O 47 Rastersondentechniken III

Zeit: Dienstag 15:45–18:30 Raum: TU EB202

O 47.1 Di 15:45 TU EB202

Optical interaction between tip and substrate in apertureless SNOM — •Ruben Esteban, Ralf Vogelgesang und Klaus Kern — Max Planck Institute für Festkörperforschungg

Scanning near field optical microscopes (SNOM) have proved able to overcome the resolution limit and study light-matter interaction in nanometer sized structures. Resolution of $\sim 10nm$ is achievable at optical and infrared frequencies using the apertureless configuration (a-SNOM), which detects the fields scattered when a sharp tip is approached to a substrate under focused illumination. We use numerical simulation to better understand the phenomena involved. In our modelling we go significantly beyond the "spherical tip" model towards realistic, extended, conical tips. We can approach the experimental, "infinite-tip" case very well, including the presence of a large background field from the tip bulk. We also simulate the behavior of an efficient demodulation scheme that helps to discriminate the field generated in the strongly localized tip-substrate interaction. Good qualitative agreement with experimental measurements is found.

O 47.2 Di 16:00 TU EB202

Scattering scanning near-field optical microscopy on anisotropic dielectrics — •Susanne Schneider, Stefan Grafström, and Lukas Eng — Institute of Applied Photophysics, University of Technology Dresden, D-01062 Dresden

Scattering scanning near-field optical microscopy (s-SNOM) is based on the interaction between an optically scattering nano-cluster (AFM tip) and a dielectric sample. The size of the cluster defines the resolution of the microscope, which is in the order of nanometers. On this scale the optically anisotropic properties of the sample have to be taken into account, even if the sample is isotropic on the macroscopic scale.

We discuss the interaction between a cluster and an anisotropic sample using an analytical dipole-dipole model by taking the following contrast mechanisms into account:

1. The reflection on the surface of the anisotropic sample, which causes a change in the external electric field at the position of the probe.

2. The modification of the polarizability of the tip by interaction with the anisotropic sample. Here we use the image charge method for anisotropic samples, which was developed in 1997 by I. Lindell.

3. The formation of a resulting dipole which is the superposition of the tip dipole and the image dipole induced in the sample.

In these calculations not only the influence of the sample anisotropy is included but also the anisotropy that the probe may exhibit for geometrical or material-specific reasons.

O 47.3 Di 16:15 TU EB202

Resonant light scattering by near-field induced localized phonon polaritons — •Jan Renger[1], Stefan Grafström[1], Lukas M. Eng[1], and Rainer Hillenbrand[2] — [1]Institute of Applied Photophysics, University of Technology Dresden, D-01062 Dresden — [2]Nano-Photonics Group, Max-Planck-Institut für Biochemie, Am Klopferspitz 18, D-82152 Martinsried

In the vicinity of a SiC surface the scattering of light at a metallic nanoparticle shows a strong peak around the surface phonon polariton resonance of the SiC substrate [1] in the mid-infrared spectral region. Close to the surface the polarized particle couples to localized phonon polaritons. This near-field interaction shifts the peak to lower frequencies and causes a splitting into two modes for distances below 5 nm. We analyze this phenomenon by applying an accurate numerical 3D model based on the multiple-multipole method. The results are compared with the predictions of the analytical dipole model as frequently used to explain the contrast in aperture-less scattering- type scanning near-field optical microscopy. We find a qualitative agreement but the dipole model turns out to underestimate the spectral shift quantitatively, which is significant for small separations between the sphere and the SiC interface.

[1] R. Hillenbrand, T. Taubner, and F. Keilmann, Nature **418**, 159 (2002).

O 47.4 Di 16:30 TU EB202

Quantitative investigation of tip-sample interaction on single-walled carbon nanotubes in the attractive force regimes — •Makoto Ashino, Timo Behnke, and Roland Wiesendanger — Institute of Applied Physics and Microstructure Research Center, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg

The three-dimensional force field spectroscopy measurement combined with atomic-resolution dynamic force microscopy imaging has allowed us to evaluate interaction forces acting between a foremost atom of the silicon-cantilever tip and specific atomic sites of a single-walled carbon nanotubes (SWNT) [1]. Quantitative analysis using a simple Lennard-Jones (L-J) potential leads to the finding that the short-range interatomic van der Waals forces are responsible for the atomic-scale contrast. The analysis also shows that the interaction forces deviate from the L-J fits at closer tip-sample distances than that showing the maximum attractive forces. The degree of deviation is site dependent as well. Using some model calculations, we try to analyze tip-sample interactions at closer distances. By taking softness and tip-induced relaxations of SWNTs into account, we discuss the dynamic response of the SWNT to variation of the tip-sample distance.

