Friction-induced artifact in atomic force microscopy topographic images

Thales Fernando Damasceno Fernandes

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topographic images

Thales Fernando Damasceno Fernandes

Orientador: Prof. Bernardo Ruegger Almeida Neves

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“Somewhere, something incredible is waiting to be known.”

Carl Sagan
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Abstract

In Contact Mode Atomic Force Microscopy (CM-AFM), a cantilever with a sharp tip on its end is employed to acquire topographic information. Such acquisition is normally made by monitoring the deflection of the cantilever when it is in contact with the surface being scanned and using deflection variations as a feedback signal to the control electronics in order to keep the deflection constant (also known as constant force imaging mode in the literature). However, there is a major problem with this approach since, in most cases, a constant force scanning is not possible: frictional forces, besides normal forces, may bend the cantilever. Such additional bending (deflection) needs to be considered in the formulation of the problem. The present dissertation investigates how these forces (frictional and normal) can give rise to a topographic artifact when scanning along the cantilever axis direction. Such artifact is even more dramatic when the friction coefficient of the sample changes from region to region.

This effect is studied experimentally, with a sample composed of graphene monolayer atop silicon oxide. The observed artifact, caused by frictional forces, causes the graphene to appear either thicker or thinner than it really is depending on scan direction. A theoretical examination is also made both with analytical methods (Euler-Bernoulli beam theory) and a simulation on COMSOL Multiphysics package. The theory not only predicts the artifact, but also indicates how it can be completely avoided by changing the scanning angle to the perpendicular direction of the cantilever axis.
Resumo

No Modo Contato da Microscopia de Força Atômica (CM-AFM), uma alavanca com uma ponta bastante afiada em sua extremidade é usada para adquirir informação topográfica. Tal aquisição normalmente é feita monitorando a deflexão da alavanca quando em contato com a superfície a ser varrida. Usa-se a variação da deflexão como um sinal de feedback que controla a eletrônica, mantendo a deflexão constante (conhecido como modo de força constante na literatura). Porém, existe um grande problema com essa abordagem, já que, na maioria dos casos, fazer uma varredura com força constante não é possível: forças de atrito, além da força normal, podem fletir a alavanca. Tal curvatura adicional (deflexão) deve ser considerada na formulação do problema. Essa dissertação investiga como essas forças (normal e de atrito) podem dar origem a um artefato de topografia quando é feito uma varredura ao longo do eixo da alavanca. Tal artefato é ainda mais dramático quando o coeficiente de atrito da amostra muda de região para região.

Esse efeito é estudado experimentalmente, com uma amostra composta de uma monocamada de grafeno em cima de oxido de silício. O artefato observado, causado pelas forças de atrito, faz o grafeno aparecer mais espesso ou mais estreito do que realmente é, dependendo da direção de varredura. Uma verificação teórica também é feita usando métodos analíticos (teoria de vigas de Euler-Bernoulli) e simulações usando o pacote COMSOL Multiphysics. A teoria não apenas prediz o artefato, mas também indica como ele pode ser completamente evitado ao trocar o ângulo de varredura para perpendicular à direção do eixo da alavanca.
Introduction

Atomic Force Microscopy (AFM) is a technique capable of imaging matter with atomic resolution [1–10]. It works by employing a sharp tip (~100Å of diameter at the apex) mounted on a cantilever a few hundred micrometers long. When the tip is approached to the surface being scanned, the surface-tip interaction forces deform the cantilever, causing a deflection (bending) of the cantilever. Monitoring the deflection of the cantilever by means of optical reflection and computer electronics (controller + computer), when the tip is in contact with the surface, enables the acquisition of topographic information of the surface with atomic resolution. This type of operation, when the tip is in contact with the sample, is called Contact Mode (CM) [4–6]. Another type of operation is the Non-Contact Mode (NCM) [1,2,4,5,9], where the tip is oscillated above the sample and, by measuring the amplitude or frequency shift of the cantilever when the tip is in the proximities of the sample, a topographic profile is also created. In this Dissertation, only the Contact Mode Atomic Force Microscopy (CM-AFM) will be addressed.

In CM-AFM, what is monitored by means of the computer electronics is the deflection of the cantilever, or in the AFM jargon, the setpoint. Since the cantilever works similarly to a spring [11–17], there is a direct relationship between the deflection (setpoint) and the normal force, the force between the tip and the surface. Therefore, it is always possible to convert deflection to force using Hooke’s Law. The system electronics will try to keep the cantilever deflection constant, by raising or lowering the sample as its topography changes, thus operating in a constant deflection mode, or in the jargon of AFM, constant force.

One of the major problems with CM-AFM is that in the description of its operation, only the normal force enters on the analysis of the problem. This might be a major issue, since frictional forces can cause substantial deflection of the cantilever, and since this force is unaccounted in the theory of CM-AFM, unexpected results might be produced. As a consequence of such frictional forces, in regions with higher frictional coefficients, the cantilever will bend more or less, depending on the scan direction. Since this frictional force was unaccounted, the electronics will perceive this change in deflection as a change in normal force (even if the normal force did not change), and since the microscope is operated in a constant deflection mode, the electronics will move the tip to compensate these frictional
forces. In summary, what these frictional forces do is the following: sample regions with high frictional coefficient appear higher or lower than they really are depending on the scan direction. Consequently, they modify the topographic information and introduce a topographic artifact. Although this artifact is normally in the nanometer range, this might be a major problem when investigating ultrathin samples. For example, in recent years, with the discover of graphene [18,19] and other two dimensional materials like hexagonal boron nitride [20–26], molybdenum disulfide [27–29] and others [30–32], it became important to measure small structures with sub-nanometer precision. If there is an artifact in nanometer range, the measurements become unreliable.

In this Dissertation, this topographic artifact was investigated by means of both an analytical theory and finite elements simulation [33–39], using Comsol Multiphysics. It will also be seen that experimental results agree well with the predicted analytical formulae for the topographic artifact and that it is possible to eliminate this artifact by means of another scanning direction, perpendicular to the cantilever. In this geometry, there is no artifact. And as such, we propose it as a standard for CM-AFM measurements. Regardless of the force being employed and of the type of surface being scanned, it is preferable to make all measurements in this perpendicular-to-the-cantilever geometry and, as an additional bonus, Lateral Force [1–4,9] (LF-AFM) signal is also simultaneously acquired.
1 Atomic Force Microscopy

This chapter describes in more details the working principles of an AFM and how its theory is usually treated in the literature.

1.1 Microscope Setup

The basic principles of the AFM are very simple. In Fig 1, there is a basic scheme of a typical AFM microscope. The sample is mounted on top of a piezoelectric tube, capable of moving the sample in 3 orthogonal axes, or in the jargon of AFM, the scanner. The cantilever is mounted in the proximities of the sample being scanned. The laser and the photodetector that measures the cantilever deflection are also shown in Fig. 1. Finally, the system electronics, that consists of a controller for the microscope hooked up on a computer that controls the controller and displays images.

