Using the 2D Graphite Model to understand high resolution STM images of Graphite (HOPG)

Extract of the Experiment P2532000 "Atomic resolution of the graphite surface by STM"

Following the detailed instruction given in the experiments description of P2532000, you should be able

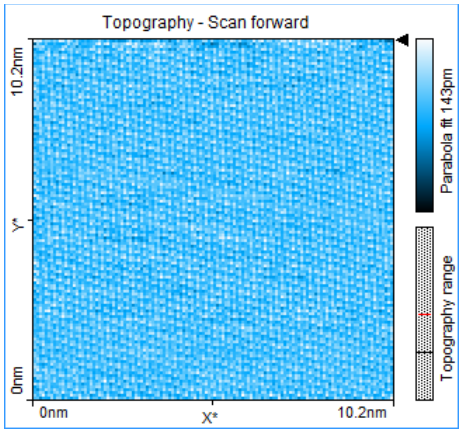

Fig. 1: Image size: 10 nm, Time/Line: 0.03 s, Set point: 1.2 nA, P-gain: 1200, I-gain: 1500.

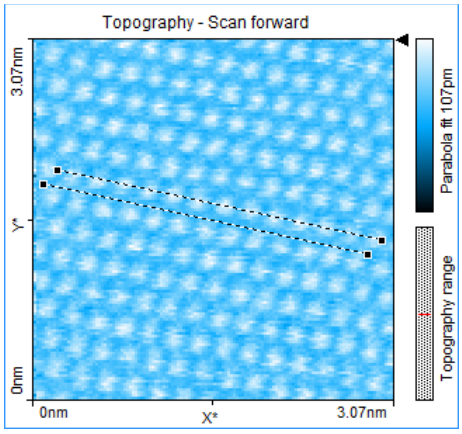

Fig. 2a: Image size: 3 nm, Time/Line: 0.03 s, Set point: 1.2 nA, P-gain: 1300, I-gain: 850. Distance between lines: d=138 pm

to observe atomic arrangements like those shown in the pictures.

The imaged data corresponds to a topographic representation of the LDOS (near the Fermi edge) of surface atoms in the HOPG sample.
Before we start to interpret the images let's have a look at the atomic arrangement of HOPG and the question what are the bright protrusions in the images we observe.

Hexagonal Structures

The lattice structure of graphite is the so called hexagonal-closest-packing (h.c.p) with a "ABA" pattern.

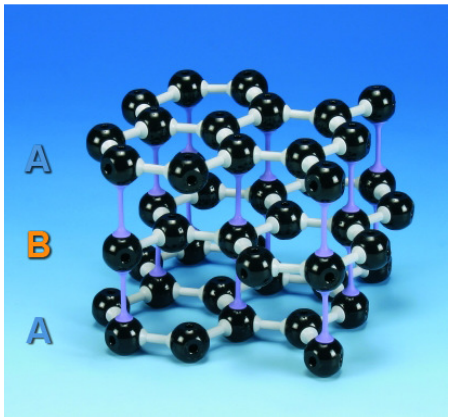

Fig. 3: PHYWE 3D model of the graphite lattice (Crystal lattice kit: graphite, 39840.00).

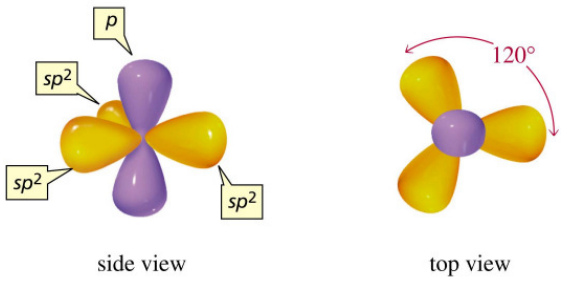

Fig. 4: Sketch of sp^2- hybridized carbon atoms.

The 3D model of the graphite lattice shows the arrangements of neighboring atoms and graphene sheets (one layer, Fig. 3).

