

Exploring the Nano-World: Friction and Light at the nanometer scale Nano3d Visualization

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Chapter 1 Introduction

Introduction

1.1 Scanning Probe Microscopy techniques

Scanning probe microscopy (SPM) covers a lateral range of imaging from 0.1 mm down to 10 pm. SPM has become an essential technique in the emerging field of nanoscience, as local experiments with single atoms or molecules can be performed. Force measurements of single chemical bonds or optical spectra of single molecules may serve as examples. Furthermore, the local probe can be used to manipulate single atoms or molecules and hence to form artificial structures on atomic scale.

The starting point of SPM was the invention of the *scanning tunneling microscope* (STM) by G. Binnig and H. Rohrer in 1982, who were awarded the Nobel prize in physics in 1986. In the STM, a sharp metallic needle is scanned over the surface at a distance of less than 1 nm. This distance is controlled by the tunneling current between the tip and the conducting surface.

Meanwhile, the family of *scanning probe microscopes* has got several members, based on a variety of tip-sample interactions. The first and most important extension of the STM is the *Atomic Force Microscope* (AFM), invented in 1986 by Binnig, Quate, and Gerber. The SFM is in principle capable to determine the topography of any surface, conducting or not. The third distinguished member of the family of SPMs is the *scanning near-field optical microscope* (SNOM), which uses short-ranged components of the electromagnetic field as tip-sample interaction.

In a standard SPM experiment, the tip is moved in three dimensions by piezoelectric actuators with a precision better than 0.1 nm. An electronic controller guides the tip at a tip-sample distance corresponding to an interaction between tip and surface. This distance is recorded by a computer as a function of the lateral position and displayed as microscopic image

1.2 Sciences at the nanometer scale

An important strength of SPM beyond topographic imaging is the manipulation of surfaces. Single atoms of the surface or adsorbates on it have been systematically moved in *STM* in order to build nanometer-sized structures. SPM has found wide applications in Surface Science, where problems like surface structure, adsorption of molecules, or local electronic properties could be studied.

Industrial applications include surface control in Material Science. Roughness and hardness are being measured on nanometer scale. Magnetic structures on data storage devices can be analyzed as well as the optical quality of coatings. The microscopic origins of friction have been investigated by *Friction Force Microscopy* (FFM). Force microscopy allows the imaging of biological materials on the nanometer scale, which are not accessible to electron microscopy due to preparative reasons.

1.3 Virtual Experiments

Within the framework of the federal program Swiss Virtual Campus, an interdisciplinary team has developed a virtual laboratory with different experiments within the context of nanoscale science. Students can work out topics of current research areas by means of virtual instruments in the field of nanoscale science. The virtual Nano-World laboratory enables a fast introduction to current research topics in nanoscale sciences in an explorative way. Students take the role of researchers and can perform their own experiments interactively over the net. The course day "Exploring the nano-world" focuses on the topics Friction Force Microscopy and Nano-Optics.

In the first two work packages the students obtain the necessary theory to perform their own virtual experiments guided by a task list. The third work package uses the nano3D web service developed in Basel which encapsulates the complex configuration of a 3D ray-tracer by an intuitive web interface. After 30 minutes the students can visualize their own achieved measurements from the previous work package

Chapter 2 Friction

Friction at the nanometer scale

Friction is one of the oldest phenomena in the history of mankind. It appears in every technical application, wherever parts are in motion. Wherever we face friction consciously, it is assumed unwanted. However, friction is a highly important phenomenon for our daily life. Without friction we could not walk, no violin would sing, no moving body would come to rest. "No screaming guitars, no gym shoes, no car races". Without friction Michael Schumacher would be a lame nobody, Moses Kiptanui a sliding clown and Jimmy Hendrix would not have been a genius musician but a disdainful slowpoke. On the other hand friction is the biggest energy annihilator of this world. Approximately 70% of all energy gets lost due to friction.

Friction has been studied since the Renaissance but anyway it is only poorly understood and therefore it counts as *Dirty Physics*. The invention of the friction force microscope and the nanoscopic laws of adhesion and friction have disproved old ideas and led to a new understanding of this highly interesting phenomenon.