The actual process of image acquisition and operation is as follows: when the cantilever starts to approach the sample, it starts to feel the interaction forces [2,5,10] between the atoms of the tip and the surface. These forces are, typically, Van der Waals forces [40,41]. The laser hits the back of the cantilever, which is reflective, and the reflected light is bounced on the 4-quadrant photodetector (Fig 2). Deflection of the cantilever is translated into a vertical difference signal on the photodetector. Thus, this detector is a very sensitive angle measurement device, capable of measuring very small deflections (angles) of the cantilever. The signal of the photodetector is monitored by the system electronics. In Contact Mode Atomic Force Microscopy (CM-AFM), the deflection of the cantilever should be constant (setpoint). For this, the electronics will try to make the signal on the detector constant, equal to the setpoint, by lowering or raising the sample by means of the piezoelectric tube. This change in height is captured by the computer and is translated into an image, which has the topographic profile of the surface.
1.2 Photodetector

As cited above, the photodetector usually has 4 quadrants as in Fig 2. The top 2 quadrants are called \( A \) while the bottom two are called \( B \), the left two are called \( C \) while the right two are \( D \). The way the photodetector measures signal is as follows: The laser spot is projected onto the photodetector, but its spot size is not punctual as represented here; it usually covers all the 4 quadrants. The laser will be more incident on some quadrants than others. So the signal of \( A - B \), the voltage difference between \( A \) and \( B \), will give how much the laser is displaced in the vertical direction of the detector. The same applies to \( C - D \) and it will indicate how much the laser is displaced in the horizontal direction. Therefore, the photodetector is a differential signal detector; it gives the difference in signal between the regions of the detector, thus providing the “location” of the laser, the region with greater intensity. This signal up-down or left-right is directly proportional to the deflection (angle) of the cantilever. Bending of the cantilever causes increase/decrease of the \( A - B \) signal, while torsion of the cantilever causes increase/decrease of the \( C - D \) signal as in Fig 3.
When operating the microscope in the CM-AFM mode, the $A - B$ signal is the only one of importance, since this is the signal used in the feedback loop and it is this signal that is maintained constant by means of the setpoint. The $C - D$ signal plays no role in the feedback loop and it is only used to acquire the Lateral Force signal [3,6,9].

![Photodetector Segments](image)

**Fig 2.** How the four quadrants of a photodetector are divided. The differential signal $A - B$ tell us the vertical position of the laser, while the signal $C - D$ tell us the horizontal position.

![Diagram](image)

**Fig 3.** How deflections of the cantilever get translated into signal. In (a), twists (torsions) in the cantilever cause the laser to go to the left or to the right. In (b), bending along the cantilever beam causes the laser to go up and down.

### 1.3 Scan Direction

Fig 4 shows a scheme of the top view of the microscope. Two directions are defined: parallel or perpendicular to the cantilever. It is also possible to scan in any other direction, forming an angle with these, but they are unimportant and, here, only those two will be compared, since other directions are linear combinations of these two.

While scanning in the direction parallel to the cantilever axis, the cantilever moves in the left to right direction, while in the perpendicular direction, the cantilever moves in the top to bottom direction, according to the geometry shown on Fig 4. So while scanning, in
whatever direction, there will always be two images. These, in the jargon of AFM, are called trace and retrace or also forward and backward direction images. These two directions are acquired simultaneously\(^1\) in two channels by the microscope.

![Diagram showing the parallel and perpendicular scan directions.](image)

**Fig 4.** The definition of the Parallel and Perpendicular scan directions. Parallel being along the axis of the cantilever, and perpendicular being perpendicular to the axis. This figure also shows the top view of the experimental setup.

There is a clear symmetry in the forward/backward direction of the perpendicular direction (mirror symmetry on the \(x\) axis, the axis along the cantilever), while there is an asymmetry in the parallel direction. The symmetry in the perpendicular direction can be thought as a more similar signal in the forward/backward channels; in the parallel direction there is an asymmetry in the geometry, this can be an indicator that the signal will be dissimilar, and it is further explored in a qualitative argument in section 2.1 Qualitative Understanding.

Normally, it is a matter of choice, or taste, to choose between these two directions (perpendicular and parallel), or as a matter of fact, any angle at all. What is usually done is to opt for the default direction of the specific microscope; some have perpendicular as a default direction, while others have parallel. Some microscopes also have the default feature of

\(^1\) The microscope works in this back and forth manner, scanning from left to right and then right to left, one scan channel is acquired in the travel from left to right and the other channel is acquired in right to left travel. The two channels are acquired sequentially in this manner, alternating between single lines acquisition.
showing both channels (forward and backward), while others usually only show a single channel. It is usually a good choice to choose the default configuration of the microscope, since it usually gives more stable and precise measurements, since this direction is used more often. But it is not a good idea to choose blindly any direction without further reason to do so, for the commodity of being default. As a good practice, it is always wise to see both channels (forward and backward) and compare them; if they yield equal results, then it is likely that the topography is being properly imaged.

A quote from B. Bhushan [10], “Topographic measurements are made at any scanning angle. At a first instance, scanning angle may not appear to be an important parameter. However, the friction force between the tip and the sample will affect the topographic measurements in a parallel scan (scanning along the long axis of the cantilever). Therefore a perpendicular scan may be more desirable. Generally, one picks a scanning angle which gives the same topographic data in both directions; this angle may be slightly different than that for the perpendicular scan.”.

While it is fairly well known that friction can alter topographic information on parallel scan, it is not yet well understood how friction influences the topography and by how much. What is usually done, if there is any mismatch between forward and backward images, is to simply choose another scanning angle that gives no mismatch. Also, there is no consensus or even a standard of which direction should be used in the literature, or even worst, any guidelines to always acquire both channels. Notwithstanding, in the literature, it is known that, in a parallel scan, the measurements can suffer from artifact, this geometry is still in use, even with the shortcoming of not acquiring Lateral Force measurements simultaneously.

1.4 Lateral Force Microscopy

Lateral Force Microscopy (LFM) [3,6,9] is a technique of the family of techniques of Scanning Probe Microscopy (SPM) [2,4–6,8–10] that acquires information on frictional forces. It can be acquired simultaneously with the signal of CM-AFM. For it to work properly, the scan direction needs to be on the perpendicular geometry, since the cantilever needs to twist as explained below. While the tip scans the surface, regions with different frictional coefficients will give rise to frictional forces with different magnitudes. High frictional coefficient regions will deform (rotate, twist) more the cantilever than low frictional
coefficient regions. This can be seen in Fig 5: when the tip passes a region with different frictional coefficient, it will be more twisted and will deform more, thus augmenting the $C - D$ signal on the photodetector. This signal $C - D$ is translated as a LFM image that can be interpreted in a quantitative way to determine the frictional coefficient of the surface. The only problem with this technique is the determination of the torsional spring constant, the constant that translates rotation of the cantilever to force by means of Hooke’s Law (for twist). Its determination is not as simple as the bending spring constant, where several methods, as thermal tuning [42–49], Sader Method [43,46,49], or others [44–46,48,49] can be used. In order to determine the torsional spring constant, it can be used the Sader Method for torsion [49], or other methods [50–56].

**Fig 5.** The basic operation of LF-AFM. Regions with high friction will twist the cantilever, rotating it. While regions with very low friction will not deform the cantilever significantly.

### 1.5 Force Curve

The photodetector signal (deflection) is normally in Volts. Therefore, a way to translate this signal in Volts to a signal in Newtons is needed and this is done by means of a Force Curve,. In this way, it is possible to know the interaction forces between the tip and the sample surface.

In Fig 6 shows a typical force curve. The cantilever is lowered (red curve) onto the sample and then raised (blue curve). In $A$, the cantilever is lowered from a large distance from
the sample; in $B$ it starts to feel the interaction forces between the system cantilever-sample and suddenly jumps into contact, (into what is called in the AFM jargon snap-in); in $C$, the cantilever is in hard contact with the sample and the forces onto the cantilever are repulsive, so it starts to deform; in $D$ the cantilever is being attracted by the sample while distancing from it, this attractive force may be dominated by the contamination layer that it is present in air $[1,2,5,7–9]$ and forms a water meniscus (see Fig 10), and in the AFM jargon it is called capillary force; in $E$ the attractive forces are not enough to bend the cantilever any further and the contamination layer ceases to have a meniscus and it breaks, suddenly jumping out of contact with the surface, or in the AFM jargon, snap out. It, then, retreats to $F$ to start the cycle over if desired.

