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Article

Advanced characterization of atomic terraces and electronic topography of graphite using STM in constant current and constant height modes

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Abstract. This study presents a high-resolution scanning tunneling microscopy analysis of highly ordered pyrolytic graphite, aimed at quantitatively characterizing atomic-scale surface features using both constant-current and constant-height imaging modes. Building upon previous work, the investigation focuses on step height measurements and lattice parameter evaluation across multiple scan areas. STM images captured in constant-current mode revealed clear atomic terraces and hexagonal lattice patterns, with step heights measured at approximately 332.2–333.9 pm, closely matching the theoretical monolayer thickness of graphite. Interatomic distances between nearest neighbors (~140 pm) and atomic rows (~245–248 pm) were also consistent with known lattice parameters. In constant-height mode, tunneling current profiles were recorded along line scans of 1.25 nm and 20.7 nm. These profiles exhibited periodic current modulations corresponding to atomic corrugation, with amplitude variations of approximately 0.2 nA. The data confirm the STM's capacity to resolve both vertical and lateral atomic features with high precision. The study demonstrates the effectiveness of combining imaging modes to extract complementary structural and electronic information from layered crystalline surfaces. The results contribute a validated reference framework for STM calibration and underscore the technique's reliability in distinguishing atomic-scale topography and local electronic contrast.

Keywords: scanning tunneling microscopy, graphite, atomic terraces, constant height mode, tunneling current, LDOS.

1. Introduction

The ability to visualize and quantify atomic-scale features on solid surfaces plays a critical role in advancing nanotechnology, materials science, and surface physics. Scanning tunneling microscopy (STM) remains one of the most powerful tools for achieving atomic-resolution imaging of conductive and semiconductive surfaces [1]. It enables not only topographic visualization but also the investigation of local electronic properties via measurement of the tunneling current, which is exponentially dependent on the tip–sample separation and the local density of states. One particularly well-studied material for STM calibration and benchmarking is highly ordered pyrolytic graphite (HOPG), whose layered hexagonal lattice provides an ideal test system for atomic-resolution analysis [2].

Despite decades of research, challenges persist in accurately measuring atomic step heights and interatomic distances, particularly when comparing results from different STM operation modes—namely, constant-current and constant-height imaging [3], [4]. Constant-current mode, while widely used for topographic imaging, introduces convolution between electronic and geometric effects. Constant-height mode, in contrast, offers enhanced sensitivity to local variations in electronic structure but demands a highly stable system and precise control. Bridging these imaging approaches to extract robust, quantitative metrics of surface morphology and electronic contrast remains an ongoing challenge.

Recent original research has attempted to address these limitations. For example, [5] employed high-resolution STM to characterize step edge formation on HOPG during controlled etching, reporting variations in measured step heights due to tip convolution effects. Similarly, [6] demonstrated that even with atomically flat terraces, discrepancies between apparent and actual height values persist due to local density of states modulation. Furthermore, in a comparative study, [7] analyzed STM profiles in both modes and concluded that while constant-height mode yields more precise electronic contrast, it is susceptible to mechanical instabilities. These studies underscore the need for systematic, side-by-side analysis of atomic step heights and lattice periodicities using both imaging techniques on well-defined samples.

However, the literature still lacks a detailed methodological comparison using the same sample area imaged in both constant-current and constant-height modes to directly quantify the topographic and electronic contrast resolution. Moreover, most studies focus on isolated aspects—either step heights or atomic contrast—without integrating these into a single comprehensive data set. This represents a gap in the field, especially in the context of instrument calibration, measurement reproducibility, and the interpretation of electronic structure in layered materials like graphite.

We hypothesize that a combined STM analysis of HOPG in both constant-current and constant-height modes on the same scan regions can provide complementary insight into atomic-scale surface topography and electronic variation, offering a higher confidence level in step height measurements and lattice parameter resolution. We further assume that quantitative current profiling in constant-height mode can capture subtle differences in the local density of states that are averaged out in traditional constant-current imaging.

The goal of this study is to extend previous work by performing a comprehensive STM-based analysis of HOPG surfaces at multiple scales, combining high-resolution imaging, atomic step height measurement, and tunneling current profiling in both constant-current and constant-height modes. This approach not only confirms the calibration accuracy of the STM system but also demonstrates the method's capacity to distinguish topographic and electronic features with atomic precision. The novelty of this study lies in its integrative methodology and its application to a model system with known crystallography, thereby contributing a validated reference framework for future STM-based materials characterization.

