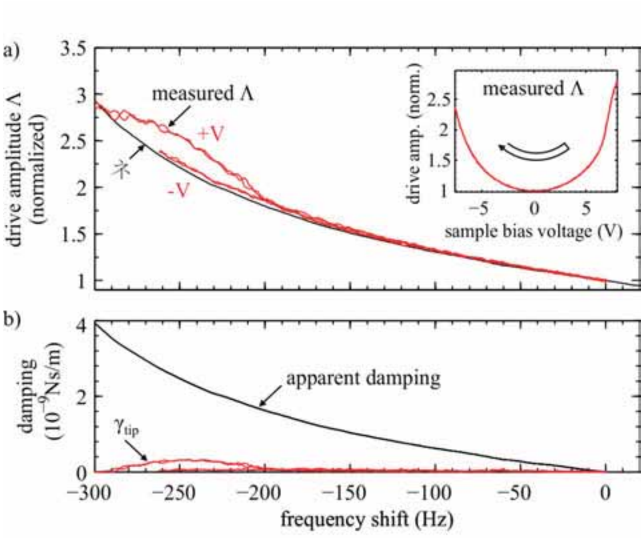
Experiments and theoretical calculations of dissipative forces in FM-AFM often disagree by several orders of magnitude. These discrepancies have repeatedly been attributed to instrumental artifacts, the cause of which remains elusive. We demonstrate that the frequency response of the piezoacoustic cantilever excitation system, traditionally assumed flat, can actually lead to surprisingly large apparent damping by the coupling of the frequency shift to the drive amplitude signal, typically referred to as the "dissipation" signal. Our theory [1], based on a recent derivation presented in the context of liquid environments[2], predicts problems in vacuum environments such as the large quantitative and qualitative variability observed in dissipation spectroscopy experiments, as well as contrast inversion in the drive amplitude signal observed at step edges and in atomic-scale imaging. The magnitude of apparent damping can escalate by more than an order of magnitude at cryogenic temperatures. We present a simple non-destructive method for correcting this source of apparent damping.



The normalized drive amplitude Λ was measured while sweeping the sample bias voltage twice as shown in the inset, and the same data is replotted *vs* measured frequency shift. The drive amplitude predicted for a conservative interaction (ネ) is plotted and shows that most of the measured drive signal is an instrumental artifact. b) The true damping was recovered (γ_{tip}) using the theory derivef in [1]. Assuming a flat piezoacoustic excitation transfer function would have resulted in additional apparent damping, also plotted, *and* the true damping (γ_{tip}) would have been overestimated by almost 3 ×.

[1] A. Labuda, Y. Miyahara, L. Cockins, P. H. Grütter, *submitted* (2011)
[2] A. Labuda, K. Kobayashi, D. Kiracofe, K. Suzuki, P. H. Grütter, H. Yamada, AIP Advances, *accepted* (2011)

POSTER SESSION II ABSTRACTS

Investigation of Point Defects at the $TiO_2(110)$ Surface by 3D-AFM

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[2]Center for Research on Interface Structure and Phenomena (CRISP), Yale University, USA
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The catalytic properties of surfaces are inherently related to their structural and electronic properties. In particular, forces extending from surface defects to the surrounding medium govern the local chemical reactivity and reaction paths at the surface. The recently introduced three-dimensional atomic force microscopy technique (3D-AFM) [1,2] provides quantitative surface force information that could advance our understanding of the related catalytic surface reactions.

We investigated different point defects of the rutile $TiO_2(110)$ surface, which is a commonly studied model catalyst. Our ultrahigh vacuum microscope [3] was operated at liquid nitrogen temperature using a tuning fork sensor that allows simultaneous measurement of the frequency shift and tunnelling current in the three spatial dimensions. From these data, we recover the surface force field experienced by the tip around defects with atomic precision, which ultimately reflects the defect's effect on the local chemical activity. To gain complementary information about the electronic surface properties, the simultaneously recorded tunnelling current was evaluated. On this poster, we present our preliminary results as force and current maps at constant tip-sample distances for different types of surface defects on the $TiO_2(110)$ surface.

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Force and Current Spectroscopy with Atomically Defined Tips

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Simultaneous force and current spectroscopy is used to study the electrical and mechanical properties of metal-metal and metal-molecule-metal junctions in the contact formation and nanoindentation regimes (Figure 1). A combined ultra-high vacuum (UHV) scanning tunneling microscope (STM) and atomic force microscope (AFM) with static force sensing is used for these studies [1]. Samples consist of Au(111) and Au(111)-C_{60} thermally evaporated on mica substrates and mounted on glass cantilever beams with a reflective Au coating. The cantilever beam acts as a force transducer with a spring constant in the range of 50-200 N/m and is detected by differential interferometry.

Experiments are carried out using probes which have been atomically characterized using field ion microscopy (FIM) [2]. Tips are fabricated by DC electrochemical etching of W(111) or W(110) wire in KOH or by AC electrochemical etching of Ir(100) in $CaCl_2$ followed by zone polishing under and optical microscope. These tips have typical radii of curvature between 3-20 nm (Figure 2). In addition, single atom tips of Ir can be prepared by e-beam evaporation. These well-defined probes are particularly suited for the detailed study of contrast mechanisms in STM imaging of metal surfaces [3].

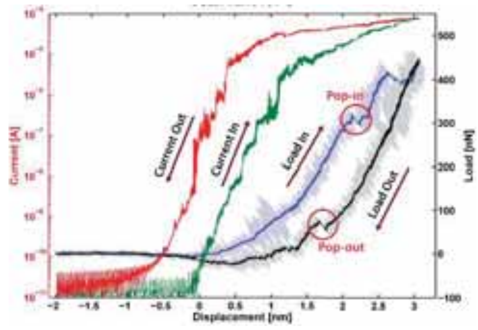

Figure 1: Simultaneous force and current nanoindentation measurement of W(111)/Au(111)

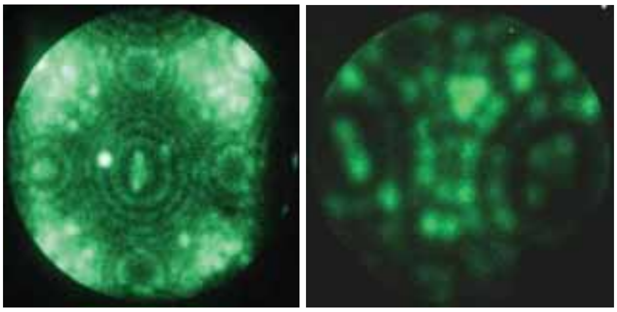

Figure 2: FIM images of Ir(100) and W(111) tips with radii of 16 and 3.2 nm, respectively

[1] Y. Sun *et al.*, PRB 71, 193407 (2005)
[2] A.-S. Lucier, H. Mortensen, Y. Sun, and P. Grutter, PRB 72, 235420 (2005)
[3] W.A. Hofer, A.J. Fischer, R.A. Wolkow, P. Grutter, PRL 87, 236104 (2001)

How do *you* calculate chemical interactions from Δf(z)?

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The extraction of consistent quantitative information about short-range chemical interactions between tip and sample in NC-AFM requires extreme prudence. This process typically consists of two parts: removing the long-range interaction component, and converting the frequency shift data, Δf(z), into interaction force, F(z), and/or energy, U(z). To a newcomer to the field of NC-AFM, rigorous consideration of the fallibility of these vital procedures seems overlooked in many cases, questioning the reliability of quoted values. Here we take a critical look at the variety of techniques employed, identifying key instances where a cautious approach is required most.

In many experimental configurations, removing the long-range interaction component is accomplished by fitting inverse power laws to either Δf(z) or F(z)/U(z). Some reported Δf(z) fits imply unphysical interaction potentials, whilst others are physical but ultimately unrealistic. Faithful fitting to an inverse power requires the inclusion of *all* long-range interaction data before the point where short-range interactions become significant. Here we describe a procedure to accurately identify this point.

The conversion of Δf(z) to F(z) and U(z) is well understood [1], however some aspects of the implementation of these formulae are over-looked, for example, the inclusion of flat noisy tail data can lead to spurious interaction forces and, in particular, energies at all tip-sample separations. Indeed, we show here how U(z) curves are much more susceptible to imprecise data analysis than F(z) curves. Fig. 1 demonstrates this point by showing F(z) curves with similar peak forces but very different peak interaction energies.

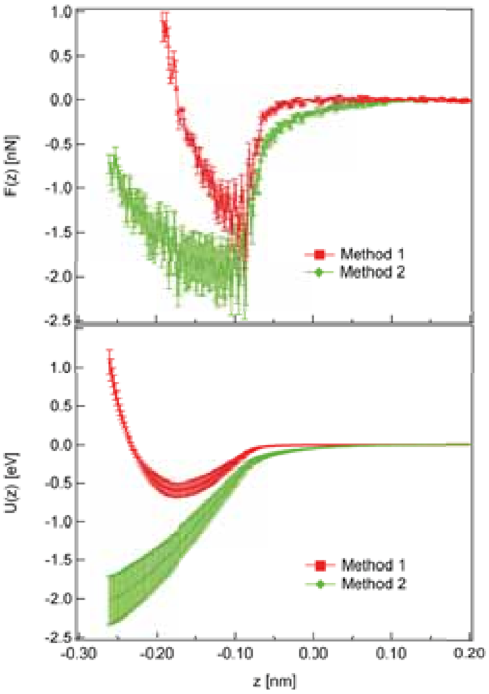

Figure 1. Examples of F(z) and U(z) curves for the interaction between a Si tip and an adatom on the Si(111)-(7x7) surface obtained by converting the same Δf(z) data using different long-range interaction subtraction methods. Similar peak attractive forces are obtained (in agreement with Ref. [2]), but wholly different peak energies are observed (the peak energy of method 2 agrees with Ref. [3]).

[1] J. E. Sader, S. P. Jarvis, Appl. Phys. Lett., 84, (10), (2004)
[2] M. A. Lantz, H. J. Hug, R. Hoffmann et al., Science, 291, (5513), (2001)
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P.II-04

Interaction-free measurement with tunnelling microscope

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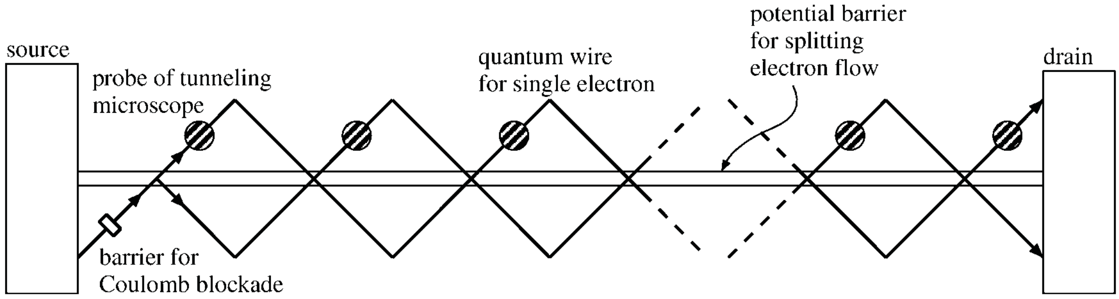
In this presentation, we propose a method for implementing the interaction-free measurement (IFM) with the tunnelling microscope. The discussions about the IFM begin to exist and develop from the following problem stated by Elitzur and Vaidman: “Let us assume there is an object that absorbs a particle (for example, a photon) with strong interaction if the particle approaches the object closely enough. Can we examine whether or not the object exists without its absorption?” The reason why we do not want to let the object absorb the particle is that it might lead to an explosion, for instance. Kwiat et al. find an experimental method for realizing the IFM [1]. They put the absorbing object in an interferometer which consists of many beam splitters, and inject a photon into it to examine whether or not the object exists. In Kwiat et al.’s scheme, the quantum Zeno effect plays an important role.

In the current presentation, we try to construct Kwiat et al.’s interferometer for the IFM, using an electron, quantum wires and a probe of the tunnelling microscope. Making use of the effect of the Coulomb blockade in a tunnelling-barrier, we can let electrons travel along the quantum wire one by one with a constant time interval. Then, we put the probe of the tunnelling microscope as the absorbing object into the interferometer, which is formed from the quantum wires and a potential barrier for splitting a current of electrons.

In our method, we replace the absorbing object with the probe of the tunnelling microscope. This prescription gives us the following advantage: Varying the distance between a tip of the microscope and the quantum wire, we can adjust the probability that the probe captures the electron, at ease. The dependence of the success probability of the IFM on the rate at which the probe captures the electron is investigated in Refs. [2, 3]. We try to examine this dependence precisely with referring to the Ref. [4], which shows the simulation method of Kelvin probe force microscopy.



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[2] H. Azuma, Phys. Rev. A, 68, (022320), (2003)
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A low temperature AFM tailored for lowest-noise qPlus operation

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At low temperatures, the quality factor Q of a qPlus sensor can reach values of around 200,000. At the sensors resonance frequency f_0 = 32kHz, an external vibration with an amplitude z_{noise} will cause an oscillation of the sensor with an amplitude $z_{\text{qPlus}} = z_{\text{noise}} \cdot Q$ [1]. For amplitudes in the 50pm regime, used for the detection of short range forces [2], z_{noise} has to be smaller than 25fm. While many commercial microscopes are available in the, home built microscopes do not need to sacrifice signal to noise ratio (SNR) in order to accommodate a wide variety of users. The presented microscope is therefore developed with a strong focus on mechanical stiffness to enable smallest oscillation amplitudes in a high Q environment.
Vertical approach motors are often based on a design idea by Pan [3]. For these microscopes, the coupling of the moving part of the coarse approach is not constant through the pathway of the approach. We overcome this by introducing a so called “Inverted Pan Design”. Furthermore, we have sacrificed the comfort of having an in-situ sensor change in order to strengthen the connection between the force sensor and the piezo to maximum performance. The whole Microscope will be implemented into a bottom-loading ^{4}He cryostat from Cryovac via an eddy-current damping stage.

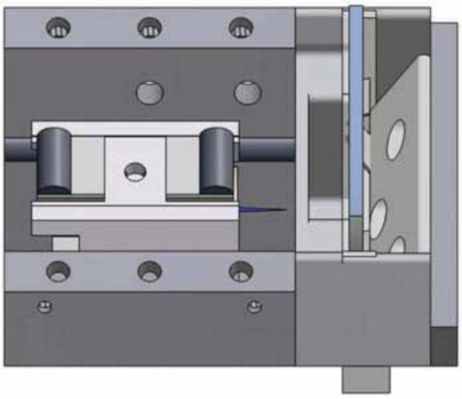

Fig 1: Schematic of the Coarse Approach
In contrast to the standard design according to Pan, the slider is much smaller than the housing around it, assuring a constant clamping force over the whole pathway.
The sensor (indicated as the blue pin) is directly mounted onto the tube piezo, sitting inside the slider

[1] F.J. Giessibl, (2003) Rev. Mod. Phys., Vol. 75, No. 3
[2] J. Welker, et ., (2011) arXiv:1106.3018v1, submitted to Appl. Phys. Lett.
[3] S.H. Pan, (1993), International Patent Publication Number WO 93/19494

What are the sources of frequency noise in NC-AFM ?

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It is now well established that frequency noise (as opposed to amplitude noise) is the main limiting factor for improving the signal to noise ratio in NC-AFM [1]. This noise has been considered in a number of works [1-4] and the main conclusion was that two sources of noise have to be considered (excluding environmental noise such as vibrations, thermal drift or electromagnetic perturbations): (i) The *thermal frequency noise* that arises from the thermo-mechanical fluctuations of the cantilever and (ii) the *deflection sensor frequency noise* that depends on the method used to measure the oscillation of the cantilever (i.e. beam deflection, interferometry, piezoelectricity- or piezoresistivity-based methods).
Recently a third frequency noise, called oscillator noise was introduced, in particular to discuss the noise in situations where the quality factor Q is low [5]. Here, we demonstrate that this contribution is not necessary. We derive the expression of the frequency noise in an idealized but still realistic situation and compare the resulting analytical expressions with numerical simulations performed with a virtual AFM [6]. In all the different cases considered (high/low Q, large/small measurement bandwidth), the agreement is excellent. It is essential in these calculations to take into account the closing of the positive feedback loop that drives the cantilever. This simple analysis is based on well-known results obtained in different research areas on noisy harmonic oscillators. We hope that it will allow clarifying the situation in the NC-AFM context.

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P.II-07

Combined SIMS-SPM instrument for high sensitivity and high resolution elemental 3D analysis

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State-of-the-art Secondary Ion Mass Spectrometry (SIMS) instruments allow producing 3D chemical mappings with excellent sensitivity and spatial resolution [1]. However, several important artefacts arise from the fact that the 3D mappings do not take into account the surface topography of the sample. The traditional 3D reconstruction assumes that the initial sample surface is flat and the analyzed volume is cuboid. The produced 3D images are thus affected by a more or less important uncertainty on the depth scale and can be distorted. The situation becomes even more complicated as the topography changes during the ion bombardment.

In order to correct for these artefacts, we have integrated a specially developed scanning probe microscopy (SPM) system into the analysis chamber of the NanoSIMS50 (Cameca) at the CRP-GL. This system includes a new high-precision sample stage, a scanner with a range of 100µm in x and y direction and a dedicated SPM head which can be operated in the static and dynamic AFM as well as in KPFM modes [2]. Topographical information gained from scanning probe measurements taken before, during and after SIMS analysis are used to accurately reconstruct the actual 3D analyzed volume. The prototype instrument, the dedicated software and first results will be presented in this contribution.

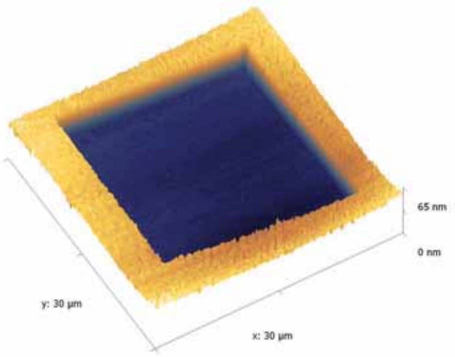

Figure 1: SIMS crater on PVC on a silicon wafer images by dynamic AFM. The area of the crater is 25µm× 25µm and the depth is 40nm.

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The NanoWizard® 3 – The Most Flexible, High Resolution AFM With True Optical Integration

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The NanoWizard® 3 represents the latest in AFM technology. The new Vortis™ controller series uses the latest FPGA architecture to guarantee highest digital performance. Fast signal acquisition and control, advanced feedback and analysis are key components of a modular and ultra flexible controller. The high-speed data acquisition makes the controller perfect for time resolved force spectroscopy, higher harmonics imaging or high frequency cantilever use. Cantilever calibration by thermal noise method up to 3.25 MHz is unique.

HyperDrive™ is a soft sample imaging technique in liquid which provides sub-nanometer lateral resolution with minimal tip-sample interactions and works with off-the-shelf cantilevers. This is made possible by the new optics and electronics of the NanoWizard® 3 AFM head, which gives the lowest noise level in the cantilever deflection detection system available commercially.

The NanoWizard® 3 maximizes stability, performance and ease of handling for samples in fluid and for full integration with optical microscopy. This enables the simultaneous acquisition of high quality AFM images with optical imaging, under physiological conditions. This is critical as for biological samples, whether cells or molecules, extra information from optical signals can be vital to interpreting the AFM images. This can be fluorescent markers of certain components, for instance, or structural information from optical phase contrast or DIC.

The unique DirectOverlay™ software for the JPK NanoWizard® systems uses the tip location to calibrate accurately the optical images and integrate them into the AFM software for direct AFM navigation. In addition, exact, quantitative correlation of AFM and optical features is possible.

With the NanoWizard® 3, AFM imaging and force spectroscopy can also be combined simultaneously with high end optical techniques such as confocal LSM, FCS, FRET, FRAP or TIRF. The Vortis™ controller allows direct photon counting for single-molecule experiments and extension to near-field techniques.

Flexibility is critical, as the future of modern AFM is increasingly in combining different measurement techniques and flexibility in different experiments. The range of electrical experiments such as CAFM, STM, Piezo Response, KPM, SCM etc. has been widely extended by different accessories as the boundaries between scientific disciplines provide some of the most interesting applications. The role of force measurements is also increasingly important, and this is reflected in the flexible software such as RampDesigner™, which allows free creation of force ramp movements for advanced force experiments, such as multiple force clamps.

P.II-09

Combined TEM and NC-AFM study of Al_2O_3-supported Pt nanoparticles

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Sintering, the growth of large particles at the expense of smaller ones, is one of the main causes of catalysts deactivation, since the physicochemical properties of a nanoparticle may depend strongly on its size, shape and composition. For application as heterogeneous catalysts, the nanoparticle kinks and edges often play an important role for the catalytic activity. In order to preserve these sites, it is important to stabilize the supported nanoparticles with sizes of a few nanometers during operational conditions at often high temperatures and in the relevant gas environments. A prototypical nanocatalyst system for studying coarsening consists of Pt nanoparticles supported on an Al_2O_3 material which is relevant as an oxidation catalyst in diesel and lean-burn engine exhaust after-treatment technologies.

