Scientific Report

New trends in Scanning Probe Microscopy: simultaneous tunneling and current measurements

1) Summary

The workshop 'New trends in Scanning Probe Microscopy: simultaneous tunneling and current measurements' took place at City theater of Cesky Krumlov, Czech Republic between Sunday 1st July 2012 and Monday 2nd July 2012. Workshop participation was free for any attending person of the 15th International Conference on non-contact Atomic Force Microscopy. The aim of the workshop was to gather leading scientists from the field of the SPM community to exchange ideas about the most pressing challenges and to discuss the next developments needed to anticipate the future of scanning probe techniques. Main focused was devoted to new experimental technique combining STM/AFM measurements with atomic resolution. Scientific discussion lead during the workshop included critical comparison of both STM and nc-AFM techniques. The workshop included of 6 invited talks (40 minutes) and 6 regular talks (20 minutes). In total, we had 37 participants from 10 countries (UK, Spain, Netherlands, Germany, USA, Japan, Canada, Poland, Switzerland and Czech Republic). The event was organized as a satellite workshop of the 15th International Conference of non-contact Atomic force Microscopy organized by the Institute of Physics of the AS CR in Prague, Czech Republic in July 2012. More information about the workshop is available on a webpage http://ncafm12.fzu.cz/symposium.

Among main topics addressed by the workshop were:

- Novel Instrumentation and techniques for force/current detection
- Combined force and tunneling spectroscopy
- Relation between force and current in atomic scale
- Theoretical understanding of force/current in near-to-contact regime
- Charge transfer mechanisms at the atomic scale
- High resolution AFM and STM imaging
- Theoretical aspects of scanning probe microscopy

List of invited speakers:
Richard Berndt (Universitaet Kiel, Germany)
Franz Giessibl (Universitaet Regensburg, Germany)
Nicolas Lorente (Centro de Investigaciones en Nanociencia y Nanotecnologia, Spain)
Latha Venkataraman (Columbia University, USA)
Yoshiaki Sugimoto (Osaka University, Japan)
Stefan Tautz (Julich Forschungszentrum, Germany)

2) Description of scientific meeting

The analysis, control and modification of individual atoms, molecules, surfaces and nanostructures are among the great challenges of the last few years. Nanoprobe techniques such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM) provide not only a variety of experimental information at the atomic scale, but they are also the potential to be used as an assembly tool to create potential nanoscale devices using both the contact and non-contact modes of operation. These scanning probe techniques have found wide application in nanotechnology and other research areas such as surface physics and chemistry, tribology, molecular/cell biology etc.. It is evident that the further development of these scanning probe methods will have a dramatic impact on many scientific areas.

Recently, several new experimental techniques yielding atomic resolution derived from standard AFM or STM techniques, such as Kelvin probe force microscopy and combined STM/AFM measurements, have been introduced. However, a comprehensive understanding of the whole scanning process is still lacking and remains a challenge. The control of the geometric, electronic, and mechanical properties of atomic-scale structures is a prerequisite for the understanding and fabrication of new materials and devices. In this context, the coupling between two atomically sharp nanocontacts provides tunable access to a fundamental underlying interaction: the formation of the bond between two atoms as they are brought into the atomic contact.

The aim of the workshop was to bring together leading scientists from the experimental and theoretical sides to exchange ideas needed for new horizons in the field and to discus next steps in the close future of scanning probe microscopy with special emphasis on combination of AFM and STM methods.

The first block of lectures, including 2 invited lectures given by F.J. Giessibl and Y. Sugimoto and a contributed talk given by A. Sweetman, was devoted to experimental studied of surfaces and nanostructures using simultaneous AFM/STM measurements. Particular attention was paid to correlation between tunneling current and atomic force. Also new possibilities of 3D imaging at atomic scale using both tunneling current and force was discussed. Finally, the importance of proper interpretation of experimental data obtained by SPM was critically discussed.

The opening lecture was given by Prof. F.J. Giessibl, the leading scientist in Scanning Probe field, inventor of qPlus sensor technique allowing simultaneous acquisition of tunneling current and force with atomic resolution. He provided a brief overview of recent progress in AFM/STM measurement. He critically compared both AFM and STM techniques in terms of signal to noise ratio and its capability to achieve atomic resolution or perform atomic manipulation. He provided a perspective of high resolution sub-atomic using atomic force in his contribution.

Y. Sugimoto reported in his invited talk simultaneous AFM/STM imaging at constant height, 3D force/current mapping and the conversion formula from the time-averaged tunneling current to the instantaneous tunneling current.

The relation between the chemical bonding force and the tunneling current in a semiconducting atomic-scale junction is also discussed.

