THE STM IMAGING OF THE SURFACE STRUCTURE OF GRAPHITE

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Abstract.

The scanning tunneling microscope allows us to image an atomic structures of materials. In this experiment we scanned a graphite using *easyScan STM* system and were able to obtain an image of the crystal structure of the graphite. The graphite atoms form a hexagonal closepacked structure with lattice constant of a=2.5A. From our experimental data we found it ($2.27 \pm .30$)A.

1. Introduction

The scanning tunneling microscope was invented by Nobel laureates G.Binnig, H.Rohrer and their colleagues at the IBM Zurich Research Laboratory in 1981.^[1] This technique allows us to image a material surface and now days it is used even to modify a material in an atomic scale. Quantum mechanics show that a particle, such as an electron, can be described by a wave function, has a finite probability to penetrate through classically forbidden barrier. The wave function for the particle, inside of the 1D rectangular barrier, is,

$$\psi \propto e^{-kz}$$
, where $k^2 = \frac{2m\phi}{\hbar^2}$ and m -mass of the particle, ϕ - work function. (1)

Therefore, the transmission probability or the tunneling current, I, is [2]

$$I \propto e^{-2kz} \,. \tag{2}$$

In STM, a sharp metal tip is brought very close, in order of a few nanometers, to a surface of the sample , so that the wave functions of the tip and the sample overlap, thus enabling electrons to tunnel through the potential barrier when a bias voltage is applied to the tip. The vacuum gap between the tip and the sample serves as potential barrier. Fig.1. shows the principle of the STM. For tunneling between two electrodes with a voltage V across the gap, only the states within V or below the Fermi level , E_F , can contribute to tunneling. Other states can not contribute either because there are no electrons to tunnel at higher energy, or the exclusion principle at lower energy. The electrons, which are near the Fermi level, have higher transmission probability. Thus STM tunneling current is carried by those electrons. $^{[2]}$

The work function in the equation (1) is defined as $\phi = E_F - V$. The Fermi level diagram is shown in Fig.2.

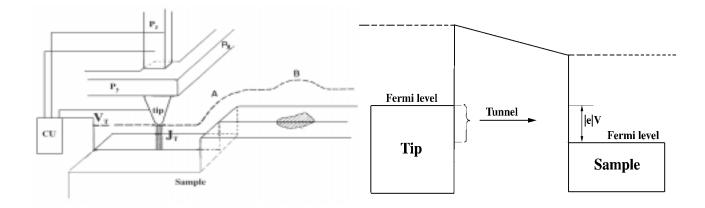


Fig.1. The pseudodrivers P_x , P_y scan the head over the sample's surface. The control unit (CU) applies the bias voltage V_T to the P_z pseudodriver, so tunneling current J_T is kept constant for this voltage. Dashed line presents tip movement and B is chemical inhomogeneity. [2]

Fig.2. Energy level diagram of the tip and the sample with an applied bias V. In this case the the tip is charged negatively, so that the energy level of the tip is shifted upward.

In our experiment we had used a graphite as a sample and obtained an surface image of it. The graphite has a hexagonal close-packed crystal structure, with a lattice constant of a= 2.5A. (please see Fig.3.) Based on our images, we were able to calculate a lattice constant of the graphite crystal.

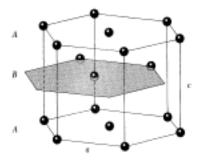


Fig.3. The hexagonal close-packed structure of the graphite. The lattice parameters a and c are indicated, where a-is basal plane (not the lattice constant) and c-is magnitude of the primitive axis a_3 . [3]

2. Measurement.

We used easyScan STM system manufactured by Nanosurf AG, Liestal, Switzerland. This equipment is shown in Fig. 4.

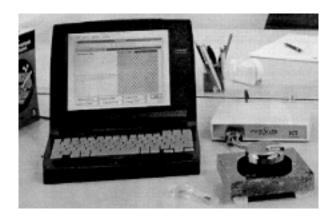


Fig. 4. The easyScan STM system.

The tip voltage of .05V was applied to the platinum tip. We used constant current mode throughout this experiment. Since the tunneling current is very sensitive to the distance between the tip and the sample, by keeping the feedback current constant the distance between the tip and sample is also kept constant

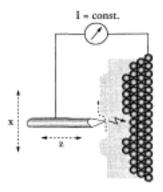


Fig. 5. The scheme of the topography.

and the tip follows the sample's surface structure, which can be observed using z-offset value of the easyScan software. The current value was set at 1nA. The used P-Gain, the proportional feedback value, and I-Gain, the integral feedback value of the z distance controller, values were 11-16 depending on the quality of the tip, where 16 is the highest gain corresponding to the best tip we had.

In most of the measurements, the image was obtained at z-value of .78-1.56 nm and we set the time per line at .068 seconds, because of the high sensitivity of the scan head to temperature variations, where fraction of the tenth of 1C can cause change of several nanometers in the length of the scanning head.

The sample was, as stated above, HOPG (highly orientated pyrolytic graphite).

3. Results and discussion.

The obtained images are shown in Fig.6.-7.