In this study we address the effect on sintering of the shape of Pt nanoparticles supported on planar, amorphous Al_2O_3. Characterization of the size and shape of the Pt nanoparticles has been done by combining transmission electron microscopy (TEM) and non-contact atomic force microscopy (NC-AFM), because of the great complementarity between these techniques. TEM measurements very accurately give the nanoparticle diameters while AFM measurements give the height. It is suggested that the Al_2O_3-supported nanoparticles adopt size-dependent 3D geometrical shapes after thermal ageing and additionally, it is suggested, that the height-diameter ratio exhibits a surprising decrease with the nanoparticle size. This size-dependence of the shape may influence the ripening process in several ways.

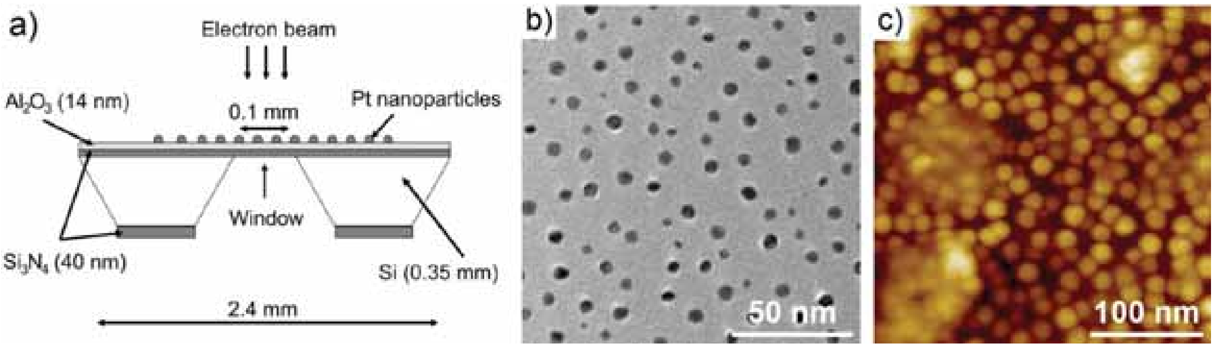

Figure 1: **(a)** Pt nanoparticles supported on a Si wafer with an amorphous and electron transparent Si_3N_4 window. **(b)** TEM and **(c)** NC-AFM images of the Pt/Al_2O_3 sample after aging in a tube furnace in 1 bar 0.2 % O_2 in N_2 for 3 hours at 650 °C.

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Force Control and Bandwidth: Enabling Faster AFM imaging in Survey, Screening and Dynamics Applications

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Since the invention of Atomic Force Microscopy (AFM) by Binnig & Quate the AFM's broad potential for imaging and characterization of numerous physical surface properties on the nano scale has been somewhat offset by it's slow imaging speeds when compared to other common microscopy techniques (optical, SEM, TEM). Therefore, the AFM is sometimes seen as a "specialty tool", powerful when other suitable techniques are not available.

The ability of the AFM's feedback loop to follow the sample surface faster is determined by the sum of the individual system component transfer functions. Different components get taxed more by different sample properties.

To overcome the limitations in imaging speed, in a general, non-sample specific way, the characteristics of all system components must be optimized to support the higher speeds, without compromising data quality, tip-sample force control, available scan sizes, or overall usability of the system.

Once this is achieved, a number of applications areas become attractive, in some cases even enabled:

- Surveying an unknown, heterogeneous sample to explore and document it's representative morphologies
- Screening a large number of similar class samples to characterize certain metrics on the nano scale and how they depend on sample variables, and
- Dynamics studies of processes on the nano scale, often in the area of molecular biophysics.

Survey Applications require ultimate data quality, a suite of imaging modes, unrestricted scan ranges, and easy sample navigation; Screening Applications require multi sample automation capabilities; Dynamics Applications require continuous trade off between data quality and time resolution, and efficient time series processing. For all applications, small probe availability, tip life, and cost are important factors, to go beyond the proof-of-concept stage.

We will show how we have addressed this range of challenges in our FastScan system, and will present the latest examples of the achievable results, in the areas of Survey, Screening, and Dynamics.

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Local Potential Measurements of Nanoparticles with Different Surface Charges in Liquid by Open-loop Electric Potential Microscopy

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Local potential distribution at a solid/liquid interface plays important roles in various processes. To understand the mechanism of these processes, it is critically important to directly measure local potential distribution in liquid with nanoscale resolution. Kelvin probe force microscopy (KFM) has been used for local potential distribution measurements in air and vacuum. However, KFM cannot be used in liquid due to electrochemical reactions and redistribution of ions and water caused by the application of ac and dc bias voltages between a tip and a sample.

To overcome this problem, we have recently developed a method to measure local potential distribution in liquid, which is referred to as open-loop electric potential microscopy (OL-EPM). In this method, only an ac bias voltage with a relatively high modulation frequency is applied between a tip and a sample. Owing to the slow time response of electrochemical reactions and redistribution of ions and water, the application of ac bias voltage with a high modulation frequency does not cause the problems observed in KFM measurements in liquid. Potential values are calculated from the amplitudes of the first and second harmonic cantilever oscillations induced by the ac bias voltage. In the previous study [1], we demonstrated that nanoscale local potential distribution can be measured by OL-EPM in electrolyte solution

In this study, to quantitatively evaluate the validity of the potential values measured by OL-EPM, we have measured surface potential of nanoparticles with different surface charges deposited on an HOPG surface. The topographic image [Fig. 1(a)] reveals the existence of the positively charged particles with a smaller diameter (~25 nm) and the negatively charged particles with a larger diameter (~50 nm). The corresponding potential image [Fig. 1(b)] shows that the average of the potential values measured on the positively charged particles is 70 mV higher than that measured on the negatively charged ones. This potential difference (~70 mV) approximately agrees with their zeta potential difference (~55 mV). These results demonstrate that OL-EPM has a capability of quantitative measurements of local potential distribution in liquid.

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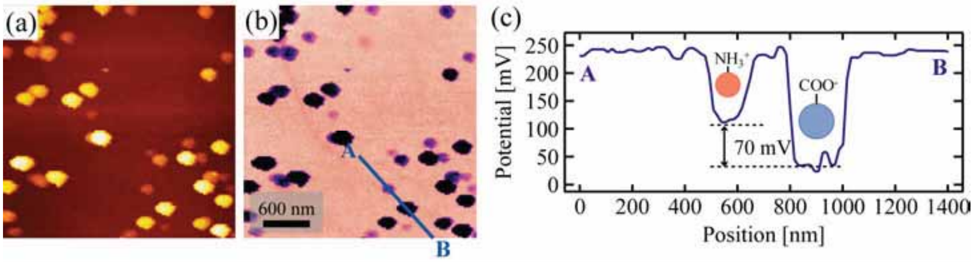

Figure 1. (a) Topographic and (b) potential images of positively and negatively charged nanoparticles on HOPG taken in 1 mM NaCl solution. (c) Potential profile measured along Line A-B in (b).

All digital PLL-based control system for high-frequency AFM cantilevers

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In a recent work by Roukes et al. [1], piezoresistive cantilevers with reduced dimensions and several tens of megahertz resonance frequency were used to increase the force sensitivity. In order to control such cantilevers in noncontact atomic force microscopy (NC-AFM), we propose an all digital and tunable control system which detects a 0.1Hz frequency variation for input frequencies ranging from 20kHz to 60MHz. The upper limit is well beyond the maximum one presented (15MHz) in [2]. This control system continues the development in our previous works described in [3] and [4]. It is based on a Phase Locked Loop (PLL) to detect the frequency shift which is used for the tip-surface distance control. Furthermore, an amplitude proportional integral controller (APIC) was implemented which drives the cantilever at its resonance frequency. The control system is connected to the microscope by means of a home built ADC/DAC daughter card. External inputs are added to the system for configurability purpose. They are set by the user via a graphical interface located on the host personal computer which is linked to the control system via an Ethernet connection managed by a microprocessor. The latter and the control system are implemented in a *Stratix III EP3SL150F1152C2* FPGA development board.

In order to validate the developed system, a $1V_{P\text{-}P}$ amplitude sinewave signal with 60MHz frequency was provided to the PLL. It is frequency modulated with a rate of 50Hz and a frequency deviation of 0.1Hz. A Tektronix oscilloscope DPO2012 has been used for the measurements. Fig. 1 shows the output of the PLL and demonstrates the ability of the system to detect 0.1Hz frequency shift.

In combination with the new high-frequency piezoresistive cantilevers, NC-AFM will provide high-speed scanning at all temperatures and in all environments with an improved sensitivity compared to traditional beam deflection.

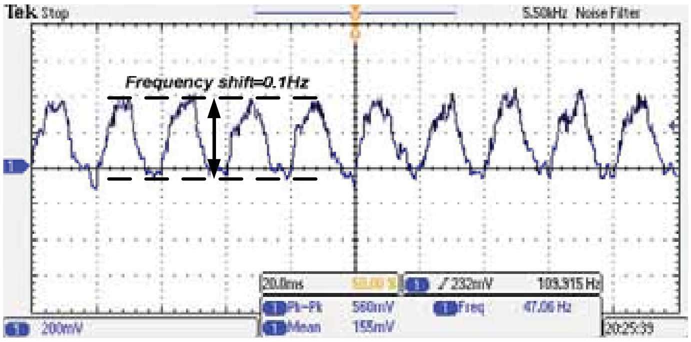

Fig. 1. Mesured output with $\boldsymbol{f_0}$**=60MHz**, f_{mod}=50Hz, Frequency shift(Fs)=0.1Hz

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P.II-13

Determination of cantilever stiffness from dimensions and eigenfrequencies

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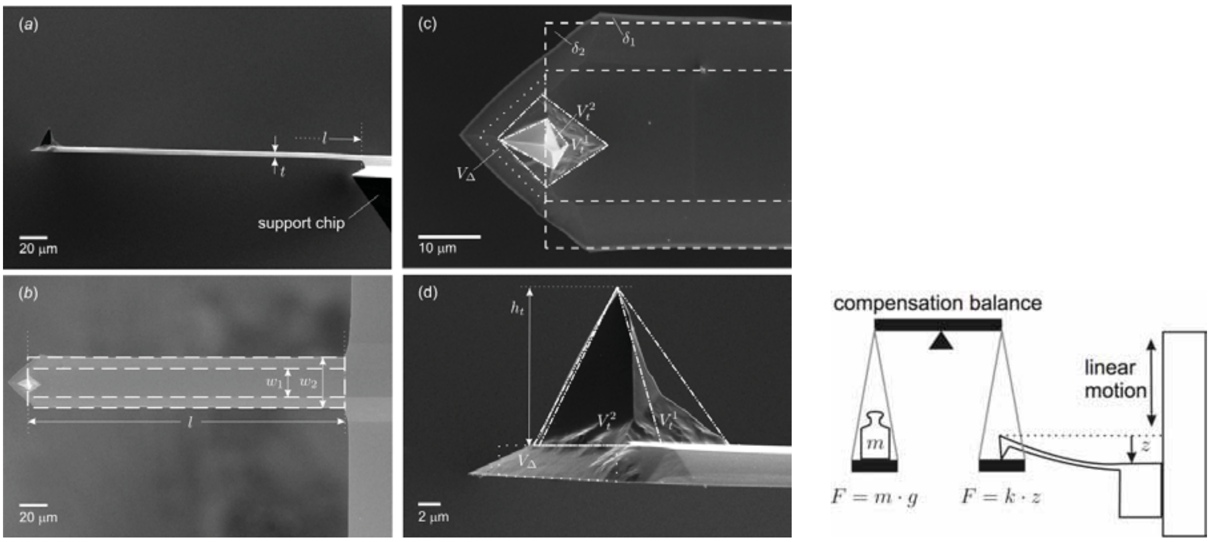
We discuss the non-destructive determination of the stiffness of silicon cantilevers with tips as used for non-contact atomic force microscopy under ultra-high vacuum conditions from the knowledge of cantilever dimensions and eigenfrequencies [1,2]. Results are verified by measurements with a tip-destructive precision method.

The calculation of the stiffness is based on dimensions derived from scanning electron microscope micrographs (left panel in figure), optical microscopy or interferometry. This yields stiffness values with an accuracy not better than 30% as the result depends on the thickness of the cantilever that is experimentally difficult to be determined. The accuracy margins can be reduced to 9% when the measured fundamental eigenfrequency is included in the calculation and a tip mass correction is applied. The tip mass correction can be determined from the eigenfrequencies of the fundamental mode and the first harmonic mode [3].

Spring constants determined by the dimensional analysis are verified by results obtained with an ultra-precision instrument determining the cantilever stiffness from a force-bending curve. This method is based on a force measurement with an ultra-precision balance and moving the cantilever with a nanopositioning device (right panel in figure) and yields an accuracy better than 5% when operated under well stabilized environmental conditions.



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Quantification of noise in NC-AFM systems for UHV applications

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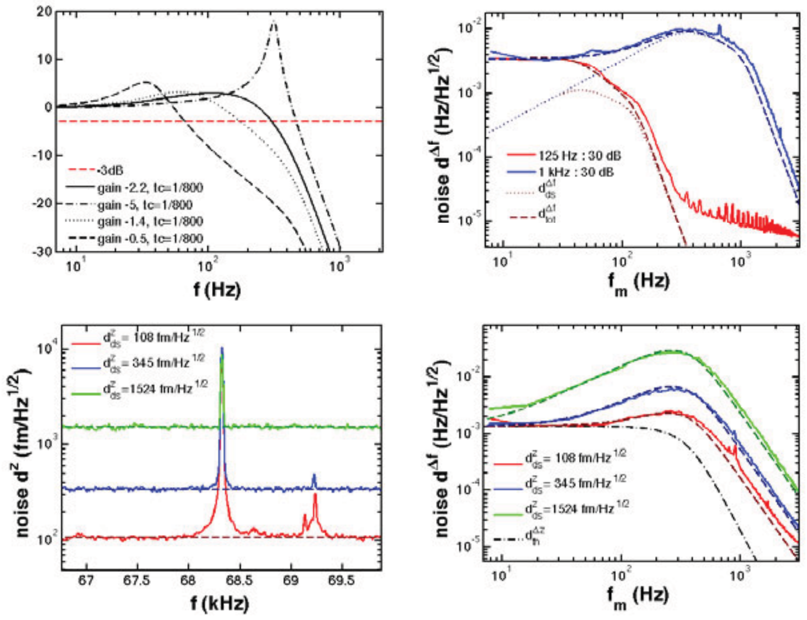
The total noise in the frequency shift signal Δf of NC-AFM measurements consists of thermal noise determined by the temperature and cantilever properties and instrumental noise from the detection and signal processing systems [1]. We investigate the deflection noise spectral density d^z at the input of the PLL demodulator as well the frequency noise spectral density at the output $d^{\Delta f}$ in dependence of cantilever properties and settings of the signal processing electronics. Prerequisite to a quantification of noise figures is the calibration of the cantilever deflection signal as well as the knowledge of the PLL demodulator transfer function.

Here, we study the transfer function of a RHK PLLpro 2 with different settings for the filter cut-off frequency and PLL loop gain and time constant settings. To quantify the cantilever oscillation amplitude and the deflection noise, we use a non-contact method based on the normalized frequency shift [2]. From the transfer function (upper left panel of figure) and the measured deflection noise spectral density (lower left panel), we derive predictions for the frequency noise spectral density (right panels) for various filter settings and different levels d^z_{ds} of detection system noise [1]. Predicted frequency spectral noise densities well agree with measured ones. When operated with appropriate parameters, a fully characterised system with low noise signal detection allows operation at the thermal noise limit with a significant bandwidth.



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Measurement of intrinsic cantilever properties from thermal noise

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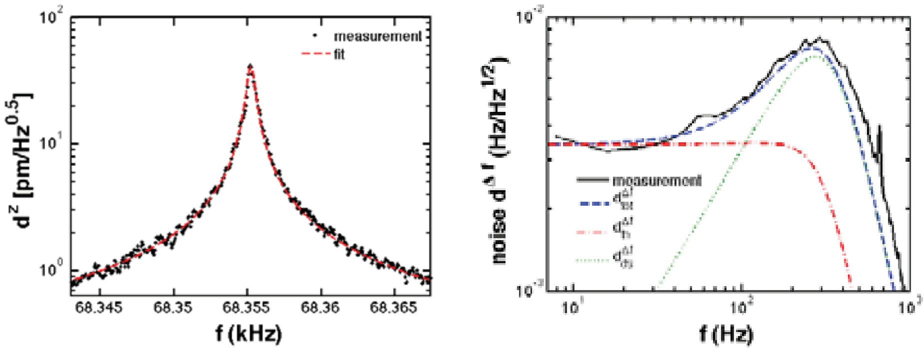
We investigate a method to determine the eigenfrequency f_0, the intrinsic quality factor Q_0 and the stiffness k from the cantilever deflection noise density $d^z{}_{\mathrm{th}}(f)$ as a function of frequency of a thermally excited cantilever in an ultra-high vacuum environment [1]. While a fit of the function of the deflection noise density to the experimental data (left panel in figure) is straightforward, the precise determination of cantilever properties requires great care in experimentation. The precision of the f_0 value as derived from the peak position is of the order of 0.1% and solely limited by thermal drift. The Q_0 value can be determined from the fit with a precision of 10 %, however, its reproducibility may strongly be forged by a mounting loss [2]. Most delicate is the determination of k derived from the fit of the $d^z{}_{\mathrm{th}}(f)$ curve. This measurement requires a calibration of the deflection measurement and utmost care has to be taken to avoid any excitation of the cantilever other than by thermal noise. Furthermore, the dynamic analysis of the fundamental resonance yields k_0 and has to be corrected to yield the static stiffness k [3].

As an alternative, we introduce an approach to determine dynamic stiffness that is based on a measurement of the frequency noise density $d^{\Delta f}{}_{\mathrm{th}}(f)$ at the output of the PLL demodulator. This approach requires separate measurements of the eigenfrequency and the effective quality factor but can easily be extended to higher order eigenmodes as the spectral analysis of $d^{\Delta f}{}_{\mathrm{th}}(f)$ can mostly be restricted to frequencies below 100 Hz and does not require high spectral resolution. We measure cantilever properties for the first harmonic mode and relate the respective dynamic stiffness k_1 to the stiffness k_0 of the fundamental mode and the static value k [3].



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Measuring Wear by Friction Force and Dynamic Force Microscopy

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In every product, one can observe wear on the moving parts during their lifecycle. The economic costs of wear are billions of dollars every year. Therefore, reducing the wear is the goal in every device and production process even though the microscopic origins of wear process have not been completely understood. With the invention of the friction force microscope (FFM) 1987, one gets a tool to examine friction and wear on the nano-scale. While the wear of the sample surface can easily be measured via the change of the sample's topography [1], it is not possible to measure the tip's wear simultaneously in a direct way.

From an experimentalist's point of view, tip wear is a well-known effect from everyday experience as a blunted tip reduces the resolution of the microscope. To quantify the tip's wear, it is possible to image the cantilevers tip in a scanning electron microscope (SEM), but this is a very time consuming procedure. For many experiments it is also not practicable, because the tip has to be transferred from the FFM to the SEM, which rules out the continuance of the wear experiment.

For measuring nano-scale wear of the tip, we introduce a new technique combining friction force and dynamic force microscopy. We are using the FFM for "weighing" the cantilevers tip mass. As the cantilevers resonance frequency depends on mass of the tip, we can measure the increase (the tip picks up some material from the sample) or decrease (wear of the tip) of the tip's worn mass down to some picograms due to the resonance frequency shift of the cantilever [2]. By attaching a small sphere to the upper end of the cantilever's tip we can detect the nano-wear of several material combinations with this approach [3].

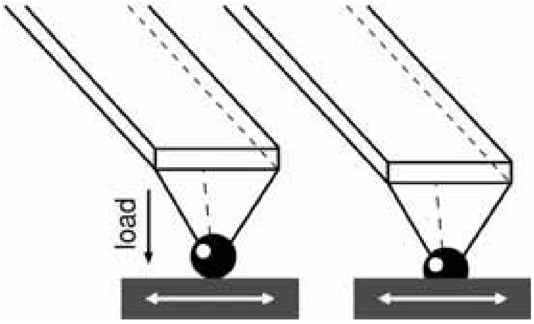

Fig. 1: Experimental setup

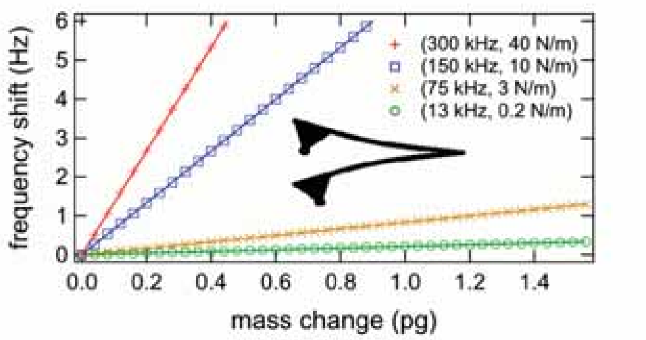

Fig. 2: Frequency shift depending on the mass change

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qPlus-based low-temperature STM/AFM: Built up and first experiments

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In recent years low-temperature scanning tunneling microscopy (STM) and spectroscopy have been very successfully applied to study electron transport through individual molecules. However, STM investigations are limited to conducting substrates and the experimental data is determined by both the geometry and the electronic structure of the sample in a complex and often ambiguous manner.