Fig 6. A typical force curve. In red it shows the cantilever being lowered and in blue it being raised.

The inclination of this curve (Fig 6) is called in the jargon of AFM sensibility. Since the signal of the photodetector ($y$ axis) is in Volts, and the travel distance of the cantilever, $Z$-Position, ($x$ axis) is in nanometers, the sensibility is expressed as the ratio of the two: Volts per nanometer. Since the cantilever behaves as a spring $[11,12,14,17,57–59]$ (its behavior with low deflection is linear), it is possible to use Hooke’s Law as $F = k\Delta x$. Using the sensibility and Hooke’s Law, it is possible to express the force on the cantilever in function of the setpoint (in Volts) as $F = Sk\Delta V$, where $\Delta V$ is the setpoint, it follows from $\Delta x = S\Delta V$. With these formulas, it is possible to convert a reading in the photodetector ($A - B$ signal) to a force on the cantilever.

However, there is a major problem with this conventional CM-AFM approach since, in most cases, a constant deflection scanning is not possible: frictional forces, besides normal forces, may bend the cantilever. Such additional bending (deflection) needs to be considered
in the formulation of the problem. The present work investigates how these forces (friction and normal) can give rise to a topographic artifact when scanning along the cantilever axis direction.

Since now there are two forces on the cantilever tip, a normal force and a frictional force, it is not possible to uniquely determine the force on the cantilever solely on its deflection, since its deflection is partially caused by the normal force and the other part by the frictional forces.
2 Topographic Artifact

This chapter investigates, in depth, how to model the Contact Mode in AFM to account for frictional forces and how these forces may affect topography measurements. An analytical theory is developed based on structural mechanics and a finite elements simulation on COMSOL Multiphysics 4.4 is also carried out. At the end of this chapter, some guidelines on how to do CM-AFM avoiding artifacts are proposed.

2.1 Qualitative Understanding

By making a Force Curve (section 1.5 Force Curve) and, therefore, determining the sensibility of the system cantilever-microscope\(^2\), it is possible to link a force with a deflection with the knowledge of the spring constant. This is a one to one map, since it is a quasi-static situation. The cantilever is static and is in a concave deflection as shown in Fig 7a.

In Fig 7b, the cantilever is moving in the backward direction (moving to the left), therefore the frictional forces on the tip will be to the right; this force will bend the cantilever more, leaving it with a more concave deflection. In the forward direction, Fig 7c (moving to the right), the frictional forces will be to the left, and this force will try to unbend the cantilever, leaving it in a less concave deflection. Here, for the sake of illustration, it is shown the deflection as convex, but, in reality, it would still be concave, but less than in Fig 7b.

\(^2\) This sensibility may change if measurements were made in different days, since the sensibility is highly correlated to the laser and its location on the back of the cantilever. Changes in the spring constant, if any, are insignificant and in the range of the expected error of the measuring instruments.
Fig 7. Qualitative picture of the topographic artifact. In (a), the cantilever is lowered to the surface while in a static situation (no scanning). Figure (b) shows a scan in the backward direction (to the left), so friction is in the opposite direction (to the right). Figure (c) shows a scan in the forward direction (to the right), so friction is to the left. In (b) the cantilever is more bent than in (a), while in (c) it is less bent than in (a).

In all 3 cases (Fig 7a-c), it is assumed the normal force to be equal and only the friction changes. As stated before, CM-AFM is a technique of constant deflection: the setpoint specifies a deflection (a reading in the photodetector) and so, when scanning in Contact Mode, it is expected that the deflection of all 3 cases to be equal (to the setpoint). In order to keep this deflection constant, the microscope lowers or raises the cantilever, thus diminishing or increasing the normal force. As a consequence, for case b to have the same deflection as in a, the cantilever will need to be raised, lowering the normal force. While in c, the cantilever will need to be lowered, to increase the normal force and achieve the expected cantilever bending (setpoint).

Although there is no height difference on the surface, in b the surface will appear to be higher, and in c it will appear to be lower than it really is. As a consequence, in a sample surface with two regions with different frictional coefficients: one very high, while the other very low, in the low friction coefficient region, the cantilever will behave as image a, while in the high friction coefficient region, it will behave as b or c, depending on the scanning direction (backward or forward). In such a case, a completely flat region, but with different
frictional coefficients may appear as a hole or as a hill in the topography image depending on scanning direction used.

2.2 Experimental Results

An experiment was carried out in order to verify this artifact using the setup of Fig 9: a graphene monolayer (~ 1\text{nm}) is on top of a wafer of silicon with a layer (~ 300\text{nm} thick) of silicon oxide. Graphene has a very low frictional coefficient [60–64] (as does graphite [65–67]), while silicon oxide has a larger friction coefficient with the AFM tip [68]. A cantilever was used to scan in the parallel scan direction and both channels of topography (backward and forward) are acquired. The experiment was done with increasing setpoints (“Forces”) and the graphene height is measured in each step. Subsequently, the same experiment is repeated, with the same forces, but in the perpendicular scanning direction and the results are summarized in Fig 8.
Fig 8. Top Panel: Experimental data of the height of the graphene in function of the setpoint (force) for 4 different scans. Both forward (trace) and backward (retrace) scanning directions for the perpendicular and parallel directions. Bottom Panel: Topographic image of the graphene used in the experiment. (a,b) constitute a low force regime for the parallel geometry, (c,d) constitute a high force regime for the parallel geometry, (e,f) constitute a high force regime for the perpendicular geometry.
As shown in Fig 8, the graphene layer appears either as higher or lower in the parallel scan direction, and its height increases/decreases with the applied force. But, in the perpendicular scan direction, the graphene height is constant, regardless the force or scan direction used. In section 2.1 Qualitative Understanding, it is explained that regions with high friction appear higher in the backward direction (the scanner need to be raised) while regions with high friction in the forward direction appear as lower (the scanner need to be lowered). But in Fig 8 the graphene height in the backward direction is being decreased, while the height in the forward direction is being increased: apparently, the opposite of what is explained in 2.1 Qualitative Understanding. The reason for this is very simple: graphene has almost no frictional coefficient, so its height will be practically equal in both forward and backward directions. What is really happening is as follows: the silicon oxide substrate is appearing as higher in the backward direction, but the graphene stays the same height, so as a net result, the height of the graphene minus the height of the silicon is decreased. For the forward direction, it is the opposite: the silicon is appearing lower, but the graphene is at the same height, so the height difference between the two appears greater. So it is not actually the graphene that is changing (or appearing to change) its height, but the silicon oxide substrate itself. The artifact occurs when there are regions with different frictional coefficients, affecting more regions with higher friction.
Fig 10. Water meniscus. When the tip is near the sample, the contamination layer (mostly water) forms a meniscus. This meniscus is the principal reason for the adhesion forces in a standard Force Curve.

In the parallel scan of Fig 8, no artifact is expected at zero force, since zero force means no friction (assuming a standard model of friction $F_{fric} = \mu N$, where $N$ is the normal force). But, as shown, the graphene height is changed even with low (zero) force. But even in low forces, there still exists a force of adhesion (capillary forces) caused by the water meniscus (Fig 10). This force is caused by a thin water meniscus formed due to impurities, air humidity, etc [2,3,5,7]. When moving the cantilever, the tip is dragging this meniscus, thus exerting a force (a frictional force) and this is why there is an artifact even with low forces. Since the artifact occurs even with low forces, this additional force is enough to yield significant contributions.

