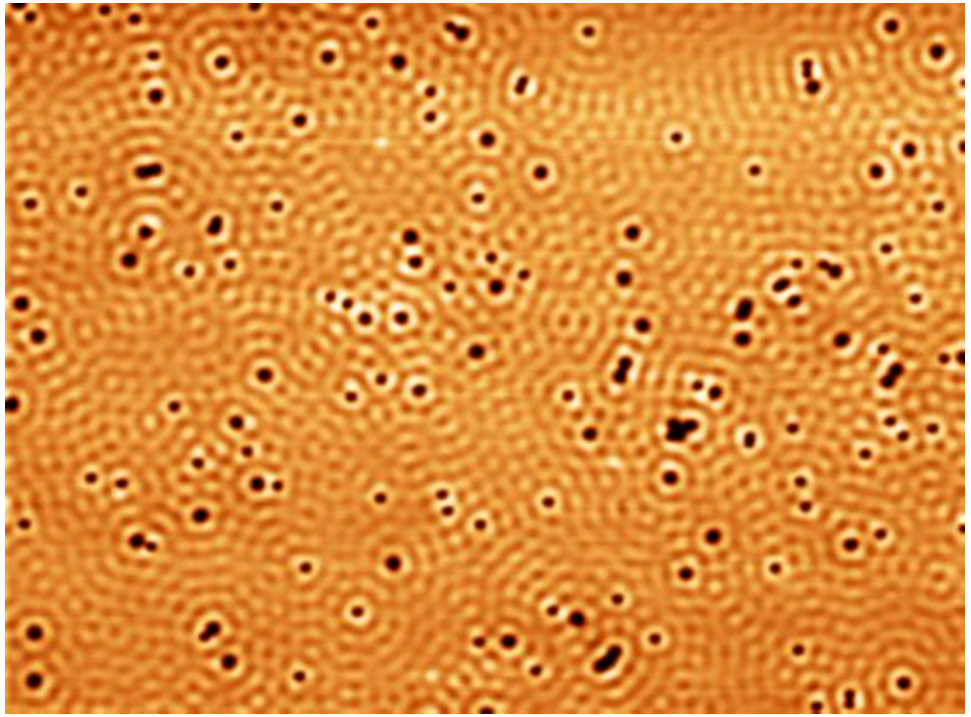
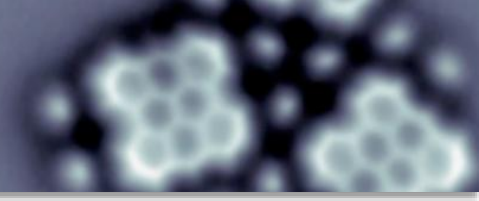
# PHYS-E0411 – Exercise 5

# Surface state dispersion of Cu(111) with STM



Markus Aapro & Xin Huang
25.2.2021

# Contents



Background and theory

- Principles of STM and STS
- Physics of surface states
- Measuring surface state dispersion with STM

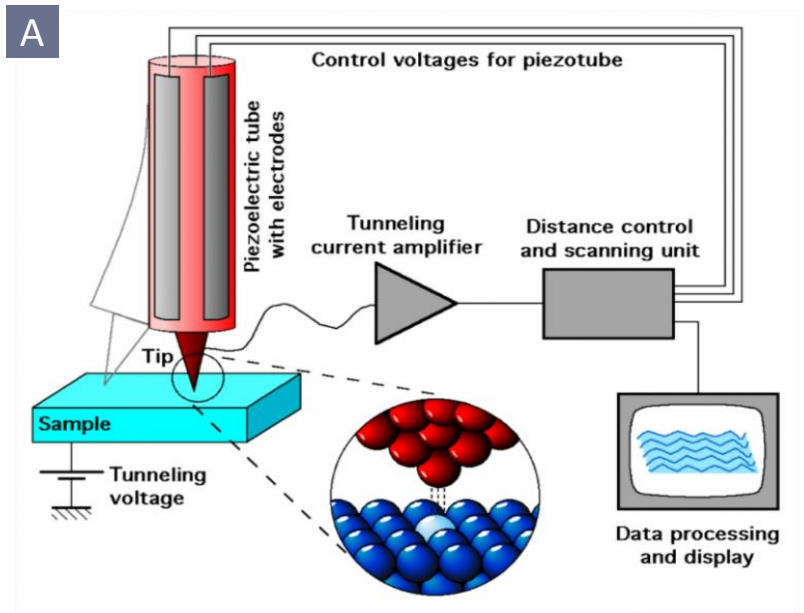
Experiment

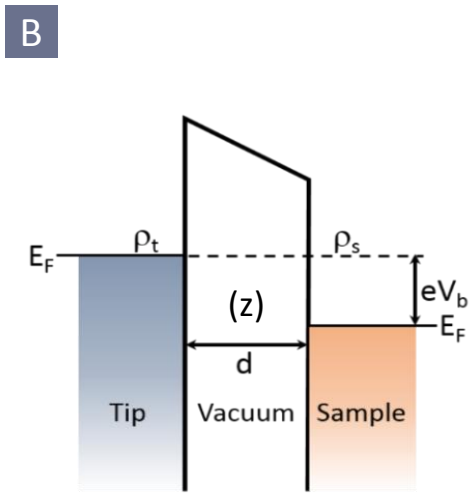
- Some necessary equipment
- Sample preparation
- Operating the STM

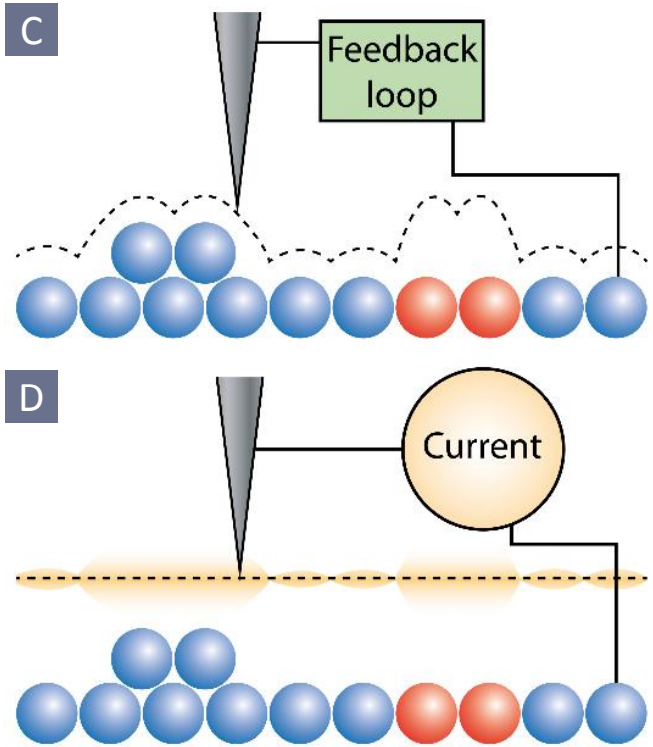
Data analysis

- Scan data: Gwyddion
- Point spectra: SpectraFox

# Scanning tunneling microscopy




Tunneling probability at a small bias voltage:

$$T := \frac{|\psi(z)|^2}{|\psi(0)|^2} = e^{-2\kappa z} = \exp\left(-2z\frac{\sqrt{2m\phi}}{\hbar}\right)$$

Tunneling current:

$$I(V_b) \propto \int_0^{V_b} \rho_t(E - eV)\rho_s(E)T(E,V,d)dV$$

c) Constant current
d) Constant height

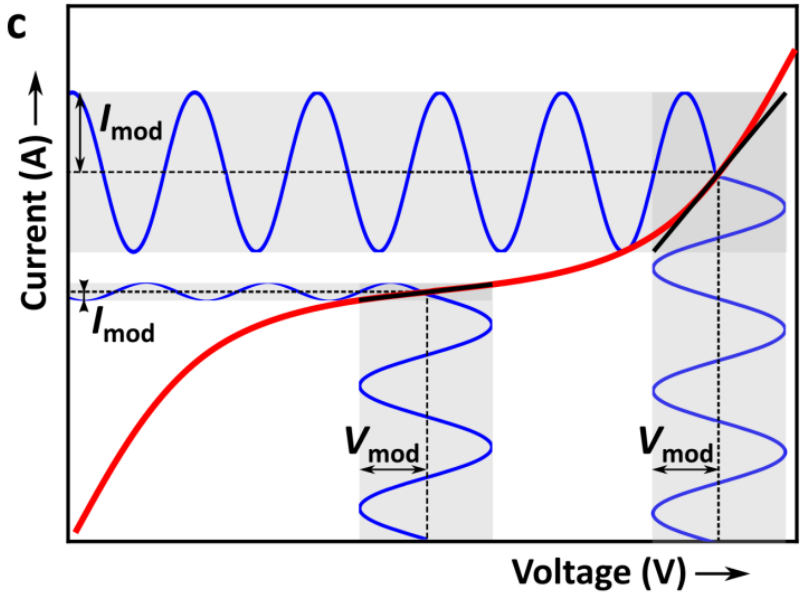
# dI/dV and the local density of states

$$I(V_b) \propto \int_0^{V_b} \rho_t(E - eV)\rho_s(E)T(E,V,d)dV$$

Assuming

- Constant tip DOS
- Low temperature
- Constant T (“small” bias V)

$$\Rightarrow \quad dI/dV_b \propto \rho_s(eV_b)$$



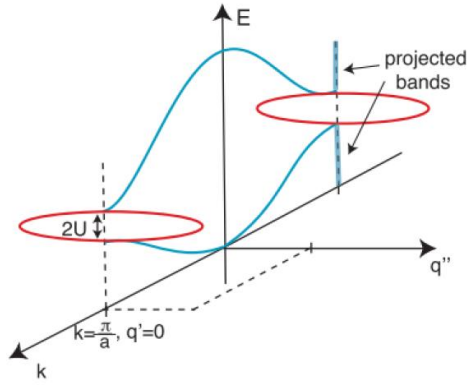

M. Slot, PhD thesis:
https://dspace.library.uu.nl/handle/1874/381147

Lock-in technique: measure dI/dV with voltage modulation

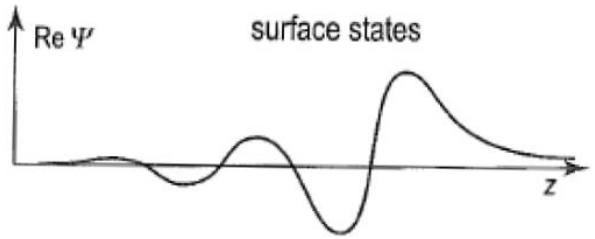
$$I(V_b + V_m \sin(\omega t)) \sim I(V_b) + \left.\frac{dI(V)}{dV}\right|_{V=V_b} \cdot V_m \sin(\omega t) + \cdots.$$

# Physics of surface states

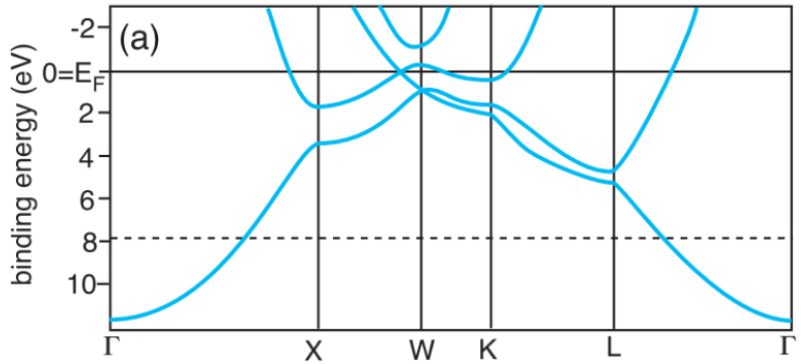
A




B




C

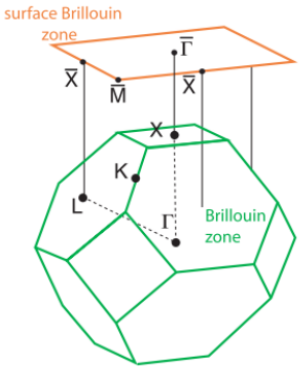



Bulk wavefunction: $\psi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})u_{\mathbf{k}}(\mathbf{r})$