To overcome these two limitations we planned to experimentally implement force detection as an additional measure in molecular electronics. To this end a combined low temperature STM /AFM has been built up. The force detection scheme is based on the qPlus-sensor [1]. The scanner is based on the SPS Createc design and the qPlus has been integrated following the design of Gerhard Meyer [2].
On our poster we present first measurements that demonstrate the performance of the machine at low temperatures. We show high-resolution constant height Δf-images as well as Kelvin Probe Force spectroscopy data acquired with oscillation amplitudes well below one Ångstrom. Simultaneously, tunnelling current images are recorded down to the sub-pA regime.

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NanoXAS - Combining Scanning Probe and X-Ray Microscopy for Nanoanalytics

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NanoXAS is a novel x-ray microscope combining x-ray spectroscopy with scanning probe microscopy. While the first one gives access to chemical information, the second reveal the sample topology. We report the first results combining x-ray transmission and atomic force microscopy imaging at the same time.

The instrument uses Fresnel zone plates to focus x-rays (100 – 1800 eV) onto a semi-transparent sample which is raster scanned through the beam. A scanning probe microscope (SPM) is looking on the down stream side of the sample. In complement to the material contrast arising from the x-ray transmission chemical sensitivity, topology, magnetic forces, elasticity, friction, conductivity may be collected using the SPM. Scanning transmission x-ray microscopy (STXM) images have been recorded using the AFM tip to measure the transmitted x-rays allowing the record of the topological image in mean time. Furthermore the SPM tip could be used to collect the photo-emitted electrons produced upon x-ray absorption in the sample with high lateral resolution.

A few examples will be shown to demonstrate the principle (polymer blend, nanodots).

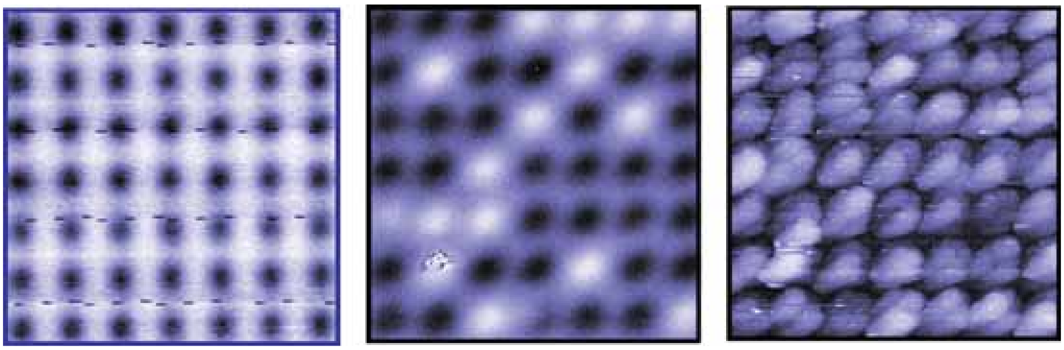

Fig. 1: *Co/Pt dot array (images size: 2x2μm^2, dots size: 120nm) imaged in the NanoXAS instrument showing STXM x-ray transmission (left), MFM magnetization (center) and AFM topography (right). All images were taken in-situ on the same area.*

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P.II-19

Reflection from diffraction grating etched onto the backside surface of AFM cantilever increases the force sensitivity

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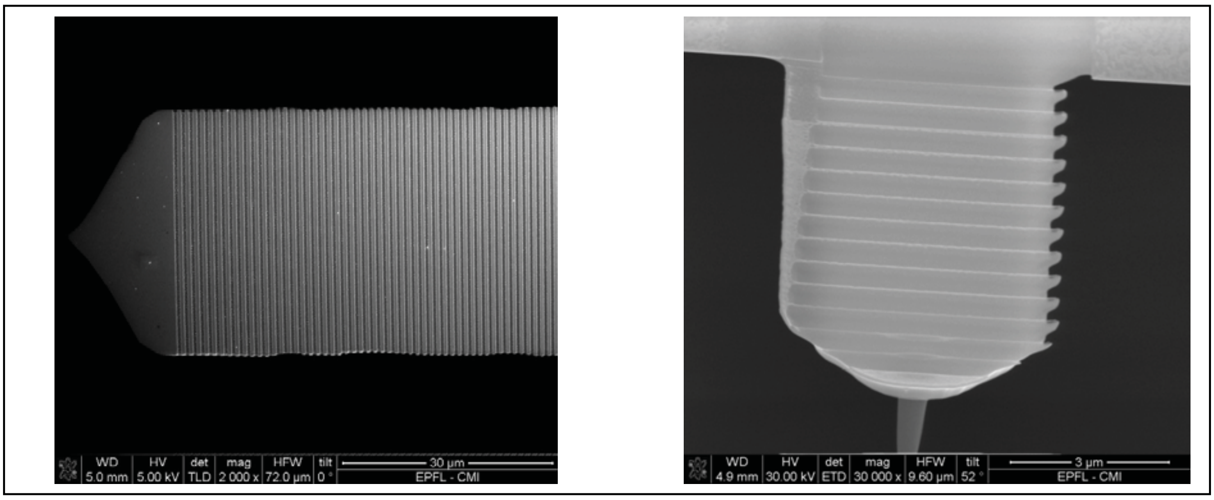
If a reflecting diffraction grating is prepared onto backside of a standard cantilever for atomic force microscopy, and diffracted light is used to monitor the angular position of the cantilever, the diffraction grating equation $d(\sin\vartheta - \sin\vartheta_0) = n\lambda$ shows that the derivative $d\vartheta / d\vartheta_0 = \cos\vartheta_0 / \cos\vartheta$ becomes much larger for small angles of incidence ϑ_0 and large angles of reflection of the diffracted beam ϑ. Correspondingly, the force sensitivity can be improved by few times when an appropriate detection scheme is used [1]: this approach does not give an improvement for a split detector but is important for position-sensitive (duolateral) detector, cf. [2]. (Note that the theoretical detection limit for the latter method is a few times smaller [2]). The first demonstration was performed with a one micron period d amplitude diffraction grating etched onto the backside of an Al-coated cantilever (see SEM image in Fig. 1 left), for the experiments in air and an analogous 600 nm-period grating for the experiments in water; special liquid cell was elaborated for the latter experiment, He-Ne with the wavelength λ=633 nm was used. Further applications of the method include the preparation of gratings onto very small cantilevers (see Fig. 1 right), where the measurements with the diffraction-type reflected beam enable to eliminate the background noise signal due to the reflection of light beam from the sample surface, which is extremely important for these small efg4cantilevers designed for ultra-fast scanning. Preparation of gratings of special forms can enable also to get a sensitivity improvement with the exploitation of the most standard split detectors, and it should be noted that much more cheap grating preparation methods, e.g. by “nanoprinting”, also exist. Additional advantage is the possibility of the simultaneous use of different orders of diffraction for the cross-check and noise reduction.



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Trimodal Tapping-Mode Atomic Force Microscopy

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We have commissioned a trimodal tapping-mode AFM method [1,2], by incorporating control of a third cantilever eigenmode into the already established bimodal tapping-mode scheme [3]. The new eigenmode is controlled using a phase-locked loop [4] and provides frequency shift contrast, in addition to the topographical and phase contrast obtained with bimodal tapping-mode AFM (see instrumentation schematic in Figure 1a). In general, we find that the higher-order phase and negative frequency shift exhibit similar behavior, in agreement with harmonic oscillator dynamics [1], although deviations from this trend are often observed, such that all available contrast channels should be complementary in the measurement of material properties. To further understand the higher-order contrast and to develop guidelines for selecting the controls schemes that would be most useful to include in a trimodal operation, we performed a series of bimodal imaging and spectroscopy experiments comparing the ability of higher eigenmodes to map conservative and dissipative tip-sample interactions under open-loop (OL), constant-excitation phase-locked-loop (CE-PLL) and constant-amplitude phase-locked-loop (CA-PLL) operation [5]. In each case we calculated the virial and dissipated power, and found that the OL and CE-PLL schemes provide similar information, while the CA-PLL scheme explores a broader range of interactions, especially for softer samples, due to its constant sensitivity to tip-sample forces.

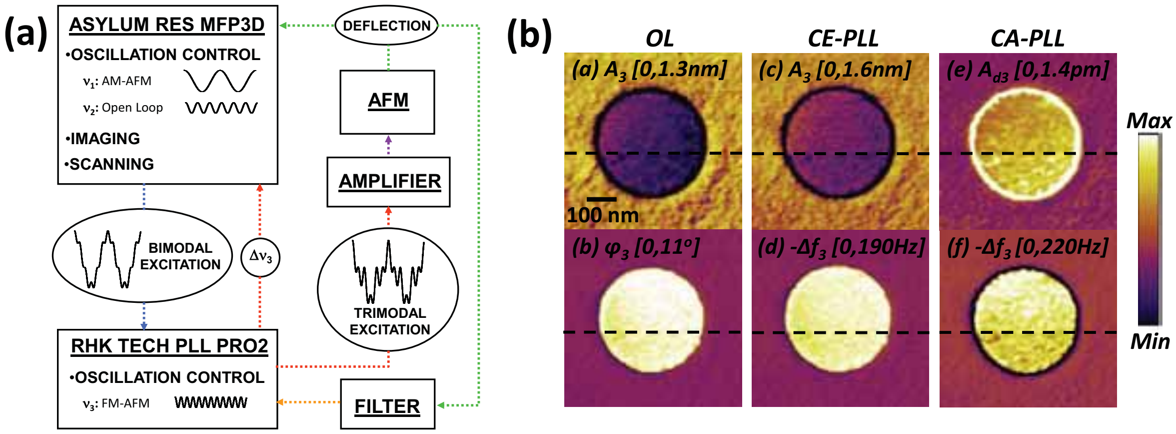

Figure 1. (a) Instrumentation schematic; (b) typical higher-eigemode contrast for two-component polymer sample under three different excitation schemes.

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P.II-21

Silicon AFM probes for dynamic AFM with sub-nanometre amplitudes

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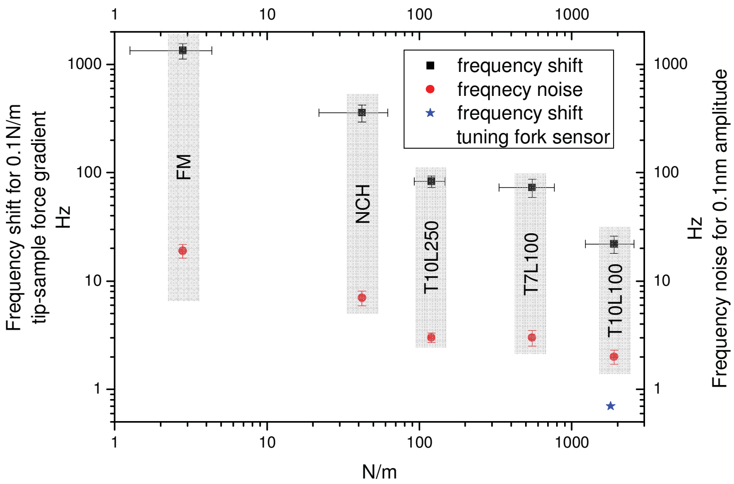
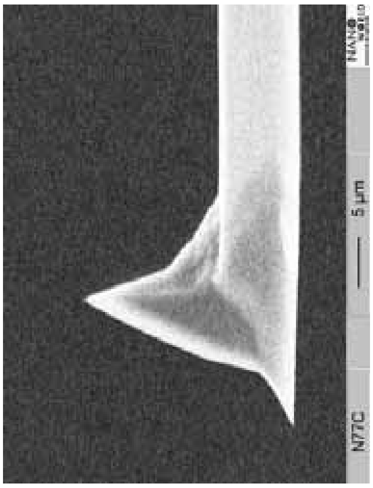
Dynamic AFM with extremely small oscillation amplitudes of the probing tip has shown its potential for atomic and even sub-atomic resolution [1]. By adjusting the oscillation amplitude to the regime of short-range forces the impact of long-range forces on the detection mechanism can be suppressed effectively [2]. This AFM technique requires extremely sensitive cantilever detection methods capable to resolve changes in the sub-nanometre oscillation amplitude such as frequency modulation (FM-AFM) techniques. Moreover, for stable operation the bending forces of the cantilever must be able to overwhelm the attractive tip-sample forces. An empirically limit for avoiding of such "jump-to-contact" instabilities is kA > 200nN [3] whereas k is the force constant of the cantilever and A is the amplitude of oscillation.

Therefore, dynamic AFM with sub-nanometre amplitudes (A < 1nm) requires cantilevers with a force constant larger than 200N/m. We present the design, realization and characterization of batch fabricated monolithic silicon cantilever probes with integrated sharp tips with force constants of 120N/m, 550N/m and 1900N/m enabling a stable operation with amplitudes down to 1Å. Even in case of the stiffest cantilever the expected frequency shift due to a 0.1N/m constant force gradient of the tip-sample interaction is in the order of 20Hz, well above the thermal noise of 1.6Hz at a typical measurement bandwidth of 100Hz. Due to small cantilever dimensions the first resonance frequency is more than one order of magnitude larger than for previous approaches based on tuning fork probes [1]. As consequence the sensitivity (frequency shift) is significantly improved.





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The effect of different tip preparations on force distance curves

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An accurately defined scanning tip is of utmost importance in non contact atomic force microscopy (nc-AFM). Both, the geometric structure tip profile and the tip surface contamination have an influence to the tip sample interaction. In addition a good working STM-tip is not necessary a good AFM tip. Therefore we have used different techniques of *in-* and *ex-situ* tip preparation and compare these by spectroscopy and topography measurement.

The tips (W) are chemical etched with an NaOH-Solution. After the etching process the tip will be placed into the vacuum system. The tips can be sputtered head on by ion bombardment with Ar^+ ions in situ. In the course of the sputtering process the tip will be cleaned from adsorbates and oxides. To assure the sharpness of the tip, SEM-images (scanning electron microscope) were taken before and after the sputtering process. In general the tips will be further prepared by field emission, in front of Ag(111) surface.

Force spectroscopy measurement with unsputtered and sputtered tips on various substrates such as the 7x7 reconstruction of Si(111) and the Ag-√3x√3-Si(111) reconstruction reveal significant different spectra.

Design and construction of a 300 mK, 10 Tesla, UHV facility for AFM

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In atomic force microscopy and spectroscopy the force sensitivity and energy resolution scales with √T as well as the minimal detectable dissipated energy. To increase the sensitivity or to observe certain phenomena, which only occur below a critical temperature, experiments have to be performed in cryogenic environments. Up to now low temperature experiments with atomic resolution are mainly performed using liquid helium, whereby temperatures down to 4.2 K can be achieved. Here the design and construction of a 300 mK instrument will be presented. Since we are mainly interested in magnetic experiments, the cryostat is also equipped with a superconducting 10 T magnet.

The 3He cryostat is a Heliox system from Oxford Instruments and is similar to an already existing STM [1]. It possesses a movable UHV-compatible insert with a 1K-pot constantly refilled via a flexible capillary from the main He bath. It can be pumped with an external rotary pump to reduce the temperature from 4.2 K to less than 2 K, which is required to condense the 3He. The small 3He reservoir, to which the microscope body is attached, is located below the 1K-pot. After condensation the rotary pump can be turned off (single shot modus). By pumping with a vibration-less charcoal-filled sorption pump a temperature of 300 mK can be reached.

The microscope body is based on a rigid and reliable design (Hamburg design with interferometric detection [2, 3]). However, for faster thermalization its body is metallic. For in-situ tip and sample exchange the microscope is lowered into a UHV chamber, because it cannot be accessed in its measuring position due to the presence of a 10 T solenoid. For preparation purposes, two additional side chambers are attached to the central cryostat chambers. In addition, facilities to deposit molecules and atoms onto a cold substrate located in the sample holder of the microscope also exist.

We will present the realization of the instruments based on the above described design concept as well as some first test results. Particularly, the material selection due to thermal requirements, the use of a strong magnet and the low temperatures as well as machinability for microscope parts will be discussed.

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Sapphire-based multi-environment AFM tips

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It has been shown that frequency modulation atomic force microscopy (FM-AFM) is a powerful tool for probing various samples not only in UHV, but also under ambient conditions and in liquid environments [1,2]. Sharp, stable and non-reactive tips are even more important for FM-AFM in air and liquid than in UHV, because the usual tip preparation methods (eg. Field emission or Electron-beam bombardment) are not available.

We are using tuning fork based sensors in the qPlus configuration, and are pursuing to build sharp, chemically inert tips. We demonstrate that we can produce sharp tips from bulk sapphire crystals, suitable for ambient, liquid and vacuum environment. We are showing the capabilities of these tips in a qPlus configuration for AFM in liquids The stability of the bulk sapphire tips is demonstrated by force lithography on calcite in liquid. Furthermore, we demonstrate the feasibility of in-situ coating these sapphire tips with iron, such that they can then be used e.g. for MFM experiments. As it is possible to attach any kind of tip material on to the qPlus sensor, we are in principle able to produce various kinds of coated tips.

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P.II-25

Towards in-situ Creation and Characterization of Graphene Devices

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We are working towards the all in-situ (UHV) creation and characterization of high quality nano-graphene devices on insulating templates. Our new 2nd generation Nanostencil/ Dynamic Force Microscope provides the capability of depositing nanostructured epitaxial ruthenium as a graphene growth template on insulating sapphire substrates [1]. The system is integrated in-situ with a high-resolution UHV scanning electron microscope, and with a 4-point nanoprobing station for electrical device characterization.

In the Nanostencil, patterns are defined by pre-fabricated stencil masks written into Si-nitride membranes using focused ion beam milling, and are transferred onto arbitrary substrates by UHV evaporation through these masks. The stencil technique is mainly limited my mask fabrication, and to date 30 nm line width has been demonstrated [2,3]. Compared with previous systems, our new Nanostencil system has improved positioning controls and the option to use a closed loop scan table for scanning in mixed static and dynamic patterning. We demonstrate the use of the Nanostencil to pattern a catalytically active thin film of ruthenium on sapphire [1], to generate in a second step high quality, nanostructured epitaxial graphene by high-temperature exposure to ethylene [3,4,5]. The nanostructured metal templates offer the possibility to grow graphene from a catalytic metal surface across adjacent insulating (sapphire) areas, thus providing a simple approach to electrically isolated, patterned graphene nanostructures. Additional masks can be aligned with these patterns to build up additional device elements, such as gate dielectrics and interconnects. The DFM integrated with the Nanostencil is used to inspect the patterned nanostructures on both metallic and insulating supports.

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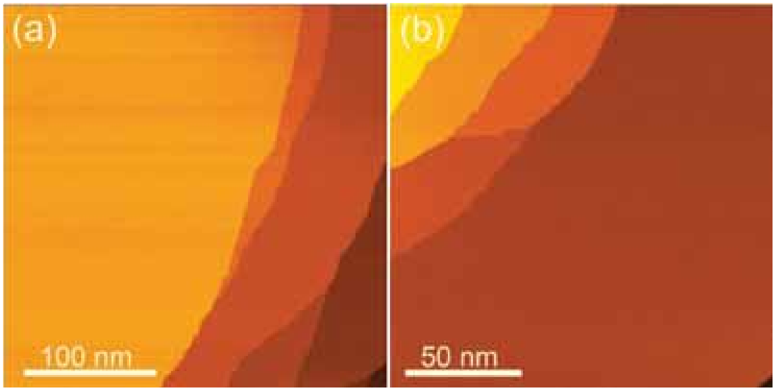

Fig. 1. (a) Overview STM image showing the surface morphology of the epitaxial Ru film grown on Al_2O_3 and the continuous graphene layer formed on it. (b) Zoomed image of the graphene/Ru moiré structure for epitaxial Ru/Al_2O_3.
Bias +0.5 V, current 1 nA.