This is a remarkable result due to the cantilever used, with a very large length (374 µm). And, as will be seen later (section 2.4.3 Topography Artifact), the greater the length of the cantilever, the more pronounced will be the artifact.
Fig 11. Topographic image a graphene flake under different scanning forces in a parallel scanning. (a-c) constitute a topographic image of the forward direction while (d-f) the backward direction for a parallel scan direction. In (a) and (b) have normal force of 2 nN; in (c) and (d) of 59 nN; in (e) and (f) of 157 nN. As can be seen from (a-f) the graphene appears as a hole in the backward direction (d-f) and gets higher in the forward direction (a-c).

Fig 8 shows that these additional frictional forces caused by adhesion do not affect the height of the graphene in perpendicular scanning, and that its height is constant. And this height is the true height of the graphene.

Fig 11 shows the graphene (topography) under different scanning forces in a parallel scanning configuration. Figures a-e constitute topographic images of the forward direction,
while d-f, the backward direction. Images a and b have a normal force of 2 nN; c and d of 59 nN; e and f of 157 nN. As can be seen from images a-f, the graphene appears as a hole in the backward direction d-f and gets higher in the forward directions a-c. These images were acquired with a short cantilever and with a high spring constant, so there would be (almost) no artifact in low forces, but there would still be an artifact with higher forces. Here, the frictional forces caused by the adhesion forces are not enough to cause substantial artifacts in low force, but are still present and change the topography slightly.

The experimental difficulties in dealing with high forces are that the graphene may break or curl on itself, as shown in the lower right of Fig 11.

This artifact is a serious issue, principally in recent years, with the advances in two dimensional materials [32]. Although the Contact Mode is being used less often than in the early days of AFM, as it is preferable to use less intrusive techniques as the Non-Contact Mode, or the Tapping Mode [4,5], it is still a useful tool for nanomanipulations [2,3,5]. As the tip is in hard contact with the surface, it is possible to modify it by applying different forces on certain regions, therefore modifying it locally. If any artifact is produced during these nanomanipulations, the results become non reproducible, or biased to a particular direction used. Since not only the topography is affected, the normal force also changes from scanning angle, the forces being reported on a nanomanipulation experiment may underestimate or overestimate the real applied force.

2.3 Simulation

A series of simulations were done using Comsol Multiphysics 4.4 using the module of Structural Mechanics in both 2D and in 3D. The Beam Module\(^3\) was also used to better compare the results of the Euler-Bernoulli model (a more in depth description of these models are done in the Theory chapter).

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\(^3\) The beam modulus uses the Euler-Bernoulli beam equations and gives the same results as the Structural Mechanics module. Its great advantage is its computational speed, since there are far less degrees of freedom. Specific data from the beam modulus are not shown, but give the same behavior with the same precision as the Structural Mechanics modulus.
A typical contact cantilever is simulated (length of 300\,\mu m), but its aspect ratio does not match a real one (if this were done, with a thickness of 4\,\mu m, it would be very hard to properly see the images of the cantilever, the stresses and deflection, so the thickness of the cantilever is exaggerated a bit). The Young modulus of the cantilever is adjusted to give a spring constant of \( 1\,nN/nm \) for simplicity (since the model is linear in the loads, these conversion constants are unimportant for the result and only useful for a better view of the simulation).

Three forces are acting on the tip of the cantilever along the 3 axis. Since these forces cause a moment (torque) on the cantilever that further causes it to bend; they are subdivided in further cases. The force perpendicular to the axis along the surface can cause a torsion of the cantilever and can also bend it, so this force is divided in 2 cases: a torsion one (where there is no bending, Fig 12c) and a bending (where there is no torsion, Fig 12d). The force along the axis of the cantilever can compress\(^4\) the cantilever and also bend it, Fig 12a. The compression will be orders of magnitude smaller than any other displacement. Therefore, it will be considered that there is no compression and treat this as only a bending case. The normal force (perpendicular to the surface, Fig 12b) can cause only bending, so there are 4 cases to simulate: 3 bending and 1 torsion.

Since the model is linear, the principle of the superposition can be used to simulate each case separately and their net effects combine. In this way, the general case of an arbitrary load on the tip in an arbitrary direction (this is done also in the theory) can be considered. Also, it is only necessary to simulate positive or negative forces, since the model is linear and the displacements are zero at zero force, so the displacements need to be asymmetric at zero (odd function), as indeed they are.

\(^4\) A force along the axis of the cantilever can also cause a compression of the cantilever along its axis. This compression will not deform the cantilever along directions perpendicular to its axis, unless the force is excessive, then it will also cause buckling and possible failure of the cantilever. This deformation at the end of the cantilever be proportional to \( L/TWE \), which is a very small quantity. For its derivation follow the section 2.4.1 Euler-Bernoulli Beam Theory and assume that there is a \( x \) displacement \( U(x) \) and balance the equation to the external force \( F_x \), similar to (6), but using force balance instead of moment. This analysis is available in any good book of structural mechanics.
Fig 12. Scheme of the 4 cases to simulate. (a) consists of the force $F_x$, (b) consists of the force $F_z$, (c) consists of the force $F_{yM}$ (torsion case), (d) consists of the force $F_y$ (bending case).

2.3.1 3D Model

The results are as follows: in Fig 13, the force $F_x$, along the $x$ axis (Fig 12a scheme), causes a bending of the cantilever. The color map on the cantilever is the von Mises stress [69–72], which gives information of an equivalent stress acting at that point by all forces (normal and shear stresses) in all directions. As can be seen, the tip of the cantilever displaces more and has a higher stress. This large deformation of the tip is expected, since the simulation was done with a point load. However, according to Saint-Venant's Principle [38,39,73], the difference of a point load (idealized) and a distributed load (reality) becomes small the further away from the load, so the displacements along the beam are more accurate, while the displacements near the tip are less accurate because of the point load. Nevertheless, the deformations of the tip are unimportant here, since, usually, the deformation of the cantilever is much greater and will dominate the final configuration. The contribution of the tip due to the point load artifact is small and can be safely ignored.
Fig 13. Von Mises stress on the cantilever. Force on the tip along the x axis. Deformation factor: 5000.

Fig 14 shows the effect of bending due to the force $F_y$, along the y axis (Fig 12d scheme). Since only the bending that this force produces is of interest, the point of appliance is on the end of the neutral axis\(^5\) instead of the tip. This force causes the same moment along the z axis as it would cause if it were on the tip, but it does not cause any moment along the x axis (torsion), so it gives the behavior of only the bending caused by the force $F_y$ on the tip.

Fig 14. Von Mises stress on the cantilever. Force on the neutral axis along the y axis. This is the bending deformation caused by the y force. Deformation factor: 6000.

Fig 15 shows the deformation caused by the normal force $F_z$ along the z axis (Fig 12b scheme). Compare its difference with the force $F_x$ (Fig 13): it causes a much larger displacement (10 times larger) and the stresses are also distributed differently. With the force

\(^5\) See section 2.4.1 Euler-Bernoulli Beam Theory for an explanation about the neutral axis.
$F_x$, the stresses are more uniform along the beam (Fig 13), while with $F_z$, it decreases with the distance to the tip (Fig 15). Also the tip displacement is not as large as in Fig 13, but the high stress on the tip demonstrates the consequences of the point load.

Fig 15. Von Mises stress on the cantilever. Force on the tip along the $z$ axis. Deformation factor: 700.

Fig 16 shows the torsion effect of the force $F_y$. It is added an opposite force on the end of the neutral axis (Fig 12c scheme) for the sum of the forces to be zero, so this added force cancels the bending caused by the force on the tip, but there still is a torque being applied (but with no bending). In this way, it is possible to separate the effect of torsion from the bending (Fig 14). This torsion will tend to rotate the cantilever, giving no displacement of the neutral axis along the 3 axis. It only twists along the axis, as expected from a circular shaft with very low forces [16,35,74–77].