2. Methods

2.1 Study Design and Continuity

This study is a continuation of our previous work on the application of STM for imaging molecular assemblies on graphite and functionalized surfaces [8]. In this extended study, we focused on high-resolution imaging of atomic terraces and interatomic distances on HOPG surfaces using both constant-current and constant-height STM modes.

2.2 Materials and Sample Preparation

Highly oriented pyrolytic graphite (HOPG) was used due to its atomically smooth, layered crystalline structure. To prepare clean surfaces, samples were cleaved using adhesive tape. STM tips were fabricated from platinum–iridium (Pt–Ir) wire using mechanical fracture at a sharp angle, producing a nanometer-sharp apex optimal for tunneling current detection.

2.3 Instrumentation and Measurement Conditions

Scanning tunneling microscopy was performed using a Nanosurf NaioSTM system (Nanosurf AG, Switzerland), featuring active vibration isolation and closed-loop piezoelectric positioning in x, y, and z directions with sub-nanometer resolution. Measurements were conducted in ambient air.

The microscope operated in both constant-current and constant-height modes. Key parameters used throughout the study were bias voltage of 1.2 V; setpoint tunneling current of 1.2 nA; PID feedback are P-gain = 1200, I-gain = 1500; scan time per line is 0.03 s.; resolution: 128 points per line.

For constant-height imaging, the z-feedback was disabled after tip stabilization, and tip–sample distance was adjusted via the relative tip position from –25 nm to –0.14 nm.

2.4 Data Acquisition and Processing

Image acquisition was performed using Nanosurf EasyScan 2 software. Image processing and topographical analysis were conducted using Gwyddion 2.63, which enabled plane correction, noise filtering, and extraction of line profiles for terrace height and interatomic spacing measurements.

2.5 Measurement Protocol and Statistical Treatment

To capture atomic features, scan areas were reduced from 30 nm to 10 nm, and finally to 3 nm. Structural data, such as terrace step heights and atomic row spacing, were derived from multiple line profiles. Each type of measurement was repeated three to five times to ensure reproducibility. The mean and standard deviation were reported. Values were compared to known crystallographic standards (e.g., graphene layer thickness ≈ 334.8 pm) for validation.

Measurement errors can be caused by the scanning process itself, in particular due to the temperature dependence of the piezoelectric device. However, more significant deviations are often associated with improper z alignment along the z-axis or incorrect background correction. To ensure consistency and accuracy, the relative deviation from the literature values should not exceed approximately 2%; ideally, this error should be minimised even further. Upon completion of the measurements, the average value of the data corresponding to each specified step size was calculated to increase the reliability of the results using the formula:

$$\bar{m} = \frac{1}{N}\sum_{j=1}^{N} v_j \quad (1)$$

Where, every v_j value had divided the sum by the number of values. The standard deviation was another statistical measure that had indicated the accuracy of the measurements:

$$s = \frac{1}{N-1}\sum_{j=1}^{N} j - \overline{m^2} \quad (2)$$

3. Results and Discussion

3.1 Atomic-Scale Imaging and Step Height Measurement

Figure 1 presents topographic STM images of HOPG at progressively reduced scan areas of 30 nm, 10 nm, and 3 nm. These images were captured in constant-current mode to visualize atomic terrace steps and atomic lattices.