[1] M. Ashino *et al.*, Phys. Phys. Lett. **93**, 136101 (2004).

O 47.5 Di 16:45 TU EB202

First-priciples simulations of NC-AFM image contrast on InAs(110) surface — •Vasile Caciuc[1], Hendrik Hölscher[1], Stefan Blügel[2], and Harald Fuchs[1] — [1]Physikalisches Institut der Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

In the present contribution we report *ab initio* pseudopotential calculations based on density functional theory to investigate the non-contact atomic force microscopy (NC-AFM) image contrast on InAs(110) surface. The foremost tip structure is modeled by a SiH_3 tip. The influence of long-range van der Waals forces on the simulated AFM images due to the macroscopic part of the tip was taken into account by an empirical model. The effect of the tip-induced surface relaxations on the calculated forces was investigated for the tip above As and In atoms. The displacement curves corresponding to these vertical scans exhibit an hysteretic behaviour. At the tip-surface separations where the instability induced by this hysteresis is not present, the force curves obtained for relaxed (due to tip-sample interaction) and unrelaxed InAs(110) surface exhibit the same qualitative behaviour. From the calculated forces on a large number of grid points in real space (≈ 1300) we obtained maps of constant frequency shifts. The overall structure and the corrugation of the simulated NC-AFM images are in good agreement with the experimental results and allow us to explain the experimentally observed features of the image contrast mechanism on the basis of the calculated short-range chemical tip-sample interaction forces.

O 47.6 Di 17:00 TU EB202

Tip Models and Surface Atoms in DFT Simulations of AFM Scans — •Vladan Buš and Josef Redinger — Center for Computational Materials Science, Institut f. Allgemeine Physik, Vienna University of Technology, Getreidemarkt 9/134, 1060 Vienna, Austria

Non-contact Atomic Force Microscope operated under ultra-high vacuum conditions is able to display atomic features of insulating or semiconductor surfaces. Oscillations of the cantilever are influenced by forces acting between the surface atoms and the probe tip. In the close-to-contact operation region and for small amplitudes, forces describing the on-set of chemical bonding stand behind the contrast formation in this experiment.

We employ the DFT VASP code, using PAW and PW91 GGA, to simulate probing of surface atoms of GaAs(110) and Si(100) surfaces with a Si tip. Changes in structure during the approaching and withdrawing move lead to abrupt changes in normal and lateral forces and cause a hysteresis in the interaction energy.

O 47.7 Di 17:15 TU EB202

Q-Control in der dynamischen Kraftmikroskopie — •D. Ebeling[1], H. Hölscher[1], U.D. Schwarz[2], B. Anczykowski[3] und H. Fuchs[1] — [1]Center for Nanotechnology (CeNTech) und Physikalisches Institut, Universität Münster — [2]Department of Mechanical Engineering, Yale University, New Haven, USA — [3]nanoAnalytics GmbH, Münster

Der Cantilever kann in der dynamischen Kraftmikroskopie sowohl als extern angeregter als auch als selbsterregter Oszillator betrieben werden. Das so genannte Q-control kombiniert beide Ansätze und erlaubt eine aktive Modifikation der Dämpfung des Federbalkens und damit der Güte des Systems [1]. Diese Eigenschaft kann auf verschiedene Arten genutzt werden, um die Möglichkeiten der dynamischen Kraftmikroskopie zu verbessern.

Wir präsentieren eine Analyse des Q-controls in der dynamischen Kraftmikroskopie. Basierend auf der analytischen Lösung der Bewegungsgleichung geben wir explizite Formeln an, mit denen man die relevanten Parameter wie Verstärkungsfaktor, Phase und Amplitude berechnen kann. Anhand der eingehenden Analyse dieser Formeln lassen sich die bekannten Vorteile des Q-controls (wie z.B. Kontrolle des Q-Faktors, erhöhte Scangeschwindigkeit, Reduktion der Spitze-Proben Kräfte) erklären. Zum Schluss vergleichen wir die theoretischen Ergebnisse mit den experimentellen Resultaten.