2.1 Macroscopic friction

In high school physics the phenomenon of friction is reduced to the classical friction laws of Leonardo da Vinci, Guillaume Amontons, Leonard Euler und Charles Coulomb. Leonardo da Vinci made experiments on an inclined plane. He found that friction is independent on the area of contact. Amontons did experiments on a horizontal surface and measured the friction force with a spring. He found that friction is proportional to the normal force and independent on the area of contact. He called the proportional factor friction constant. While Leonardo tested static friction Amontons dealt with kinetic friction. It was found by Leonhard Euler that one has to distinguish between static and kinetic friction, because it is not possible to cause a slow motion by slowly increasing the angle of an inclined plan. Also Coulomb looked at the phenomenon of friction. He built an experiment, which allowed to measure kinetic friction for different speeds. He found that friction is independent on the velocity.

1) law of Leonardo (da Vinci):

Friction is independent on the area of contact

2) law of Euler and Amontons:

Friction is proportional to the loading force

3) law of Coulomb:

Friction is independent on the velocity

2.2 Microscopic Friction: Deformation of asperities

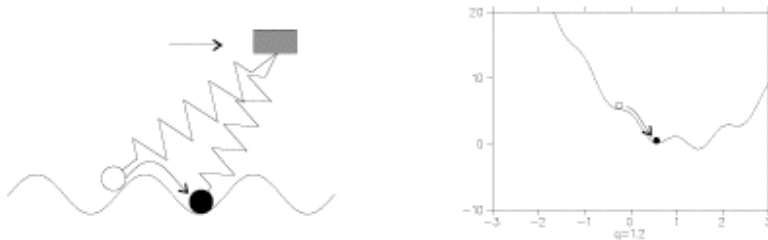
Even a surface, which appears to be flat on a millimeter scale may contain micrometer scale asperities i.e., the surface is rough. If we bring two surfaces in contact, only these asperities really touch each other. Friction is due to the interaction between the asperities of the different surfaces and the resulting energy dissipation is due to the interaction of these asperities. The real area of contact is therefore a few orders of magnitude smaller than the apparent area of contact. This important fact has to be taken into account while modelling a friction process.

Wear of the material is one possible reason of friction. Though, if you calculate the rate of wear by means of the mechanical work you have to close that the wheels of a locomotive would be destroyed after a few kilometers of use.

2.3 Friction at the nanometer scale

When a tip is dragged over a periodic potential through an elastic medium (symbolized as a spring), at certain positions of the support the tip may undergo sudden jumps. It is impossible to drag the tip in a fully controlled way. Hence the tip is unable to follow the support at any slow speed.

The Tomlinson model consists of a particle in a periodic potential. At a certain position of the support, the position of the tip becomes unstable and a sudden jump occurs. The right picture shows the local potential of the tip for a fixed support position. Note that the potential varies with the support position.



In two dimensions the Tomlinson mechanism becomes much more complicated. The tip may take a totally different path than the support.

2.4 Friction Force Microscopy

The invention of the Scanning Probe Microscopy had a deep impact into tribology. It was possible to perform friction experiments under very well defined conditions. It is possible to perform single asperity – friction experiments in a highly controlled way.

Since the poorly known environment conditions were the main problem of friction physics, a new age in this field began. In scanning force microscopy a very small tip attached on a cantilever is drawn across a surface. The surface is systematically

scanned line by line. The tip is bended by the forces between the tip and the surface. This motion of the tip is detected with the laser beam deflection method.

The cantilever can be bended in two ways:

- longitudinal deflection gives information about the topology of the sample
- torsion of the lever gives information on friction between the tip and the sample

The longitudinal deflection is caused by the different force as a function of the distance between tip and sample. It measures therefore mainly the topology of the sample. A friction force acting on the tip yields a torsion of the cantilever. In an FFM experiment therefore the torsion of the cantilever is recorded. It is quite easy to compute the amount of dissipated energy. The energy which is needed to move the tip over a distance ds is given as $dW=F ds$ where F is the Friction force. The amount of dissipated energy is hence given by the area of the friction hysteresis during one friction loop.

2.5 Applications of Friction Force Microscopy

Book: Friction and Rheology on the Nanometer Scale, E. Meyer, R.M. Overney, K. Dransfeld, T. Gyalog

- Material-specific contrast of friction force microscopy
 - Langmuir-Blodgett films
- Anorganic thin films
- SAM on SAM
- Friction in outer space

2.6 Virtual Experiments: Friction Force Microscopy

Start with the experiments: <http://labor.nano-world.org/>

First measurement

Play around with the parameters and try to get a feeling for the controls and features of the instrument. Compare your different measured images with the results of your colleagues.