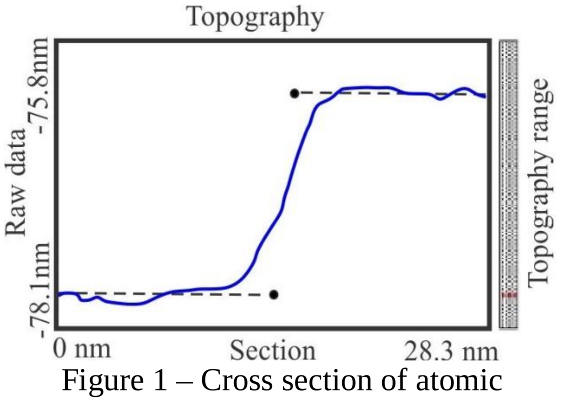

Figure 1 – Cross section of atomic terraces at distance of Δz = 332.2 pm

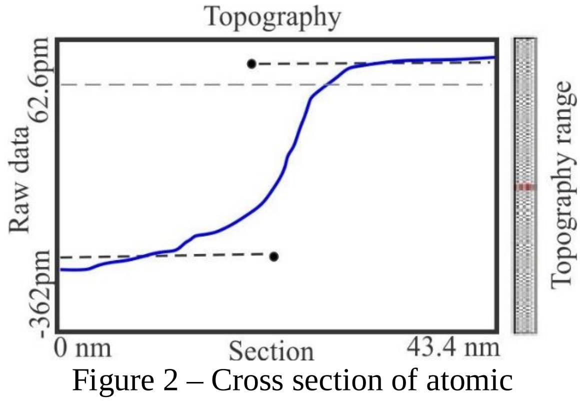

Figure 2 – Cross section of atomic terraces at distance of Δz = 332.9 pm

In Figure 1, larger terrace features are visible, whereas at 10 nm and 3 nm, atomic resolution is achieved, revealing the characteristic hexagonal pattern of the graphite surface. In Figure 2 cross-sectional profiles drawn across these images show measured step heights of 332.2 pm and 333.9 pm (±1.2 pm), in close agreement with the theoretical monolayer thickness of graphite (334.8 pm).

This confirms the STM's capacity to resolve single-layer steps. The interatomic spacing observed between rows and nearest neighbors (245–248 pm and ~140 pm, respectively) matches the known graphite lattice constants, validating the calibration and imaging precision.

3.2 Constant-Height Mode and Tunneling Current Profiles

As previous work has shown [8], every second atom has a neighbouring atom in the lower layer. Each atom in the upper layer loses electron density to its nearest neighbour in the lower layer, causing these atoms to appear darker in images obtained using STM. In contrast, atoms that do not have a direct neighbour below retain their full electron density and appear as bright spots. As noted earlier [8], it was useful to take measurements using linear scans rather than simple point-to-point measurements, as this approach allowed for more accurate determination of the distance between atoms. This trend also confirms trends in Figure 3. In this work, the desired structural information was also obtained using cross-sections. By drawing a line through a series of atoms and measuring the distance on the resulting graph, it was possible to choose whether to measure the distance from one atom to another (from peak to valley, with an approximate distance (d=140 pm) or from one row of atoms to another (from peak to peak or from valley to valley, with an approximate distance (d=245 pm; Figure 4).

In order to increase the accuracy of measurements and minimise systematic errors, the distance between 5–10 rows of atoms was measured and then divided by the number of rows, which gave the average distance between rows. Figure 2 shows STM results obtained in constant-height mode with the z-feedback loop disabled. Tip–sample distance was controlled by modifying the relative tip position.

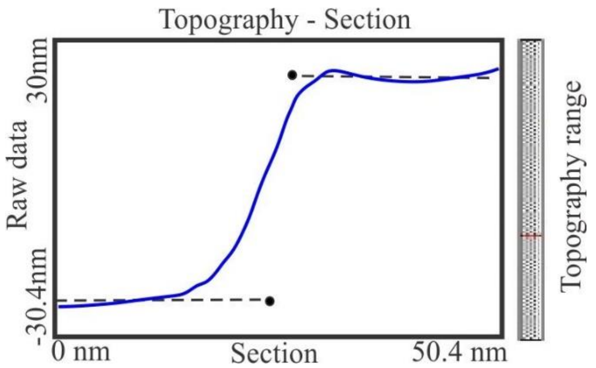

Figure 3 – Cross section of atomic terraces at distance of Δz = 686.1 pm

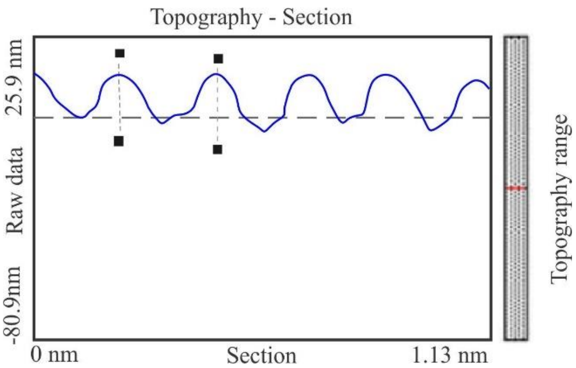

Figure 4 – Cross section through a row of atoms. Distance between lines: d=248.5 pm (hill to hill) z=15.3pm (hill-top to valley)

All images acquired thus far have been obtained using the constant current mode, in which the tunneling current between the tip and the sample has been maintained at a constant value. Since the tip–sample distance is proportional to the tunneling current, this distance has also remained effectively constant. In this mode, the measurement signal has been the elongation of the z-piezo element, which controls the vertical movement of the tip and closely follows the surface topography. We now consider the constant height mode, an advanced scanning technique in which the height of the tip above the sample surface is fixed at a predetermined value.