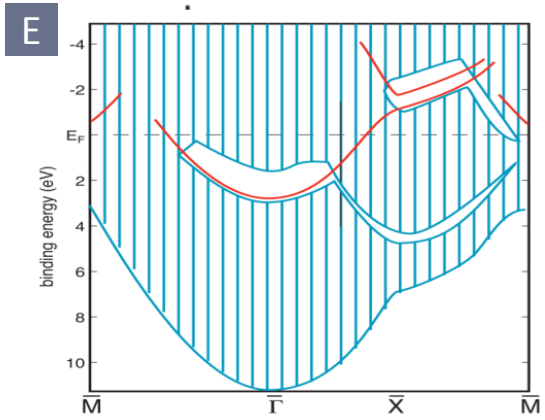
Generalized wavefunction: $\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}_\parallel}(\mathbf{r}_\parallel)e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel}e^{-\kappa r_\perp}$

κ is a complex wave vector perpendicular to the surface

D




E




True surface state is not degenerate with any bulk states
→ Surface states must lie in the projected band gap of the bulk electronic structure

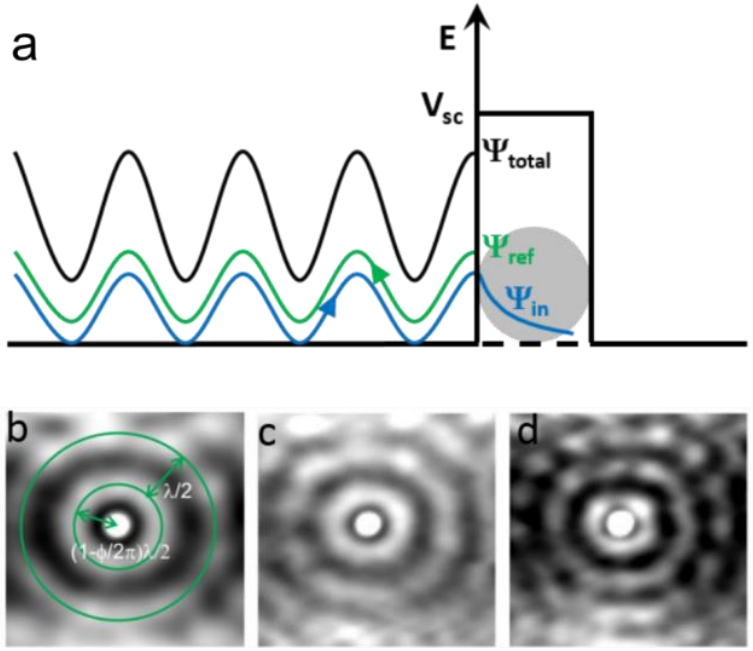
Brillouin zone and projected band structure of Al(111)

# Measuring surface states with STM/STS

Scattering from impurities causes interference
→ Standing waves (Friedel oscillations)

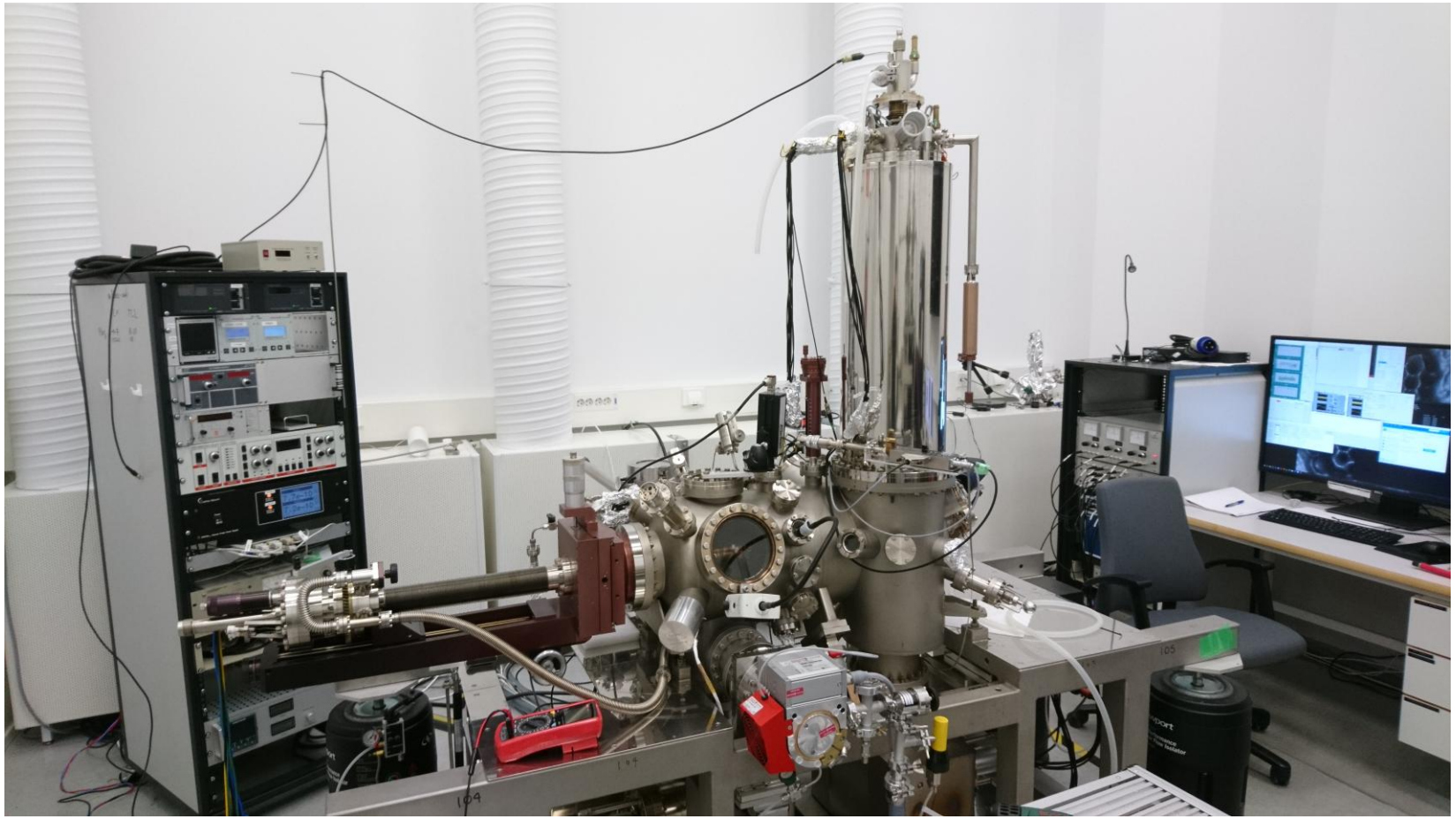
Measure dI/dV while scanning at constant height
→ Surface state wavelength at a given bias (energy)

Repeat at several bias voltages
→ Surface state dispersion




(a) One-dimensional schematic of scattering of an electron wavefunction due to a scatterer shown by a grey circle representing potential barrier of height $V_{sc}$. The wavefunctions have been shifted vertically up for clarity. (b-d) $dI/dV_b$ maps recorded in the vicinity of a Cu adatom on Cu(111) surface at (b) -300 mV, (c) -200 mV, and (d) -100 mV. Antinodes of the standing waves are shown by green circles in (b).

# In the lab…



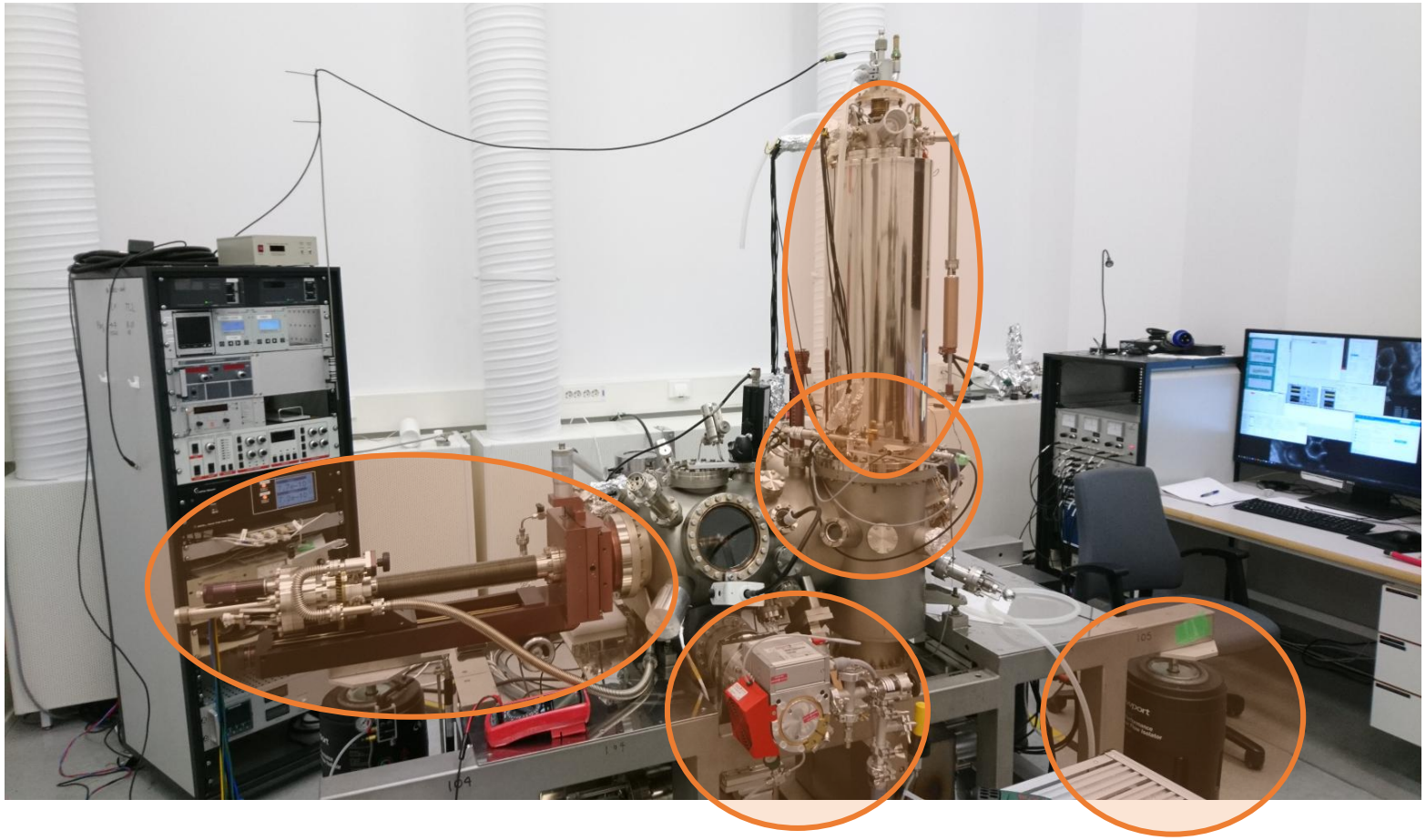
Low-temperature scanning tunnelling microscope (LT-STM)

Manufacturer: Createc

Temperature: 5 K

Pressure: UHV (< $1x10^{-10}$ mbar)

# Equipment and their purpose



Low temperature
- Liquid nitrogen and liquid helium cryostat

Sample preparation
- Evaporators, sputter gun, manipulator, heater

Ultra high vacuum
- Ion pumps, turbo pumps, scroll pumps

Mechanical isolation
- 10 m concrete block on base rock, air legs, springs, eddy current damping

Signal processing
- Preamplifier, filtering, DSP

# Sample preparation

Clean the Cu(111) crystal
- Ar/Ne Sputtering
- Annealing (~600 °C)
- Repeat 2-3 times for best results

