PeakForce Tapping™ (PFT) and ScanAsyst™ (SA) are two Atomic Force Microscope (AFM) imaging techniques that have been recently introduced by Bruker. In this application note we will explain the underlying physical background, fit PFT into the framework of existing AFM modes, and show the benefits of these new modes through application examples.

**Why Were AFMs Previously Difficult to Use?**

Let’s examine briefly the actual workflow necessary to run an AFM experiment. A typical session starts with sample preparation and AFM mode selection. The latter sometimes dictating the former. Once the sample is ready, the AFM has to be set up (i.e., the sample has to be mounted, the scan mode selected, a tip inserted, and the detection system aligned). After that, the system has to be brought into “feedback” and the feedback constantly tuned by the operator according to the scan conditions to ensure proper operation. Following the successful acquisition of an image it has to be analyzed and presented.

If one analyzes this typical workflow across applications and user experience, the crucial step is the actual adjustment of the AFM feedback parameters. It is by far the most time-consuming and nuanced part of an AFM experiment, and thus offers the most potential benefit to the user for automation. In short, ScanAsyst automatically provides you with consistent, expert-quality results independent of user experience.

To put the capability of ScanAsyst into context, it is useful to examine the existing AFM scan modes to better understand how ScanAsyst, and its underlying mode PeakForce Tapping fit into the modes hierarchy.

**Fundamentals of AFM Operation**

In atomic force microscopy a sharp probe is brought into close proximity to a sample. Probe and sample are subsequently moved relative to each other in a raster pattern, and a quantity is measured in a serial fashion at discreet locations (pixels). Figure 1 shows a schematic of a probe in an AFM system.
The external disturbance is the tip-sample interaction as measured through the cantilever displacement sensor. The setpoint value is a user input that determines the magnitude of the tip-sample interaction. For example, in conventional AFM the setpoint represents the imaging force. The resulting error signal (or difference between the setpoint and actual value) is processed by a Proportional-Integral-Differential (PID) feedback controller that drives the z-piezo to minimize the error signal, thereby realizing the desired setpoint.

**Contact Mode**

Contact mode is the easiest AFM mode to understand, and it is also the fundamental basis of such additional modes as Scanning Capacitance Mode (SCM), Scanning Spreading Resistance Mode (SSRM), etc. A typical AFM cantilever is shown in figure 3.

The cantilever and tip are typically manufactured as one unit from silicon. Common dimensions are about 100µm for the length of the cantilever, with <10nm for the tip radius and springs constants from 10mN/m to 100N/m. The tip itself can have various coatings to enable its sensitivity to a certain interaction to be measured – ranging from a metal for conductivity to a ligand for biological specificity. Any interaction between the tip and sample surface is measured by monitoring the displacement of the free end of the attached cantilever. There are several schemes to accomplish that task, including beam-bounce, capacitive sensor, interferometry. A beam-bounce scheme, where a laser beam is reflected off the cantilever into a segmented photodetector is arguably the most common and established for a variety of reasons. The fixed end of the cantilever can be mounted either static or on a small actuator to enable dynamic imaging modes. During operation the cantilever/probe is part of a modified classical closed-loop feedback system (see figure 2).

The tip-sample gap (G) is G = Z-D. D is the deflection of the free end of the lever caused by tip-sample interactions. (For a closer look into tip sample interaction look into Mie potential in common physics textbooks.) G is directly proportional to the applied force action on the cantilever.

The small (angular) movement of the lever is commonly measured by a laser beam that is reflected off the cantilever and directed onto a split photodetector, as shown in figure 4. With that setup, the lever motion becomes proportional to the movement of the laser beam on the split photodetector amplified by B = 3s/l, with s being the distance between the cantilever and photodetector, and l the cantilever length. It is, however, important to note that one can not simply increase the distance from the cantilever to the detector to achieve more sensitivity. By increasing the distance, the spot size of the beam on the detector also increases, in turn making the actual sensitivity of the system independent of l and proportional to 1/s.
A basic AFM operation, which helps explain contact mode, is the force-distance curve. Here the cantilever is brought from a location above the surface but within the range of the z-piezo \((Z < Z_{\text{piezorange}})\) toward the surface until the tip contacts the surface. Any further movement of the z-piezo toward the sample surface will result in an upward deflection of the lever and/or sample deformation. The z-scanner position is commonly generated by a triangular waveform applied to the z-piezo. A schematic of a force curve is depicted in figure 5.

It should be noted that to obtain a force curve, the z-feedback normally used to keep the cantilever deflection constant has to be turned off. Points 2 and 4 describe two important occurrences in a loading curve. These are the points where the force generated by the tip-sample interaction force is not balanced by the restoring force of the cantilever, i.e., \(dF/dx > k\) at point 2. Setpoint denotes the deflection value used for the z-feedback. To convert the vertical axis from the photodetector output in volts to units of force, the system must be calibrated. The first step is to calibrate the photodetector output to the actual cantilever displacement, commonly referred to as “deflection sensitivity.” That step is simply carried out on a hard sample with the assumption that the tip-sample gap is zero \((G=0)\). The vertical axis now has the units of length. The second step is the determination of the cantilever spring constant. Force curves in themselves can reveal a variety of sample properties, such as adhesion and compliance. As an aside, there is an imaging mode called Force-Volume that is based on pixel-by-pixel analysis of force curves, however, due to its slow speed, it is not often used. The most common use of force curves is in combination with any of the forms of SPM imaging in a “point-and-shoot” fashion.