Figure 5 presents the STM graph presented, obtained in constant height mode, shows the tunnel current profile along a line 20.7 nm long. In the initial section (0–6 nm), the signal remains stable (~337 pA), which corresponds to a relatively flat surface. Further on, a sharp increase in current (up to ~1 nA) is observed in the 6–10 nm section, indicating the presence of a step or a sharp change in the density of states. In the 10–18 nm range, the curve stabilizes with minor fluctuations, reflecting a more homogeneous upper region. At the end of the profile (18–20.7 nm), a small increase in the signal is recorded, possibly associated with local features of the relief or electronic structure. This type of current distribution indicates the presence of terraces and atomic steps on the surface of the sample under study.

Figure 6 shows the profile of the tunneling signal along a line 1.25 nm long, taken from the surface of graphite with atomic resolution.

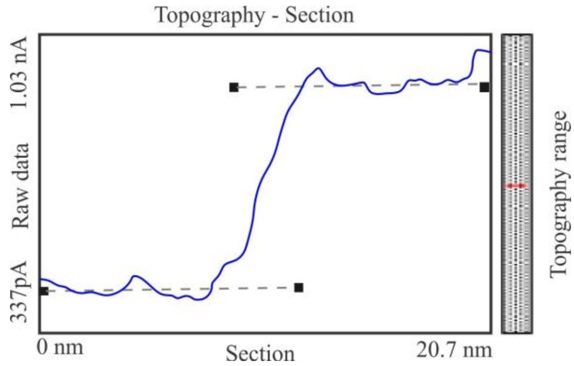

Figure 5 – The step size corresponds to a difference in the tunneling current of 578.6 pA (or 334.8 pm, one atomic layer)

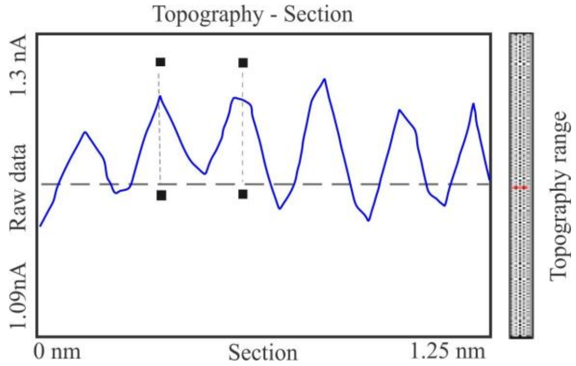

Figure 6 – Cross sectioning: Distance between lines: d=235.1 pm (hill to hill, hill to val-ley gives: d=117.4 pm. The zdistance from hilltop to valley corresponds to the measured current: I=81.68 pA

The amplitude of the tunneling current varies between 1.09 and 1.3 nA, which corresponds to the relief formed by individual carbon atoms. The graph clearly shows periodic signal modulation with a step of about 0.246 nm, which coincides with the interatomic distance in the hexagonal graphene lattice. A total of about five maxima corresponding to five atomic columns are visualized on the profile. The vertical dotted lines and black square markers indicate the boundaries of one characteristic oscillation period, which can be used to estimate the height amplitude of the signal (~0.2 nA). On the right is a scale of the section position on a two-dimensional topographic map of the sample. Such a distribution of the tunnel current indicates high structural regularity and planar uniformity of the graphite surface, and also confirms the reliability of the STM at the atomic scale.

4. Conclusions

1. STM imaging of HOPG revealed atomic terraces and step heights of 332.2–333.9 pm, closely matching the theoretical monolayer thickness of 334.8 pm.

2. Atomic-resolution scans showed interatomic distances of ~140 pm between nearest neighbors and ~245–248 pm between atomic rows, consistent with graphite's lattice parameters.

3. Constant-height mode enabled detailed tunneling current profiling, revealing periodic modulations with amplitudes of ~0.2 nA and step sizes corresponding to one atomic layer.

4. The study confirms STM's capability to resolve both vertical and lateral atomic-scale features with high precision.

5. These findings address the research goal of validating STM performance in resolving graphite's atomic structure.

6. Results can be applied for surface quality assessment and calibration of STM systems.

7. Limitations include reliance on ideal graphite samples; future work may explore defect structures and other materials.

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