Calibration

Take a picture of the KBr surface. Their interatomic distance is 0.4 nm. You may use this number to calibrate your scanner. (Tip: zoom in and turn the surface so that the atomic lattice is parallel to the line sections.) The friction force is calibrated through the scale-control. Estimate the spring constant of the cantilever by watching the slope in the LineSection

Attention: You can only see the Br Atoms.

Calculation of the torsional spring constant using REM data

Compute the torsional spring constant of the given cantilever (Available at the company Nanosensors.) The spring constant is approximatively given through:

$$c_t = \frac{Gwt^3}{3h^2l}$$

8 (10)

Here c_t denotes the torsional spring constant.

The cantilever used in the simulation is given by the following parameters:

Thickness: $t = 3'000 \text{ nm}$
Width: $w = 53'000 \text{ nm}$
Length of tip: $h = 12'500 \text{ nm}$
Length of Lever $l = 450'000 \text{ nm}$
Shear modulus $G = 5 \times 10^{10} \text{ N/m}^2$

Calculation of the torsional spring constant by FFM

Compute the spring constant of the cantilever through the slope of the sawtooth of your friction profile.

Remember that $F_{lat} = \frac{Signal}{Gain} \cdot 10nN$

Dissipation

Measure the dissipated energy per friction cycle by computing the area included in the friction hysteresis loop. (Tip: You have to take a backward and forward image using the same parameters.)

Calculation of the Friction Force

Calculate the mean friction force using the Data Analysis toolbox. The mean friction force can be extracted using the statistics over the line section. Cut off the starting ramp!

Dependence on the Spring constant

You may change the spring constant of the cantilever by typing the command:

```
command=set name=springconstant value=65
```

How does the friction change with increasing spring constant?

Understanding atomic friction by the Tomlinson mechanism



Make some free experiments with the Playing Tomlinson Applet.

Perform different measurements with different spring constants and try to find the phase transition to the superlubric phase. Derive the friction force from the hysteresis volume for a “superlubric” spring constant.

Take Pictures of Critical Curves for $v_2=0; 0.1; 1; 1.5$ using scanning angles (0, 30 45) for Noise=0.

10 (10)

Useful Equations

Always

$$F_{lat} = \frac{Signal}{Gain} \cdot 10nN$$

2D-Analysis

$$x = \frac{Scale}{256} \cdot \Delta x$$

$$y = \frac{Scale}{256} \cdot \Delta y$$

Line Section Analysis

$$d = \frac{Scale}{256} \cdot \Delta x$$

$$\Delta F_{lat} = \frac{\Delta y}{Gain} \cdot 10nN$$

Chapter 3 Light

Light at the nanometer scale

Benefits of Optics

Sensitivity: Single photons, single molecules

Selectivity: fluorescence, filters

Spectroscopy: Chemical composition

Optics (appearance or look in ancient Greek) is a branch of physics that describes the behavior and properties of light and the interaction of light with matter. Light is electromagnetic radiation with a wavelength that is visible to the eye, or in a more general sense, any electromagnetic radiation in the range from infrared to ultraviolet.

Resolution in optical microscopy, the diffraction limit implies that optical resolution is ultimately limited by the wavelength of the light. Before the advent of near-field optics it was believed that the diffraction limit imposes a hard boundary and that physical laws strictly prohibit resolution significantly better than $\lambda/2$. However it was found that this limit is not as strict as assumed and that various tricks allow us to access the evanescent modes of the spatial spectrum. In this chapter we will discuss fluorescence microscopy a specialized type of confocal microscopy.

3.1 Single Molecule Fluorescence Microscopy

In the case that a plane wave is totally reflected at an interface, an evanescent wave on the other side of the interface appears. An evanescent wave is an electromagnetic wave that decays exponentially with distance. Evanescent waves exist only at interfaces between two medias.

In fluorescence microscopy a focused laser beam excites a fluorescence part on a biomolecule. The reemitted light contains information about the orientation of the molecule adsorbed on top of a surface. Prior knowledge is associated with the type of molecules that are used to label specific parts of a biological specimen. The knowledge of the absorption and emission properties of these molecules makes it possible to substantially increase resolution.