In summary, it can be seen from these simulations that the force $F_z$ is the one that, by far, gives the biggest displacement on the cantilever. Also, the qualitative difference between the forces $F_x$ and $F_z$ is that force $F_x$ gives a more uniform stress along the cantilever, while for force $F_z$, the stresses increase from the end of the cantilever (where the tip is) to the beginning of the cantilever (where it is pinned). It is shown that the torque on the cantilever twists the plane about the neutral axis. So the displacement along the neutral axis is zero.
Fig 16. Von Mises stress on the cantilever. Torque on the tip caused by the y force. This torque is created by applying a force on the tip and counter-balancing this force on the end of the neutral axis with the opposite force. In this way, the sum of the forces is zero, but the torque is different from zero. Deformation factor: 5000.

In order to better understand the cantilever deformation, the x, y, z deformation of the cantilever with the forces $F_x, F_y, F_z, F_{yM}$ will be plotted. The forces $F_x, F_y, F_z$ cause only bending as Fig 13, Fig 14 and Fig 15 show, respectively, while the force $F_{yM}$ causes torsion (Fig 16). The plots are as follows (the $u, v, w$ displacement in Comsol corresponds to a displacement $u$ in the directions $x, y, z$, respectively):

Fig 17, Fig 18 and Fig 19 show the x, y, z displacements of the neutral axis, respectively. The results from the simulation are compared with the analytical solution (see section 2.4 Theory). The graphs show the normalized displacement\(^6\) (displacement per applied force) and, since the model is linear for a ramp of forces, they give the same normalized displacement. For a particular displacement in a specific force, it can be multiplied the normalized displacement by the desired applied force.

Fig 17 shows displacement along the x axis. The only force that causes any (but small) displacement is the $F_x$ force. This displacement is the compression of the cantilever along its length and, being very small, can be ignored, as stated previously. There are no further displacements caused by other forces since the axis shown is the neutral axis.

---

\(^6\) The maximum force used was 100nN, the forces where ramped from 0 to this maximum force using 13 values. The graphs show each displacement divided by their respective force and all of them give the same normalized displacement. Since the number of simulation points was very large, just a few points are shown in the graphs for better visualization.
Fig 17. Normalized x displacement along the neutral axis.

The y displacement is shown on Fig 18. Since the forces $F_x$ and $F_z$ are perpendicular to this axis, there is no displacement for them. The only force that can cause displacement along the y axis is the force $F_y$. Since the torque rotates the cantilever, there is no displacement for it (as stated earlier), so the only contribution for this displacement is the bending component of the force $F_y$. 

Fig 18. Normalized y displacement along the neutral axis.

The z displacement is shown in Fig 19. The only two forces that cause bending moments (torque) along the y axis are $F_x$ and $F_z$. The force $F_z$ causes a displacement 10 times greater than the force $F_x$. This is as expected since the normal force $F_z$ has a bigger lever length.

The actual relationship between the two displacements is: the $F_z$ force causes a $z$ displacement $2L/3h_{tip}$ times greater than the force $F_x$. For the actual simulation this is exactly equal to 10. For more information on the geometric parameters and the theory see section 2.4.1 Euler-Bernoulli Beam Theory.
The results in Figs. 17, 18 and 19 show how the neutral axis deforms, which is one of the most important parts of the model. This served as way to compare theory with simulation with great agreement, since in the theory (section 2.4 Theory) will be described how the neutral axis is displaced. But another piece of information is also interesting: the position of the tip. Since the tip is in constant contact with the surface, it is important to know how it is displaced. The z position of the tip should be constant along a flat surface (it does not leave the surface), so the amount of the tip displacement in a constant deflection mode shows how much the scanner will compensate so the tip does not move. In practice, the scanner moves the base of the cantilever, but in the theory the base is pinned (it does not move). So, to convert theory to reality, it is necessary to translate the cantilever in such a way for the tip to be constantly in contact with the surface, simulating, therefore, a real scan where the scanner is really moving the cantilever.

The x displacement of the tip is shown in Fig 20. Since the force $F_y$ is perpendicular to this axis, it will cause no displacement. The forces $F_x$ and $F_z$ cause a bending around the y
axis, so, even though the neutral axis is not displaced, points above or below will rotate\(^8\), so they have a \(x\) component of displacement. As expected, the force \(F_z\) gives a much larger displacement\(^9\) than the force \(F_x\), since it produces a larger bending. As seen in Fig 13 and Fig 15, the force \(F_x\) deforms the tip more (due to the point load) than the force \(F_z\), this additional deformation caused by the use of a point load instead of a body load, or a surface load, is in reality an artifact, and therefore, overestimates the displacement in the \(x\) axis. The theory does not account for this artifact and, therefore, it predicts a smaller displacement, as shown by the simulated and theoretical curves for the force \(F_x\) in Fig 20.

\[
\text{Tip x Displacement}
\]

![Tip x Displacement](image)

**Fig 20.** \(x\) displacement of the tip.

The \(y\) displacement of the tip is shown in Fig 21. As expected, only the force \(F_y\) (due to bending and torsion) causes a displacement. The bending caused by the force \(F_y\) is the same kind of bending (the equations are isomorphic) caused by the force \(F_z\), but with the roles of

\[8\] \text{See Fig 35 for a better view of this rotation.}

\[9\] The theoretical ratio between the \(x\) displacement of the force \(F_z\) by the force \(F_x\) is \(L/2h_{\text{tip}}\), which in this case is 7.5.
width and thickness interchanged. Since the cantilever appears thicker in this view, there is far smaller displacement. The torsion also causes y displacement, since it rotates around the neutral axis and points distant from the neutral axis rotate it in the zy plane.

**Fig 21.** y displacement of the tip.

The z displacement of the tip is shown in Fig 22. It gives the same behavior as the z displacement of end of the neutral axis (Fig 19), since points displaced above or below are displaced by the same amount\(^\text{10}\).

---

\(^{10}\) In the section 2.4.1 Euler-Bernoulli Beam Theory, it is shown that the z displacement of any point of the cantilever is the same as the displacement of the neutral axis.
Fig 22. z displacement of the tip.

Fig 23 shows the von Mises stress of the zy plane at the tip caused by the torsion of force $F_y$. There are two regions of high stress caused by the two forces (remember, there is a force at the neutral axis to eliminate bending). It can be seen clearly that the torque will only rotate the plane sections of the cantilever.
Fig 23. The von Mises stress for the 2y plane at the neutral axis (on the tip) for the torsion. Deformation factor 3000.

Fig 24 shows the same graph as Fig 23, but with the total displacement\textsuperscript{11}. It follows a circular profile around the neutral axis, showing that this torsion only causes rotation. This type of figure is very similar to a circular shaft, as it has the same circular pattern. Therefore, for this case, it is accurate to use a theory of circular shafts for a cantilever, instead of a more sophisticated torsion theory such as St. Venant Torsion Theory [78–81] or Prandtl Torsion Theory [13,15,33,82,83].

\textsuperscript{11} The total displacement is the modulus of the vector displacement $\mathbf{u}$. 

30
Fig 24. Total displacement of the zy plane section at the tip caused by torsion.

Fig 25 shows the same kind of graph as Fig 24, but showing only the x displacement. As it can be seen, even for the highest force in the simulation, 100nN, there are x displacements of a few picometers, which are irrelevant in AFM. Usually, when dealing with non-circular shafts, the warping of the plane sections need to be accounted. Here, however, there is no significant warping of the plane sections, showing, as previously stated, that the theory of circular shafts can be safely used to deal with the deformation of an AFM cantilever.
Fig 25. $x$ displacement of the $zy$ plane section at the tip caused by torsion.