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This research was carried out at the Center for Functional Nanomaterials, Brookhaven National Laboratory (BNL), which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

Open Source SPM Software GXSM and a very affordable DSP MK2-A810

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We present the latest developments and features related to the open source SPM control software project GXSM [1,2,3] and related Digital Signal Processing (DSP) with a dedicated analog interface "SignalRanger MK2-A810" [3,4]. Major enhancements were made under the hood providing dynamic data resolution, a improved high resolution mode for all outputs together with optimized scan and probe vector calculations. The DSP Control control interface now can be customized depending on experiment needs for a better work flow. Also new is a digital generated, but analog added Z-slope-compensation signal to get rid of sample tilt within Z data. A new real time "feature" (atom, molecule, etc.) tracking mode was added to the Vector Probe (VP) engine. This now allows to program real time sequences for tracking. The per default provided mechanism is based on a gradient up or down seek on a dual radius search algorithm. New modes allow sub-dividing a spectroscopic probe run to optimize for time and eliminate "energy" ranges of no interest – this is in particular useful for full spectroscopic image maps to save time. Will show examples of full spectroscopic image mapping and analysis of Aromatic Diisocyanides on Au(111) (see Fig 1.) by J. Zhou, P. Zahl, D. Stacchiola, Y. Li, P. Sutter, M. G. White.
Coming soon: Signal Ranger MK3 support by GXSM and also on the way is a included capability of running a full digital PLL using a advanced frequency detection algorithm; capable of up to 70kHz – very suitable for tuning fork DFM systems. Also a new: a high precision High Voltage Amplifier made by SoftDB with embedded DSP for advanced SPM functionality and digital full scale offset management and real time signal monitoring.

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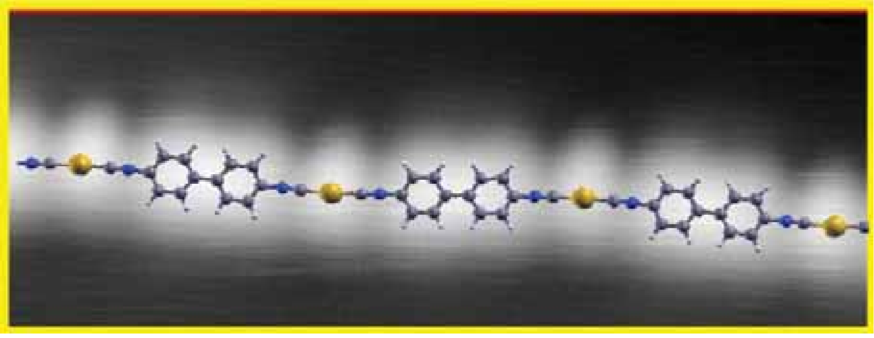

Fig. 1.: Superposition of a DFT calculated structure of a $[BPDIAu]_n$ molecular chain onto a STM image acquired at 5K and a bias of -1.6 V. Image size: 5.4 x 2.2 nm^2.

This research was carried out at the Center for Functional Nanomaterials, Brookhaven National Laboratory (BNL), which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

Long Range Tip Sample Forces using a FIM Characterized Tip

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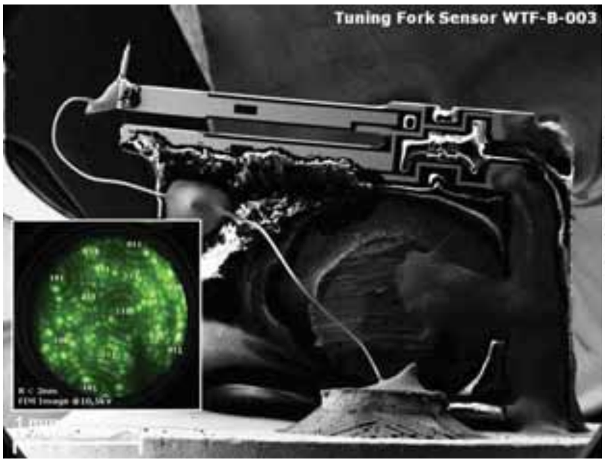
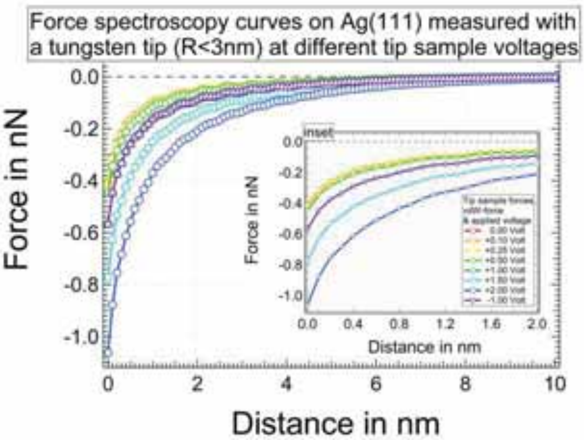
Since its invention non-contact atomic force microscopy (ncAFM) is the state of the art method to investigate surfaces with atomic resolution. Beyond imaging, the interaction forces between the probing tip and the sample can be measured with the so called force spectroscopy. For the correct comparison of these measurement results with predictions from simulation experiments, both interaction partners need to be known with atomic precision. In 1951 the Field Ion Microscope (FIM) [1] was presented for the first time which is able to image metal tips with atomic resolution in real time. The implementation of the tuning fork sensor in the "qPlus" design [2] with its metal tip to ncAFM allows the combination of these two techniques, AFM and FIM.

In our experiments we measure tip-sample force interactions curves using a tungsten tip characterized at the atomic level with a home build FIM. Force curves where acquired with a commercial tuning fork LT-AFM from Omicron. The combination of both microscopy techniques, i.e high sensitivity for the AFM operation and high voltages necessary for FIM, poses special requirements to the fragile tuning fork sensor. With our etching technique, based on the double lamellae technique [3], we gain ultra sharp tip radii (R<3nm) suitable for FIM (see inset of left picture below) as well as AFM with atomic resolution.

Here we focus on the full spectrum of long range forces measured in our experiment (see right picture below) with an atomic scale characterized tungsten tip. The individual force contributions, contact potential, van-der-Waals forces and electrostatic forces can be separated and compared with predictions from theoretical models [4], where the experimental tip shape and radius are known with molecular precision.





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Split quartz tuning fork sensor for enhanced sensitivity force detection

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For application of tuning forks (TF) in atomic force microscopy, it is important to measure reliably the motion of the prong where the probe tip is mounted, in order to correctly control tip/sample distance, and at the same time, to obtain the highest quality factor Q, to improve measurement sensitivity. The first request is not satisfied by a standard TF, motivating for instance the introduction of the “qPlus sensor” [1] where one of the prongs is immobilized. The second request, instead, is not satisfied by the qPlus sensor, while it is fulfilled by a perfectly balanced TF, that is, where the two prongs have the same mass, spring constant and dissipation coefficient. This condition is hardly obtainable by a TF with a probe applied to one of the prongs, leading to an increased mass and dissipation coefficient of the prong.

The above considerations have motivated us to explore an approach, already pointed out by other groups for different purposes [2,3], where a split TF is realized, with the electrical connection between the two prongs in antiparallel, like produced at the factory, is interrupted, and piezoelectric signals produced by the two prongs are addressed separately. The device produced in this way can be modeled in a more accurate way than the original TF, since interaction between the two prongs becomes purely mechanical, by removal of their electrical connection. With such device, the signal of each of the prongs, and particularly of the one supporting the probe, is measured separately in an accurate way.

In this work we show the experimental realization of such approach, as well as how the obtained result can be correctly described by a dynamical model where it is necessary to consider energy dissipation associated to the motion of the center of mass. Our analysis has shown which of the approximation customarily used in TF modeling can be justified or not.

An example of application of this configuration is represented by a kind of “Q control” realized by driving one prong by a given frequency and the other one by the signal produced by the first one. Depending on the amplification level of the signal driving the second prong, the effective Q can be regulated within a wide interval.

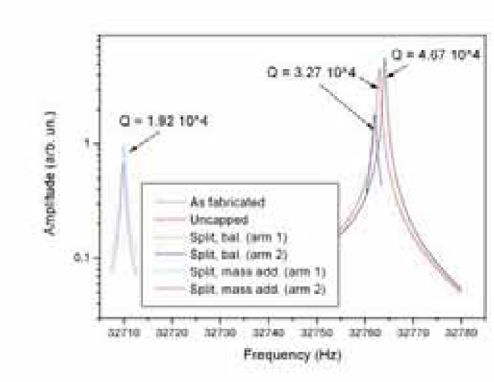

Figure 1: Q factor of a standard TF, of a split one, with or without a tiny mass on arm 2.

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Hybrid AFM, STM, and Near-Field Microwave Microscopy

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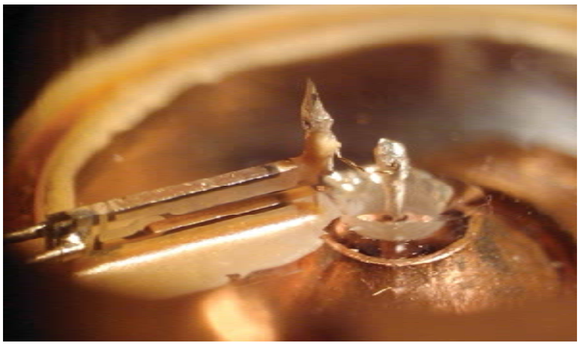
We present an update on our research into the development of a hybrid microscope which combines near-field microwave microscopy (NFMM) with AFM, STM, or both.

NFMM most frequently finds applications in the characterization of the GHz frequency dielectric properties of bulk and thin film materials [1]. In this talk, we present our work towards expanding the capabilities of NFMM beyond this traditional role. In previous work, we have shown that NFMM can be used to obtain atomic resolution images of conducting samples by combining it with scanning tunneling microscopy; the imaging mechanism in this case is GHz frequency alternating current through the STM tunnel junction [2]. We have also used NFMM to image magnetostatic spin wave modes in a ferromagnetic disk using scanning ferromagnetic resonance spectroscopy. Most recently, we have explored the domain structure and conductivity switching in multiferroic $BiFeO_3$ thin films using a single instrument which can simultaneously perform NFMM, AFM, and STM.

The microscope is based on a two-port resonant microwave cavity operating at 2.5 GHz with a quality factor of ~500. Coupling the resonator to a probe tip produces GHz frequency electric and magnetic fields confined to the region around the probe tip. The interaction of these fields with the sample produces a shift in the resonant frequency and quality factor of the resonant cavity. Tip-sample distance is typically maintained using the DC tunneling current on conducting samples, or using a tuning fork based AFM for non-conducting samples.



An image of the probe tip for the hybrid NFMM, AFM, and STM. A Pt-Ir STM tip is mounted at the end of a quartz tuning fork. A soft gold wire couples the tip to a microwave resonator and allows for measurement of the tunnelling current.

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Ultra-sensitive bias dependence of force-distance curve and hysteresis measured on single Pb adatom on Pb (111)

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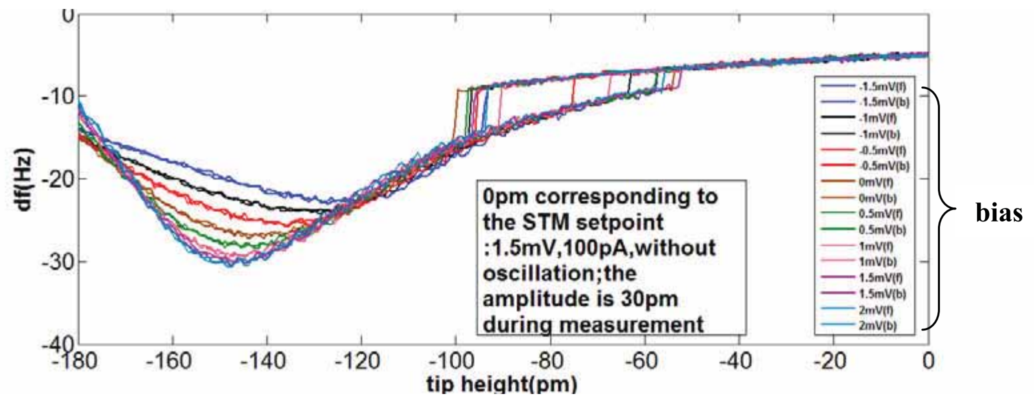
Using a Q-plus based NC-AFM, we observed hysteresis in the force-distance curve as well as in the simultaneously obtained tunneling current-distance curve measured on single Pb adatom grown on Pb (111) surface. The width of the hysteresis decreases with the increasing of oscillation amplitude, which is consistent with the model of N. Sasaki and M. Tsukada1. The 'real' two turning points of the hysteresis were determined by the tunneling current-distance curve with zero oscillation amplitude being (STM mode). The energy dissipation involved in the hysteresis, which was found to be 40 meV, was obtained from the step in the excitation-distance curve by using large oscillation amplitude (at least the same as the distance between the two turning points of about 100 pm). More interestingly, with small amplitude (e.g. 30 pm), the part of the force-distance curve closer to sample than the two turning points changes dramatically with bias in the scale of only 1 mV. We suggest that the adatom jumps to one of the bi-stable states between surface and tip, which makes the electrostatic shielding of surface charge on the adatom weaker. Consequently, the short-range electrostatic force becomes dominant and sensitive to bias.



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P.II-31

MgO on Ag(100): A simultaneous STM/AFM study

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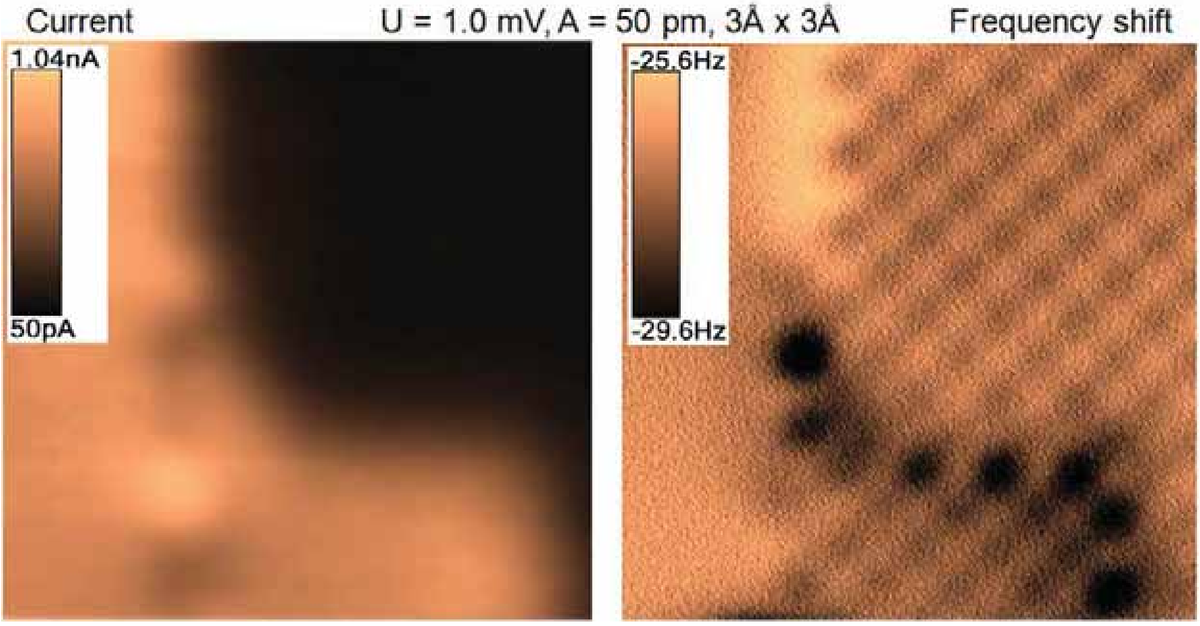
MgO is a promising decoupling layer for the study of electronically isolated atoms and molecules on surfaces. The electronic and structural properties of MgO on Ag(100) have been studied by STM [1], AFM [2] and KPFM [3]. Here we performed constant height imaging on small MgO islands to record frequency shift and current simultaneously at low bias voltages. Frequency shift images show atomic corrugation of the MgO lattice, whereas, as expected, there is no atomic contrast visible in the current data.

Two different types of islands are normally observed. When MgO is grown on an Ag(100) crystal with sub-monolayer coverage the islands are usually on top of the Ag surface or embedded within the Ag lattice. Here we report upon a bias dependent contrast in STM images within single islands which are embedded in the Ag surface. The two different regions are also distinguished by STS measurements. Constant height frequency shift images above both regions show an attractive boundary at the interface between them.



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Development of nc-AFM/STM using a tuning fork quartz force sensor

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Invention of an easy-to-use force sensor with high sensitivity is one of central issues in nc-AFM. Quartz is one of promising materials for it; Giessibl successfully introduced the q-Plus sensor of a quartz tuning fork [1]. The quartz sensor has advantages in respect to self-sensing of a change in its resonance frequency in high accuracy with its high Q value, and to its temperature stability, and furthermore to its high spring constant to avoid jump-to-contact with a sample surface. In this study we construct an ultra-high vacuum (UHV) microscope with the quartz force sensor operated in nc-AFM and STM with a field ion microscope/field emission microscope (FIM/FEM) to evaluate a tip on the force sensor. To excite the sensor in a straightforward way, we adopt a self-excitation method. To decrease an AC current signal due to the capacitance of the sensor and the capacitance coupling around the sensor [2], we construct a compensation circuit to cancel out the signal to attain a better S/N ratio.

We used a quartz tuning fork (Epson Toyotem, f_0 = 32.768 kHz), and one prong of the fork was attached to a ceramic holder with epoxy resin. An electrochemically etched Pt-Ir (8:2) tip was attached at the end of the other prong. An equivalent circuit of the fork is shown in fig. 1. In use of inverse piezoelectricity to excite the fork at its resonance frequency, the resonance curve exhibited asymmetric owing to an AC coupling through capacitance C2, as shown in fig. 2(a). Thus, we used a pulse transformer to generate both of an excitation AC signal and the AC signal with a phase of 180° to that. We adjusted the output of a current amplifier, placed near the AFM head in UHV, to be zero by changing the value of a variable capacitor in a frequency range at off-resonance. As the result, we obtained a symmetric resonance curve shown in fig. 2(b), and the noise due to the AC coupling was less than the white noise level. The sensitivity of the senor was 3 μV/pm at the output of the amplifier, which was evaluated from the normalized frequency shift with respect to a change in amplitude, and from a noise spectrum using a lock-in amplifier. Using this system we obtained atom-resolved frequency shift images in the mode of dynamic STM for a Si(111)7x7 surface, as shown in fig. 3. We will discuss the imaging mechanism of the Si surface with a metallic tip.

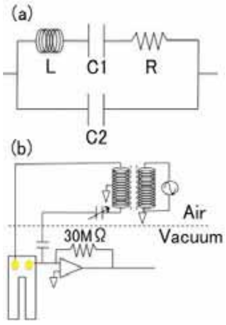

Fig. 1 (a) equivalent circuit of a quartz tuning fork, and (b)compensation circuit to cancel the capacitive coupling.

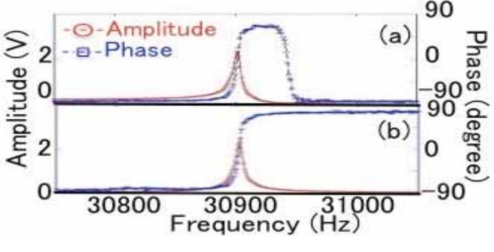

Fig. 2 Resonance and phase curves (a) without the cancel circuit, and (b)with the cancel circuit

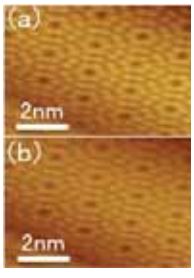

Fig. 3 (a)Dynamic STM image, and (b) Δf image.

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P.II-33

Small-amplitude FM-AFM using a Si cantilever with very high stiffness and very high resonance frequency

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Smaller amplitude operation of the oscillating cantilever enables higher spatial resolution in FM-AFM since sensitivity of the frequency shift to the short-range interaction force is increased. A force sensor with high stiffness (k) should be used to avoid the jump-to-contact instability and to ensure the small amplitude operation. As force sensors, a quartz tuning fork (qPlus sensor) [1] and needle sensor (Kolibri sensor) [2] have been used to realize the small amplitude operation. However, it is a disadvantage for qPlus sensor and Kolibri sensor to be unable to fabricate those with various stiffness k and/or resonance frequencies f_0. As a result, the force sensitivity is limited by the low resonance frequency f_0 in qPlus sensor and by the extreme high stiffness k in Kolibri sensor.

In this study, we theoretically and experimentally investigate the enhancement of the force sensitivity by using a Si cantilever with very high k and very high f_0. From the theoretical study, we found that the minimum detectable force gradient for small amplitude operation is approximately proportional to the ratio of the stiffness to the resonance frequency (k/f_0) and the noise density of the deflection sensor (n_{ds}) (Fig. 1). This means that to enhance the force sensitivity for small amplitude operation, the force sensor with low k (k >1000N/m) [1] and high f_0 as well as the deflection sensor with low n_{ds} are required. By the numerical simulation, as shown in Fig. 1, we found that the Si cantilever (circle ●) (k=2000N/m, f_0=1MHz, n_{ds}=60fm/Hz$^{1/2}$) has very high force sensitivity, compared with the qPlus sensor (triangle ▲) (k=1800N/m, f_0=33kHz, n_{ds}=20 fm/Hz$^{1/2}$) and the Kolibri sensor (rectangle ■) (k=540kN/m, f_0=1MHz, n_{ds}=1fm/Hz$^{1/2}$). Then, we experimentally verified the enhancement of the force sensitivity using a maicro-fabricated Si cantilever with k=2000N/m and f_0=1MHz. We demonstrated the stable atomic resolution imaging and the high sensitive force spectroscopy measurement with a small amplitude on Si(111)7×7 surface at room temperature. It should be also emphasized that the micro-fabricated Si cantilever has a small tip apex, which is suitable for enhancing the force sensitivity to the short-range interaction. Thus Si cantilever with very high k and very high f_0 significantly improves the spatial resolution in FM-AFM.