In order to map the dipole orientation of arbitrary oriented single molecules it is desirable that all three excitation field components (E_x, E_y, E_z) in the focus are of comparable magnitude. It has been demonstrated that this can be achieved by annular illumination for which the centre part of the focused laser beam is suppressed [B. Sick, B. Hecht, and L. Novotny, PRL 85 4482-4485 (2000)].

The Electromagnetic Field may be calculated:

$$\mathbf{E}(\rho, \varphi, z) = \frac{ikf e^{-ikf}}{2} \sqrt{\frac{n_1}{n_2}} E_{\text{inc}} \begin{pmatrix} I_0(\rho, z) + I_2(\rho, z) \cos 2\varphi \\ I_2(\rho, z) \sin 2\varphi \\ -2iI_1(\rho, z) \cos \varphi \end{pmatrix}$$

$$I_0(\rho, z) = \int_0^{\theta_{\max}} d\theta \sqrt{\cos \theta} \sin \theta (1 + \cos \theta) J_0(k\rho \sin \theta) e^{ikz \cos \theta}$$

$$I_1(\rho, z) = \int_0^{\theta_{\max}} d\theta \sqrt{\cos \theta} \sin^2 \theta J_1(k\rho \sin \theta) e^{ikz \cos \theta}$$

$$I_2(\rho, z) = \int_0^{\theta_{\max}} d\theta \sqrt{\cos \theta} \sin \theta (1 - \cos \theta) J_2(k\rho \sin \theta) e^{ikz \cos \theta}$$

In contrast to classical microscopy the fluorescence part of the biological specimen or molecules contains an induced dipole moment. Through interaction between this dipole moment and the electric field of the laser beam a set of different characteristic patterns can be observed. The characteristic patterns allow a conclusion of the orientation of the observed dipole.

Single molecule excitation patterns: A sample with isolated single molecules is raster scanned in the focal plane of strongly focused laser beam. For each pixel, the fluorescence intensity is recorded and encoded in the grey scale. The excitation rate in each pixel is determined by the relative orientation of local electric field vector and molecular absorption dipole moments to be reconstructed from the recorded patterns.

Further information to nano optics can be found in *Principles of Nano-Optics*, Cambridge University press, in press (2005) by Lukas Novotny & Bert Hecht

3.2 Virtual Experiments

Exercise 1: E-Field Patterns: Orientation of single molecules

Coordinate System definition at:

http://www.nano-world.org/WS03_04/0300SNOM/content/0500angles

Generate a set of pictures describing the E-Field pattern for the “cube angle pairs”:

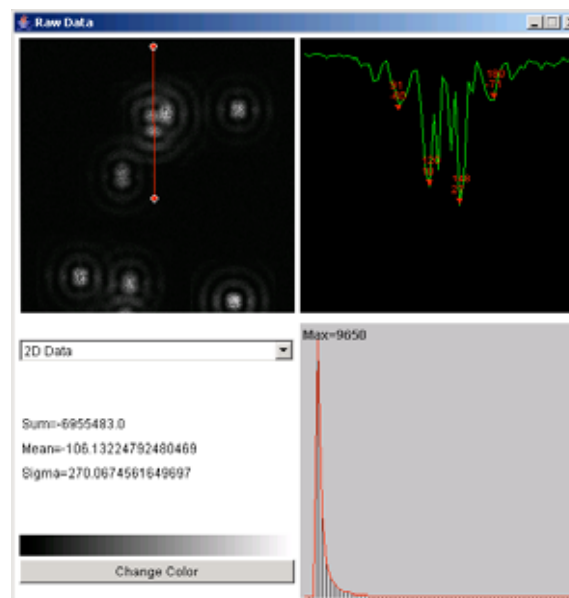
Theta	Phi
90	
0	-90
	0
	90
	180
-90	

Try to get the angles theta and phi for the following measurements:



Exercise 2: Analyze a picture of a dipole field

2.1 Measure an image using the simulation. Take 5 dipoles and try to identify their angles theta and phi by making use of the results of exercise 1.



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2.2 Using the analysis toolbox, generate a line section through the middle of dipole. Calculate the intensity ratio between the neighbouring maxima compared to the main maximum.