A graphene sheet consists of carbon atoms (black balls in the 3D model) in their sp^2- hybridized state with an angle of 120° for each bonding in the x-y-plane (Fig. 4). These are covalent bonds (indicated with white connection pieces) from atom to atom within one

layer (C_6-rings). From one layer to the other only electrostatic interactions take effect (Van der Waals forces). In the 3D model this loose connection from p-orbital repulsion is indicated by the violet connection pieces. The distance between two adjacent graphene sheets in the graphite lattice is 0.3348 nm (334.8 pm) (see Fig. 21).

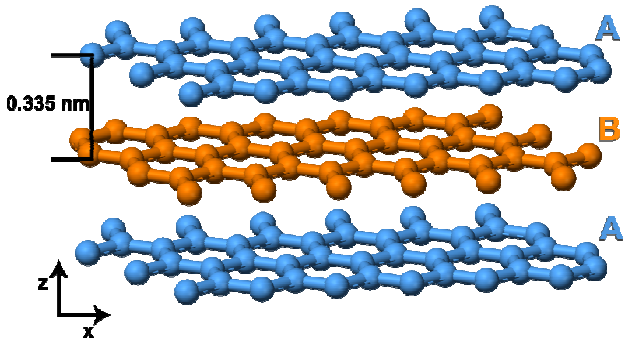

Fig. 5: 3D sketch of the graphite lattice structure (side view).

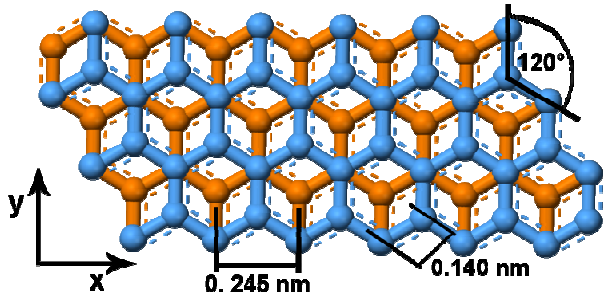

Fig. 6: 2D sketch of the graphite lattice structure (top view).

The second aid you can use to get along on the atomic scale is the **2D model of graphite** (09620-00, Fig. 7).

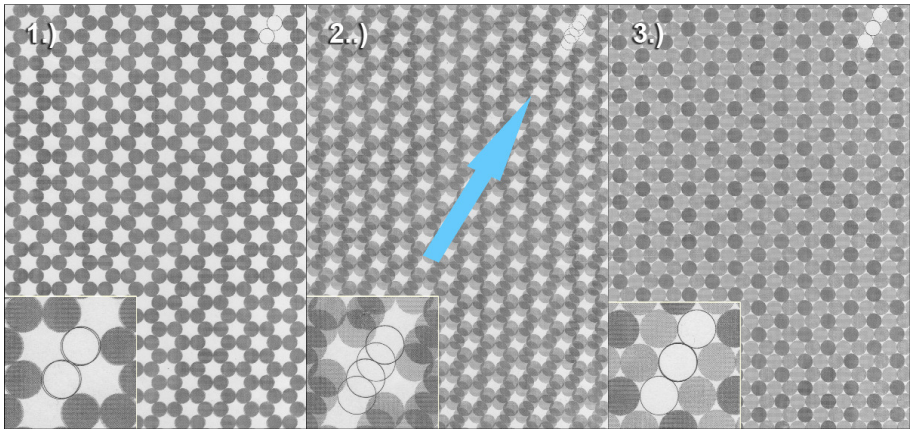

Fig. 7: 2D model of the graphite surface atoms and an underlying graphene sheet (top view) (09620-00).

Start by bringing the foil matching on top of the paper, the marker should show two circles. Then translate the foil diagonally. Afterwards the markers should show three circles indicating that you translated correctly. The atoms from the surface layer with a neighbor in the layer below appear darker as those without a direct neighbor, they appear brighter. This view corresponds to the imaging data of your HOPG sample you collect with your STM. Every second surface atom is imaged.
The distance between two rows of atoms of the same type is 245 pm. From one atom to its next neighbor, this distance is 140 pm (Fig. 6).