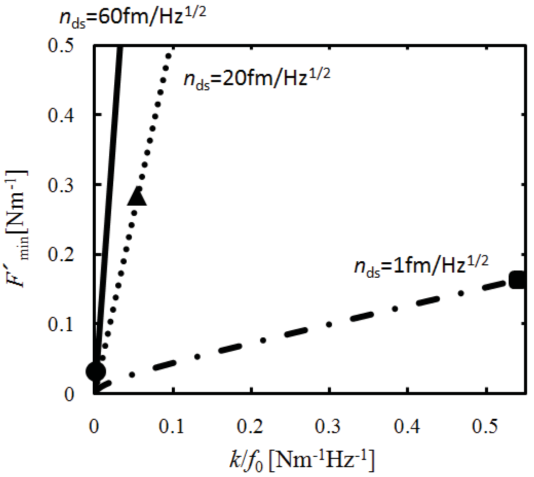

Fig. 1 Minimum detectable force gradient as a function of the ratio of the stiffness to the resonance frequency. A=0.2nm, Q=10000, and B=1kHz.

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The role of van der Waals versus chemical forces in atom identification

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Atomic force microscopy (AFM) measures long- and short-range interactions. Sugimoto et al. [1] recently demonstrated chemical identification of atoms by AFM using the short range forces. Separation of long and short range forces was not necessary 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. Previously, Lantz et al. [2] reported a chemical contrast between the corner adatom unfaulted and the center adatom faulted on the non-uniform Si(111)-7×7 surface. However, like the varying vdW forces at step edges, the corner holes on Si(111)-7×7 surface might lead to a spatial alteration in the vdW forces. Because the corner atoms are close to the corner holes, it is expected that the vdW attraction for corner adatoms is smaller than for center adatoms.

We therefore performed a simulation of the van-der-Waals force on the Si(111)-7×7 surface showing a small effect of the spatially varying vdW force. We investigated experimentally the contribution of the in-plane local spatial variation, e.g., the corner holes, to the long range vdW force with measurements on Si(111)-7×7 in constant height mode with oscillation amplitudes from the picometer to the nanometer range. The measurements revealed a chemical contrast that is much stronger than the varying vdW contribution and confirmed the results of Lantz, et al. In addition we found small variations among the other adatom types that are partially tip dependent.

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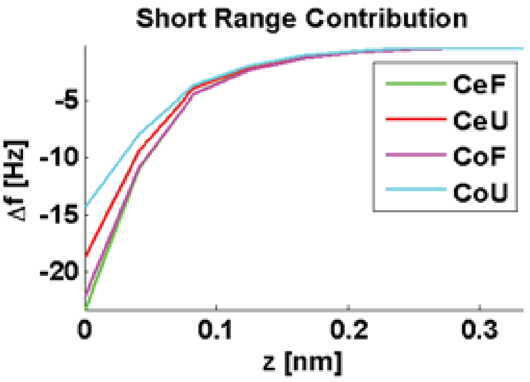

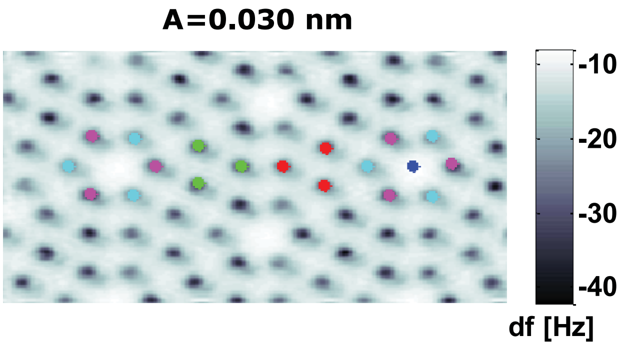

FM-AFM on Epitaxial Graphene in Air with the qPlus Sensor

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Yamada et al. [1,2] have shown that it is possible to obtain atomic resolution on cleaved mica and calcite in water with frequency-modulation atomic force microscopy (FM-AFM). These impressive results were acquired with a setup that enabled them to get very low deflection noise density, which is decisive for atomic resolution.

We have approached the problem of ambient condition imaging with quartz tuning fork based (qPlus) cantilevers. We tried to simplify our setup by using very stiff cantilevers (spring constant of 4300 N/m) with small amplitudes (some Ångstroms). Independent of the cantilever, small amplitudes appear to be necessary for high resolution imaging.

Results made in air with the frequency-modulation force microscopy mode on epitaxial graphene, grown on SiC (0001) [3], are presented. A previously unreported structure was imaged on the graphene surface. Domains of wrinkles, spaced uniformly 5.6 nm apart were found atop the graphene surface and are formed along the lattice directions of the hexagonal graphene structure.

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P.II-36

Exploring the Scale of a Tunnel Current Induced Phantom Force

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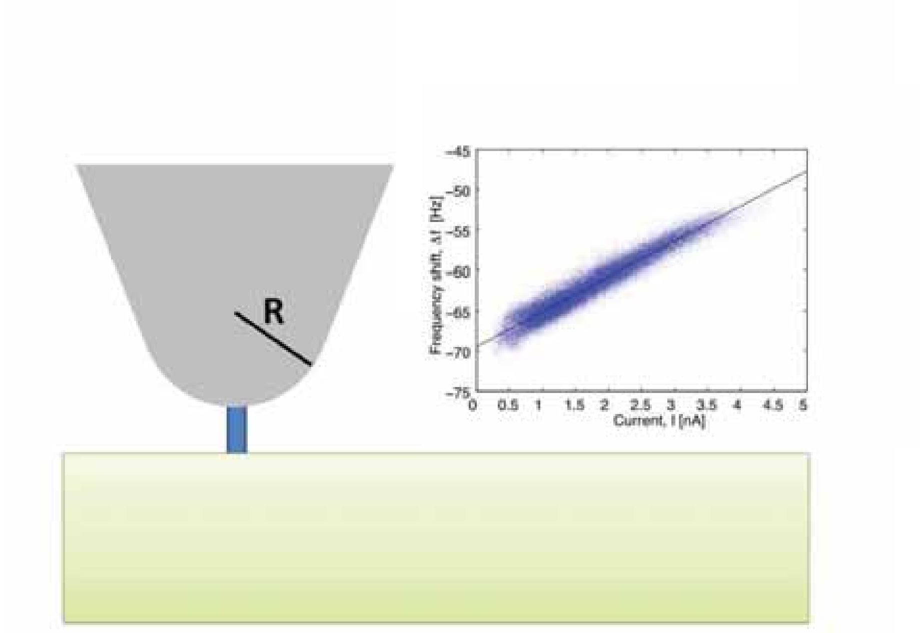
The phantom force is a repulsive force contribution observed when performing simultaneous AFM and STM, dependent on sample resistivity, the average tunnel current <*I*> and the bias voltage V_{bias} [1]. The origin of this apparent repulsive force is a reduced electrostatic attraction due to the current flow and the limited sample conductivity leading to a reduced voltage across the tunnelling gap. While the model presented in [1] includes a very short-range decay of the voltage from the point where the tunnel current enters the sample, a long-range decay of the voltage would cause a strong dependence of the phantom force with respect to the tip radius. In this contribution, we measure the effect of the macroscopic tip shape on the phantom force.

The macroscopic tip shape was determined by fitting $\Delta f\,(z)$ spectra to a model of a parabolic tip incorporating only van der Waals forces [2,3]. Then, we recorded constant-height images to extract a relation between the average tunnel current <*I*> and the frequency shift Δf. This apparently-repulsive linear relation characterizes the phantom force. There was no clear influence of the macroscopic tip shape on the phantom force, which corresponds well with our proposed model.



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Huge & Complex Dissipation Signals from Small & Simple NC-AFM Scans

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Our extensive theoretical investigation confirms experimental findings that huge dissipations (>1eV per cycle) can occur during NC-AFM imaging even at 5K and, along with experimental results, we conclusively show that even whilst there may be poor (or misleading) topological contrast, dissipation signals can still provide clear atomic resolution.

The debate as to the cause of dissipation and to whether or not dissipation gives true atomic resolution has gone on for many years with different models and mechanisms suggested to explain the 0.1-1eV dissipation signals many experimentalists have recorded [1,2]. Therefore we present here not a mechanism for dissipation to occur but instead an interpretation and practical utilization of dissipation signals.

Experimentalists have performed NC-AFM imaging on the Si(001)-c(4x2) surface at 5K and, even at such low temperatures, still recorded dissipation exceeding 1eV per cycle. Most interestingly, at a frequency set shift in which the topology indicates that dimers are being manipulated during imaging, the dissipation signal clearly displays the original structure of the surface. The dissipation signal also has very good contrast of approximately 0.7eV between the smallest and largest signal recorded during a single scan. Fascinatingly, our results both confirm the experimental findings and uncover a very complex architecture behind the dissipation signals across the dimers. This means that the dissipation signal could, in fact, also be use to derive information in situations where the topology (frequency shift) signals on its own cannot.

So we discuss here the nature of forces between the tip and surface during a line scan and calculate the dissipation for several points along the dimer over several tip-surface separations. In all instances the DFT method is implemented with the SIESTA code, using a localized numerical basis set and GGA Perdew-Burke-Ernzerhof (PBE) density functional.

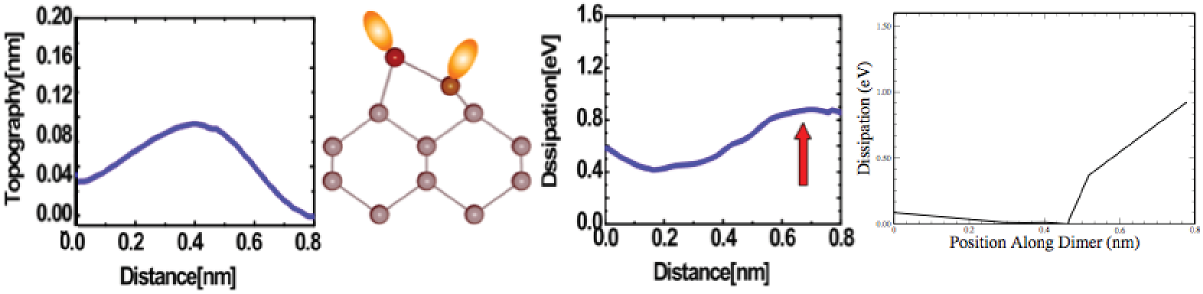

Fig. 1: Line scan across a Si(001)-c(4x2) dimer (left to right: experimental topology scan [2], cartoon of scan line, experimental dissipation signal [2], calculated dissipation signal.

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A numerical FM-AFM for image calculations of adsorbed molecules

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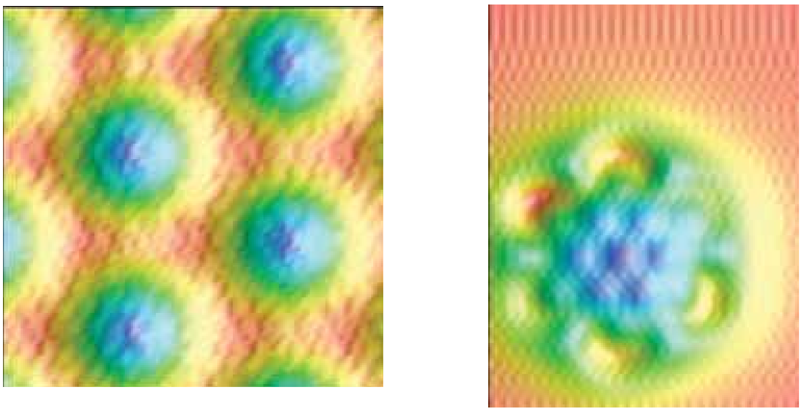
We present here a numerical frequency modulation AFM (FM-AFM) for image calculation of individual molecules adsorbed on different surfaces.

First, we describe the FM-AFM behaviour including three control loops [1]: PLL loop, amplitude controller, distance controller. The operation of each of these loops is detailed with schematics. This numerical tool allows to understand and to predict the theoretical behaviour of FM-AFM. It is able to work at large (~ 10 nm) and small amplitudes (~ 0.02 nm as for the Qplus sensor), and at constant Δf or at constant height [2]. For instance, we are able to reproduce numerically the analytical results obtained by F. Giessibl [3].

Second, we calculate the interaction between the FM-AFM tip and a molecule adsorbed on a surface in order to study its behaviour in this tip-surface environment. The first results deal with images of graphene and silicon carbide surfaces. These images show us the maximum of corrugation on each surface in the static mode (with no relaxation/deformation). Then, single molecules (as C_{60} and hexa-benzocoronene) are placed on both surfaces and imaged in static mode. At the moment, we are adding relaxation in the FM-AFM code by inserting an energy minimization stage coupled to a molecular dynamic code. This will allow us to study the behaviour of molecules in a tip-surface junction via energy dissipation study.



Calculated FM-AFM images of graphene surface (left) and a single HBC molecule adsorbed on graphene surface (right).

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P.II-39

Modelling NC-AFM Resolution on Corrugated Surfaces

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Key developments in NC-AFM have generally involved atomically flat crystalline surfaces. However, many surfaces of technological interest are not atomically flat. SiO_2 grown as gate dielectric on Si wafers, for example, is amorphous and exhibits stochastic surface roughness. Precise measurement of this roughness by AFM has become controversial due to the widespread use of SiO_2 as a support for exfoliated graphene, which may be probed with UHV STM (yielding full atomic resolution by several groups). Controversy arises when STM measurements of graphene/SiO_2 are compared with AFM measurements of the bare SiO_2 substrate [1,2], because AFM measurements of SiO_2 generally show a much smoother topography than STM of graphene/SiO_2. Motivated by the experimental difficulty in measuring SiO_2 surfaces, we propose a model to gain insight on this issue.

NC-AFM generally represents topography as a contour of constant frequency shift. Here we discuss the issues which arise when the surface is corrugated at relatively small length scales (our best measurements of SiO_2 yield a correlation length of 8-10 nm). We develop a continuum model which explicitly accounts for the corrugated substrate (modeled as a sinusoid) and obtain the response of a spherical tip to van der Waals interactions. As a function of tip radius, these long-range interactions integrated over the tip volume can produce significant flattening of the topographic contours. As an extension of the basic model, we incorporate a "front atom" and consider resolution as the strength of the front atom interaction is varied in relation to the integrated contribution of the tip. Preliminary results indicate a strong requirement for small tip radius, and a breakdown of the usually-assumed Hamaker force law for a sphere interacting with a flat surface ($F \sim A_H R/z^2$).

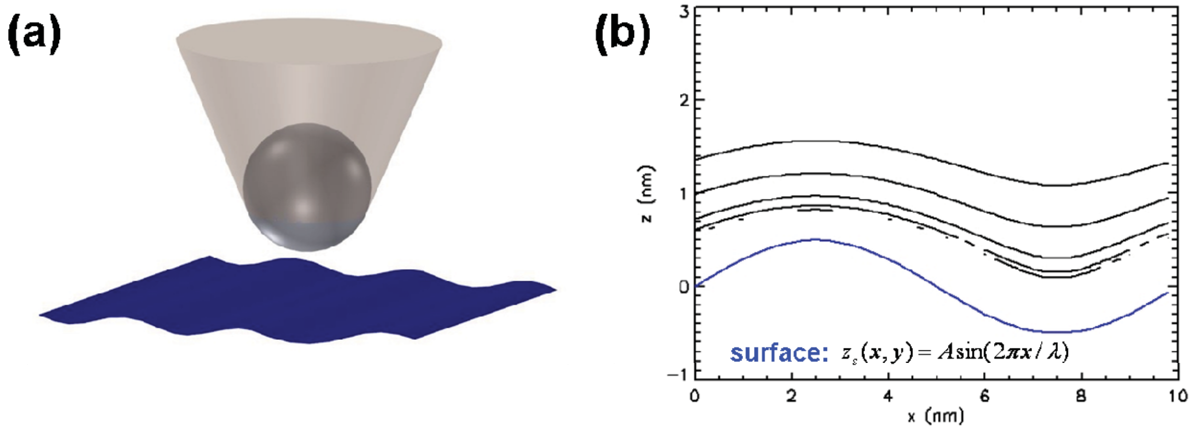

Figure 1: (a) Schematic of continuum model geometry with sinusoidal surface and spherical tip. **(b)** Contours of constant frequency shift, showing attenuation of surface corrugation.

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Wavelet coherency and phase analysis of cantiler oscillations

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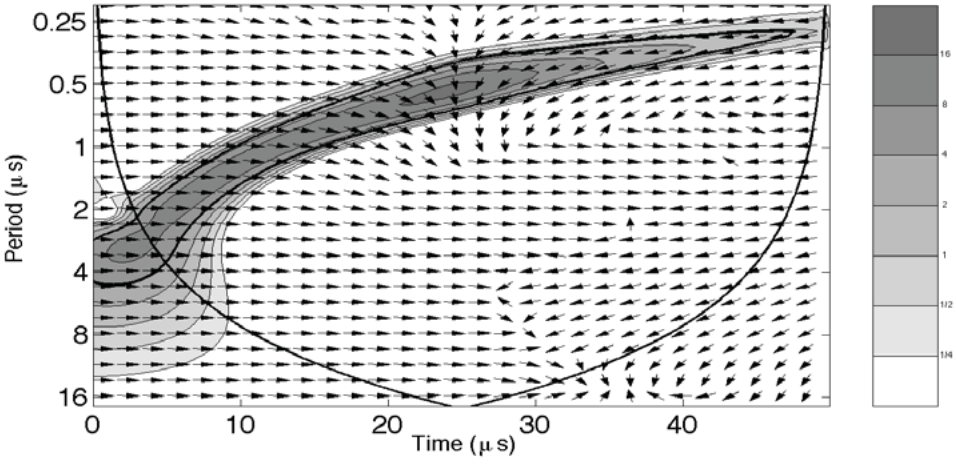
Wavelet analysis has been used to characterize the time-frequency response of a thermally excited cantilever in dynamic force spectroscopy [1-3]. In these previous works, the focus was on the power spectral density evolution in time. Here, a wavelet cross-correlation technique is presented that utilizes the inherent phase information residing within the complex Morlet transform. Measurements of phase differences between two time series, i.e. between the cantilever response signal and the driving signal, yields information on the phase delay between oscillations as a function of frequency. Moreover, wavelet cross-correlation quantify the coherency relation between the cantilever response and the driving signal. The example in the figure highlights the characteristics of wavelet cross-correlation [4]. An oscillator with a free resonant frequency f_0=1 Mhz and Q=4 is excited with a driving frequency that sweeps the frequency interval $0.1f_0<\Delta f<1.9f_0$ in 50 μs. The oscillator phase relations with the driving frequency are displayed simultaneously with the (cross wavelet) power spectral density (represented in scales of grey, identifying the time series common power) as a function of time and the instantaneous period (the inverse of instantaneous frequency). Phase arrows indicate the phase relationship of the oscillator with the driving sinusuoid (pointing right: in-phase; left: anti-phase; down: oscillator leading driver by 90°). Note that the power peak no longer overlaps with f_0 (period 1μs) and edge effects are delimited by continuous lines. Phase analysis techniques are of great interest, expecially in low-Q environments. The present study points out the possibility to obtain a phase analysis as a function of time and frequency, that could be useful in dual mode excitation techniques, band excitation methods and fast force spectroscopy techniques, providing time-frequency phase maps specific to different surface interactions. Examples of the ongoing experimental activity will be commented.



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Soft material liquid AFM simulator

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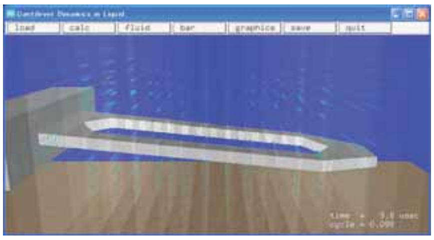
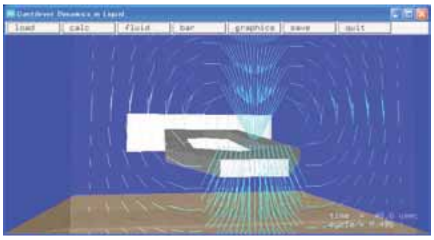
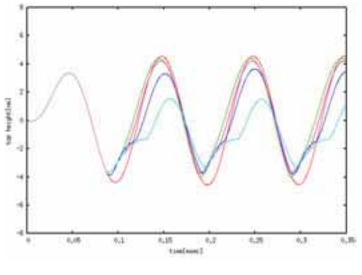
We have developed simulator to analyze of cantilever oscillation in liquids, and dynamic AFM analyses of visco-elastic samples in liquids can be performed. This numerical simulator calculates an elastic cantilever oscillation combined with fluid dynamics of liquids as well as the tip-sample interaction force.