Insert into STM, cool down to 4 K

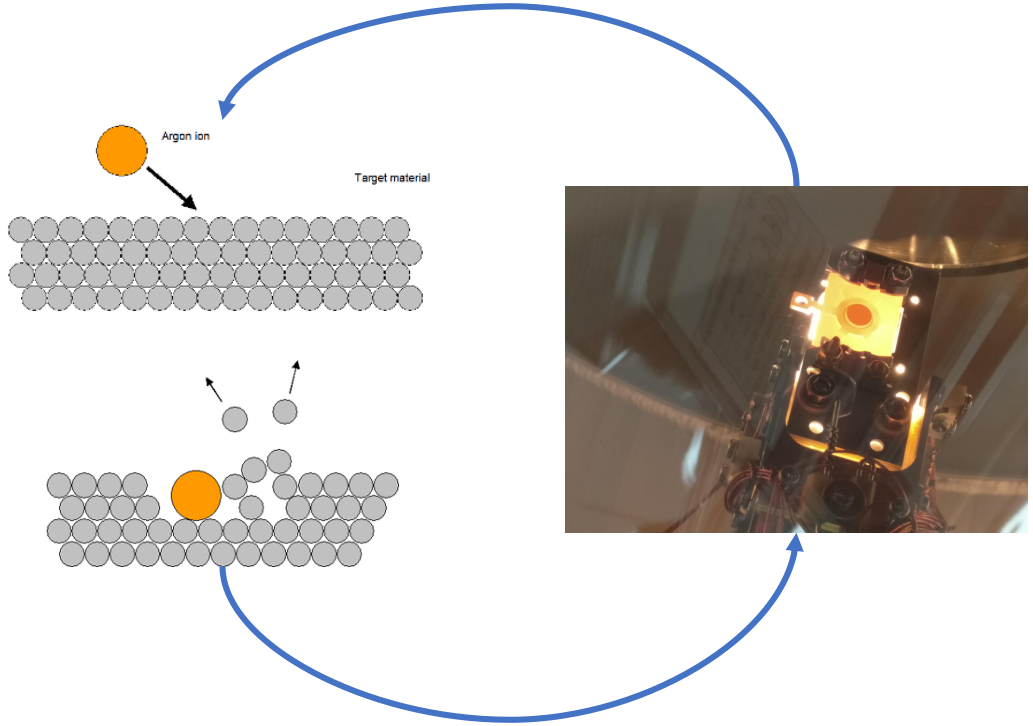
Leak CO into STM chamber, open shutter into STM

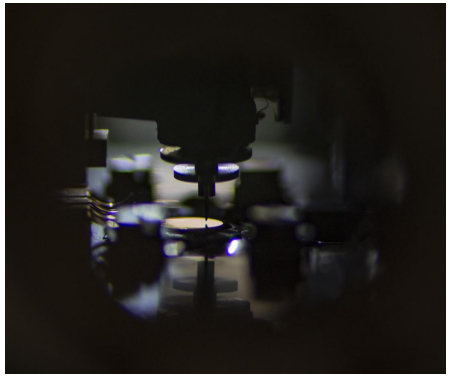
Pump excess CO out of the vacuum

Wait for sample to cool down (from ~20 K)

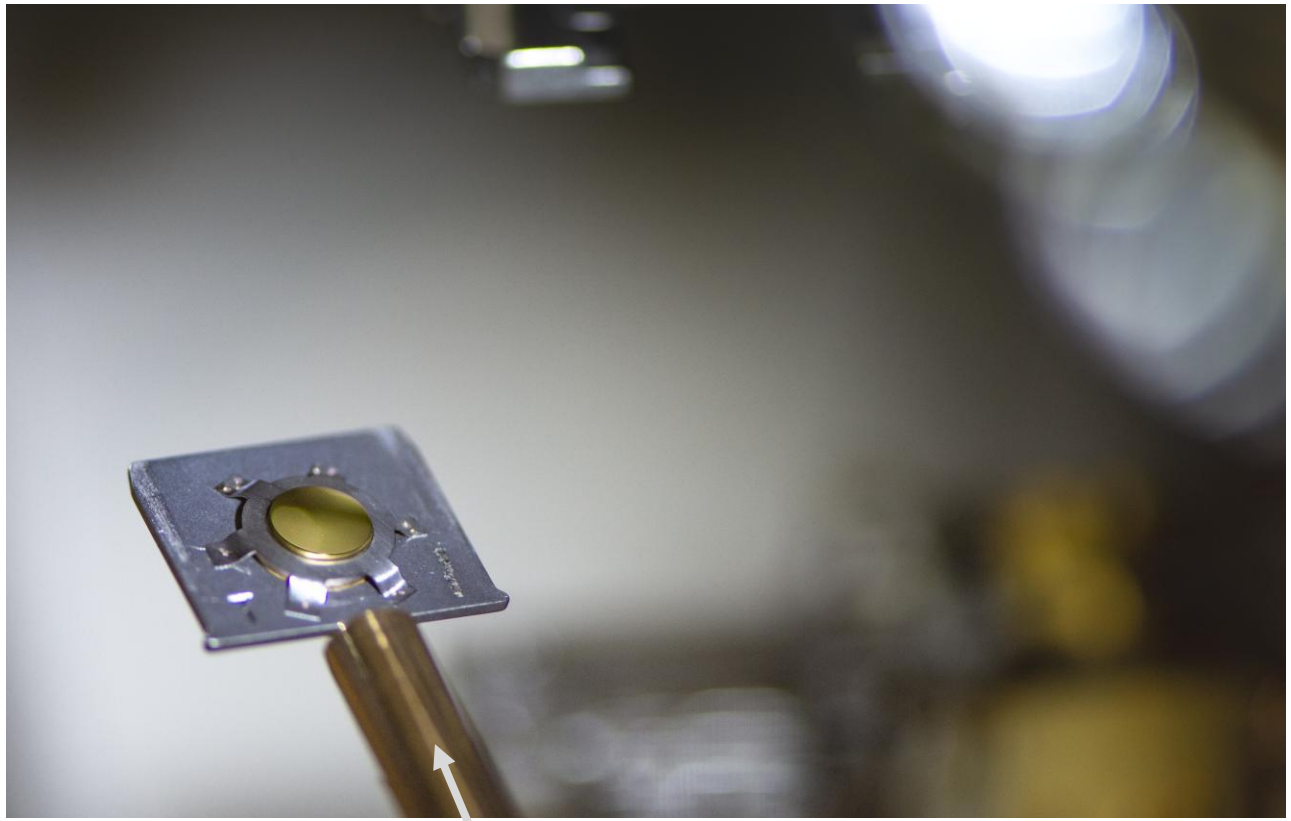
Approach with the STM tip

Start scanning!



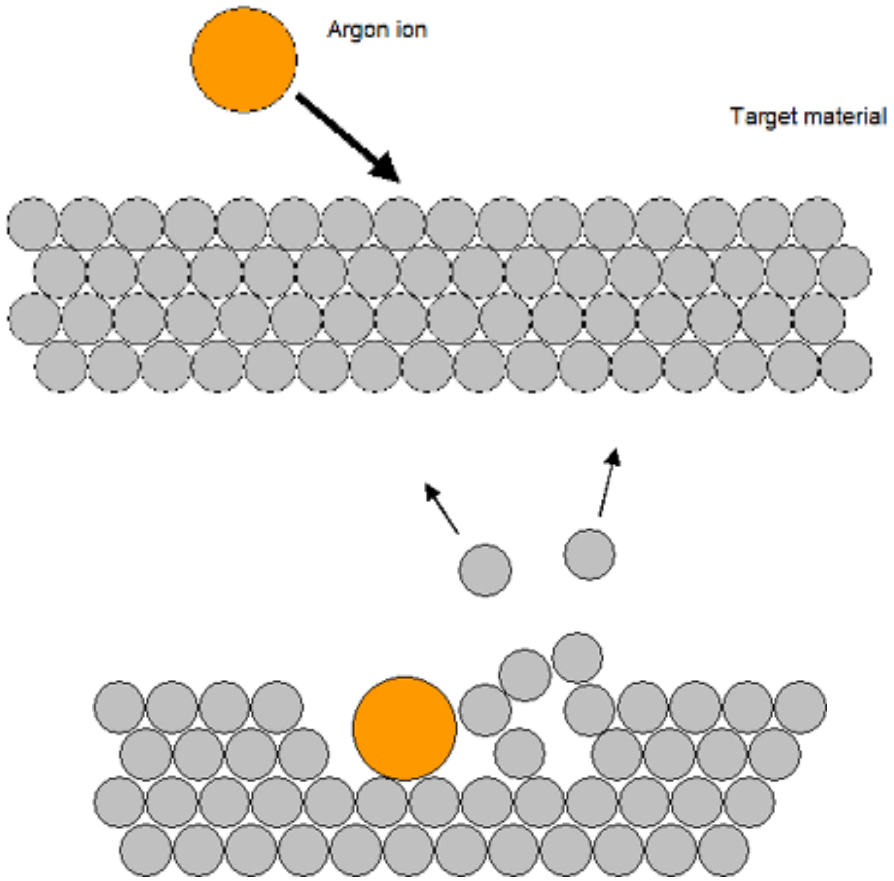
# Moving samples in UHV



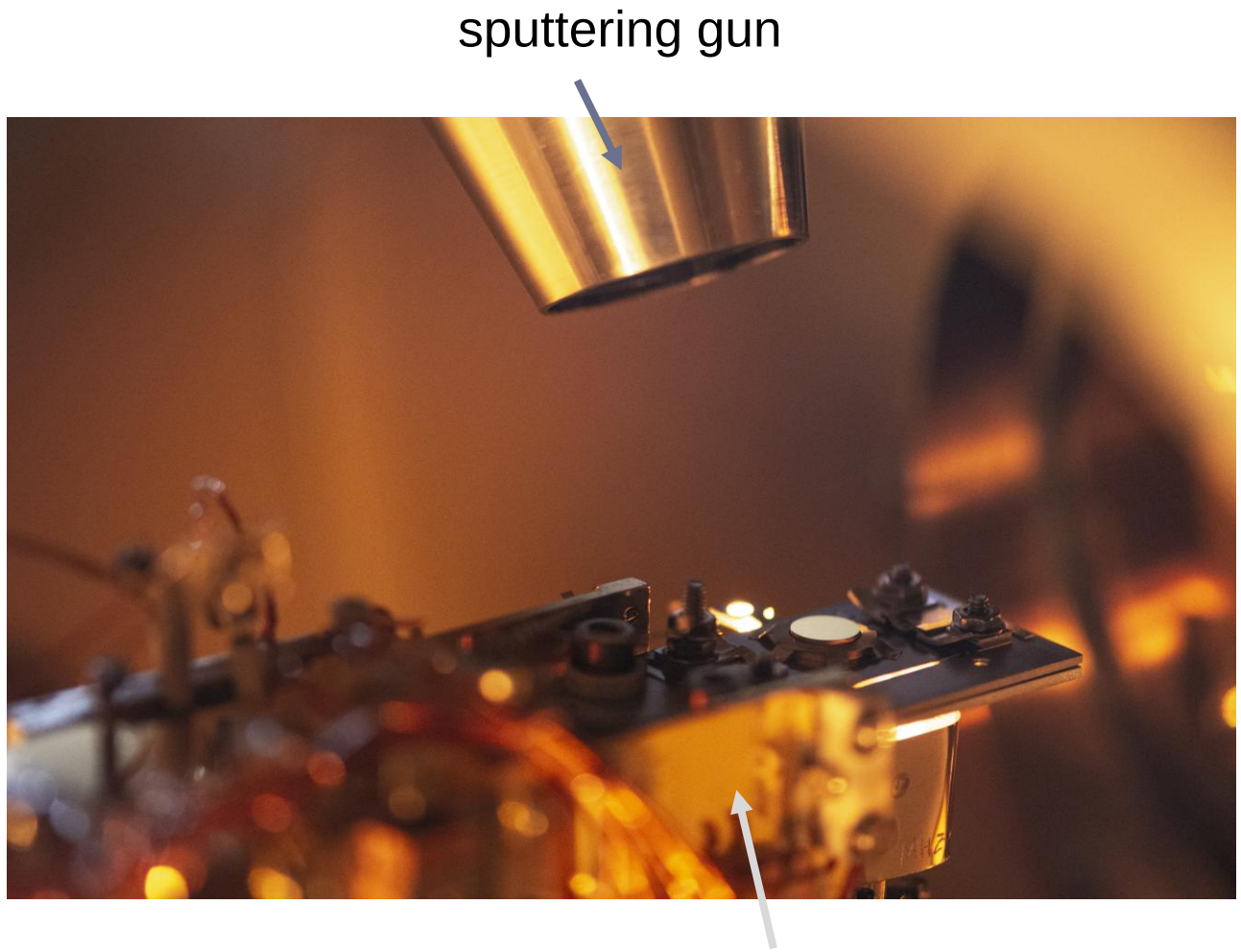
Transfer rod

Sample mounted on a sample plate (W, Mo, Ta etc)