A. Sweetman reported detailed study of silver-terminated silicon surface, Ag-Si(111)-(√3x√3)R30 (Ag-√3) by means of simultaneous AFM/STM measurement. Using qPlus NC-AFM/STM in constant frequency shift feedback and acquiring tunnel current simultaneously, he and co-workers were able to unambiguously determine the origin of the features in NC-AFM by comparing the proposed STM and AFM contrast mechanisms.

L. Venkataraman introduced powerful experimental techniques used to measure these properties in single molecule circuits using a custom-built conducting atomic force microscope under ambient conditions. In following she reported simultaneously measured conductance and force across single Au-molecule-Au junctions in order to obtain complementary information about the electronics and structure in these systems. Finally, she showed how the simultaneous measurements of forces can be used to demonstrate effects related to quantum interference in single-molecule junctions.

N. Lorente introduced magnetic inelastic electron tunneling spectroscopy (IETS), where electron currents can induce magnetic excitations in molecular nanostructures. He discussed in details the theoretical predictions for inelastic magnetic tunneling obtained with a one-electron approach and with a many-body theory including Kondo-like phenomena. He demostrated that the inclusion of inelastic effects in the impurity leads to an enhancement of the electronic coherence and hence of the Kondo temperature contrary to what is found when inelastic effects of the substrate are included.

Ch. Lotze reported detailed study of a model bi-stable molecular system using dynamic force spectroscopy. The effect of current-induced stochastic fluctuations of conductance was correlated with fluctuations in force. In this experiment, they identified the last from both, frequency shifts and energy dissipation measurements, picturing a regime in which electrical transport and mechanical motion are coupled.

F.S. Tautz illustrated the benefits of combining force with current detection when molecules are in the transport path between the STM tip and the surface. Two experiments were considered: (1) a molecular wire is lifted up between tip and surface as the tip retracts from the surface, (2) a sensor molecule is present in the tunneling junction, yielding very high lateral image resolution as the tip is scanned across the surface in near contact (scanning tunneling hydrogen microscopy, STHM). In particular, the possibility to form molecular junction consisting of only a single molecule by means of SPM has been reported by S. Tautz. The formation of molecular junction between STM probe and molecule/surface interfaces has been revealed by simultaneous measurement of the tunneling current and the chemical force. This combination opens a completely new way to study single-molecule junctions.

P. Pou presented a combined experimental and theoretical study on the influence of the atomic thermal movements on both the STM and the FM-AFM images of a Si tetramer on the Si(111)-7x7 surface at room temperature. In this contribution, the author showed importance of dynamical motion to understand experimental observation. In particular, a complex molecular dynamic as well as energy barrier calculations disclosed that, at room temperature, the tetramer is moving between 4 nonequivalent solutions (each one corresponding to a different Si tetramer atom being the highest). Therefore, the STM is in fact sensing an average of the different atomic configurations resulting in images displaying a symmetric structure.

Finally T. Arai reported the relationship on the resonance state between the force and the current between a Si tip and a Si(111)7x7 by measuring the changes in the force and the current with decreasing tip-sample separation. By analyzing the curves, they were able to extract the relationship between the force and the time-averaged current on the resonance state.

In the second session on Monday, R. Berndt gave an invited talk titled “Single and bimolecular contacts: conductance and forces”. Using low-temperature scanning tunnelling microscopy he described in details investigation of the conductance of molecules adsorbed on surfaces. Going beyond the tunnelling range, he explored closer tip-molecule distances in the contact regime where currents of several microamperes are passed through the junction. He showed, in his talk, that the detailed electrode geometry and the molecular structure and bonding drastically affect the conductance.

The last block of the workshop has been devoted to 3 regular talks addressing possible influence of nc-AFM measurements by presence of tunneling current and detailed understanding Kelvin Force Probe microscopy. The block was open by Z. Majzik, who discussed a correlation between the apparent barrier height and the local contact potential difference at the atomic scale. In particular, he reported simultaneous site-specific AFM/STM measurements using a qPlus sensor on the prototypical Si(111)–7×7 surface with low coverage of atomic hydrogen. In the contribution, he demonstrated how the chemical force, the apparent barrier height and local contact potential difference change according to the tip-sample distance and atomic site.

A. J. Weymouth demonstrated a dominating effect that the tunnel current can have upon AFM imaging. While it is common practice in NC-AFM to apply a bias voltage between the tip and sample in order to decrease the attractive long-range electrostatic force, when the sample and tip are not insulating, this can induce a tunnel current. The voltage drop of this current can be significant due to the large areal current density, affecting the electrostatic force and inducing a “phantom” atomic contrast in AFM images. In his contribution, he presented force-bias spectra on silicon surfaces, discussing the breakdown of the Kelvin parabola and the influence of the phantom force upon determining local contact potential differences.