Exercise 3: Long time behaviour

Take a new sample (withdraw and approach) and try to describe the long time behaviour of the fluorescence of the dipoles over 1-2 hours.

Chapter 4 nano3d

Interactive 3D Visualizations

3D-Visualizations and animations appears in every day situations like sending a email or watching the weather forecast. The game and movie industry using 3D-Visualization in their products since several years. Different open source Frameworks open the 3D technologies in a convenient way for scientific visualization. This chapter deals with the open source 3D visualization program PovRay and nano3d a webinterface for nanoscale science developed at university of Basel.

nano3D: <http://nano3d.nccr-nano.org>

Povray: <http://www.povray.org>

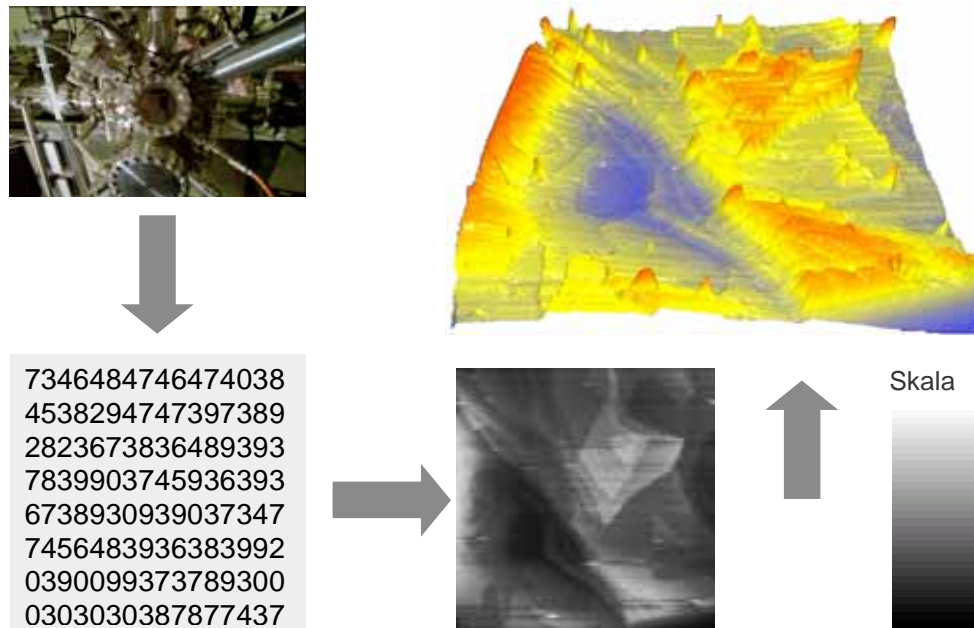
Tutorial: http://www.f-lohmueller.de/pov_tut

Povray Examples:
http://www.oyonale.com/oy_en.htm



4.1 3D rendering techniques for surfaces

The outcome of all different scanning probe are parallel collected channels of 2D maps. Line by line interaction potentials, reaction of the distance controller or collected photons are recorded in different channels. The standard representation of these results are grey scale map, darker color means less interaction. 3D representation of scanning probe measurements can help to pronounce specific results in stronger way than a greyscale representation.



Quick Start Povray: From a grey scale image to a 3D representation

The Persistence of Vision Ray-Tracer, or POV-Ray, is a free ray tracing program available for a variety of computer platforms. POV-Ray internally represents objects using their mathematical definitions; all POV-Ray primitive objects can be described by mathematical functions. This is different from many other 3D computer modeling packages, which typically use triangle meshes to compose all objects. POV-Ray primitives are usually more accurate than their polygonal counterparts. Objects that can be described in terms of spheres, planar surfaces, cylinders, tori and the like are perfectly smooth and mathematically accurate in POV-Ray renderings, whereas polygonal artifacts may be visible in mesh-based modeling software. POV-Ray primitives are also simpler to define than most of their polygonal counterparts.