Fig 26 shows the 3D profile of Fig 25 with the deformations along $z,y$ disabled, since they are much smaller. If the 3 displacements were shown simultaneously, it would be impossible to see the warping of the plane sections, since it is has an effect orders of magnitude smaller.
In summary, it was shown that the force $F_z$ causes a bending 10 times greater than the force $F_x$ or $F_y$, and that these last two have the same order of magnitude deflection. In reality, the deformation of the force $F_x$ will be greater than that of $F_y$, because the cantilever is much thinner than the values used in this simulation (for the purpose of visualization, the thickness used in the simulations is 2 to 3 times greater than what is usually encountered in practice). But the major fact remains: the deformation caused by $F_x$ should not be discarded and should be considered in practice. It gives 10% of the deformation of $F_z$ and this value is very significant.

The force $F_{yM}$ causes torsion of the cantilever and this torsion only twists the cantilever, it does not displace the neutral axis. Since it does not bend the cantilever, it does not cause any deformation in the $z$ axis. A torsion does not change the deflection of the cantilever, and thus, does not change the reading on the photodetector, and the same occurs with the force $F_y$, which does not cause additional bending around the $y$ axis (upward, as the $F_x$ and $F_z$). So it does not contribute with the deflection either.
With these results, it is safe to ignore the torsion from the model, since it does not have any role in the topography artifact (additional z displacement).

2.3.2 2D Model

Since, as shown in section 2.3.1 3D Model, the only important forces in the creation of the topography artifact are the $F_x$ and $F_z$ in the parallel scan direction, then, performing a 2D simulation only (a slice of the 3D model) is enough to investigate all the relevant effects. Doing so has great computational advantages, since a 2D model is considerably faster than a 3D model. 2D simulations were done based on the 3D simulations and the results compared with the theory.

Fig 27 and Fig 28 show the von Mises stress of the forces $F_x$ and $F_z$. As it can be seen, the behavior is the same as the 3D model (Fig 13 and Fig 15). The major difference is that the tip is less deformed in comparison to the 3D case, giving more realistic results.

Fig 27. Von Mises stress on the cantilever. Force on the tip along the x axis. Deformation factor: 3000.

Fig 28. Von Mises stress on the cantilever. Force on the tip along the z axis. Deformation factor: 400.

Fig 29 and Fig 30 show the neutral axis x, z normalized displacement. The behavior is exactly the same as Fig 17 and Fig 19.
Fig 29. Normalized x displacement along the neutral axis.

Fig 30. Normalized z displacement along the neutral axis.
The tip $x, z$ displacement is also simulated in Fig 31 and Fig 32, respectively. Here, the difference between the 3D model, Fig 20 and Fig 22, is that the theory agrees much better with the simulation, since as stated previously, there is not as much deformation on the tip due to the point load, so the results are more accurate near the tip.

Fig 31. $x$ displacement of the tip.
2.3.3 2D Model, Constant Deflection

Since it was demonstrated that the 2D model is a valid replacement of the 3D model, it is now possible to simulate a dynamic AFM measurement. For this, it will be assumed that the frictional force ($F_x$) along the cantilever axis is proportional to the normal force ($F_z$); i.e., the standard formula for friction, $F_x = \mu F_z$ is assumed to hold [84]. Negative values of $\mu$ will be allowed to simulate both scans directions: forward and backward.\footnote{For more details see section 2.4.2 Constant Deflection.}

The simulation is run in such a way that the normal force $F_z$ is modified in order to keep the deflection constant, while the friction coefficient $\mu$ is being ramped up. In this way, a constant deflection can be attained with varying normal and frictional forces.

Fig 33 shows the deflection angle at the end of the cantilever, calculated for different frictional forces (shown as varying frictional coefficient). This angle is calculated from the
curl of the displacement and the simulation is run in such a way to make this angle equal to 0.01°.

![Deflection Angle Graph]

**Fig 33.** The deflection angle at the end of the neutral axis as a function of the frictional coefficient.

Fig 34 shows how the normal force $F_x$ varies as a function of the frictional coefficient. When the cantilever is moving in the forward direction (negative $\mu$), the normal force is greater; while in the backward direction (positive $\mu$), a smaller normal force is observed. The force at $\mu = 0$ is the setpoint and can be defined using a force curve. As it can be seen, it follows the same qualitative behaviors as explained in section 2.1 Qualitative Understanding. It is remarkable that the normal force can change up to 10% above or below the setpoint depending on the scan direction and frictional coefficient (for this particular cantilever). If a precise force is needed in an experiment, the normal force is being overestimating in the forward direction and underestimated in the backward direction. As it can be seen, the theory correlates well with the simulation.
Fig 34. Normal force $F_z$ in function of frictional forces.

Fig 35 shows the z displacement of the end of the neutral axis versus the normal force. As seen earlier, the z displacement of the tip is the same as the z displacement of the neutral axis. So, this graph is a direct evidence of the topography artifact, since it is a constant deflection simulation, and it shows how much, depending on the friction, the scanner will need to travel for it to keep constant deflection. Fig 36 shows the same graph, but as a function of the frictional coefficient.
**Fig 35.** z displacement of the neutral axis end versus normal force.

**Fig 36.** z displacement of the neutral axis end versus frictional coefficient.
Fig 37 shows an animation on how the frictional forces can alter the z position while maintaining constant deflection and also how the stress changes.

(a)

(b)

(c)

**Fig 37.** Different frictional forces applied on the tip while maintaining constant deflection. (a) forward scan direction, friction to the left; (b) no scanning, no friction; (c) backward scan direction, friction to the right. Note: for better visualization the forces on the tip are not to the same scale, they only show direction, not magnitude. Also in (a,c) a shadow image (b) is shown for comparison.

### 2.4 Theory

The study of the deformation of a cantilever can be found in any book about Structural Mechanics, Mechanics of Materials or Structural Engineering [11–17,33–37,57–59,69–72,74–83,85]. Here, it will be derived the cantilever deformation when there is a load applied to its tip. It will only be considered a deformation by a force along the axis of the cantilever (a parallel geometry), since, in this case, there is no torsion and the model simplifies drastically (and the artifact can still be accounted for).
2.4.1 Euler-Bernoulli Beam Theory

The Euler-Bernoulli Beam Theory [11,12,14,17,57,59,85] will be used for the bending deformation. The geometry of the cantilever is shown in Fig 38: notice the tip of the cantilever is a square pyramid. This model is used since it is the simplest to implement and the geometric factors of the tip are absent: it is only specified by the tip height $h_{tip}$. The shape of the tip can slightly change the results, but, here, its effect will be considered irrelevant and the only important geometric factor of the tip is its height.

![Fig 38. Geometric parameters of the cantilever.](image)

*Fig 38. Geometric parameters of the cantilever. T is the cantilever thickness, L is the cantilever length, W is the cantilever width, and $H_{tip}$ is the tip height.*

The principal aspect of the Euler-Bernoulli Beam Theory is that plane sections remain plane and normal to the neutral axis (the neutral axis is an imaginary axis where the stresses are zero).

A deformation of the cantilever results in a strain that can be calculated from this displacement as follows\(^\text{13}\):

$$
\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (1)
$$

Where $u_i$ is the displacement of the cantilever in the $i$ direction, $\varepsilon_{ij}$ is the strain tensor and $i, j = x, y, z$ the axis.

\(^{13}\) See Appendix A.
The displacements $u_i$ can be calculated from Fig 39 and Fig 40, where only loads in the $zx$ plane are considered and there is no displacement in the $y$ direction (parallel scan).

**Fig 39. Bending deformation of the cantilever.** As it can be seen, plane sections remain plane and perpendicular to the neutral axis.