Measurements on atomic arrangements

Keep in mind that you can't see every atom of a C_6-ring (as a bright spot), but every second. Use the 2D model of the graphite surface to compare it with the images you took (also see Fig. 7). Every second atom has a neighbor in the layer beneath it. Each atom from the upper layer loses electron density to the direct neighbor in the layer below it, making them to appear darker in STM images. Atoms without a direct neighbor in the layer beneath have the full electron density and appear as bright spots.

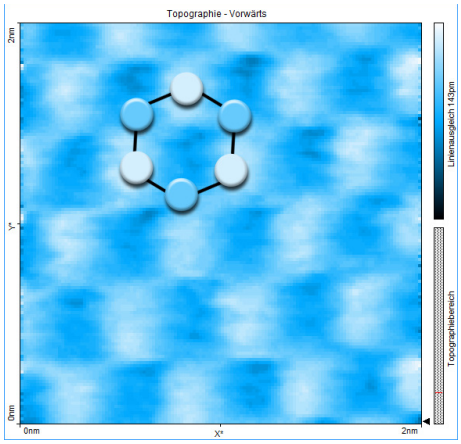

Fig. 2b: Hexagonal pattern reveals electronic and topographic structure of surface atoms

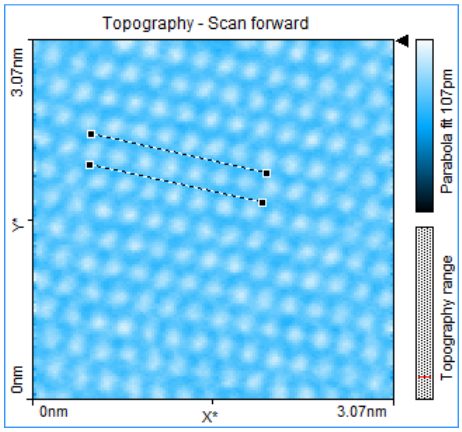

Fig. 8: Distance measurement. Distance between lines: d=252.7 pm

Due to the accuracy of measurement values it is useful to do measurements with lines (“Measure Distance”) instead of a measurement from point to point (“Measure Length”).
Now determine the spacing between atoms: You can either draw lines for the measurement between neighboring atoms (Fig. 2 and 6) or between atoms of the next following row (Fig. 6 and 8).
It is also possible to gain the desired information from a cross sectioning. Draw a line through a row of atoms and do the distance measurement in the graph image. Here you can decide again if you want to measure from one atom to the other (hill to valley, distance approx. d = 140 pm) or from atom row to atom row (hill to hill see Fig. 9 or valley to valley, distance approx. d = 245 pm).

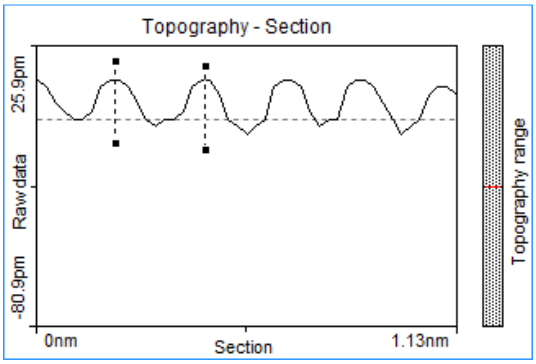

Fig. 9: Cross section through a row of atoms (see Fig. 17). Distance between lines: d=248.5 pm (hill to hill). Δz=15.3 pm (hill-top to valley).

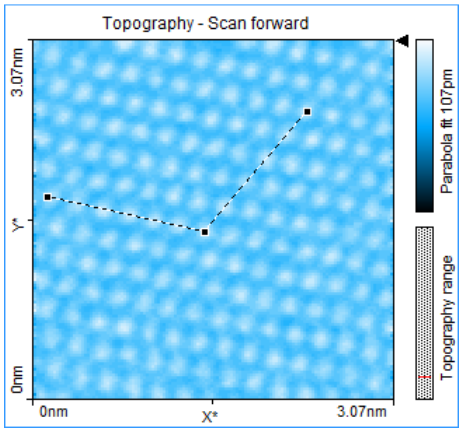

Fig. 10: Angle measurement. Angle between lines: α=118.8

To further increase the accuracy of your measurement and reduce systematic errors, measure the distance of 5 to 10 rows and divide it by the number of rows and you also end up with the distance from row to row. For example a single measurement in Fig. 9 gives a distance from row to row of d=248.5 pm, doing the same measurement over 5 rows (d=1231.5 pm) reduces this value to d=246.3 pm.
Do the measurements as exact as possible, minimal differences in the line drawing (only a few pixel) can make a big difference in your resulting values. To further support your results do a quick estimation of mean values (see above) from at least three to five measurements (more will increase the accuracy even further).

