PHYS-E0411 – Exercise 5

Surface state dispersion of Cu(111) with STM



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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 currentd) Constant height

dl/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)

$$\implies dI/dV_b \propto \rho_s(eV_b)$$

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

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



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

Physics of surface states



True surface state is not degenerate with any bulk states

 \rightarrow 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) d/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



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

Low temperature

 Liquid nitrogen and liquid helium cryostat



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





Sample manipulator

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)



CO leak valve

Shutter/door (inside)

After CO deposition



Collecting dI/dV maps

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

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Sc	an1	Scan2	DSP	Tip-For	m	Lock-in	Panel	Info				1
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Collecting dl/dV maps

Lock-in parameters

- Frequency: 595 Hz
- Amplitude: 30 mVpp

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Scan1 Scan2 DSP Tip-Form Lock-in Panel Info	
Lock-In (Stopped)	
Frequency[Hz] 595.0 ~ Amplitude[mVpp]*30.000 ~	
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Start_Display_Lockin_Output >>	6 - 2.174E-14 V
	8 1.174E-14 V
Amplitude[Vpp] - Lockin (1xF)- Phase[Deg]	10 1.74E-15 V
X [Vpp] - Lockin (1xF)- Y[Vpp]	128.26E-15 V
0.000 0.00	14
	162.826E-14 V
Amplitude[Vpp] - Lockin (2xF)- Phase[Deg] 0.000 0.00	183.826E-14 V
X [Vpp] - Lockin (2xF)- Y[Vpp] 0.000 0.00	-4.826E-14 V
	dl/dV map of CO molecules on Cu(111)



- 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

Image: Search Size Modified Image: Search Size Modified Facettest.gwy Image: Search Gata.3d 49.1 k8 22/08/16 Image: Search Gata.3d 49.1 k8 22/08/16 Image: Data Gata.gwy 12.6 k8 20/12/08 Image: Data Gata.gwy 7.4 M8 20/12/08 Image: Data Gata.gwy 1.3 M8 20/12/08 Image: Data Gata.gwy 1.3 M8 20/12/08 Image: Data Gata.gwy 1.1 M8 11/04/15 Image: Data Gata.gwy 1.1 M8 11/04/15 Image: Data Gata.gwy <td< th=""><th>Ç</th><th></th><th>Open File</th><th></th><th></th><th></th><th></th><th></th><th></th></td<>	Ç		Open File						
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Gwyddion: Finding the step height

- 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

Tools

×

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



180

(128.3 nm, 0.2 nm): -9719.8 pm = -9.720e-009 m



— Profile 1

X



-9.48

-9.50

-9.52

-9.54

-9.56

-9.58

9.60

9.62 9 64 9.66

9.68

-9.70

9 72

9.74 -9.76

-9.78

-9.79

Gwyddion: CH maps, dl/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 dl/dV channel (Voltage) from Data Browser

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Gwyddion: 2D FFT

- 1. Correct the plane and shift minimum data value to zero
- 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

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	50 nm

Opening .VERT files: SpectraFox

- Navigate to data folder
- Open data-browser
- Set X axis to Bias (V)
- Set Y axis to dl/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 dl/dV)
- See the Matlab functions provided in MyCourses