**Fig 40. Zoom of Fig 39.** It shows the displacement vectors from the non-deformed to the deformed geometry.

In Fig 39, $w(x)$ is the deformation of the neutral axis (dotted line) and $\theta = \arctan w'(x) \cong w'(x)$ is the angle that this curve makes with the horizontal axis.
From Fig 40, the point $A$ is displaced to the point $A'$ and follows that $|OA| = |OA'| = z$, since plane sections remain plane (also for simplicity the Poisson ratio is considered zero). It follows then that $u_x = \overrightarrow{BA'}$ where the $u_x(x, y, z)$ is the $x$ displacement of the element in the position $(x, y, z)$. If bending occurs upward, there is a negative (positive) displacement above (below) the neutral axis. For a downward bending, the opposite behavior is observed.

Since $|BA'| = z \sin \theta$, it follows that $u_x = -z \sin \theta \approx -z \theta \approx -z w'(x)$. The displacement in the $z$ direction is equal to the displacement of the neutral axis plus the length of the segment $|BA| = z(1 - \cos \theta)$:

$$u_z = w(x) + z(1 - \cos \theta) \equiv w(x)$$  \hspace{1cm} (2)

Expressing the displacement as a vector (using $\cos \theta \approx 1$ for small angles):

$$\mathbf{u}(x, y, z) = -z w'(x)\hat{x} + w(x)\hat{z}$$  \hspace{1cm} (3)

Using the formula for the strain (1), the only non-null component is $\varepsilon_{xx}$ that is equal to:

$$\varepsilon_{xx} = -z w''(x)$$  \hspace{1cm} (4)

The cantilever is made of a linear isotropic material and its elastic properties are specified by its Young Modulus $E$. By Hooke’s Law, it follows that:

$$\sigma_{xx} = E\varepsilon_{xx} = -E z w''(x)$$  \hspace{1cm} (5)

For concave bending regions above the neutral axis ($z > 0$), the cantilever will be compressed, while regions below it will be expanded, hence the minus sign in $\sigma_{xx}$.

This stress (5) will cause an internal moment $\mathbf{M}$ (torque) calculated with help from Fig 41 to be:

$$d\mathbf{M} = \mathbf{r} \times d\mathbf{F} = (x \ y \ z) \times (\sigma_{xx} \ 0 \ 0) \ dA$$

$$d\mathbf{M} = (0 \ z\sigma_{xx} \ -y\sigma_{xx}) \ dA$$  \hspace{1cm} (6)
From (6), the $z$ component of this vector may cause a bending in the $y$ direction. However, the only way to create such bending is if there was a force perpendicular to the cantilever ($y$ axis) and such force is absent. Therefore, it will only be considered the moment in the $y$ axis, which causes the bending in the $z$ direction.

Integrating the $y$ component of (6), it follows that:

$$M_y = -E w''(x) \iint_S z^2 \, dA = -EI w''(x)$$  \hspace{1cm} (7)

Where $I = \iint_S z^2 \, dA$ is the moment of area. With the calculations of the internal moment, now the torque caused by the external forces (the forces on the tip) can be calculated for a torque balance equation. The position of the tip in relation of the neutral axis is
(L 0 \(-h_{tip}^*)^{14}, so the displacement vector of a point on the neutral axis at a distance x from the fixed end is given by \((L - x \quad 0 \quad -h_{tip}^*)\). So the external moment is:

\[
M = r \times F = (L - x \quad 0 \quad -h_{tip}^*) \times (F_x \quad 0 \quad F_z) \\
M = -\left(F_x h_{tip}^* + F_z (L - x)\right)\hat{y}
\]  

(8)

Equating the internal (7) to the external moments (8), it follows this differential equation:

\[
w''(x) = \frac{F_x h_{tip}^*}{EI} + \frac{F_z}{EI} (L - x)
\]  

(9)

Solving equation (9) with the boundary condition of the cantilever being pinned (i.e. \(w(0) = w'(0) = 0\)):

\[
w(x) = \frac{F_x h_{tip}^*}{2EI} x^2 + \frac{F_z}{6EI} (3L - x)x^2
\]  

(10)

The difference in the equation (10) and the usual displacement \(w\) found in the literature [4,8,86] is the additional term dependent on \(F_x\), which is the frictional force.

2.4.2 Constant Deflection

As stated multiple times previously, CM-AFM is a technique of constant deflection, and in AFM, the term deflection is used to mean angle. Since the photodetector measures angle and the setpoint determines a deflection (a signal in the photodetector), a deflection is the same as an angle. As said previously, this angle of deflection \(\theta\) is just the derivative of \(w\) (i.e. \(w'(x)\)). This angle changes with the distance, for a setpoint it will be used the angle at the end of the cantilever \((x = L)\), since the further away from the cantilever base, the greater the angle is, and since the laser is reflected the cantilever, the greater the angle, the greater the sensibility will be. Equating this deflection \(\theta\) with a deflection setpoint \(\varphi_s\):

\[\]

\(h_{tip}\) is the tip height, while \(h_{\text{tip}}^*\) is the corrected tip height, the height of the tip from the apex to the neutral axis and is equivalent to \(h_{\text{tip}}^* = h_{\text{tip}} + T/2\), where \(T\) is the thickness of the cantilever.
It will be assumed that the frictional force \( F_x \) is proportional to the normal force (Amonton’s Law), \( F_x = \mu F_z \) [84]. Where \( \mu \) is the frictional coefficient and here it will be considered that \( \mu > 0 \) means a cantilever moving from right to left (backward direction) and \( \mu < 0 \) indicates a cantilever moving from left to right (forward direction).

The deflection setpoint \( \varphi_s \) is defined like it is usually done in AFM, by means of a force curve. In a Force Curve (section 1.5 Force Curve), the surface is approached on the same point, so the tip does not move quite as much (in the surface plane), so this problem can be regarded as a static one with no friction. In this way, the deflection setpoint can be defined by means of a force setpoint \( F_z \), and this force means a normal force that would be done if there were no friction \( (F_x = 0) \). It then follows from (11):

\[
\varphi_s = \frac{F_z L^2}{2EI} \tag{12}
\]

The normal force done while scanning at constant deflection can be found by combining (11) and (12) with the friction formula \( (F_x = \mu F_z) \):

\[
F_x = F_z \frac{L}{L + 2\mu h_{tip}^*} \tag{13}
\]

The normal force that is expected to be done, \( F_s \), is not really the force that is actually being applied, \( F_z \). Since the scan direction (the signal of \( \mu \)) changes this force, the normal force will differ from the backward direction to the forward direction, and none of those will be equal to the setpoint. Moreover, regions with different friction coefficients (modulus of \( \mu \)) will have different normal forces, even in the same scan direction. Nevertheless, despite the normal force changing from region to region and in each scan direction, the deflection will always stay constant.

The ratio of the normal forces in the backward and forward directions is:

\[
\frac{F_{\text{backward}}}{F_{\text{forward}}} = \frac{F_z|_{\mu>0}}{F_z|_{\mu<0}} = \frac{2L}{2|\mu| h_{tip}^* + L} - 1 \tag{14}
\]
This ratio is always less than 1, so in the backward direction the normal force is always smaller than the forward normal force. This is in agreement with the qualitative picture (section 2.1 Qualitative Understanding) made before and the simulation (section 2.3.3 2D Model, Constant Deflection, Fig 34). In the backward direction, the frictional forces will bend the cantilever more, so the normal force will be smaller, while in the forward direction, the frictional forces will unbend the cantilever, so the normal forces will be greater.