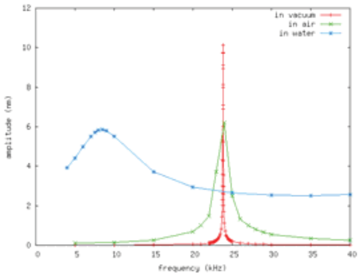
When the cantilever is oscillated in liquid, fluid around the lever is stirred, and flow field is caused. The cantilever receives the fluid pressure and viscosity. Accordingly the cantilever motion becomes complicated for fluids force and the stress due to elastic deformation of the cantilever itself. Here, the fluid model is approximated as two dimensional Stokes flow of an incompressible fluid.
When the cantilever falls down, and a probe at head of lever approaches a sample which is visco-elastic soft material, it feels a force mediated by molecules. This effect to the cantilever motion determines. Thus this simulator calculates the motion of cantilever, the frequency shift, phase images and resonant curves of cantilever can be got.

This simulator is useful to design shape of high sensitive cantilever and to help predict optimum oscillation modes. It is also possible to infer the physical properties of samples by understanding changes of cantilever oscillation state.









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Defect mediated anisotropic nanomanipulation of Au clusters on NaCl

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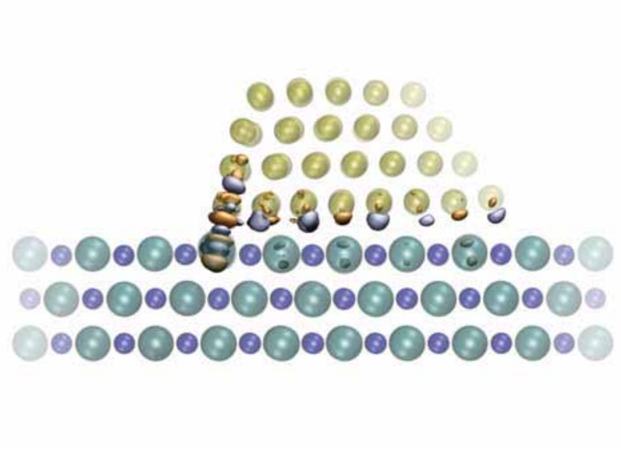
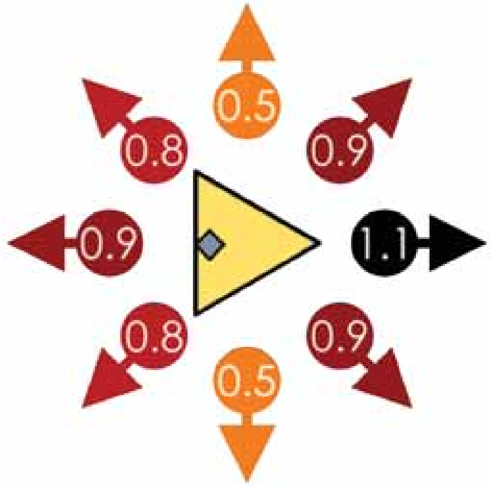
Metallic nanoclusters adsorbed on insulating surfaces and thin films are promising candidates as next generation catalysts in many industrial processes. Non-contact Atomic Force Microscopy (nc-AFM) has recently begun to be applied to these systems, potentially providing atomic resolution of the surface and the adsorbed nanoclusters. Furthermore, atomic control on the size of deposited nanoclusters and nc-AFM's ability to manipulate the clusters on the surface means one can examine the properties of clusters of specific sizes at chosen sites on the surface.

We study Au cluster manipulation on NaCl (001), a prototype system, by both experiments and simulations. On the NaCl surface, gold atoms tend to aggregate at steps and form clusters. The clusters can be detached from the steps using nc-AFM and then manipulated on the surface. Interestingly, the movement of clusters is seen to be strongly anisotropic, preferring [110] surface directions. By calculating the energy landscape of Au clusters on the surface using density-functional methods it is found that clusters are mobile on a pure NaCl surface but they bond strongly in the presence of vacancies. The anisotropy in minimum energy paths is also found to depend on the type of vacancy the clusters attach to. The anisotropic movement is likely due to the clusters attaching to a row of Cl ions in the presence of Na vacancies. Since the clusters can slide along rows of Cl ions on the surface, they prefer to move in the [110] direction. The results demonstrate how the behavior of metallic clusters on insulators during manipulation can be dominated by the interaction between the clusters and the defects found on the surface.





P.II-43

Numerical Analysis of Band Excitation Signals in Atomic Force Microscopy

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We present simulations of the Band Excitation AFM (BE-AFM) method [1], within which the cantilever is excited with a continuum frequency band in order to acquire the full spectrum of the response. The most common excitation signals used in this method are the *chirp* and *sinc* functions, none of which truly excites the cantilever at all frequencies in the band simultaneously throughout their duration. We thus seek to understand the time-dependent frequency content of these signals and its impact on cantilever dynamics (see Figure 1). The *chirp* function sweeps through the frequency band at a uniform rate, which creates a mixture of transients associated with each instantaneous excitation frequency. In the presence of strong tip-sample interaction forces or with inappropriate cantilever parameters, this creates additional peaks in the response spectrum that limit the ability to extract frequency shift and dissipation information. This is because in these cases the response does not have Lorentzian shape and the ideal harmonic oscillator concept is no longer applicable. The *sinc* function serves as a true simultaneous band excitation for only a small slice of its duration, although its response is less likely to deviate from the Lorentzian shape. However, it is not yet clear what sample information is gained or lost, depending on the chosen signal. Our future efforts will focus on exploring the relationship between response spectra and material properties, as well as on identifying true band excitation functions that are feasible to use in AFM.

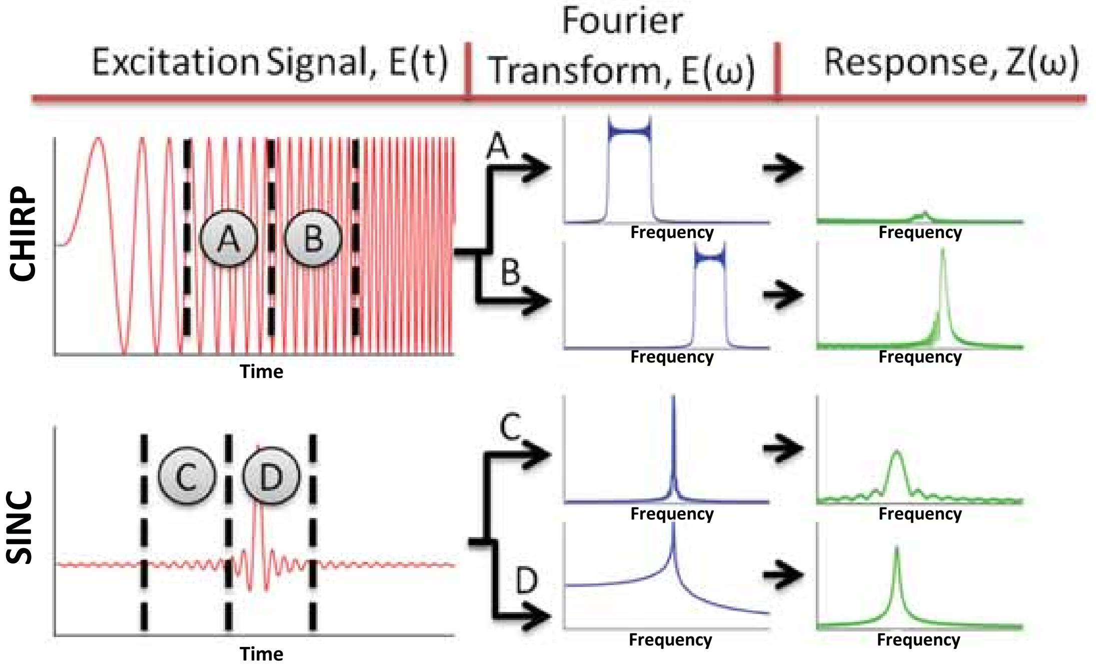

Figure 1. BE-AFM excitation signals (left), time-dependent frequency content (center) and cantilever response (right).

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Unifying theory of quantitative AFM using piezo excitation in liquids

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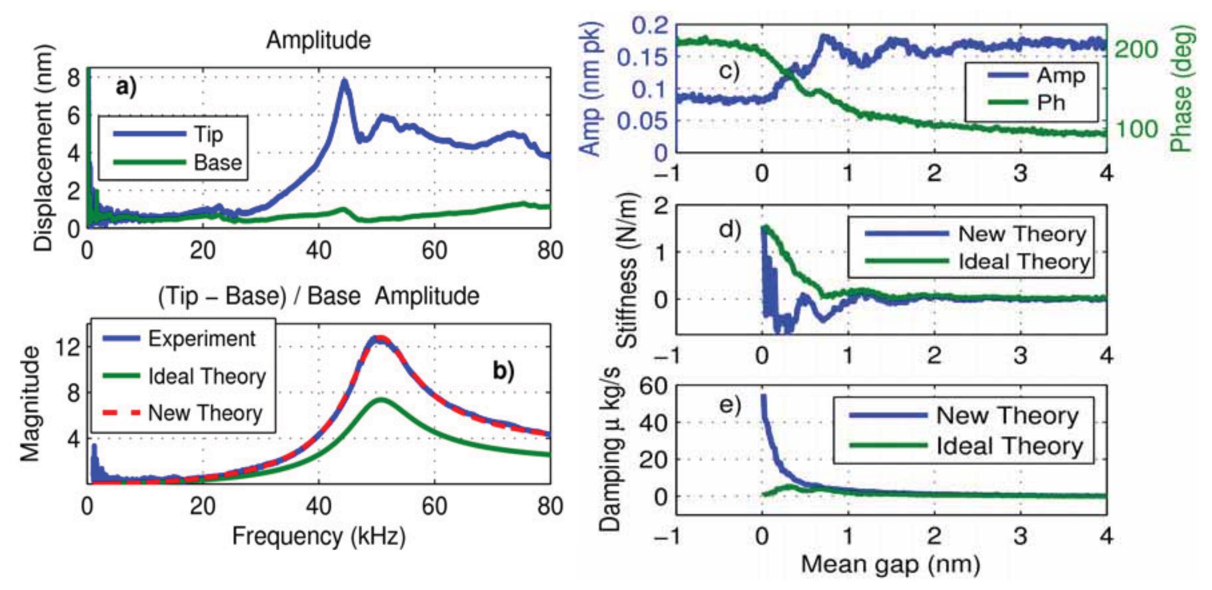
Base-excitation of cantilevers using a piezoelectric element (acoustic mode), is popular in dynamic AFM because it is inexpensive and does not require special cantilevers. Its use for quantitative force and dissipation spectroscopy relies on theoretical formulas that either implicitly or explicitly make assumptions about the magnitude of the base motion, which cannot be directly observed in most AFMs. However, in liquid environments such assumptions fail. Fig. 1(a) shows the tip and base motion of a typical acoustically excited cantilever where the base motion was measured directly using a laser Doppler vibrometer. Fig. 1(b) shows that previous formulas [1, 2] do not correctly predict the ratio between tip and base motion, which leads to a signficant error in force spectroscopy. The previous theory's prediction is incorrect because a significant component of the piezo excitation does not mechanically excite the cantilever but rather transmits acoustic waves through the surrounding liquid to indirectly excite the cantilever. Such fluid borne excitation has been postulated before [3-4], but previously it could not be quantified. In this work the authors present a method by which the base motion and fluid borne excitation can be estimated on typical AFMs based on the residual motion in permanent contact with a hard surface. This method is validated using a laser Doppler vibrometer, which can measure the actual base motion. Finally, the method is demonstrated by performing small-amplitude AM-AFM force spectroscopy on solvation shells of octamethylcyclotetrasiloxane (OMCTS) molecules on mica (Fig 1(c)–(e)). The new theory shows a difference of more than 100% in both stiffness and damping compared to the previous theory.



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P.II-45

Charge Alteration in Si(111)-DAS Surface by Atomic Force Microscopy

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This study describes charge alteration in Si(111)-DAS surface by noncontact atomic force microscopy (ncAFM) from a theoretical point of view. Recently, much attention has been attracted to Kelvin probe force microscopy (KPFM) and the mechanisms to generate local contact potential difference (LCPD) images. We are also suggesting a theoretical method for simulating the LCPD images on semiconducting samples [1], based on the ncAFM simulation method using the density-functional based tight-binding (DFTB) method [2]. This theoretical method is called the partitioned real-space DFTB (PR-DFTB) method, and is available to onset region with respect to orbital hybridization between the tip and the sample. In the region, we believe to understand LCPD with the electrostatic multi-pole interaction between the tip and the sample.

However, it is difficult to understand what is “LCPD” when the tip closely approaches a sample. Therefore, we firstly research charge alteration when the tip approaches an adatom and a rest atom on the Si(111)-(5x5)-DAS surface using the computational simulations that mimics ncAFM measurements, because KPFM is a sort of ncAFM. As a result, we obtained Mulliken charge alteration as shown in Fig. When the tip approaches an adatom of the three, Mulliken charge of the three adatom and the rest atom are hardly changed, whereas the charge converges on neutral gradually as the tip approaches the rest atom. We would like to discuss relations between the result and LCPD in our presentation.

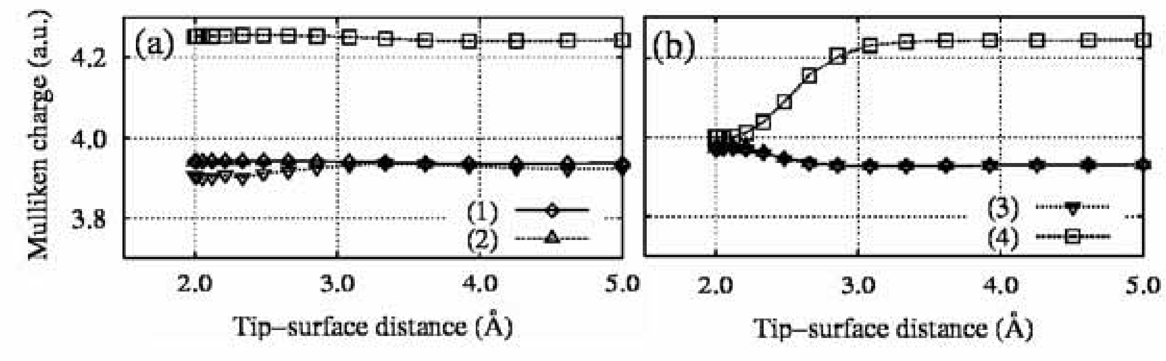

Fig: Mulliken charge of three adatom (1), (2), and (3) and a rest atom (4), when a Si cluster tip approaches an adatom of the three (a) and the rest atom (b). Mulliken charge of 4.0 is neutral, because they are Si atoms.

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Theoretical study of atomic manipulation on metals

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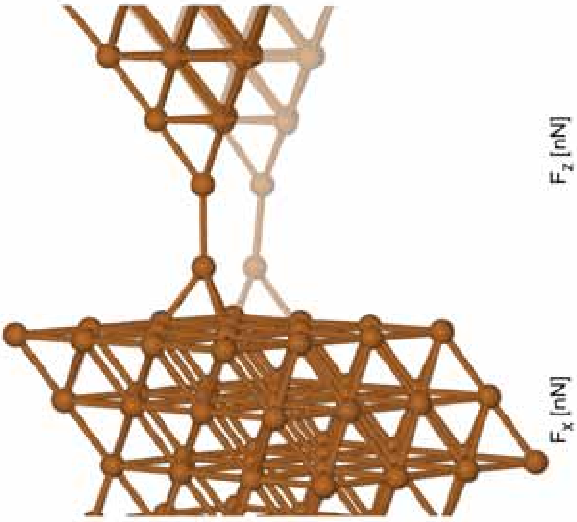
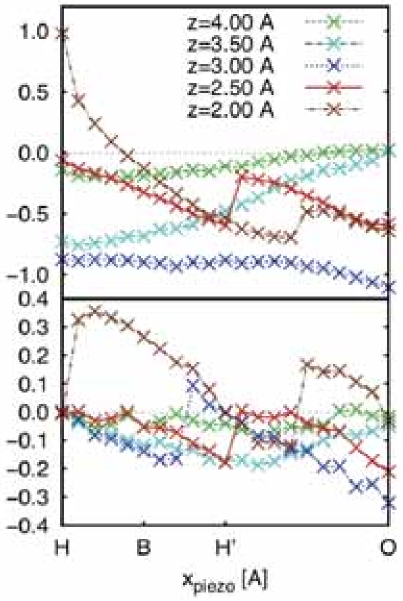
Recent progress of nc-AFM technique allowed precise control of single atom manipulation on different substrates [1]. Spatial mapping of the forces during manipulation provides the potential energy landscape of the tip-sample interaction. What is more, both vertical and lateral forces needed to move a single atom can be directly estimated [2]. Surprisingly, the experimental findings on metal surfaces [2] showed that only lateral force component plays the dominant role in single atom movement. This observation is in contradiction to observations made on semiconductor surface [3].

We carried out extensive theoretical simulations to get more insight into the manipulation of a single atom on metal surface. We combined the total energy DFT calculations with classical Molecular Dynamics using Force Field potentials. In particular, we investigated movement of a single Cu adatom on top of the Cu(111) surface as a function of tip-sample distance and chemical and atomic composition of the tip. Relation between the lateral and vertical forces exerted on adatom lateral movement will be examined. In addition, we will discuss implication of different mechanisms of lateral manipulation using static STM mode at constant height or oscillating AFM mode.





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P.II-47

Theoretical analysis of relation between force and current in the tunnelling regime

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Increasing number of precise simultaneous AFM/STM measurements has been reported last years (see e.g. [1]). The possibility of combining the powerful tools provided by scanning tunneling (STM) and atomic force microscopy (AFM) in a single instrument brings an opportunity to correlate directly tip-surface short-range chemical forces with simultaneously measured tunneling currents at the atomic and molecular scale.

Here, we discuss a simple numerical model describing the relation between the current and the chemical force in the tunneling regime (see Figure). Based on this model, two characteristic regimes can be identified according to quantum degeneracy of electronic states of tip and sample involved in the interaction process. In addition, this model will be supported by the total energy DFT simulations combined with transport Green's function calculations [3].

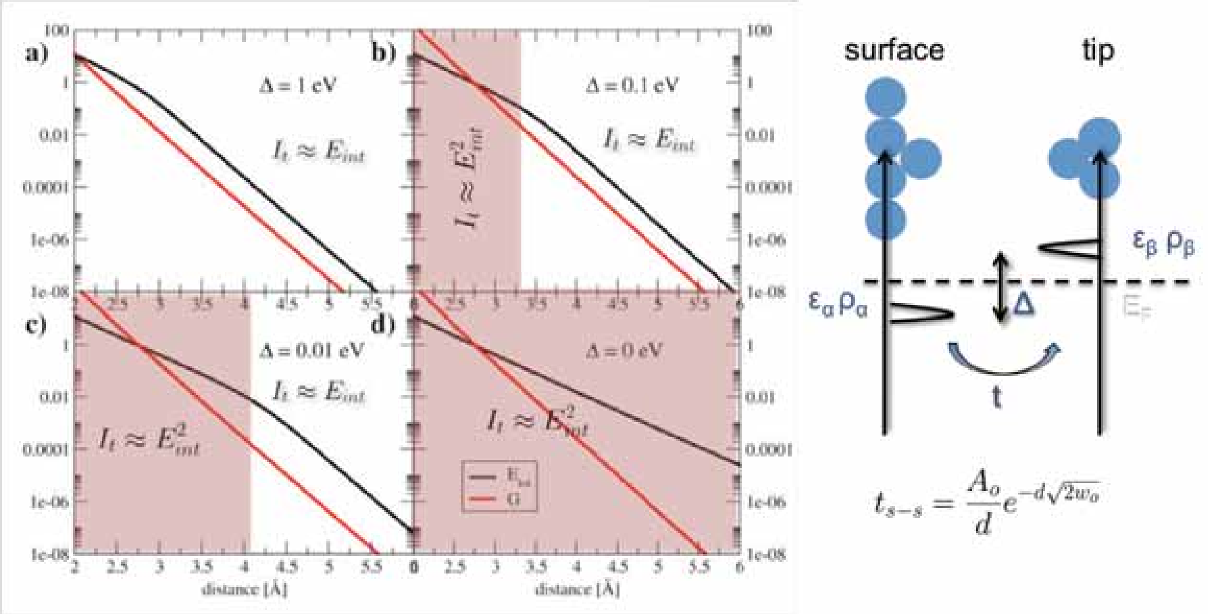

Fig. shows the relation between the current and force with the distance as a function of electronic state for a simple two-level model (right).