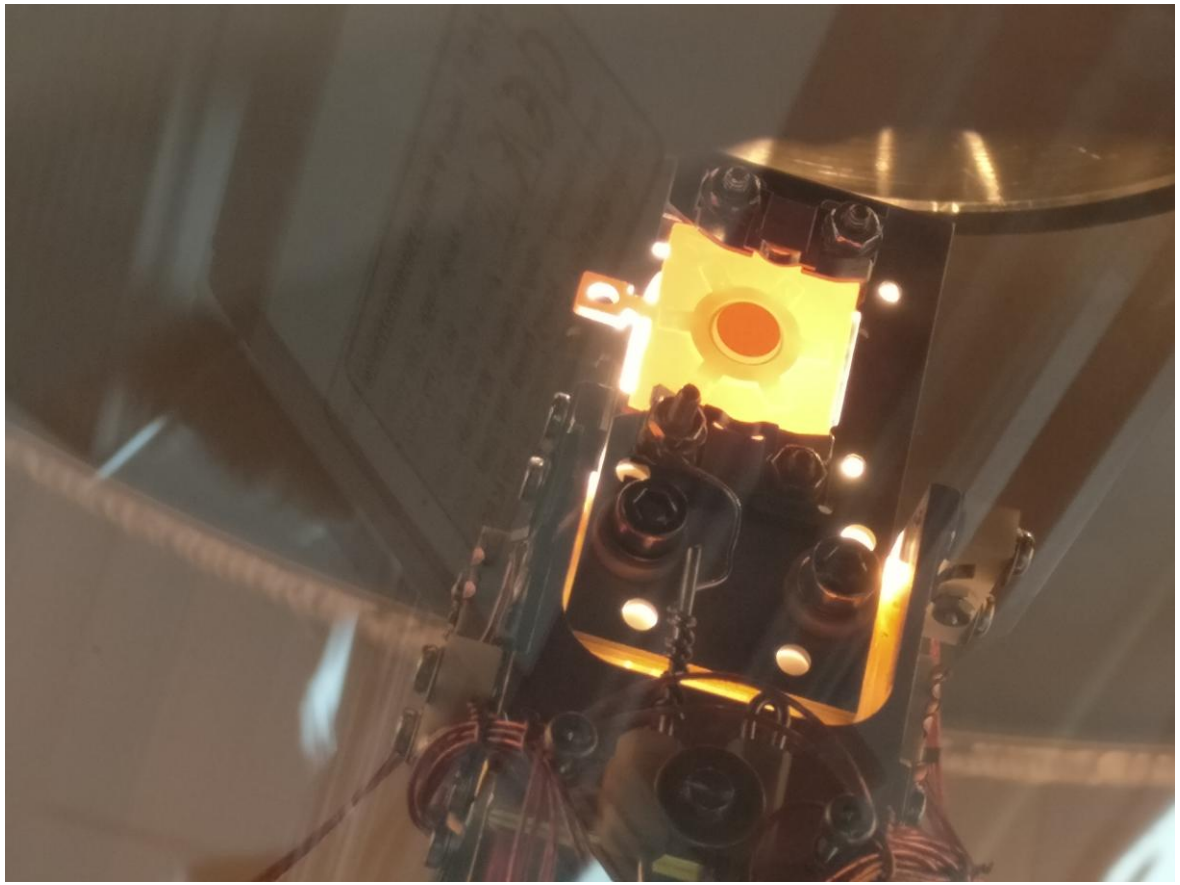
# Sample preparation – sputtering




Sputtering removes layers of material from the surface

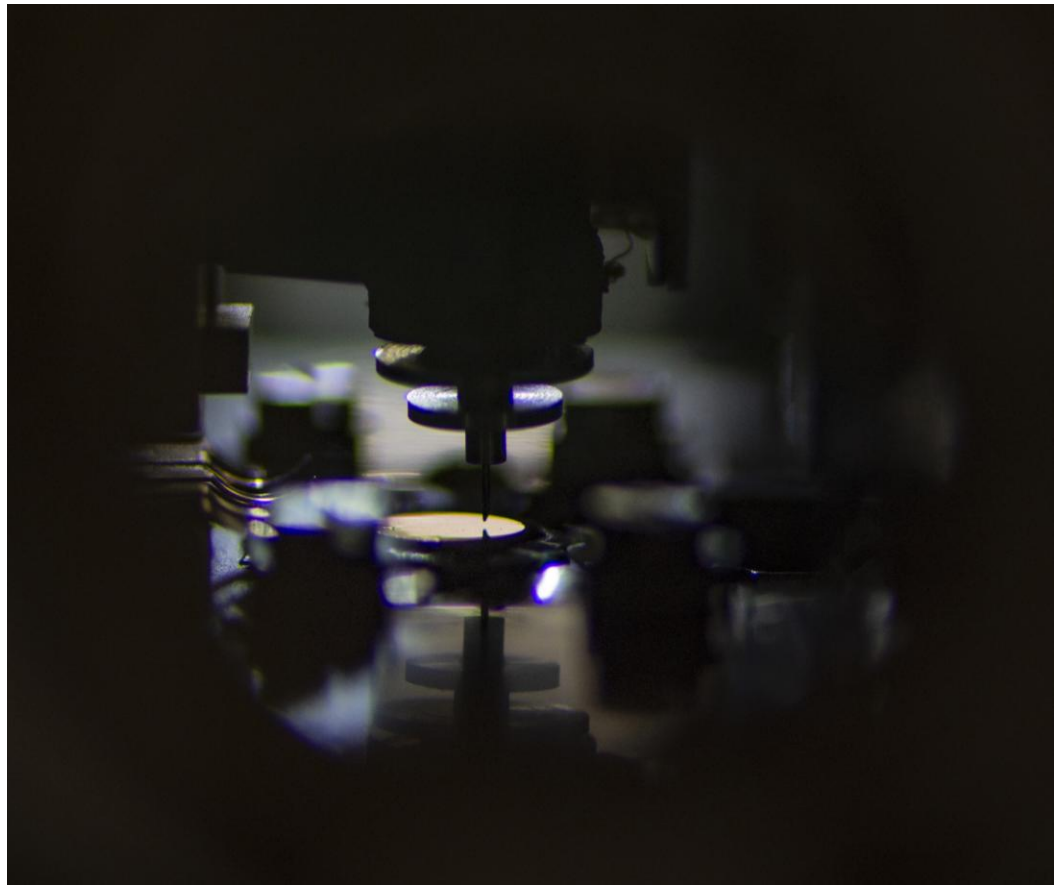


# Sample preparation – annealing

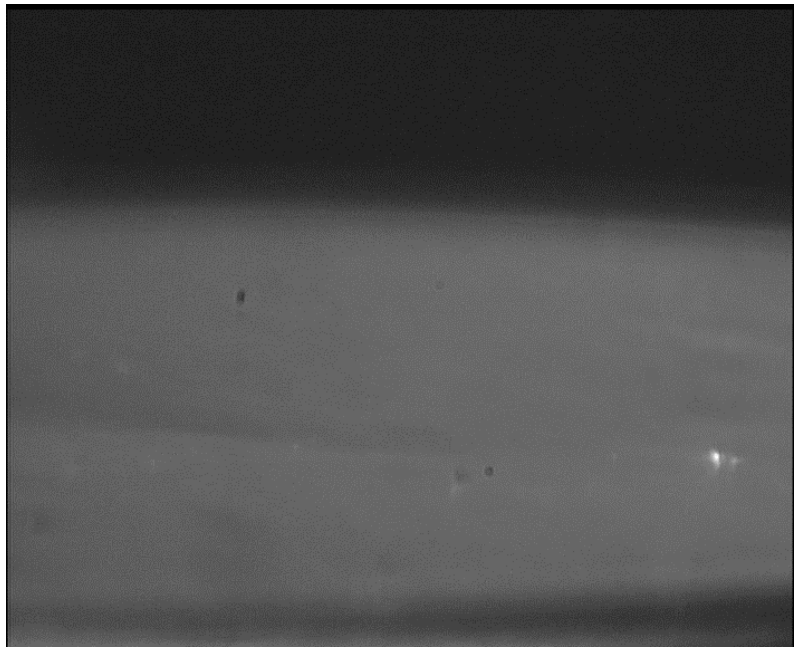


Annealing produces a flat surface

# Approaching the surface



STM tip above the Cu(111) sample



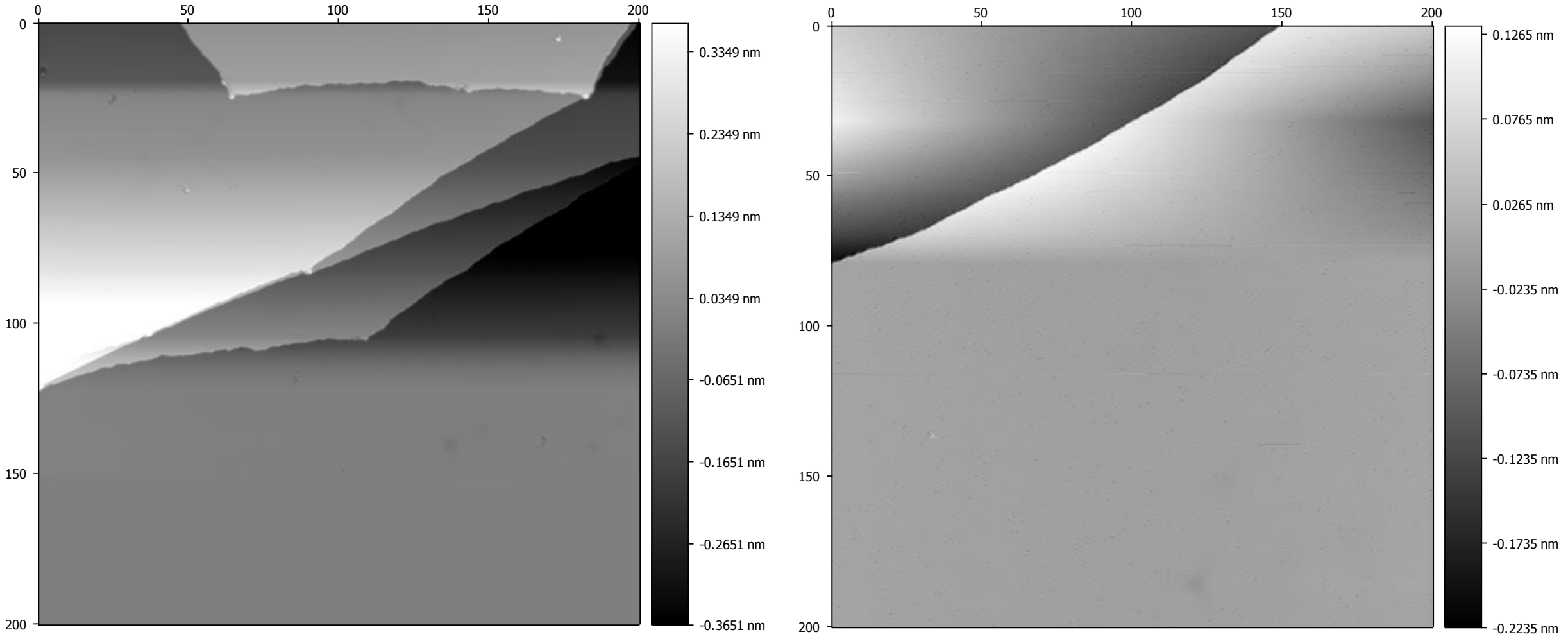
STM tip approaching surface

Mirror reflection gives the operator an estimate during coarse approach.