2.4.3 Topography Artifact

The formula for the cantilever displacement (3) is:

\[ u(x, y, z) = -z w'(x) \hat{x} + w(x) \hat{z} \]

(3)

Since the tip is in contact with the surface, it is important to know how it moves. Substituting \( w, F_x, F_z \) (equations (10) and (13)) and evaluating it on the tip \((x = L, y = 0, z = -h_{tip}^*)\).

\[
P_{tip} = u(L, 0, -h_{tip}^*) = F_s \frac{L^2 h_{tip}^*}{2EI} \hat{x} + F_s \frac{L^3(2L + 3\mu h_{tip}^*)}{6EI(L + 2\mu h_{tip}^*)} \hat{z}
\]

(15)

Comparing the z displacement of the tip, \( P_{tip} \), from a region with friction to a region without friction, as this matches the experimental setup shown in section 2.2 Experimental Results, where the tip moves from silicon oxide to graphene:

\[
\Delta h = \left( P_{tip} \bigg|_{\mu} - P_{tip} \bigg|_{\mu=0} \right) \cdot \hat{z} = -F_s \frac{L^3 \mu h_{tip}^*}{6EI(L + 2\mu h_{tip}^*)}
\]

(16)

It should be noted that there is no loss of generality when assuming one region is frictionless. In order to get the height difference between two regions of non-null friction coefficients, \( \Delta h \bigg|_{\mu_1} - \Delta h \bigg|_{\mu_2} \) can be used instead of (16).

The experimental results show that the artifact becomes more positive with the force in the forward direction \((\mu < 0)\) and more negative in the backward direction \((\mu < 0)\). From the formula of \( \Delta h \) (16), if follows that \( \Delta h > 0 \) for \( \mu < 0 \) and \( \Delta h < 0 \) for \( \mu > 0 \), as expected from the experiment.
Fig 8. Top Panel: Experimental data of the height of the graphene in function of the setpoint (force) for 4 different scans. Both forward (trace) and backward (retrace) scanning directions for the perpendicular and parallel directions.

It is more usual to use the spring constant $k$ instead of the Young modulus $E$ when dealing with AFM, also it is preferable to use the geometric parameters of the cantilever instead of the moment of area $I$. The moment of area is $I = \iint z^2 \, dA = (T^3 W)/12$. By means of Hooke’s Law in absence of friction, the spring constant can be calculated; $F_s = kw(L)$ which can be solved for $k = 3EI/L^3$. Making these substitutions on $\Delta h$ (16) and using the fact that $h^*_{tip}$ is small compared to $L$ it follows that:

$$\Delta h = -F_s \frac{\mu h^*_{tip}}{2kL} \tag{17}$$

Using the experimental cantilever parameters (length: 374 $\mu$m, width: 26 $\mu$m, spring constant: 0.075 nN/nm), if follows that:

$$\Delta h = -0.3\mu F_s \tag{18}$$

Which, in comparison to the experimental data, gives a frictional coefficient of 0.4 to the silicon oxide. The value $\mu$ found using this equation is not actually the friction coefficient of the silicon oxide, but rather the difference of friction coefficients of both materials. A formula that better express the artifact for regions with non-zero friction coefficient is:
\[ \Delta h = -F_s \frac{h_{tip}^*}{2kL} \Delta \mu \]
Conclusions

The behavior of an Atomic Force Microscope was investigated, including how the cantilever moves and how this movement is translated into an image. Using the knowledge of the cantilever deformation, it was possible to gain insight on how to properly use the microscope in the Contact Mode, and how this is far from obvious and intuitive in the literature. The lack of understanding of the frictional forces on the parallel scan in the literature was also pointed, as it is usually not mentioned (frictional forces are mainly mentioned only on Lateral Force measurements). Nevertheless, this work shows that the friction plays a major role in image acquisition, giving rise to topographic artifacts when operating in a parallel scan.

Through simulations in Comsol Multiphysics, it was possible to confirm the analytical formulas of the theory. The simulation was of utmost importance for confirming the theoretical prediction of the artifact and to better explain the experimental results, also for highlighting the major factors in the cantilever behavior: the deflection caused by normal forces are about an order of magnitude larger than deflections caused by frictional force. Nevertheless, such frictional forces can still produce height variations in the range of few nanometers depending on the circumstances. Also, the torsion of the cantilever, caused by frictional forces perpendicular to the cantilever, does not produce any additional vertical deflections. Therefore, they create no topographic artifacts and, as a consequence, the perpendicular direction should be the preferred one.

It was also seen that since frictional forces parallel to the cantilever yield additional cantilever deflections and AFM is a technique of constant deflection, these frictional forces act to change the normal force during scan (while maintaining constant deflection). Thus, depending on the scan direction acquired, forward or backward, the topographic image can change substantially. This is a major problem since, in the literature, it is usually not specified which channel was used during image acquisition. Moreover, some microscopes only acquire only a single channel and, since the user has not actually seen the other channel, the artifact may pass unnoticed.

In recent years, Contact Mode has not been used very often, as Non-Contact or Tapping modes [2,4–6,8,9] seem a better choice for topography measurements. Therefore, this artifact
may seem less relevant, but Contact Mode still is a great tool for nanomanipulation and nanomodification. These techniques of modifying matter at the nanoscale require very precise force and positioning controls. If they cannot be controlled precisely, there is little hope of successfully controlling the experiment. Since the major parameter in nanomanipulations is the force being done on the sample surface, if there is no control or methodic way of producing the same force (scan angles may vary during experiments), the results might not be as accurate as expected.

Thus, with the new insight that the preferred way to perform Contact Mode AFM is in the perpendicular direction, where it is possible to avoid any topographic artifacts and, at same time, acquire useful frictional data (using the Lateral Force AFM).
References


Appendix A

Here it will be derived a formula related to the Infinitesimal Strain Theory, available in any good book in Structural Mechanics. A geometric derivation will be given of the relationship between stress and displacement.

In Fig 42 is shown a rectangle with dimensions $dx$ and $dy$ deformed by the displacement vector $\mathbf{u} = u_x \hat{x} + u_y \hat{y}$.

The normal strain in the direction $x$ is simply the relative change in the distances of the sides of the square.

$$\varepsilon_{xx} = \frac{a'b' - ab}{ab}$$ \hfill (20)

From Fig 42 it follows directly from Pythagoras theorem:

$$a'b' = \sqrt{\left(dx + \frac{\partial u_x}{\partial x} dx\right)^2 + \left(\frac{\partial u_y}{\partial x} dx\right)^2}$$ \hfill (21)

Therefore, for infinitesimal $dx$ and linear terms of the derivatives of the displacements:

$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}$$ \hfill (22)

And, likewise, the normal stress in the $y$ or $z$ directions (not shown, but easily generalized to three dimensions) can be defined.

Next, the engineering shear strain$^{15}$ $\gamma_{xy}$ is calculated, $\gamma_{xy} = \alpha + \beta$. Its relationship with the strain tensor is simply as $\varepsilon_{xy} = \gamma_{xy}/2$.

From Fig 42 it follows that:

$^{15}$ The engineering shear strain $\gamma_{xy}$ is calculated from the change in angle from the lines $ab$ and $ac$ to the lines $a'b'$ and $a'c'$, respectively. The tensorial shear strain $\varepsilon_{xy}$ is half the shear strain because in this way the equations are symmetric and are tensorial correct; the tensorial strain $\varepsilon$ transform as a tensorial equation, but the engineering strain $\gamma$ does not.
\[ \tan \alpha = \frac{\frac{\partial u_y}{\partial x} \, dx}{dx + \frac{\partial u_x}{\partial x} \, dx} \approx \frac{\partial u_y}{\partial x} \]  
(23)

And similarly for \( \beta \). Since \( dx \) is infinitesimal so does \( \alpha \), therefore \( \alpha \approx \tan \alpha \), and it follows that:

\[ \varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \]  
(24)

Combining the formula for the normal stress (22) and shear stress (24), it follows that the stress as a function of the displacements is given by:

\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial j} + \frac{\partial u_j}{\partial i} \right) \]  
(25)

Where \( i, j \) are the \( x, y, z \) axis.

Fig 42. Infinitesimal deformation.