[1] B. Anczykowski, et al., Appl. Phys. A 66, S885 (1998)

O 47.8 Di 17:30 TU EB202

Calculation of STM images of defect and adsorbate structures on the ZnO(10$\bar{1}$0) surface — •Roman Kovacik, Bernd Meyer, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The interpretation of scanning tunneling microscopy (STM) experiments is often difficult since STM images are not a direct probe of the atomic structure of a surface but of its electronic properties. To determine STM images from electronic structure calculations we have implemented the two most common methods, the Tersoff–Haman approach and the evaluation of Bardeens tunneling formula, into the density–functional based Car–Parrinello Molecular Dynamics (CPMD) code. As first applications we have calculated STM images together with selected I(V)–profiles (scanning tunneling spectroscopy – STS) for (i) the clean ZnO(10$\bar{1}$0) surface, (ii) the surface with oxygen, zinc and ZnO vacancies and (iii) the adsorbate–covered surface considering different coverages of water molecules. Characteristic differences between the Tersoff–Haman and the Bardeen approach will be discussed, and the calculations will be compared to recent experimental results.

O 47.9 Di 17:45 TU EB202

STM induced light emission spectroscopy of individual C_{60} molecules — •Elizabeta Ćavar, Marie-Christine Blüm, Marina Pivetta, François Patthey, and Wolf-Dieter Schneider — Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

The tunneling electrons from a Pt/Ir STM tip were used as an excitation source to locally investigate optical transitions of individual C_{60} molecules. Experiments were performed with a home built STM operating in ultra-high vacuum and at a temperature of 50 K. The C_{60} molecules were sublimated on ultrathin NaCl(001) film on Au(111). Topography images revealed C_{60} nanocrystals in the hexagonal and truncated triangular form with an average side length between 30 and 80 nm and a maximal height of 4 layers. The molecules form hexagonal layers with an intermolecular distance of 1nm. Light emission spectra from individual C_{60} molecules show several peaks in the wavelength range between 670 and 900 nm which are assigned to the characteristic C_{60} luminescence.

O 47.10 Di 18:00 TU EB202

Untersuchung der Bandstruktur und der Injektionscharakteristik von Elektronen am Beispiel Niob mittels Rastertunnelspektroskopie — •Berndt Koslowski, Christof Dietrich und Paul Ziemann — Abtl. Festkörperphysik, Universität Ulm

Die Volumen-Bandstruktur von Nb wurde mittels Rastertunnelspektroskopie auf Nb(110) und Nb(100) untersucht. Zur Anwendung kamen sowohl die herkömmliche I-V-Spektroskopie als auch die selten benutzte Z-V-Spektroskopie. Letztere erweitert den adressierbaren Energiebereich auf ±5 eV. In diesem Energiebereich können viele Signaturen in der experimentell bestimmten lokalen Zustandsdichte gefunden werden, die sich kritischen Punkten der Volumenbandstruktur von Nb zuordnen lassen. Unter anderem kann eine bislang unverstandene Signatur bei +1eV auf der Nb(110) auf einen Oberflächenzustand zurückgeführt werden. Hier vergleichen wir die auf der (110)-Oberfläche gewonnenen Erkenntnisse mit der Spektroskopie auf der (100)-Oberfläche und versuchen Informationen über die Injektions-Charakteristik der Elektronen in die Elektroden abzuleiten.

O 47.11 Di 18:15 TU EB202

Visualisierung und Manipulation ferroelektrischer Domänen in Lithiumniobat mit dem Rasterkraftmikroskop* — •Tobias Jungk, Elisabeth Soergel und Karsten Buse — Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn

Lithiumniobat ist ein Ferroelekrikum, das aufgrund seiner piezoelektrischen, pyroelektrischen, elektrooptischen und nichtlinear-optischen Eigenschaften von großem Interesse für viele technische Anwendungen ist. Da die Domänenstruktur einen direkten Einfluss auf die Eigenschaften des Materials hat, ist es von besonderem Interesse diese bis hin zur kleinstmöglichen Skala zu untersuchen. Hier bietet das Rasterkraftmikroskop (RKM) die Möglichkeit der zerstörungsfreien Domänenvisualisierung auf der Nanometerskala. Wir untersuchen die Mechanismen zur Abbildung ferroelektrischer Domänen mit dem RKM in Lithiumniobat-Kristallen. Dazu wird im Kontaktmodus eine Wechselspannung an die RKM-Spitze angelegt und mittels Lock-In-Technik die lokale Antwort des Kristalls ortsaufgelöst analysiert. Die erreichte Ortsauflösung beträgt ca. 100 nm. Neben der Charakterisierung und Optimierung des Abbildungsverfahrens wird das RKM auch zur Strukturierung ferroelektrischer Domänen im Submikrometerbereich eingesetzt. Mit dem an der RKM-Spitze inhomogenen, stark überhöhten elektrischen Feld ist es möglich, gezielt Domänen zu schalten und somit künftig Strukturen für die integrierte Optik zu realisieren. *Gefördert von der DFG und von der Deutschen Telekom AG.