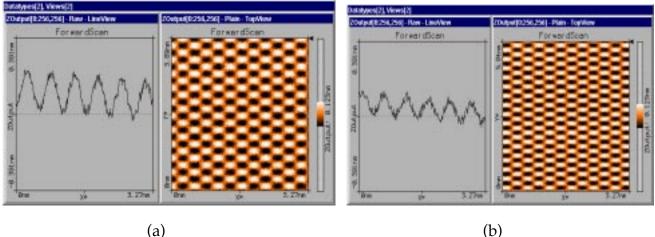


Fig.6. STM image of the graphite atoms.

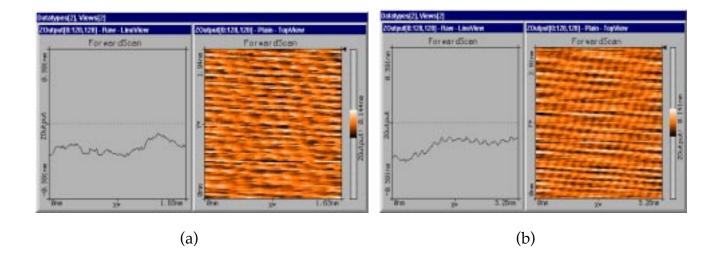
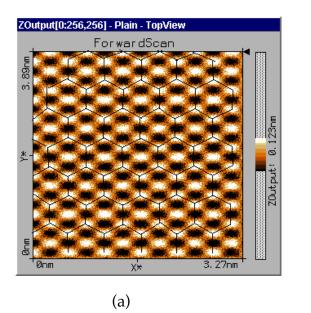


Fig.7. STM image of the graphite atoms.

Although, the one critical point in this experiment was whether the obtained image was a real image or just an electronic noise, we could easily check it by changing the scanning scale. If the image were real, the number of atoms would have changed when we change the scale, while it would have contained the same number of atoms if it were noise. This procedure is reflected in Fig. 8. Because of the temperature instability cells representing atoms are stretched and look rectangular rather than circular. The carbon atoms in our image form (white cells) hexagonal, which matches with the theory.



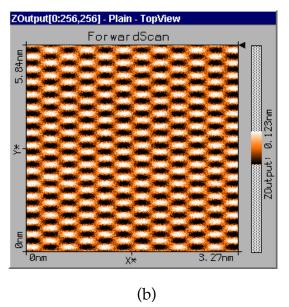


Fig. 8. The graphite surface image in two different scales. There are 10 atoms in (a), scan range of 3.89 nm, while 16 in (b), scan range of 5.84nm.

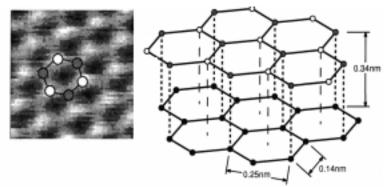


Fig. 9. The atomic image of the graphite surface and its lattice planes. [4]

Out of the lattice model of graphite one can see that there are two different positions of the carbon atoms in the graphite crystal lattice: One with a neighboring atom in the plane below (gray in Fig.9.) and one without neighboring atom in the lattice below (white in Fig.9. and also it can be seen in Fig.3.).

Consequently, the electrical conductivity of the graphite surface varies locally slightly so that the atoms without neighbors appear higher than the others. Therefore, the hexagonal in Fig.8. are twice much as the true hexagonal.

The lattice constant was measured using easyScan software and the result is shown in Fig. 10. Moreover, the analysis on data was done by using KaliedaGraph. This calculation gives us the

lattice constant of $(2.27\pm.03)$ *A*. Also the an angle for hexagonal was measured and found to be $(120.67\pm.64)^{\circ}$. The error was calculated as follows,

$$S \tan dard. deviation = \sqrt{\frac{\sum_{j=1}^{j=n} (y_j - M)^2}{(n-1)}}$$

$$M = \frac{\sum_{j=1}^{n} y_{j}}{n}$$

$$S \tan dard.Error = \frac{S \tan dard.deviation}{\sqrt{n}},$$

where y_i-is measured value, n- number of data points.

Finally the hexagonal plane structure of the graphite is drawn and it is shown in Fig. 8.

Lattice constant	Angle	Lattice constant	Angle
1.99	121	2.16	127
2.1	118	2.43	121
2.1	114	2.29	116
2.37	116	2.43	122
2.35	122	2.35	114
2.17	120	2.11	121
2.29	122	2.29	121
2.3	121	2.3	124
2.42	121	2.12	122
2.43	123	2.16	123
2.42	124	2.29	120
2.42	123	2.16	120

	Lattice constant	Angle
Minimum	1.99	114
Maximum	2.43	127
Sum	54.45	2896
Points	24	24
Mean	2.26875	120.6667
Median	2.29	121
RMS	2.27243	120.7059
Std Deviation	0.13205	3.143892
Variance	0.01744	9.884058
Std Error	0.02695	0.641744
Skewness	-0.3513	-0.62856
Kurtosis	-1.0466	0.207919

4. References

- 1. H.J.Guentherodt, R.Wiesendanger, "Scanning tunneling microscopy I", 1994.
- 2. J.Tersoff, N.D.Lang, "Theory of scanning tunneling microscopy", 1993.
- 3. C.Kittel, "Introduction to solid state physics", 1996.
- 4. EasyScan STM system software reference, 1998.