3D-visualizations are described as scenes in POV-Ray:

```
// 1.
camera {
    location <0,0,-5>          // position of the camera
    look_at  <0,0,0>          // the point it is
                              pointed at
}
```




```
// 2.
light_source {
    <500,500,-500>          // position of the light source
    rgb <1,1,1>             // colour of the light source (White)
}

// 3.
sphere {
    <0,0,0>, 1              // position of the sphere and radius
    pigment {
        rgb <1,0,0>        // colour of the sphere (Red)
    }
}
```

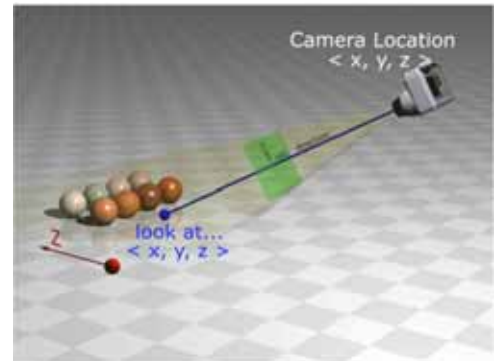
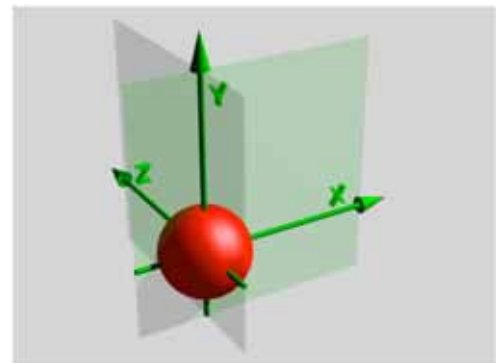
In the scene above, the camera is 5 units back from $\langle 0,0,0 \rangle$, but looking straight at it. The lightsource is 500 units to the right, 500 up, and 500 back. The sphere, which has a radius of 1 unit, has its center right on $\langle 0,0,0 \rangle$.

Additionally, the lightsource and the sphere have some kind of colour associated with them, indicated by rgb followed by another 3 numbers inside chevrons. RGB stands for "Red, Green, Blue", and these colours can be combined to produce any other colour. So rgb $\langle 1,0,0 \rangle$ is red, but $\langle 1,1,0 \rangle$ (a mixture of red and green) is yellow. Furthermore, by varying the values of each colour component, the shades can be altered further. So, $\langle 1,0,1 \rangle$ is purple, but $\langle 0.5,0,1 \rangle$ is a purple with twice as much blue as red.

In the case of lightsources, this represents the colour of the emitted light. In the case of objects, it is the colour they will be if illuminated by a pure white light $\langle 1,1,1 \rangle$.

PovRay uses a left-handed coordinate system.

For a 3D visualization of a nanostructure a minimal scene with a light source, a camera, and the surface-data (height field) is needed.

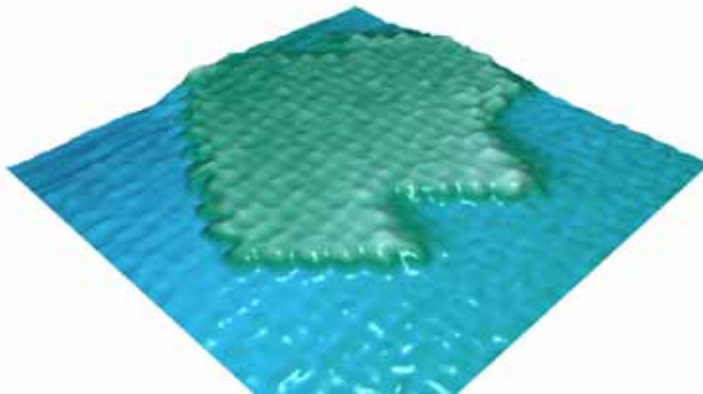


```
#include "colors.inc"
#include "textures.inc"
#declare KAMERA = <0.5,1,0.5>;

//1
light_source {
    KAMERA
    color White
}
//2
camera{
    location KAMERA
```

18 (10)

```
    look_at <0.0,0.0,0.0>
  }
  //3
  height_field{
    jpeg
    "PATH/nanosw.jpg"
    smooth
    water_level 0.0
    hierarchy off
    translate <-0.5,0,-0.5>
    texture{
      pigment {
        gradient y
        color_map {
          [0.0 color SteelBlue]
          [0.3 color SummerSky]
          [0.6 color SeaGreen]
          [1.0 color Turquoise]
        }
      }
      finish {
        phong 0.5
        ambient White * 0.5
      }
    }
    scale <1,0.1,1>
    rotate <0,180,0>
  }
}
```