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P.II-48

Multi-Scale Approach to Simulations of Kelvin Probe Force Microscopy

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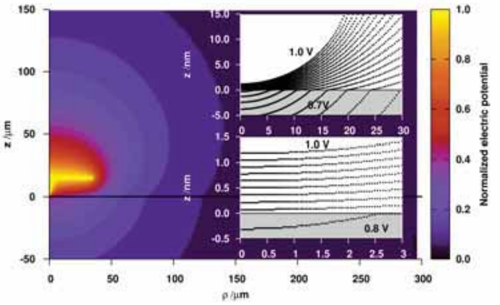
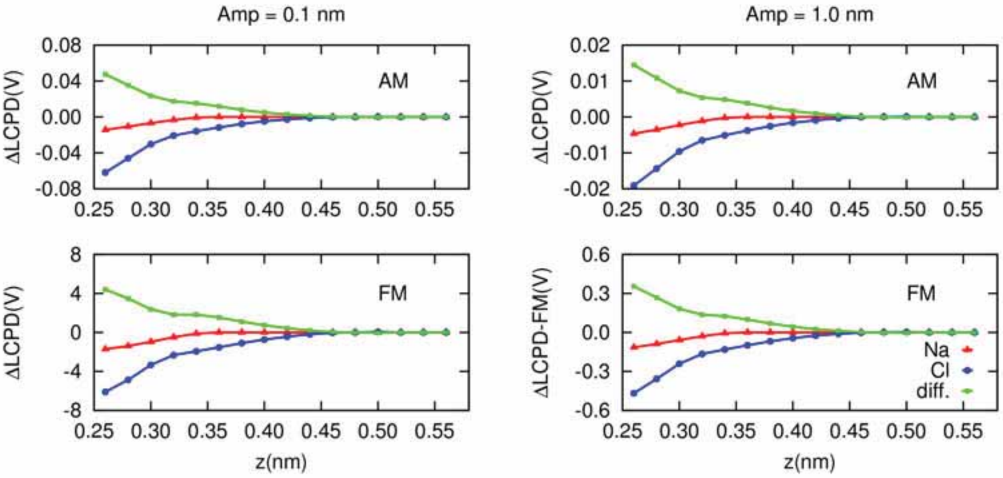
The distance dependence and atomic-scale contrast recently observed in nominal contact potential difference (CPD) signals simultaneously recorded during non-contact atomic force microscopy on conducting as well as on insulating samples has stimulated theoretical attempts to explain such effects. Especially in the case of insulators, it is not quite clear how the applied bias voltage affects electrostatic forces acting on the atomic scale.

We attack the problem in two steps. First, the electrostatics of the macroscopic tip-cantilever -sample system is treated by a finite-difference method on an adjustable nonuniform mesh. The resulting electric field near the tip apex is then inserted into a series of wavelet-based density functional theory calculations with adjustable accuracy. Results are shown for a reactive disordered silicon nano-scale tip interacting with a NaCl(001) sample. Theoretical expressions for AM and FM Kelvin signals and local contact potential differences (LCPD) are obtained by combining both contributions to the electrostatic force at the modulation frequency, and evaluated for finite tip oscillation amplitudes. In agreement with existing computations based on different tip models, site-dependent LCPD contrast arises at close distances where atomic relaxation is significant.

Figure: Electrostatic potential map around the AFM tip in three different scales (right). Calculated LCPD for AM- and FM-KPFM at two amplitudes of cantilever oscillation (below).





P.II-49

Dependence of the most probable and average bond rupture force on the force loading rate: first order correction to the Bell – Evans model

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The Bell–Evans model which predicts the linear dependence of the most probable bond rupture force F_{prob} on the force loading rate $\dot{F}$, $F_{prob} = \frac{k_B T}{\Delta x}\ln \dot{F} + \frac{k_B T}{\Delta x}\ln\left(\frac{\Delta x}{k_{off} k_B T}\right)$, is usually used to discuss the dynamic force spectroscopy experiment data. This model is consistent with the Kramers' theory of the bond dissociation rate $\lambda = C\omega_{\min}\omega_{\max}\exp(-\Delta E / k_B T)$ [1] only if one presupposes an independence of the pre-exponential factors $\omega_{\min}$, $\omega_{\max}$ in the Kramers relation on the acting force F and a linear decrease of the dissociation barrier height ΔE on this same force, and for this to be true a rather special shape of the interaction landscape is required. (Above x is a reaction coordinate, Δx is an effective barrier width, $k_B T$ is a thermal energy, and k_{off} is the dissociation rate in no-force conditions). By this reason, different attempts to generalize the model have been undertaken and, for example, Dudko *et al.* model [2, 3] based on the dissociation rate $\lambda(F) = C\varepsilon^{1/2}\exp(-A\varepsilon^{3/2})$, where $\varepsilon = 1 - F/F_c$ with F_c being some critical force value, became rather popular. This model, however, can be used only when the most probable dissociation force is rather large and approaches such value of the force when the function $\Delta E = \Delta E_0 - Fx$ or similar does not contain a minimum any more. Correspondingly, this and similar models can not be used for discussion of experiments with relatively small values of the most probable rupture force – a lot of experiments actually fall exactly into this range.

Here we present a first order correction to Bell-Evans model where the first terms of corresponding Taylor expansions for Kramers' dissociation rate are taken into account. We show that if the shape of the interaction landscape in the vicinity of its minima and maxima is given respectively by relations $U_{\min} = a_{\min}x^2 + b_{\min}x^3 + O(x^4)$ and $U_{\max} = -a_{\max}(x - x_0)^2 + b_{\max}(x - x_0)^3 + O(x^4)$, the most probable rupture force is $F_{prob} = \frac{k_B T}{x_0}(1 - \frac{\beta k_B T}{x_0})(\ln\frac{\dot{F}x_0}{k_{off}k_B T} + \frac{\beta k_B T}{x_0})$, where $\beta = \frac{3b_{\min}}{4a^2_{\min}} + \frac{3b_{\max}}{4a^2_{\max}}$ may be negative or positive. In addition to the most probable bond rupture force, an average rupture force values are also calculated. All approximations made and the range of applicability of the obtained results are carefully described and compared with those for some other models in the field as well as with the experimental data.

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Development of a KPFM simulator for microscale imaging

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Kelvin probe force microscopy (KPFM) is a powerful tool for measurement of the local surface potential of materials. In the case of the measurement with the atomic-scale resolution, we propose a simulation method based on the quantum electronic states calculation and develop an image simulator [1]. On the other hand, the imaging with larger scale resolution is also important, especially for industrial applications. Thus, we start to develop a KPFM simulator for images with micro- to submicro-scale resolution.

We adopt the boundary element method for calculating the classical electrostatic force exerted on the tip probe. After arranging a spheroidal metal tip, a substrate of metal plate, and arbitrary shaped samples of dielectric, our simulator calculates a force map under a tip bias voltage. It can also calculate the map of the local contact potential difference, which we define as the voltage on which the tip force takes a minimum value.

We show the force map calculated by the prototype version of our simulator in Fig. 1. Fig. 2 shows one of the configurations of structures in this calculation. In the future, we modify our calculation model and algorithm considering the balance of calculation accuracy and computation time. We also plan to develop a friendly graphical user interface.

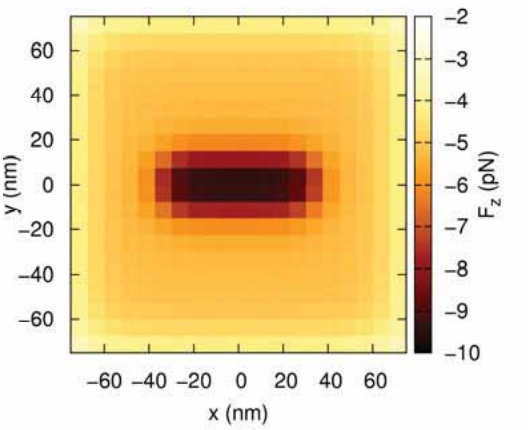

Fig. 1 The force map calculated by our prototype simulator. The tip-sample distance is 8 Ang. The tip bias voltage is +1.0 V.

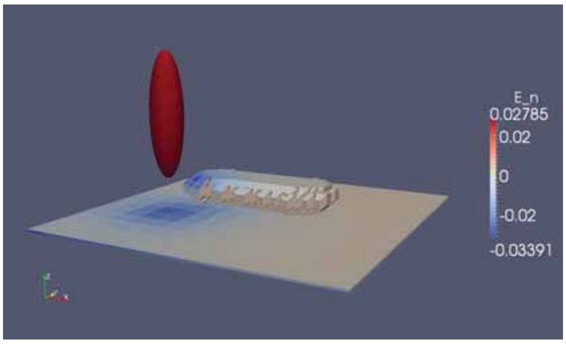

Fig. 2 A configuration in this calculation; a spheroidal tip, a plate substrate, and a sample of dielectric with relative permittivity is 1.5.

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P.II-51

Development of integrated GUI for SPM simulator

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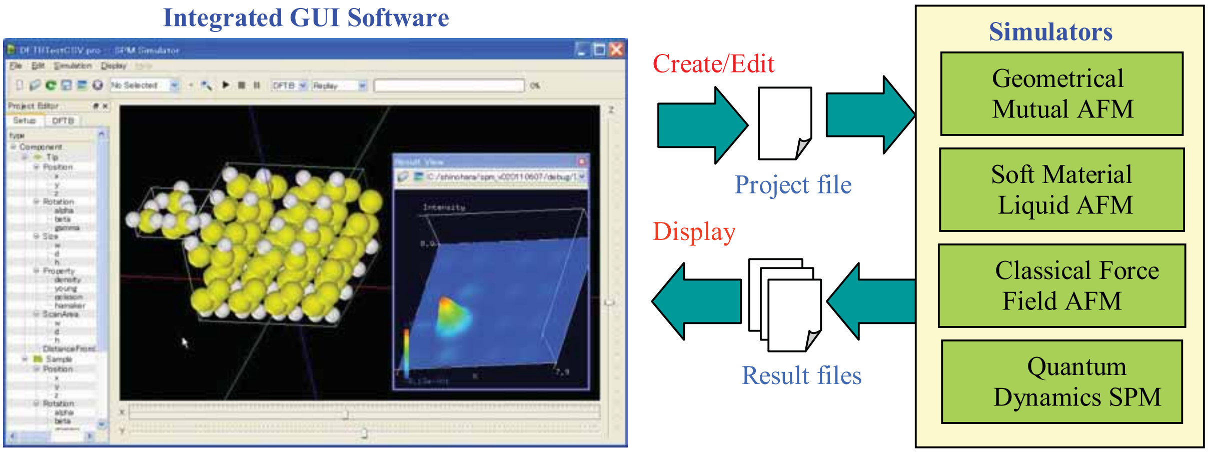
We have ever developed four SPM simulators to understand experimental images: Geometrical Mutual AFM, Soft Material Liquid AFM, Classical Force Field AFM [1][2] and Quantum Dynamics SPM [3][4]. Although there are a lot of common points about I/O among the simulators, their user interfaces were quite different because they had been developed independently.

We have developed integrated GUI software for the simulators. There are two main features in this software. One is to provide a common platform for each simulator. Thereby users can operate all simulators in the same way. The other is to lump all of the information used in our simulators as a project file, which is written by xml-format and includes tip and sample information, experimental setup conditions, parameter values for each simulator and result file paths and so on. It facilitates user's information management.

This software visualizes the contents written in a project file. Users can change the tip and sample layout and the range of scan area by directly manipulating the objects with mouse and keyboard. This feature helps users, especially beginners to create and edit project files.

A project file becomes the input into the simulators and each simulator outputs the calculated data to the file paths assigned in the project file. The software visualizes the data as 2D and 3D images and helps users to interpret the numerical results. Furthermore, the simulator visualizes tip motion and deformation of sample during simulation. The animation would have educational effects for students and beginner unfamiliar to SPM simulation.



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Computational insights into nanotribology: Antimony on HOPG

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Simulations are used to understand frictional behavior of a single asperity contact. To this end we use DFT total energy techniques adapted to accommodate van der Waals interactions [1]. One example being simulation of the recently experimentally studied motion of Sb_n nanoparticles on HOPG surface with the quest to elucidate the frictional bi-duality [2, 3]. Experimentally three clearly separated frictional dependences on contact area are observed: a) vanishing friction, b) normal friction, and c) high-friction branch.

While reproducible, the experiments alone do not provide insights into underlying physics/chemistry at the nanocontact. In order to fill the gap, large number of simulations was performed, including incommensurable Sb-HOPG interface, a range of spacer molecules, such as O_2, O, water, propane, Sb_4 clusters, oxidized antimony nanoasperities, and their combinations. These results not only provide rational for frictional behavior on all frictional branches, but in addition they also yield first realistic insights into molecular motions of these spacer particles during sliding processes as well as into chemistry at the nanosperity-substrate contact.

Transcending these results we move towards making predictions for related systems formed by replacing HOPG by chemically different substrates, such as MoS_2 or replacing the antimony nanoparticles by related nanoparticles from close vicinity in the periodic table such as Bi. These simulations may provide systematic understanding of the friction at the nanoscale and stimulate forthcoming experimental activities.

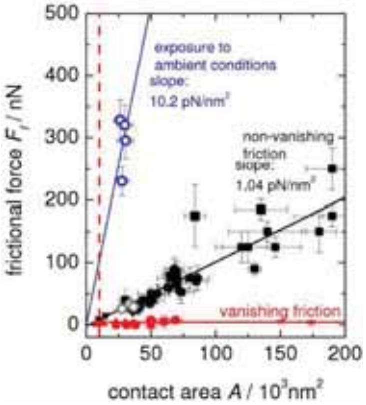
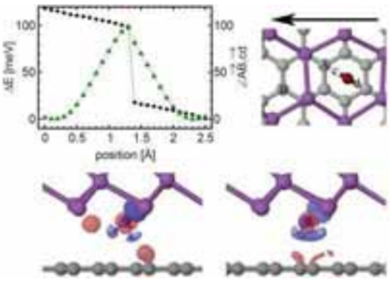


Fig.1 Left: Experimental dependence of friction force on contact area featuring double dualities. Right: Typical simulation results for a mobile spacer particle (water) locking the surfaces.



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Simulation NC-AFM Imaging and Contrast Change on Cu(111) Surface

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Simulations have been performed with the quest to elucidate NC-AFM imaging and contrast inversion observed in NC-AFM imaging of Cu(111) surface [1]. Experimentally larger attraction to atom sites was found with the tip away from the sample surface (more negative frequency shift). Upon approaching the surface the contrast was reversed. Such an image contrast, though, is only possible if the tip is able to approach the surface at very close distance. Furthermore, relation between decay length factors for tunneling currents (λ_T) and tip-sample forces (λ_F), λ_F=2 λ_T, was observed previously [2,3]. DFT simulations of force differences between top-hollow and top-bridge not only reproduce the measured behavior but also shed light on the physical reasons of the image inversion mechanism. In addition, a completely different tip apex relaxation process was found with significantly less apex deformation for a copper system, compared to gold or aluminum, which explains why the Cu surface can be imaged at very close distances. For the same reason λ_F=2 λ_T is observed, as tip and sample exhibit fairly small electronic overlap.

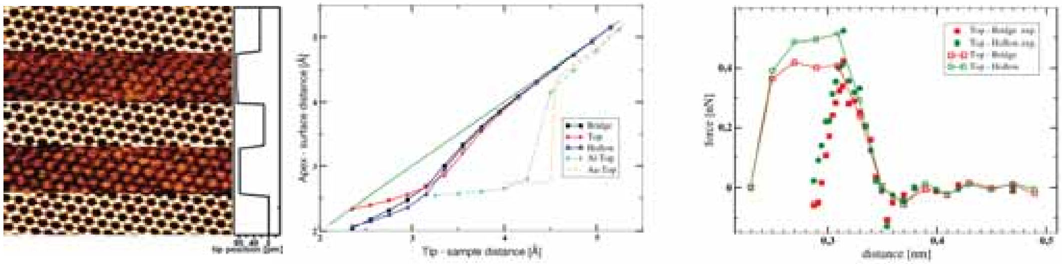

Fig.1 Left: Experimental image contrast change. Center: Tip-apex v.s. tip-sample distance, showing that Cu can be imaged at close distances, compared to results for gold and aluminum. Right: Experimental v.s. computed force differences between different sites showing sites showing that the image contrast is essentiallya geometrical effect.

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DFT analysis of combined 3D NC-AFM and STM imaging of Cu(100)-O

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Investigation of novel catalytically active surfaces requires a comprehensive experimental method for the identification and rapid characterization of prospective catalytically active sites. The powerful method of three-dimensional atomic force microscopy (3D-AFM) in non-contact mode [1] has been combined with scanning tunneling microscopy (STM) to study the oxygen-terminated copper (100) surface. Complex 3D data sets, obtained by simultaneously recording the tunneling current and the AFM frequency shift, allow for site specific quantification of forces and tunneling currents. The wealth of information obtained is promising for future applications, but the interpretation of the wide range of contrast modes requires a thorough characterization of the sources of contrast in AFM and STM imaging.

We combine DFT total-energy calculations with Non-equilibrium Green's Function (NEGF) methods for electronic transport to determine the tip-surface interaction and tunnelling current [2,3,4] for a large set of tip models in order to clarify the different contrast modes obtained in the experiments. At the outset, we obtained a stable Cu(100)$(2\sqrt{2}\mathrm{x}\sqrt{2})\mathrm{R}45^\circ$-O surface reconstruction model. Surface features were found to be in good agreement with experimental data, and the analysis of surface electronic properties enabled us to identify prospective reactive sites. The effect of tip changes on contrast modes was explored by considering tips of different reactivity. Our simulations, in comparison with AFM experimental images, identified a contaminated tip with a Cu-terminated experimental configuration. Charge density and current calculations further helped to investigate the STM imaging mode and explain the lateral shift between surface features identified separately in AFM and STM images. Consideration of different atom defect species and geometries helped us to understand detailed STM image features. The combination of conductance calculations with total energy methods provides insight into (1) the fundamentals of contrast formation in this novel experimental technique and (2) into the correlation between tip-sample forces and local chemical reactivity, factors that are essential for the further development and application of this approach to characterise catalytic activity.

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P.II-55

Classical Force Field AFM Simulator

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We have developing a product to simulate AFM imaging and this is called Classical Force Field AFM Simulator. Our aim would be to develop a practical simulator that users can get physical information of atomic-scale by using this.
Characteristics of this simulator, there are two points. First, this simulator is based on classical mechanics method. This approach is less computational cost compared to quantum-mechanical method. Second, users will be able to perform atomic-scale simulation by using this simulator that classical force field is applied to each atom.
Using this simulator, users can simulate the various systems. (For example, Organic molecular, Inorganic material and Protein, in vacuum or in water environment.)
In this simulator, deformation of the sample molecule can be considered and to obtain the stable structure of molecule, users can select from the two algorithms. These properties are different from each other. One of them, the energy relaxation method that look for stable atomic structure and calculate the force acted on the AFM probe. Generally, this method is called Molecular Mechanics (MM) method. Another is molecular dynamics (MD) method. In this approach, while solving the equation of motion for all atoms, the force acting on the probe is calculated.
Now we are developing the software to allow the users to easily operate the simulator. And, to examining the validity and usefulness of the simulator, we performed several calculations to try. (Fig.1)
This development is supported by SENTAN, Japan Science and Technology Agency (JST).

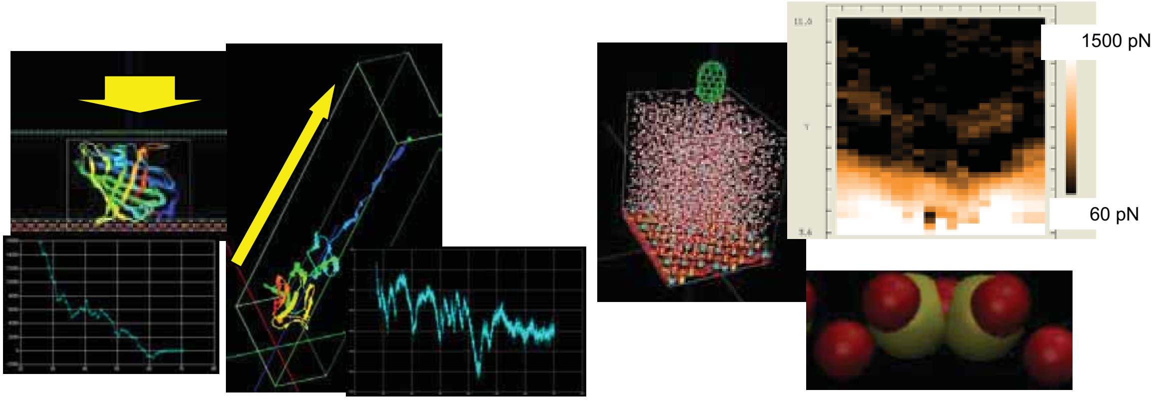

Fig.1 Examples of AFM simulation. (left) Compressing and pulling the protein. (right) AFM imaging of Mica substrate in liquids.