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561	3	1.00000E+03	0.00000E-01	2.63207E+04	1.87683E+02	-7.88280E+04
562	4	1.00000E+03	0.00000E-01	2.63271E+04	1.81475E+02	-7.88280E+04
563	5	1.00000E+03	0.00000E-01	2.63196E+04	2.05141E+02	-7.88280E+04
564	6	1.00000E+03	0.00000E-01	2.63338E+04	1.94402E+02	-7.88280E+04
565	7	1.00000E+03	0.00000E-01	2.63074E+04	1.85772E+02	-7.88280E+04
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568	10	9.91870E+02	0.00000E-01	2.62106E+04	1.90854E+02	-7.88280E+04
569	11	9.83740E+02	0.00000E-01	2.60753E+04	1.88742E+02	-7.88280E+04
570	12	9.75610E+02	0.00000E-01	2.59483E+04	1.96126E+02	-7.88280E+04
571	13	9.67480E+02	0.00000E-01	2.57805E+04	1.92850E+02	-7.88280E+04
572	14	9.59350E+02	0.00000E-01	2.56711E+04	1.88022E+02	-7.88280E+04
573	15	9.51219E+02	0.00000E-01	2.55300E+04	1.90216E+02	-7.88280E+04
574	16	9.43089E+02	0.00000E-01	2.53997E+04	2.06071E+02	-7.88280E+04
575	17	9.34959E+02	0.00000E-01	2.52615E+04	2.07086E+02	-7.88280E+04
576	18	9.26829E+02	0.00000E-01	2.51175E+04	2.03832E+02	-7.88280E+04
577	19	9.18699E+02	0.00000E-01	2.49872E+04	1.99228E+02	-7.88280E+04
578	20	9.10569E+02	0.00000E-01	2.48578E+04	1.90690E+02	-7.88280E+04
579	21	9.02439E+02	0.00000E-01	2.47103E+04	2.11172E+02	-7.88280E+04
580	22	8.94309E+02	0.00000E-01	2.45580E+04	2.22477E+02	-7.88280E+04
581	23	8.86179E+02	0.00000E-01	2.44066E+04	2.05354E+02	-7.88280E+04
582	24	8.78049E+02	0.00000E-01	2.42682E+04	2.05116E+02	-7.88280E+04
583	25	8.69919E+02	0.00000E-01	2.41051E+04	2.18084E+02	-7.88280E+04
584	26	8.61789E+02	0.00000E-01	2.39884E+04	2.21585E+02	-7.88280E+04
585	27	8.53659E+02	0.00000E-01	2.38274E+04	2.18405E+02	-7.88280E+04
586	28	8.45528E+02	0.00000E-01	2.36744E+04	2.22057E+02	-7.88280E+04
587	29	8.37398E+02	0.00000E-01	2.35155E+04	2.17125E+02	-7.88280E+04
588	30	8.29268E+02	0.00000E-01	2.33743E+04	2.30953E+02	-7.88280E+04
589	31	8.21138E+02	0.00000E-01	2.32198E+04	2.27481E+02	-7.88280E+04
590	32	8.13008E+02	0.00000E-01	2.30792E+04	2.25197E+02	-7.88280E+04
591	33	8.048/8E+02	0.00000E-01	2.29022E+04	2.2410/E+02	-7.88280E+04
592	34	7.967482+02	0.00000E-01	2.2/393E+04	2.26556E+02	-7.88280E+04
593	35	7.886186+02	0.00000E-01	2.258642+04	2.18590E+02	-7.88280E+04
594	27	7.0040000+02	0.00000E-01	2.243102+04	2.193946+02	-7.00200E+04
596	39	7 642288+02	0.00000E-01	2 210678+04	2.310/0E+02	-7.88280E±04
597	30	7 560988402	0.00000E-01	2 19513F±04	2 38792F±02	-7.88280F+04
598	40	7.479678±02	0.00000E-01	2.177708±04	2.416988±02	-7.88280F±04
599	41	7 39837F+02	0.00000E-01	2 16270F±04	2 37734F±02	-7 88280F+04
600	42	7.31707F+02	0.00000E-01	2.14724F+04	2.38525F+02	-7.88280F+04
601	43	7.23577E+02	0.00000E-01	2.13109E±04	2.46466E±02	-7.88280E+04
602	44	7.15447E+02	0.00000E-01	2.11308E+04	2.55173E+02	-7.88280E+04
603	45	7.07317E+02	0.00000E-01	2.09696E+04	2.58421E+02	-7.88280E+04
604	46	6.99187E+02	0.00000E-01	2.07802E+04	2.60134E+02	-7.88280E+04
605	47	6.91057E+02	0.00000E-01	2.06175E+04	2.64488E+02	-7.88280E+04
606	48	6.82927E+02	0.00000E-01	2.04280E+04	2.65904E+02	-7.88280E+04
607	49	6.74797E+02	0.00000E-01	2.02528E+04	2.73722E+02	-7.88280E+04
608	50	6.66667E+02	0.00000E-01	2.00519E+04	2.66485E+02	-7.88280E+04
609	51	6.58537E+02	0.00000E-01	1.98848E+04	2.66228E+02	-7.88280E+04
610	52	6.50406E+02	0.00000E-01	1.97036E+04	2.76613E+02	-7.88280E+04
611	53	6.42276E+02	0.00000E-01	1.95094E+04	2.84891E+02	-7.88280E+04
612	54	6.34146E+02	0.00000E-01	1.93074E+04	2.81789E+02	-7.88280E+04

Reference materials

Software

- Gwyddion:
- SpectraFox:
- Anaconda (Python):
- MATLAB:

http://gwyddion.net/

https://spectrafox.com/

https://www.anaconda.com/

<u>https://www.mathworks.com/</u> (University provides at <u>https://download.aalto.fi</u>)

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Thanks!