1. After the sample and STM head are cooled to ~4 K, the tip is brought close to the sample surface (Coarse approach)

2. An automatic approach routine is used to bring the tip into tunneling distance (Fine approach)

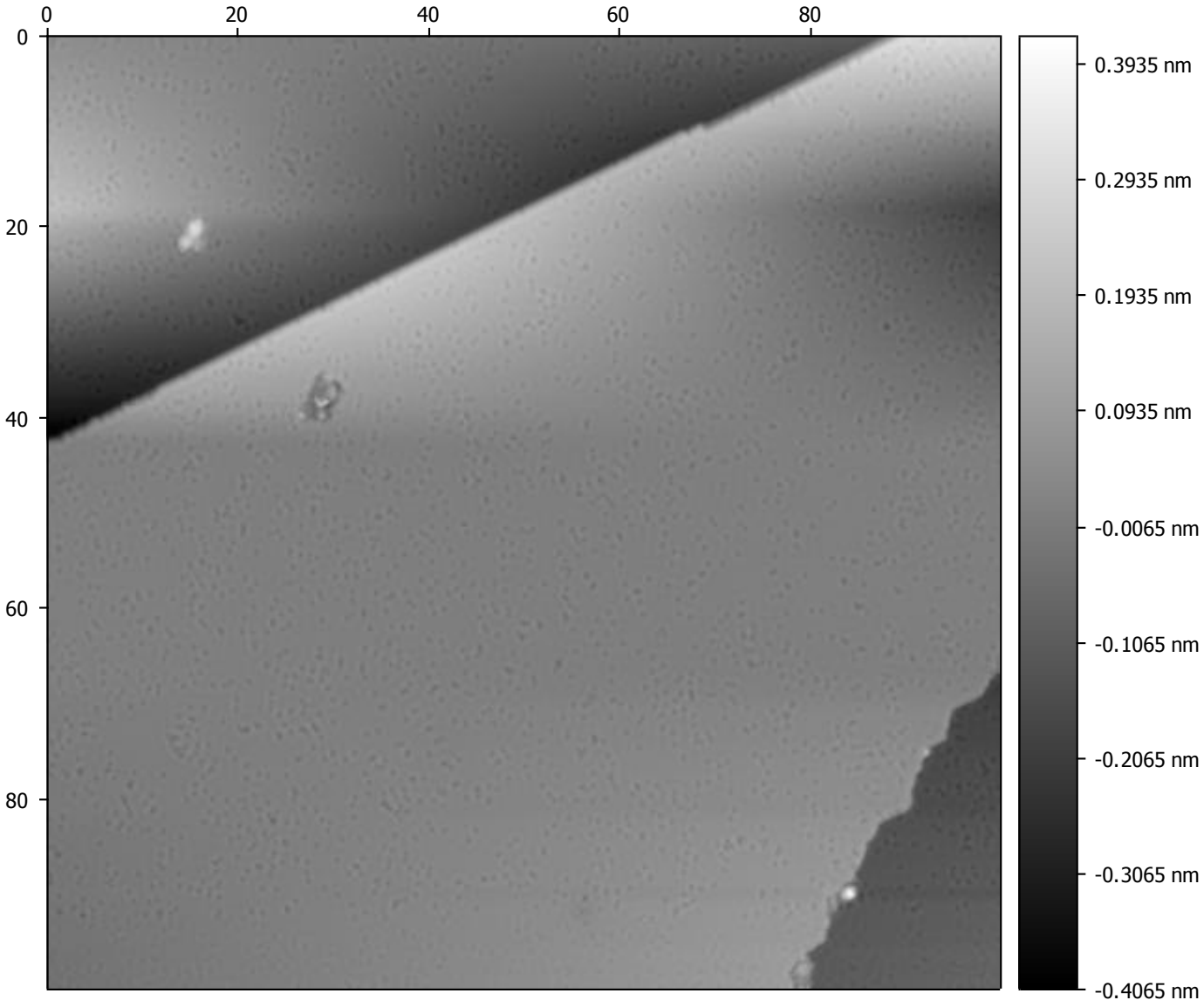
# Scan! Scan! Scan!

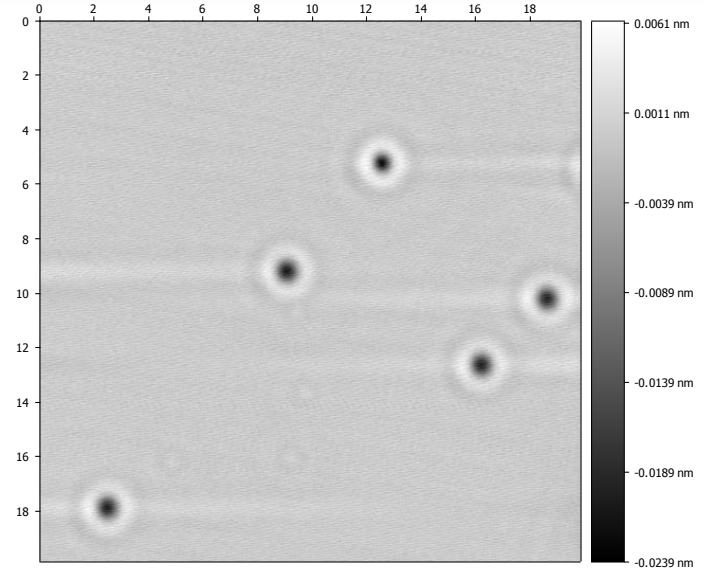


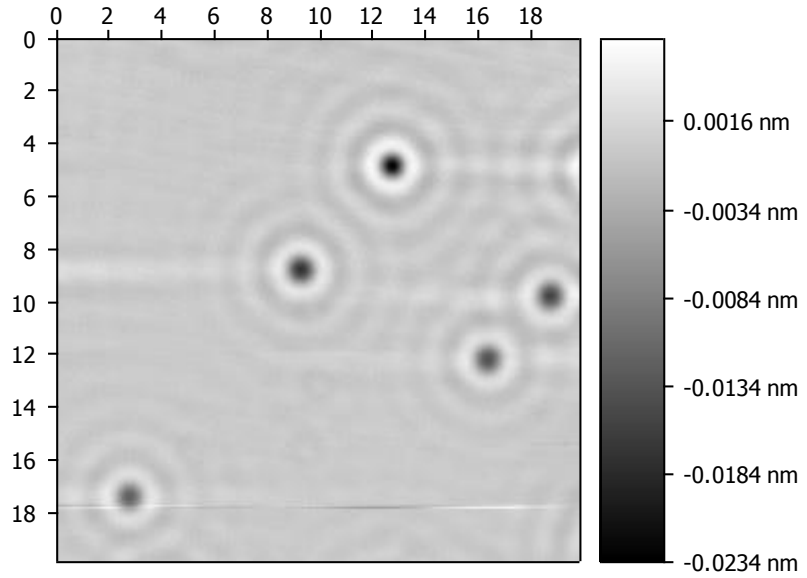

STM images of a Cu(111) single crystal

# Depositing carbon monoxide (CO)

# After CO deposition

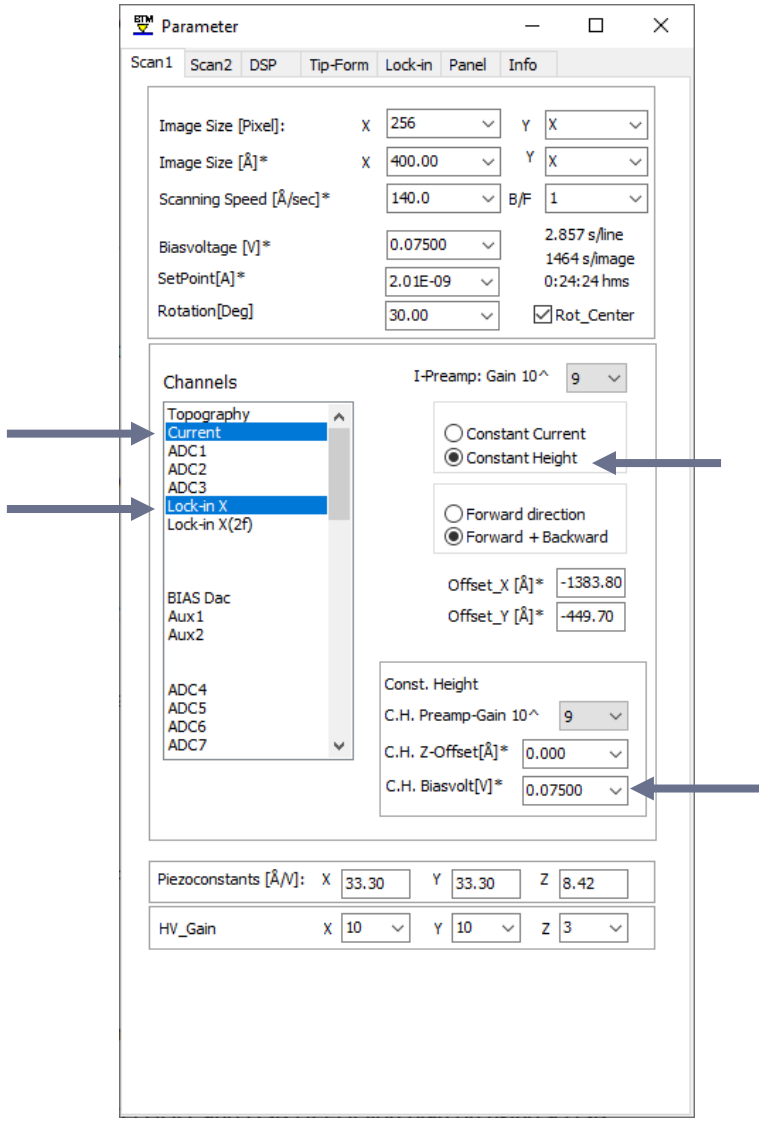


# Collecting dI/dV maps

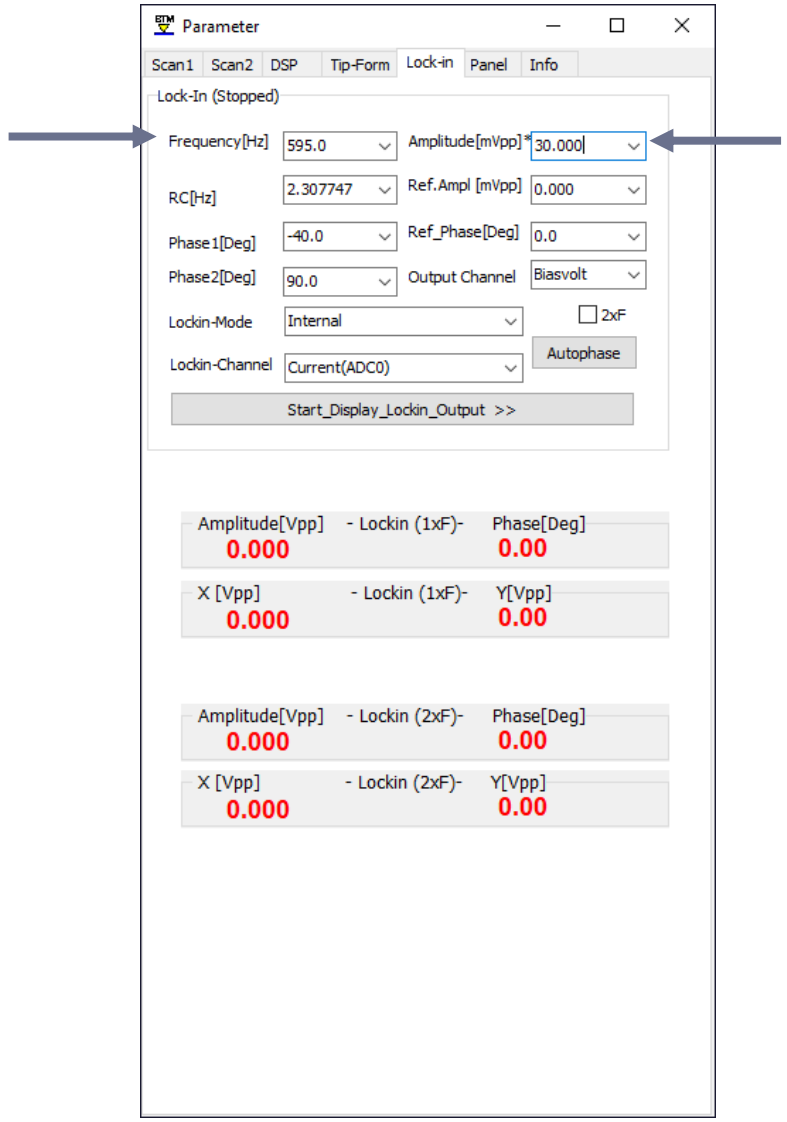
- Createc STMAFM software
- Collect the following data channels
  - Current
  - Lock-in X (dI/dV)
- Constant Height mode