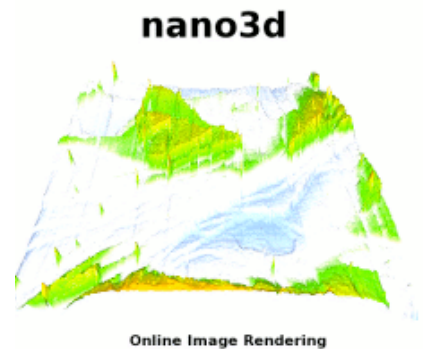


4.2 Webapplication nano3d

The web application nano3d.nccr-nano.org assists scientists with a intuitive user interface. The scientists need not to know the rather complex POV-Ray scripting language neither they have to install the rendering engine on a local computer. Only Internet access is needed to visualize the own nanostructures in 3D.

In a first step the measurements have to be uploaded as grey scale images to the nano3D server. When you access nano3d for the first time, you will receive a random ID that is stored in a cookie. All files you upload and render will be stored for that specific ID. The only way to regain access to an ID contained in a "lost cookie" is to request a custom cookie with the ID you want to access. Therefore, it is important that you write down the ID, just in case you lose the cookie. Your ID is displayed in the gallery (main page). Your ID is: aoccnncn1106315365560

Please note that your data is not well protected. If somebody knows your ID, he is able to access your files at nano3d.



Main Page

The uploaded measurements appear sorted by filenames. The 3DImage button on the left of the filename initialize a new 3D visualization, the 3dMovie button generate an animated 3D sequence, the Delete button removes the measurement data from the nano3D server. After the nano 3D server generates a new 3D image or 3D sequence the new files shows up in the right column.

Measurements				Rendered Images
cuafm138.jpg	3dImage	3dMovie	Delete	rendered.cuafm138.jpg
cuna1612s.jpg	3dImage	3dMovie	Delete	rendered.kbr.jpg
nacl_cu.jpg	3dImage	3dMovie	Delete	rendered.nacl_cu.png
kbr.jpg	3dImage	3dMovie	Delete	rendered.phorphyrin.png
nanosw.jpg	3dImage	3dMovie	Delete	rendered.kbr.png
phorphyrin.jpg	3dImage	3dMovie	Delete	rendered.si_lt.png
si_lt.jpg	3dImage	3dMovie	Delete	rendered.nanosw.png
sistep_it.jpg	3dImage	3dMovie	Delete	rendered.cuna1612s.png
dna-surf.jpg	3dImage	3dMovie	Delete	rendered.cuafm138.png
dmp_ag100_detail.jpg	3dImage	3dMovie	Delete	rendered.si_lt.jpg
DDP_C60.jpg	3dImage	3dMovie	Delete	rendered.phorphyrin.jpg
dmp_ag111.jpg	3dImage	3dMovie	Delete	rendered.cuna1612s.jpg
dsDNAoverstretched3.jpg	3dImage	3dMovie	Delete	rendered.nacl_cu.jpg
				rendered.nanosw.jpg
				rendered.dmp_ag100_detail.jpg
				rendered.dna-surf.jpg
				rendered.dsDNAoverstretched2.jpg
				rendered.DDP_C60.jpg
				rendered.dmp_ag111.jpg
				rendered.dsDNAoverstretched3.jpg

Configuration of a 3D visualization

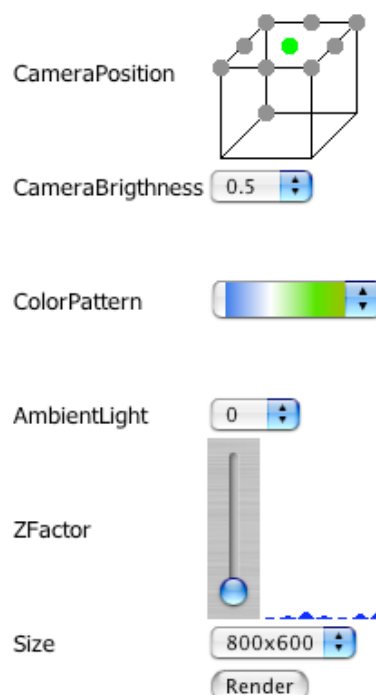
The web application nano3D provides intuitive menus to setup the 3D scenes. The camera position can be chosen by clicking on a position of the cube.