K. Yamasue introduced a new technique for imaging local dipole moments of material surfaces, so called non-contact scanning nonlinear dielectric

microscopy. He pointed out new possibilities in understanding of charging processes on surfaces and nanostructures using this method.

3) Assessment and impact of the workshop

The aim of the workshop was bring together leading scientists from the experimental and theoretical sides to exchange ideas needed for new horizons in the field and to discus next steps in the close future of Scanning Probe Microscopy. We think the workshop met this goal.

The scientific discussion between participants during the workshop initiated critical discussion of different aspects of both nc-AFM and STM measurements. In particular, possibility of high resolution imaging of complex nanostructures (such as molecules and nanoclusters) using atomic force and tunneling current was intensively discussed. Also the relation between these two quantities was under strong debate. The importance of simultaneous detection of tunneling current and atomic force in molecular and atomic contacts was frequently stressed during the meeting to better understand both transport and mechanical properties of investigated junctions.

Intensive debate was opened about complex characterization of molecular structures on surfaces using both AFM and STM techniques. It is evident that only the combination of these approaches with theoretical ones could bring the reliable analysis of molecular nanostructures on surfaces.

Inherent limitations of DFT (strong electron correlations, van der Walls interactions) have been discussed in a way accessible to the experimental audience. In addition, a discussion between presented theoreticians suggested new trends in simulations of Scanning Probe Microscopy.

The workshop joined to the 15-th International Conference on non-contact Atomic Force Microscopy. We believe that the synergy between the workshop and the conference brought benefits to both events. The transfer of knowledge between STM and nc-AFM communities stimulated further progress of both techniques. In particular, better understanding and further development of simultaneous AFM/STM technique can bring new possibilities in advanced characterization and modification of surfaces and nanostructures with atomic scale precision.

4) Annexes: Programme of the meeting & List of participants

Workshop Programme

Sunday 1/8

12:00-13:30 *Lunch together*

14:00- 14:20 Opening Ph. Moriarty and R. Perez

14:20-15:00 F.J. Giessibl

15:00-15:40 Y. Sugimoto

15:40-16:00 A. Sweetman

16:00-16:40 *Coffee break*

16:40-17:20 L. Venkataraman

17:20-18:00 N. Lorente

18:00-18:20 Ch. Lotze

Monday 2/8

9:00-9:40 F.S. Tautz

9:40-10:00 P. Pou

10:00-10:20 T. Arai

10:20-11:00 *Coffee break*

11:00-11:40 R. Berndt

11:40-12:00 Z. Majzik

12:00-12:20 A.J. Weymouth

12:20-12:40 K. Yamasue

12:40-14:00 *Lunch time*

List of participants

Convenor(s)	
Name	City, Country
Dr. Pavel Jelinek	Prague, (CZ)
Dr. Philip Moriaty	Nottingham, (UK)
Dr. Ruben Perez	Madrid, (ES)

Add a Speaker

Speakers	
Name	City, Country
Professor Toyoko Arai	Kanazawa, (JP)
Professor Richard Berndt	Kiel, (DE)
Professor Franz J. Giessibl	Regensburg, (DE)
Dr. Christian Lotze	Berlin, (DE)
- Zsolt Majzik	Prague, (CZ)
Dr. Pablo Pou	Madrid, (ES)
Dr. Yoshiaki Sugimoto	Osaka, (JP)
Dr. Adam Sweetman	Nottingham, (UK)
Professor F. S. Tautz	Jülich, (DE)
Professor Latha Venkataraman	New York, (US)
Dr. A. J. Weymouth	Regensburg, (DE)
Dr. Kohei Yamasue	Sendai, (JP)

Add a Participant

Participants	
Name	City, Country
Dr. Martin Švec	Prague, (CZ)
- Florian Albrecht	Regensburg, (DE)
- Jan Berger	Prague, (CZ)
- Yuriy Dedkov	Berlin, (DE)
- Schulz Fabian	Berlin, (DE)
- Prokop Hapala	Prague, (CZ)
- Nadine Hauptmann	Kiel, (DE)
- Tobias Herden	Stuttgart, (DE)
- Ondřej Krejčí	Prague, (CZ)
- Jan Kučera	Prague, (CZ)
- Zsolt Majzik	Prague, (CZ)
Dr. Corso Martina	Berlin, (DE)
- Emmrich Matthias	Regensburg, (DE)
Professor Alastair Mclean	Ontario, (CA)
- Martin Ondráček	Prague, (CZ)
Dr. Temirov Ruslan	Jülich, (DE)
- Maxmilian Schneiderbauer	Regensburg, (DE)
Dr. Glatzel Thilo	Basel, (CH)
- M. A. van Spronsen	Leiden, (NL)
Dr. Kaminski Wojciech	Wroclaw, (PL)
Dr. Ayhan Yurtsever	Osaka, (JP)
- Petr Zimmermann	Prague, (CZ)