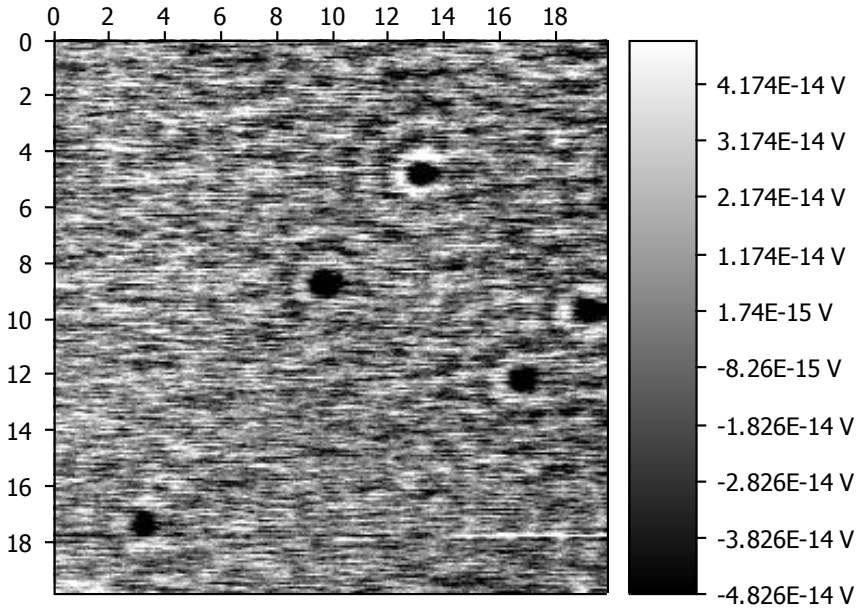


# Collecting dI/dV maps

Lock-in parameters

- Frequency: 595 Hz
- Amplitude: 30 mVpp



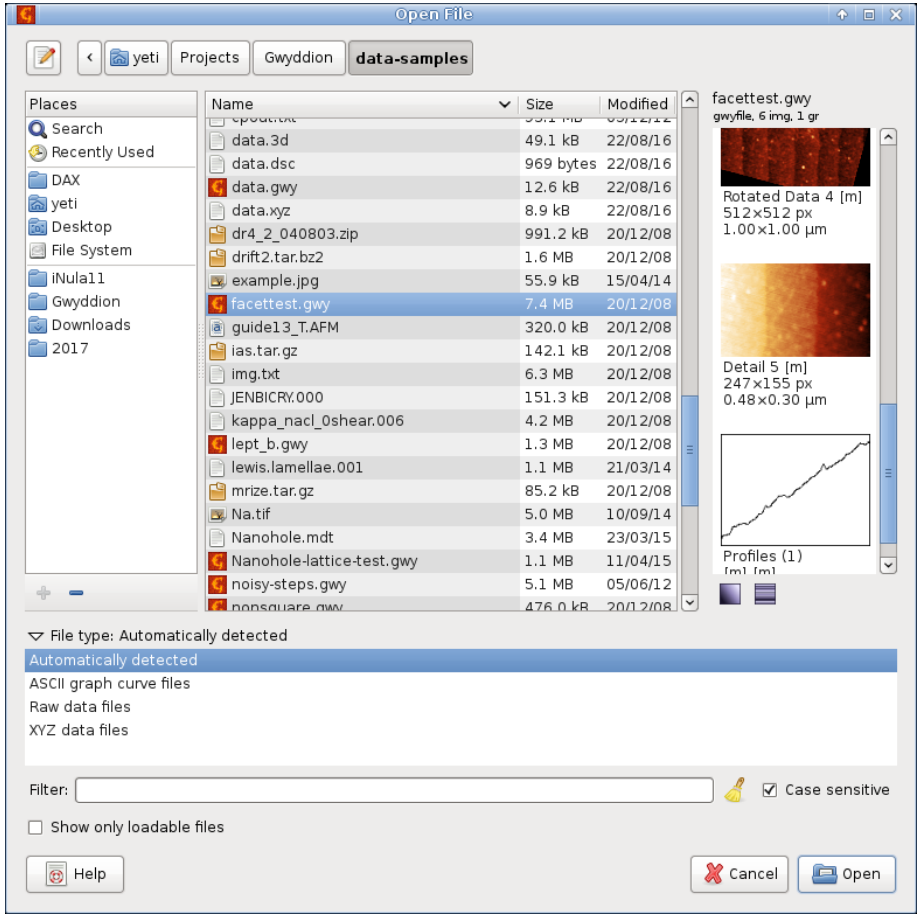

dI/dV map of CO molecules on Cu(111)

# Analysis

- Gwyddion: STM/AFM image analysis
- SpectraFox: Spectra analysis
- Python/MATLAB: Use for fitting, image generation as needed.
  - See the Matlab import functions in MyCourses

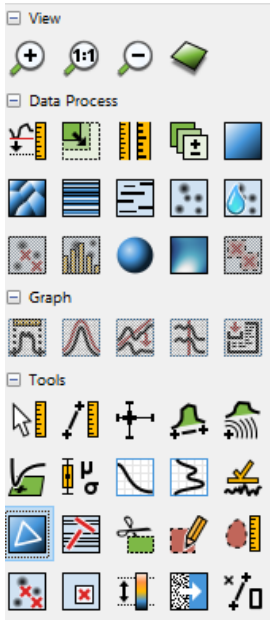
# Gwyddion: Opening .DAT files

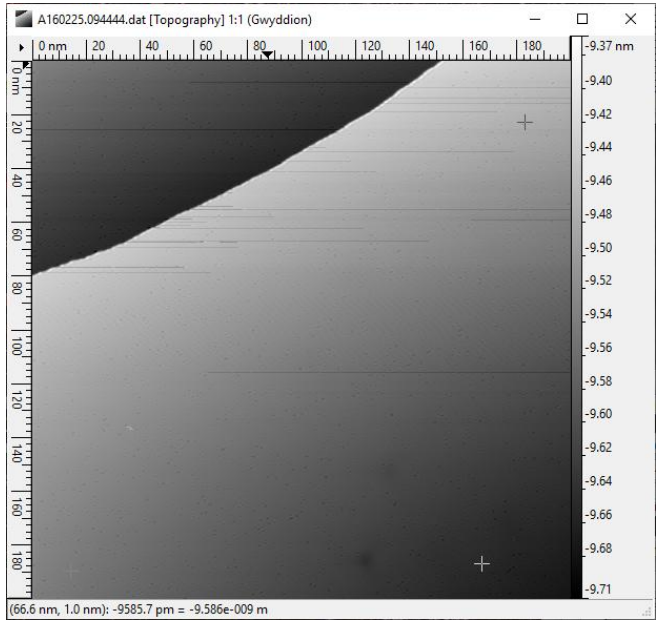
- Compatible files will be shown
- Preview of different channels shown on the right side

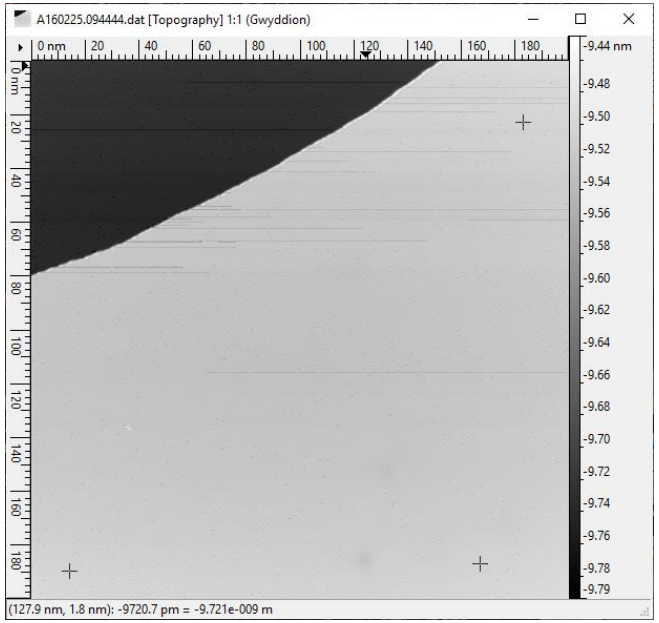


# Gwyddion: Finding the step height

1. Level the data (fit plane through 3 points)
2. Take a profile of an edge
3. Extract profile
4. Measure the height



# Gwyddion: Finding the step height

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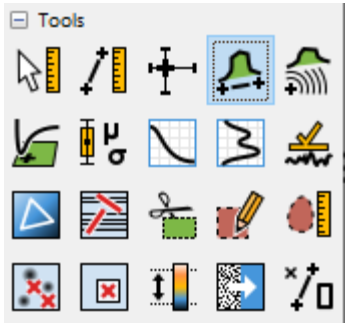
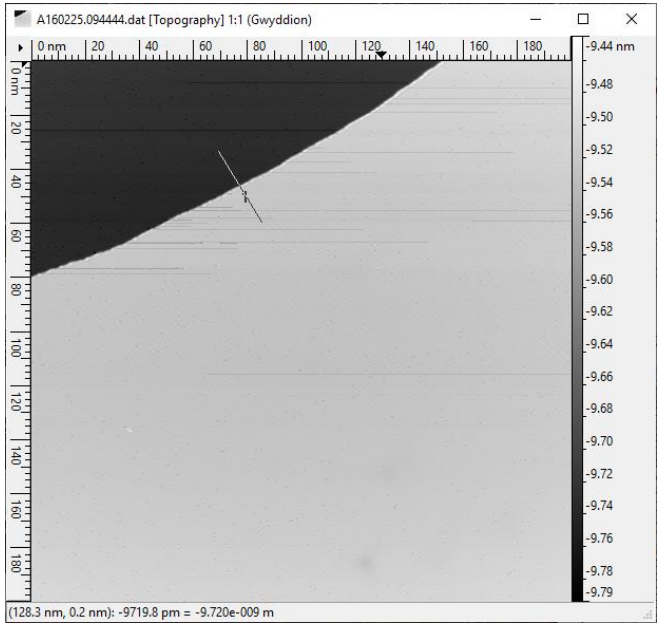
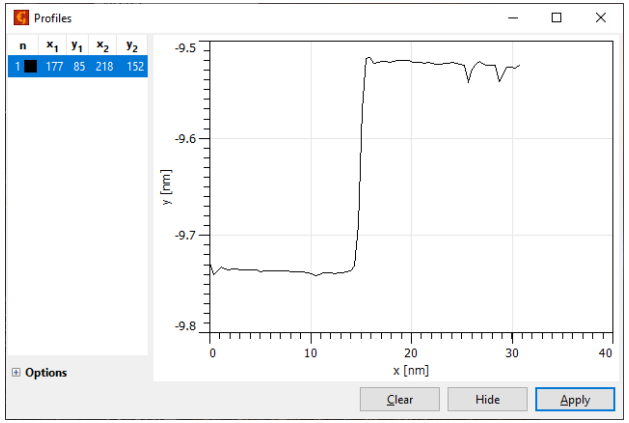
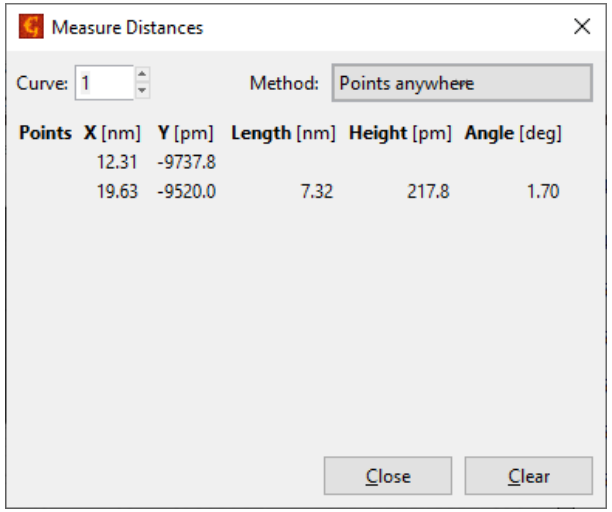
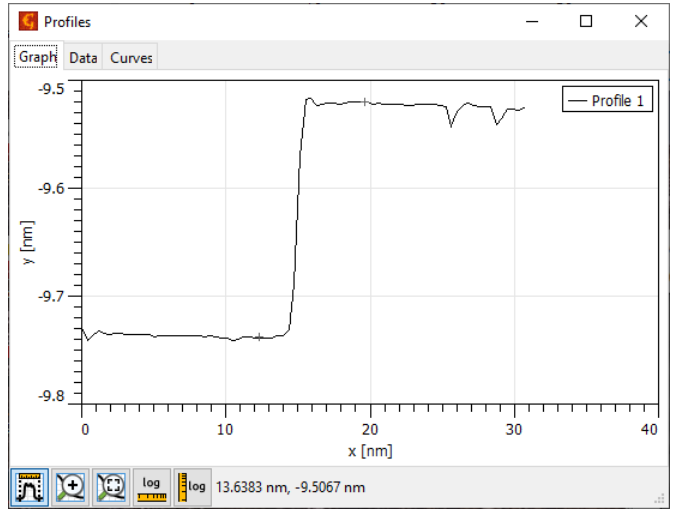
4. Measure the height