The brightness of the light source can be chosen in the drop down menu.

One of several colour profiles can be chosen

Additional ambient light let appear the some structures clearer.

The Zfactor stretch the contour profile in z-direction.



4.3 Visualization of published results

NaCl film grown on Cu(111)

Size: 9 x 9 nm

non-contact AFM / UHV Microscope Basel, Group Prof. E. Meyer

Publication:

R. Bennewitz et al. Phys. Rev. B, 62:2074, 2000.

PHYSICAL REVIEW B

VOLUME 62, NUMBER 3

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Atomically resolved edges and kinks of NaCl islands on Cu(111): Experiment and theory

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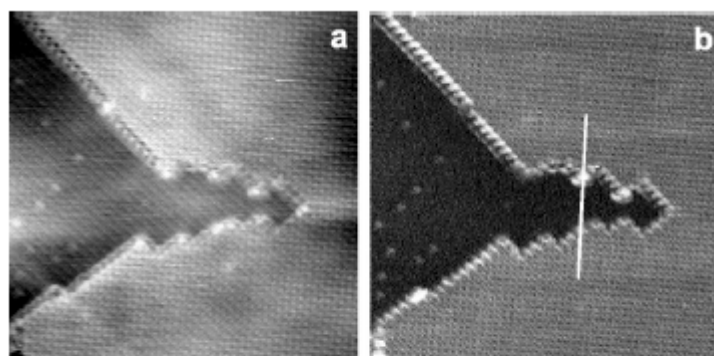
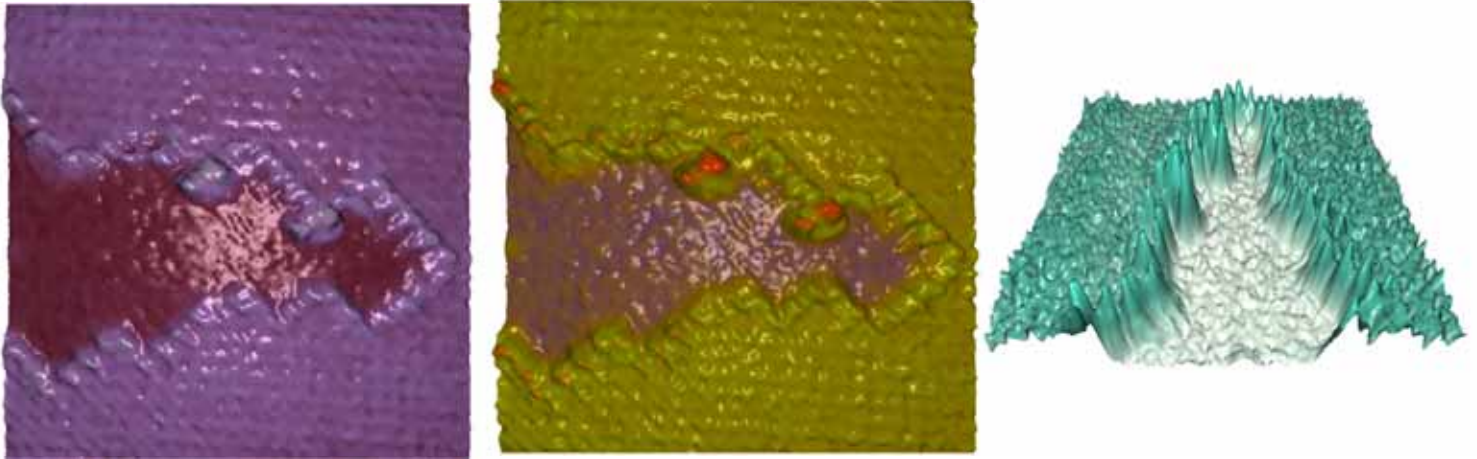


FIG. 2. (a) Enlarged topography and (b) A_{exc} images of the area mapped in Fig. 1. The image size is $18 \times 18 \text{ nm}^2$.



Radiation damage in KBr
Size: 4.86 x 4.86 nm
 non-contact AFM / UHV Microscope Basel, Group Prof. E. Meyer
 R. Bennewitz et al. Suf.Sci. 474 (2001)