The bonding angle between atoms you are able to determine by using the “Measure Angle” tool (Fig. 10).

After finishing the measurements you also have the possibility to present the data in 3D (Fig. 11) (see chapter 4.4.3 and 4.5 of the user manual). Select “3D View” in the “Select Chart Type” drop down menu. Then adjust the appearance until you are satisfied with the look:
Always click and hold the left mouse button on the 3D view chart while changing the 3D view. The surface is reduced in feature complexity as long as the left mouse button is pressed. Press the following additional keys/buttons to determine what chart property is changed:

- Surface rotation mouse left/right
- Surface tilt mouse up/down.
- Size displayed surface “Ctrl”- key + mouse up/down
- Surface position “Shift”-key + mouse up/down/left/right Z-scale magnification left mouse button + right mouse button + mouse up/down
- Light source direction (360°) “Shift”+“Ctrl”-key + mouse left/right
- Light source height (0°–90°) “Shift”+“Ctrl”-key + mouse up/down

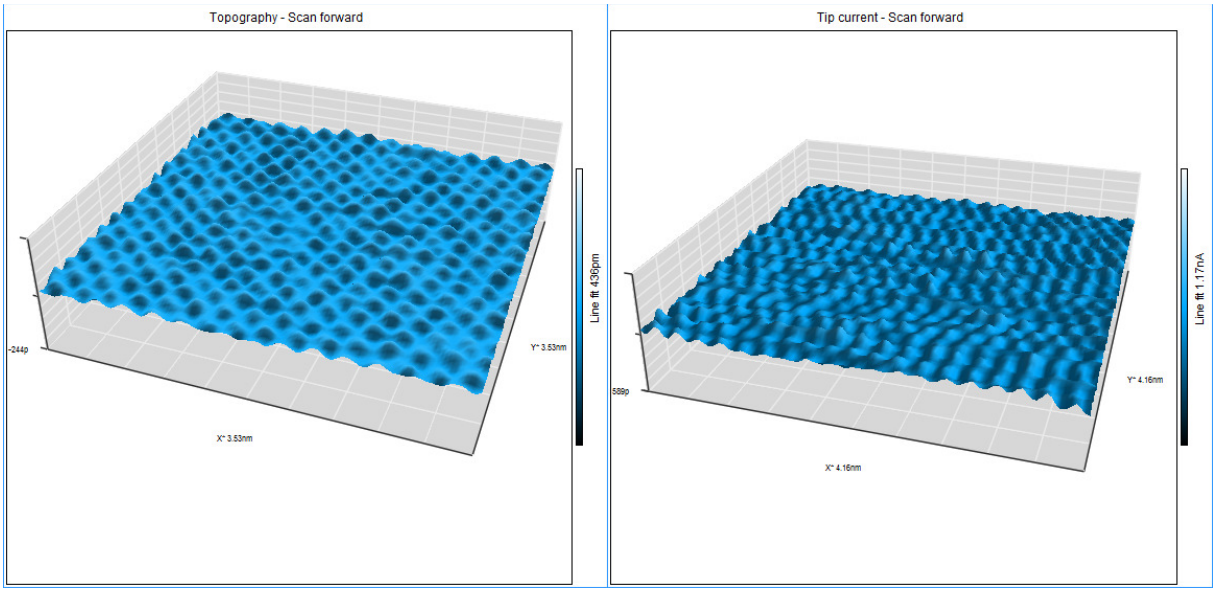

Fig. 11: 3D representation of constant current data (left) and constant height data (right).