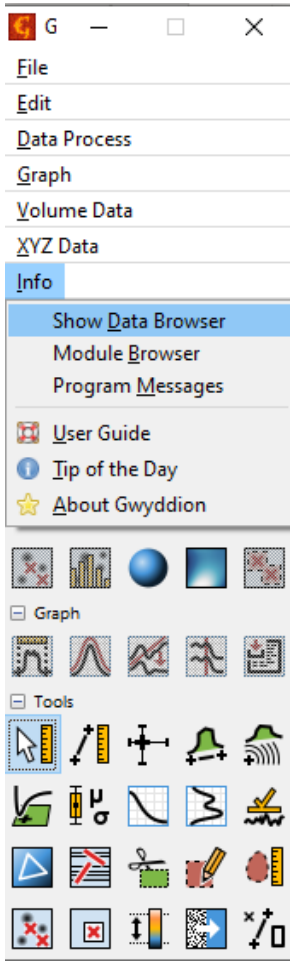



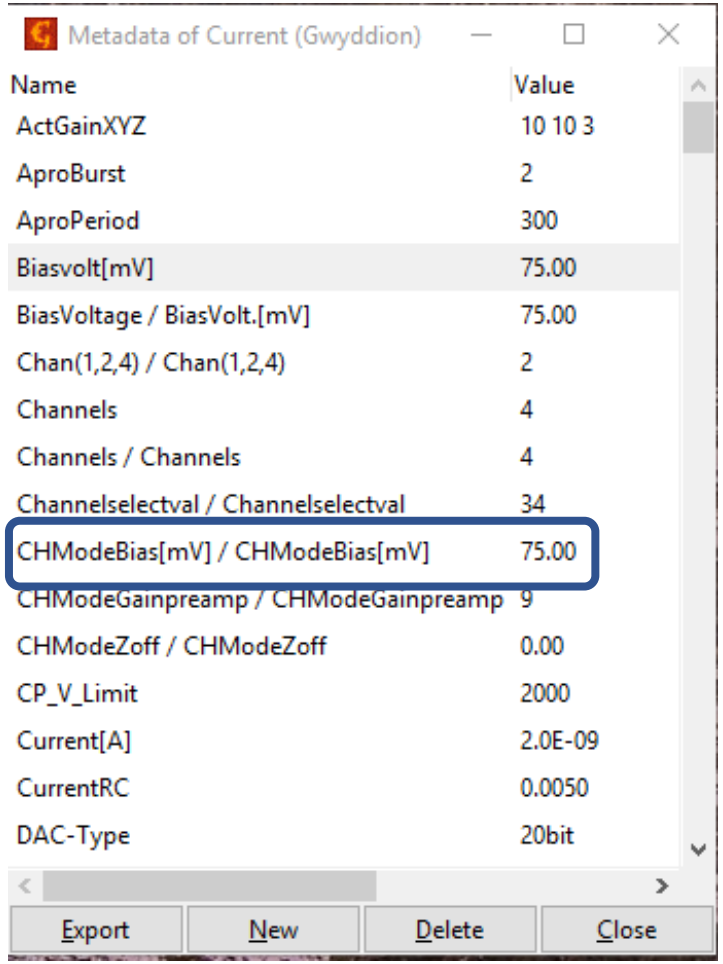



# Gwyddion: CH maps, dI/dV channel & metadata

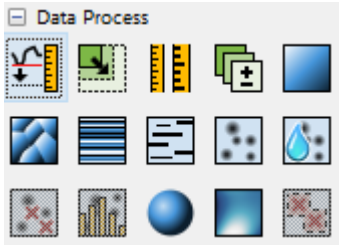
- Extract the bias voltage
  - In the Current channel window, right-click and choose Metadata browser (or press Shift+Ctrl+B)
  - Find the line CHBiasvolt[mV]
- Select the dI/dV channel (Voltage) from Data Browser

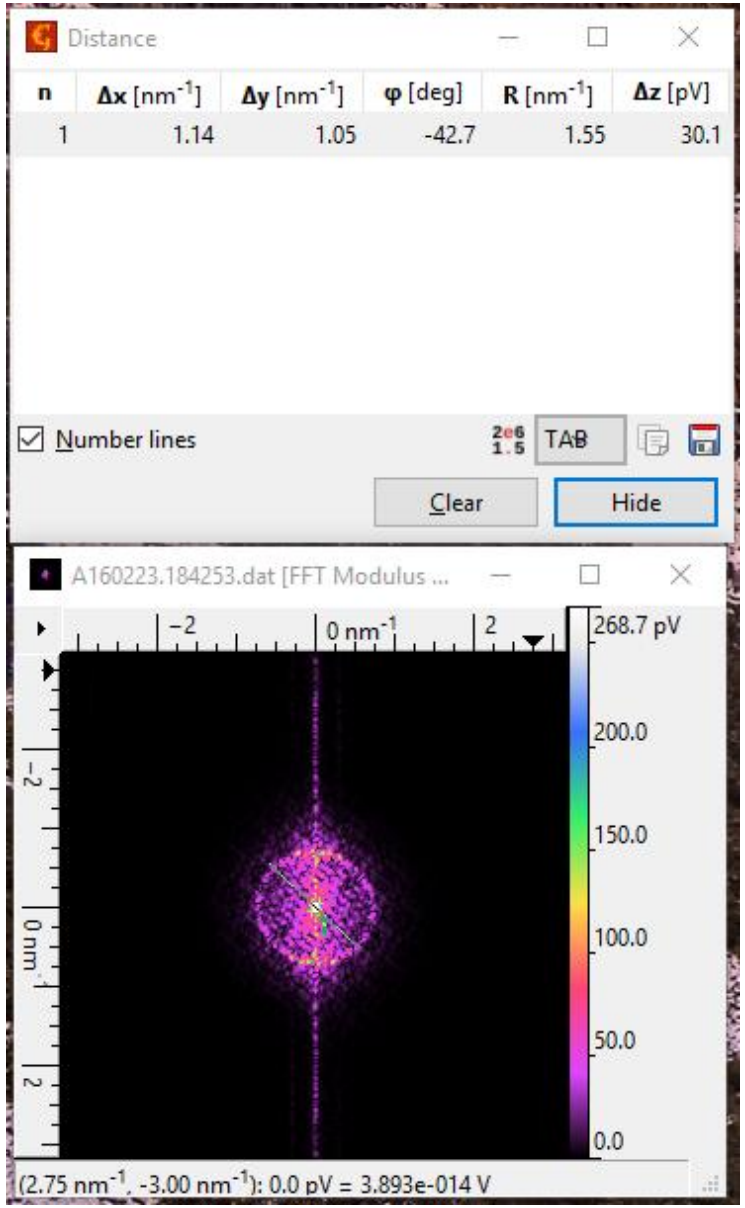


# Gwyddion: 2D FFT

1. Correct the plane and shift minimum data value to zero
2. Go to Data Process -> Integral Transforms -> 2D FFT
3. Output type: Modulus
   Windowing type: Hann
4. Click OK
5. Measure the radius of the interference ring with Distance tool

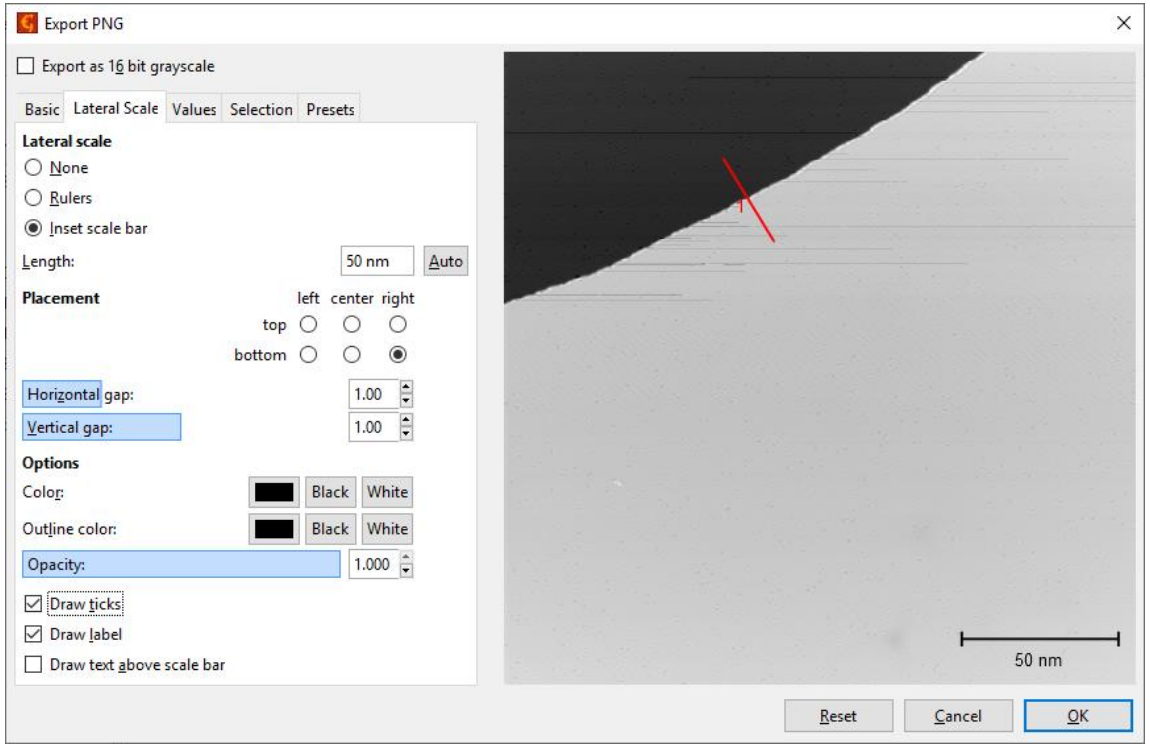


# Gwyddion: Saving figures with a scale bar

To add a scale bar:

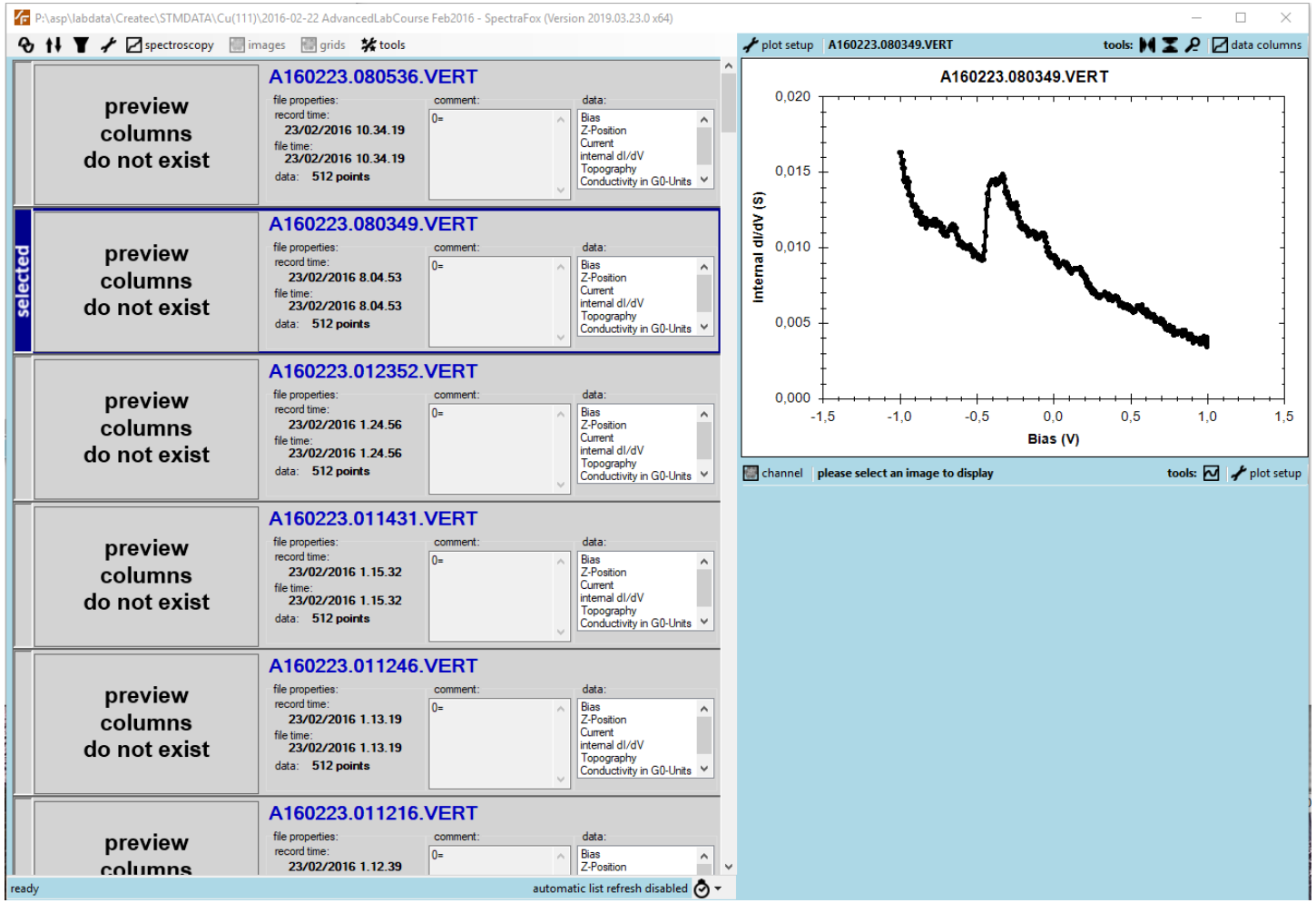
1. File -> Save As (Ctrl+Shift+S)
2. Select desired image format (PNG)
3. Select Lateral Scale tab
4. Select Inset scale bar



# Opening .VERT files: SpectraFox

- Navigate to data folder
- Open data-browser
- Set X axis to Bias (V)
- Set Y axis to dI/dV

- Matlab/Python can also interpret the data



# Opening .VERT files: Matlab/Python

- VERT files can be opened and data extracted directly (plain text file)
- Extract values from half of the values in the 1st and 4th columns (Bias and dI/dV)
- See the Matlab functions provided in MyCourses

```
DATA
      512   17556    6776      4099
0   1.00000E+03 0.00000E-01 2.63415E+04 1.79326E+02 -7.88280E+04
1   1.00000E+03 0.00000E-01 2.63370E+04 1.78216E+02 -7.88280E+04
2   1.00000E+03 0.00000E-01 2.63536E+04 2.08133E+02 -7.88280E+04
3   1.00000E+03 0.00000E-01 2.63207E+04 1.87683E+02 -7.88280E+04
4   1.00000E+03 0.00000E-01 2.63271E+04 1.81475E+02 -7.88280E+04
5   1.00000E+03 0.00000E-01 2.63196E+04 2.05141E+02 -7.88280E+04
6   1.00000E+03 0.00000E-01 2.63338E+04 1.94402E+02 -7.88280E+04
7   1.00000E+03 0.00000E-01 2.63074E+04 1.85772E+02 -7.88280E+04
8   1.00000E+03 0.00000E-01 2.63403E+04 1.97803E+02 -7.88280E+04
9   1.00000E+03 0.00000E-01 2.63342E+04 1.97415E+02 -7.88280E+04
10  9.91870E+02 0.00000E-01 2.62106E+04 1.90854E+02 -7.88280E+04
11  9.83740E+02 0.00000E-01 2.60753E+04 1.88742E+02 -7.88280E+04
12  9.75610E+02 0.00000E-01 2.59483E+04 1.96126E+02 -7.88280E+04
13  9.67480E+02 0.00000E-01 2.57805E+04 1.92850E+02 -7.88280E+04
14  9.59350E+02 0.00000E-01 2.56711E+04 1.88022E+02 -7.88280E+04
15  9.51219E+02 0.00000E-01 2.55300E+04 1.90216E+02 -7.88280E+04
16  9.43089E+02 0.00000E-01 2.53997E+04 2.06071E+02 -7.88280E+04
17  9.34959E+02 0.00000E-01 2.52615E+04 2.07086E+02 -7.88280E+04
18  9.26829E+02 0.00000E-01 2.51175E+04 2.03832E+02 -7.88280E+04
19  9.18699E+02 0.00000E-01 2.49872E+04 1.99228E+02 -7.88280E+04
20  9.10569E+02 0.00000E-01 2.48578E+04 1.90690E+02 -7.88280E+04
21  9.02439E+02 0.00000E-01 2.47103E+04 2.11172E+02 -7.88280E+04
22  8.94309E+02 0.00000E-01 2.45580E+04 2.22477E+02 -7.88280E+04
23  8.86179E+02 0.00000E-01 2.44066E+04 2.05354E+02 -7.88280E+04
24  8.78049E+02 0.00000E-01 2.42682E+04 2.05116E+02 -7.88280E+04
25  8.69919E+02 0.00000E-01 2.41051E+04 2.18084E+02 -7.88280E+04
26  8.61789E+02 0.00000E-01 2.39884E+04 2.21585E+02 -7.88280E+04
27  8.53659E+02 0.00000E-01 2.38274E+04 2.18405E+02 -7.88280E+04
28  8.45528E+02 0.00000E-01 2.36744E+04 2.22057E+02 -7.88280E+04
29  8.37398E+02 0.00000E-01 2.35155E+04 2.17125E+02 -7.88280E+04
30  8.29268E+02 0.00000E-01 2.33743E+04 2.30953E+02 -7.88280E+04
31  8.21138E+02 0.00000E-01 2.32198E+04 2.27481E+02 -7.88280E+04
32  8.13008E+02 0.00000E-01 2.30792E+04 2.25197E+02 -7.88280E+04
33  8.04878E+02 0.00000E-01 2.29022E+04 2.24107E+02 -7.88280E+04
34  7.96748E+02 0.00000E-01 2.27393E+04 2.26558E+02 -7.88280E+04
35  7.88618E+02 0.00000E-01 2.25864E+04 2.18590E+02 -7.88280E+04
36  7.80488E+02 0.00000E-01 2.24310E+04 2.19394E+02 -7.88280E+04
37  7.72358E+02 0.00000E-01 2.22712E+04 2.31070E+02 -7.88280E+04
38  7.64228E+02 0.00000E-01 2.21067E+04 2.34160E+02 -7.88280E+04
39  7.56098E+02 0.00000E-01 2.19513E+04 2.38792E+02 -7.88280E+04
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41  7.39837E+02 0.00000E-01 2.16270E+04 2.37734E+02 -7.88280E+04
42  7.31707E+02 0.00000E-01 2.14724E+04 2.38525E+02 -7.88280E+04
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44  7.15447E+02 0.00000E-01 2.11308E+04 2.55173E+02 -7.88280E+04
45  7.07317E+02 0.00000E-01 2.09696E+04 2.58421E+02 -7.88280E+04
46  6.99187E+02 0.00000E-01 2.07802E+04 2.60134E+02 -7.88280E+04
47  6.91057E+02 0.00000E-01 2.06175E+04 2.64488E+02 -7.88280E+04
48  6.82927E+02 0.00000E-01 2.04280E+04 2.65904E+02 -7.88280E+04
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51  6.58537E+02 0.00000E-01 1.98848E+04 2.66228E+02 -7.88280E+04
52  6.50406E+02 0.00000E-01 1.97036E+04 2.76613E+02 -7.88280E+04
53  6.42276E+02 0.00000E-01 1.95094E+04 2.84891E+02 -7.88280E+04
54  6.34146E+02 0.00000E-01 1.93074E+04 2.81789E+02 -7.88280E+04
```

# Reference materials

Software

- Gwyddion: http://gwyddion.net/
- SpectraFox: https://spectrafox.com/
- Anaconda (Python): https://www.anaconda.com/
- MATLAB: https://www.mathworks.com/
  (University provides at https://download.aalto.fi)

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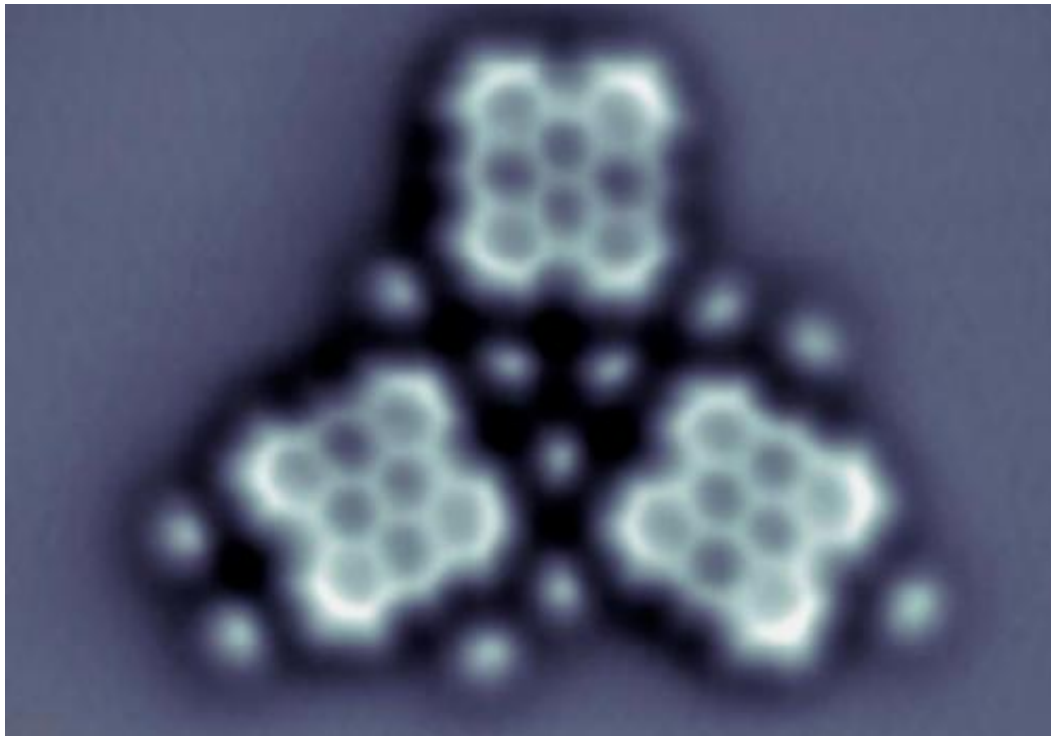

Thanks!