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Molecular dynamics at tip-water-surface junctions.

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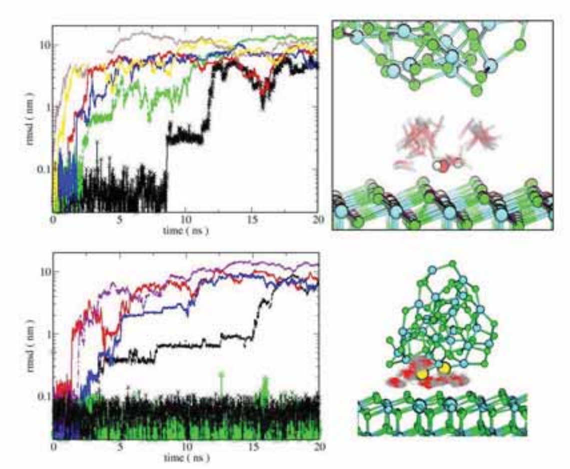
High-resolution imaging and force spectroscopy using AFM in solution opens a wide area of possible application allowing real-time and real-space imaging of surfaces in solution [1]. To obtain full benefit and provide a significant new analytical ability it is vital to understand the underlying imaging mechanism(s) that can lead to high (atomic or molecular) resolution.

Our simulations of solvated nanoparticles near surfaces show several possible mechanisms that lead to measurable force differences and image contrast over surface sites [2,3]. We used free-energy perturbation theory to calculate the free energies of nanoparticle-surface interaction. Water mediated interactions can cause significant force differences above different surface sites, and are in most cases larger, and longer ranged, than the direct vacuum-like interactions.

At tip-surface separations comparable with the diameter of a water molecule, the dynamics of water molecules located between tip and surface are found to be slowed down by over three orders of magnitude [3]. This is shown in the figure, with water residence times between tip and surface found to be > than 20 ns. These slowed dynamics leads to a situation where the approach and retraction of the tip may no longer be adiabatic, and a dissipation signal measured. With proper interpretation, measuring in this regime may throw new light on recent measurements of strongly varying frictional behaviour of confined water layers [4] and enable the measurement hydration energies of interfaces [5]. We will also present initial results of our simulations of dissipation using non-equilibrium molecular dynamics.



Root mean square deviation (RMSD) of water molecules near a blunt CaF_2 tip approaching a CaF_2 surface.
Top: RMSD for water molecules that initially have an atom within 0.3 nm of tip or surface ions when the tip is at a height of 0.61 nm. The black trace, which is stable for ~8 ns, corresponds to the highlighted molecule in the molecular structure to the right; Lower, the tip is now at 0.23 nm above the surface. Two water molecules do not diffuse over the full 20 ns of simulation.

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Acquisition of Tip-Sample Dissipation Models through Spectral Inversion

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Tip-sample dissipation has been extensively investigated within AFM. Dissipation in intermittent contact imaging modes is particularly relevant for soft viscoelastic samples, for which the dissipative forces can be a significant component of the total tip-sample interaction. Our work aims at exploring the direct acquisition of the tip-sample interaction model describing the total force as a function of the instantaneous tip position and velocity. Our approach is based on the spectral inversion method introduced by Stark et al. [1] and optimized by Sahin et al. using a Torsional Harmonic Cantilever (Fig. 1), which enhances the higher harmonics of the tip response. The research approach initially relies on numerical simulations of the THC system [3] for a range of key experimental parameters (resonance frequencies, force constants, quality factors, sample viscoelastic properties, excitation and setpoint amplitudes) and a known tip-sample dissipative model [4]. In each case, the tip-sample interaction force trajectory is reconstructed numerically as a function of position and velocity using Fourier analysis, from which analytical models are developed for sets of conditions that maximize the position-velocity phase space of the tip motion (see Fig. 1).

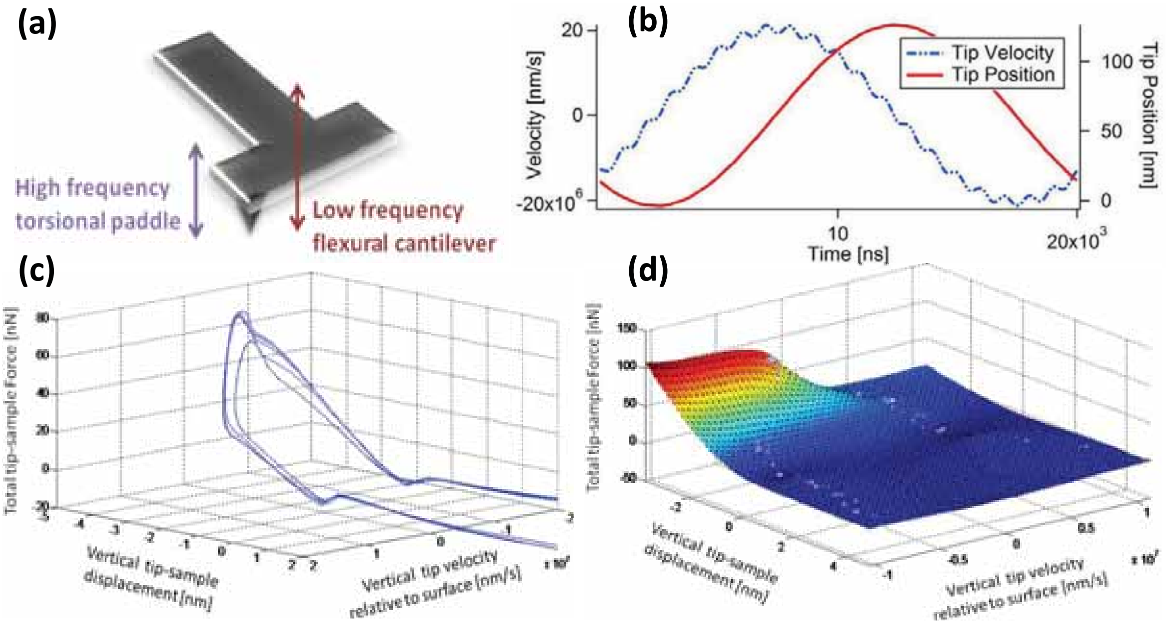

Figure 1. (a) Torsional harmonic cantilever system; (b) reconstructed tip position and velocity; (c) typical trajectories on the position-velocity-force space; (d) dissipation model surface created by combining a large number of trajectories obtained for different parameters.

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POST-DEADLINE POSTERS

Variable temperature liquid AFM reveal change in coverage of water on mica

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A variable temperature liquid AFM [1]operating in the torsional mode[2] at 1.1 MHz, revealed opening of holes on a flat ‘surface’ of mica immersed in pure water when the liquid cell temperature exceeded ca. 15 ºC. The coverage of holes increasd with temperature, eventually resulting in removal of a single layer 2.5 å in thickness. In light of former results were “ice-like” features were seen, but with low reproducibility, the phenomena observed above may be attributed to change in the layers of structured water molecules on mica at a certain ambient temperature.

A variable temperature liquid AFM with a temperature range of below freezing to boiling point was implemented. With the torsional mode at 1.1 MHz, the microscope captured an ice-like structure on mica immersed in water at room temperature. However, such images were very difficult to reproduce. When imaged with a larger scan size of around 500 nm square, opening of holes on a flat surface was observed on mica at around 15 ºC. The hole depth was ca. 2.5 å. The holes increased in number and size with temperature, and a single layer disappeared within a few degrees. The ice-like structure matched very well the ice I-h structure, were the step height is 2.5 å and the lattice pitch is 4 å. The fluctuating nature of the images implied that the features observed were not that of mica, but more likely to be that of structured water. The depth of the holes matches the step height of ice I-h, and the temperature dependent removal of an entire layer strongly suggests that it was not “peeling’ of a layer of mica, but a change in the layers of structured water molecules existing between the substrate and the tip. However, we do not know as yet the number of water layers present within the tip and the substrate. At other temperature ranges, the surface of mica immersed in pure water also revealed an unexpectedly active change in morphology, neucleation and change of coverage. We will try to identify the structure of terraces and holes, and discuss when and how ice-like structures or the substrate itself are imaged.

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Design of a Low-Temperature Ultra-High Vacuum Non-Contact Atomic Force Microscope

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Abstract

With the aim to find new routes to investigate complex surface systems, the noncontact atomic force microscope (NC-AFM) has evolved as a complementary technique in the field of scanning probe microscopy and demonstrated to be a successful surface sensitive tool with remarkable achievements such as: atomic resolution imaging on various metallic, semiconductors and also insulating surfaces [1], atomic manipulation [2] and chemical identification of individual atom on surfaces [3].

In this contribution we present the design of a low-temperature (LT), ultra-high vacuum (UHV), NC-AFM using frequency modulation (FM) detection mode. Optical fiber interferometery is used for the cantilever dynamics detection. The microscope assembly consists of two distinct parts. A fixed base, directly coupled at the bottom of a liquid helium cryostat, and a mobile base suspended by springs and decoupled from the fixed base, which comprises coarse approach elements for sample and optical fiber [4].

The operation of the microscope at LT is enabled by the top bath cryostat and additional thermal shields directly connected to the helium and nitrogen reservoirs that completely surround the microscope. The integrated shutters and optical windows in the thermal shields allow *in situ* sample and cantilever exchange, molecular/atomic deposition and also the possibility of monitoring the coarse approach of optical fiber and sample even at low temperature. Special attention is paid to the vibration isolation system and to the materials used in the construction of the microscope.

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In-situ AFM for catalysis research at high pressures and temperatures

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To address open questions in the field of catalysis, a novel AFM has been developed which allows in-situ imaging under high pressure, high temperature conditions.

The AFM scanner uses a miniature quartz tuning fork and fits in a high pressure flow reactor with a volume of 0.5 ml. The reactor is mounted in a Ultra High Vacuum (UHV) system that has been equipped with several standard tools for surface preparation and characterization. Samples can be prepared in UHV and transferred in and out of the reactor without exposure to air. To perform catalytic reactions, a wide range of mixtures of gasses can be made to flow through the reactor and a quadrupole mass spectrometer is used for the analysis of the reaction products.

In-situ images of palladium nanoparticles on an oxide support taken during the catalytic oxidation of carbon monoxide demonstrate the unique capabilities of this setup.

Measurement of atomic-scale potential variations near a LiF step

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Understanding potential variations near step edges of surfaces is of cardinal importance to control surface processes such as adsorption, growth, catalysis and friction. Ionic crystal surfaces attract the scientific attention due to their high band gap, and deposited molecules often diffuse to the step edges.[1]

We studied the potential variations near a LiF (001) step edge using bimodal dynamic force spectroscopy with the flexural and torsional resonance modes of the cantilever. The flexural oscillation is used to regulate the vertical tip-sample distance while the torsional one detects the lateral interaction. Since the lateral oscillation is affected only by site-dependent interactions, it has an extremely high sensitivity to the lateral potential variation.[2] Our measurements (fig.1) show that the vertical interaction is quite weakly modulated by the step and it does not show any strong bias dependence of the site-dependent electrostatic interaction. Contrary, the torsional frequency shift, Δf_{TR}, shows a remarkable contrast, and far away from the step (~6 nm), it has a linear dependence on the bias voltage.

In order to better understand this effect we performed atomistic calculations with the shell model, using a model LiF (001) surface with a step edge consisting of more than 36000 atoms, and an ideal $Li_{32}F_{32}$ cubic tip attached to a spherical electrode. Because the electrodes in the simulation are applied few atomic layers below the surface, while the real ones have few millimeters of insulating material on top, an effective bias was computed with finite elements methods, taking into account the shape of the whole cantilever. After relaxing the surface at different bias voltages, we evaluated the gradient of the Coulomb potential at the tip's position and found the same linear trend seen in the experiment. We can map this result to the atomic displacement and polarization at the step edge (fig.2).

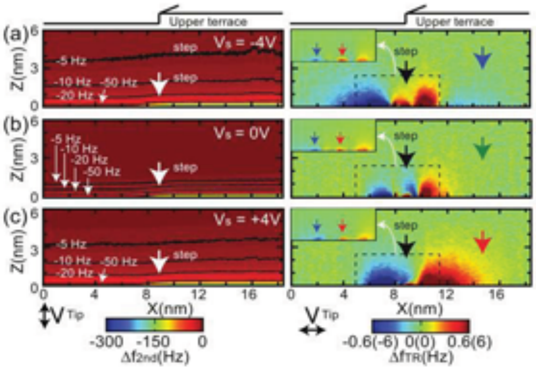

Figure 1. Bimodal DFS map across the step

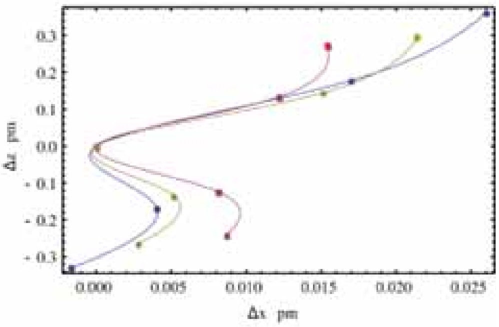

Figure 2. Calculated atomic displacement and polarization.

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Dear conference participant,

Every year, the organizing committee of the NC-AFM Conference Series arranges for a possibility to publish results presented at the conference in a high-quality journal. The goal is that the NC-AFM community is provided annually with a collection of papers assembled in one issue that give a comprehensive overview over the current state-of-the-art of this rapidly developing field. Due to the high visibility of these Speical Issues in the NC-AFM community, paper published in this series are highly cited.

Udo Schwarz, Associate Editor
Beilstein J. of Nanotechnology

In order to continue this tradition, the organizing committee has this year teamed up with the Beilstein Journal of Nanotechnology. This new, peer-reviewed, open access journal publishes high-quality original articles on all aspects of nanoscience and nanotechnology. It provides a unique platform for rapid publication, highest visibility, and worldwide impact, and I am cordially inviting you to contribute an article to the planned special NC-AFM 2011 issue. I know that many of you will have reservations publishing in an open-access journal, especially if it is new, but there are good reasons why I hope you will support this effort:

- In recent years, many of the established scientific journals have dramatically increased their subscription fees charged to libraries and universities with the effect that many smaller institutions had to discontinue their subscriptions to select journals. For the Beilstein Journal of Nanotechnology, however, there are no fees for authors and readers and no page charges or charges for color - the Journal is completely funded by the Beilstein-Institut, a German non-profit foundation, as a service to the scientific community.

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- While articles submitted to the NC-AFM Special Issue will be published online on an ongoing basis (i.e., no wait once your article has been accepted), they are additionally viewable as a group (i.e., a "virtual special issue"), allowing a series to develop with time. When the series is finalized, we will print it as a hardcopy special issue that we will distribute to all authors, all conference participants, and a large number of scientists working in this field. For broadest dissemination of your results, you can even provide us with further names and addresses we may not have on file when you submit your article (please include them into your cover letter) and we will send additional hardcopy issues to these individuals free of charge.

When you submitted a contribution to this conference, you should have already received a printed copy of a recently published Thematic Series (the issue "Preparation, properties and applications of magnetic nanoparticles") that was send to you by regular mail. This was done so that you are able to convice yourself about the quality and the high standards of Beistein's Thematic Series. More details about the aims and scope of the Journal and the Editorial and Advisory Boards can be found at the Journal's web site at www.bjnano.org, where you can also find the instructions for authors and a description of the submission process. Articles for the special issue can be submitted any time (please address your cover letter to the editor-in-chief Thomas Schimmel and indicate that your submission is for the NC-AFM 2011 Special Issue so that he can forward it to me), but the official deadline is set to two months after the end of the conference, on

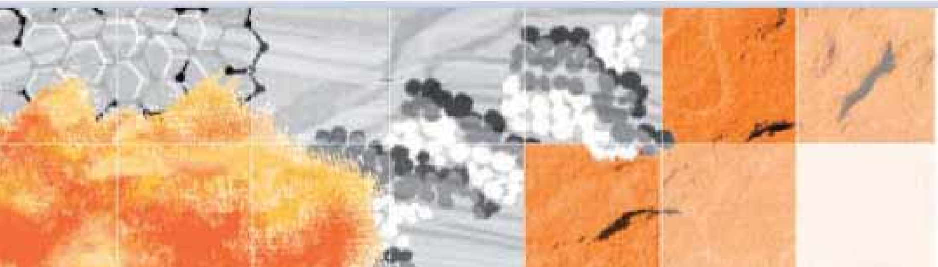
Tuesday, November 22, 2011

On behalf of the NC-AFM 2011 Organizing Committee, I cordially invite you to submit a manuscript. Take full advantage of true Open Access Publishing to disseminate your results with maximum impact and contribute to progress in the NC-AFM community. Of course, we hope that you will continue to send us your most exciting results in the future for publication so that we can make this non-profit, free service to the scientific community a success for the years to come. If you have any questions, don't hesitate to ask me during the conference.

Yours sincerely,

U. Schwarz

Udo D. Schwarz
Associate Editor, Beilstein Journal of Nanotechnology
Editor NC-AFM 2011 Special Issue



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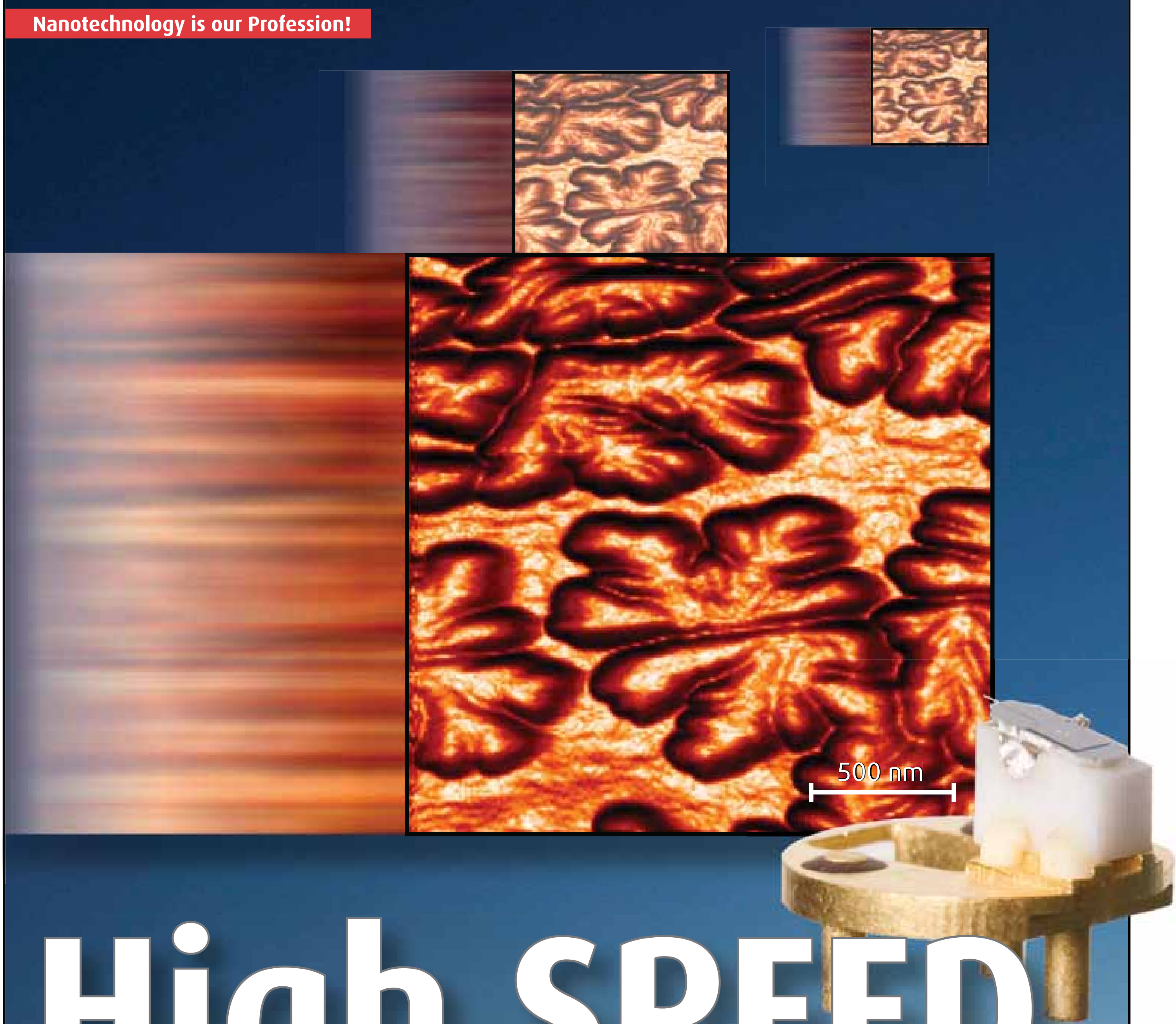
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