Contact mode imaging is carried by simply keeping the setpoint (point 3 in the force curve diagram) constant while raster scanning the tip and sample relative to each other. The movement of the z-piezo then becomes the sample topography that is plotted as a function of xy. The user has to make sure that the feedback loop is fast enough to allow the z-piezo to respond to changes in sample topography but slow enough to avoid oscillations of the system. Even though reasonably easy to operate, contact mode has the inherent drawback that lateral force exerted on the sample can be quite high. This can result in sample damage or the movement of relatively loosely attached objects. A solution to that problem was to oscillate the cantilever during imaging, which led to TappingMode™ Imaging.

**TappingMode**

The solution to the problem of having high lateral forces between the cantilever and surface, but still maintaining very high lateral resolution, is to having the tip touch the surface only for a short time, thus avoiding the issue of lateral forces and drag across the surface. This mode was hence referred to as TappingMode AFM. In TappingMode operation, the cantilever is oscillated at or near its resonance frequency normal to the sample surface. Typical amplitudes of oscillation are in the range of tens of nanometers, and thus very small compared to the cantilever length.
In order to explain TappingMode operation, it can be useful to examine the dynamics of operation. Assuming air damping is the dominant factor, the movement of the cantilever can be described using the (sinusoidal) driven damped harmonic oscillator model:

\[
m* \frac{\partial^2 z}{\partial t^2} + b \frac{\partial z}{\partial t} + k z = F_0
\]

with \(m^*\) being the effective mass of the cantilever, \(z\) the displacement of the lever, \(b\) the damping coefficient, \(k\) the spring constant, and \(F_0\) the driving force \((F_0 = k A_0)\). With the natural frequency:

\[
\omega_0 = \sqrt{\frac{k}{m^*}} \quad \text{and the relaxation time} \quad \tau_0 = \frac{m^*}{b}
\]

one can write the amplitude of the lever as:

\[
A(\omega) = \frac{A_0}{\sqrt{1 - \left(\frac{\omega}{\omega_0}\right)^2} + \frac{1}{\left(\omega_0 \tau_0\right)^2} \left(\frac{\omega_0}{\omega}\right)^2}}
\]

An important parameter to consider here is the quality factor “Q” of the system. Q is the ratio of the energy stored in the system divided by the energy loss per cycle. In the case of a lightly damped system, the Q can be written as \(Q = \frac{\omega_0}{\tau}\). The maximum amplitude at resonance then becomes: \(A_r = A_0 Q\).

A typical response curve of a cantilever is shown in figure 6. Typical TappingMode operation is carried out using amplitude modulation detection with a lock-in amplifier. This means a frequency close to the cantilever resonance is selected, and the tip-sample spacing is changed to maintain a constant cantilever amplitude without changing the drive frequency. Similar to contact mode, the movement of the \(z\)-piezo when plotted as a function of \(xy\) becomes our sample topography.

It is important to emphasize that we are not measuring a direct force in TappingMode. The curve shown in figure 7 is constructed by adding the short range repulsive and long range attractive forces.

When the probe approaches the sample, it experiences an attractive force and is pulled toward the surface until contact is made. From that point on, the attractive interaction forces dominate the response. The probe can then be retracted and additional information can be extracted from that trace. The TappingMode AFM, while experiencing these interactions, does not actually measure this force curve, nor the direct forces between the tip and the sample for that matter. The TappingMode AFM oscillates back and forth on this curve, interacting without being in direct control of the force, and reporting only an average response of many interactions though the lock-in amplifier. One can certainly measure the reduction of cantilever amplitude as tip and sample approach each other, as is shown in figure 8, but it must be understood that each point on that curve represents an average value and not a single interaction.

While this is in no way detrimental to basic imaging, it restricts the information beyond sample topography that can...
be gained and unambiguously assigned to a certain sample property. This is unlike the previously shown force-distance curve, during which one has direct control and is able to extract useful sample information.

Additionally, the inherently unstable feedback situation in TappingMode operation makes it quite difficult to automate some of the scan adjustments. Forces can vary when going away from a steady-state situation. This will occur while scanning rough surfaces, as the amplitude error at the sharp edges can correspond to interaction forces one order of magnitude higher than that of steady-state. Amplitude error incurred force is the leading cause of tip damage, and such damage occurs because the feedback is not directly controlling interaction force. On samples exhibiting high adhesion forces, a tip amplitude has to be selected that is high enough to ensure that the tip is actually leaving the sample surface. The higher the tip amplitude, the higher the energy stored in the lever and subsequently the imaging forces (see Appendix for a simple example). Operation in fluids suffers from drift due to temperature changes and/or changing fluid levels.

At this point, we have established that the adjustment of the feedback system is a task that is essential to achieving reliable information from the AFM. It is easier to control a contact mode scan when compared to a TappingMode scan due to the added complexity of the oscillating system. While past attempts have been made to adjust imaging parameters automatically in TappingMode, no method has proven competitive with an experienced user for the broad range of samples commonly studied with AFMs. This is because TappingMode operates at cantilever resonant frequency, where the cantilever dynamics are relatively complicated. For example, the cantilever dynamics can be dramatically changed by changing the amplitude set-point. This causes the highest usable gain to change, which in turn requires the optimal set-point to change. Additionally, the tapping dynamics depend strongly on the sample properties. A well-tuned feedback loop for the soft part of the sample can cause feedback oscillation for the hard part of the sample, rendering optimization of the parameters for every part of the sample very difficult. Furthermore, the long time constant (milliseconds) of the cantilever resonance also prevents instantaneous optimization at each imaging point. Finally, the direct force control of contact mode imaging and thus added information available are lost in TappingMode. TappingMode does however offer the undeniable benefit of lateral force free imaging, which has made it the dominant imaging mode in AFM to date.

**PeakForce Tapping**

PeakForce Tapping operates similarly to TappingMode in that it avoids lateral forces by intermittently contacting the sample. However, it is very different from TappingMode in that it operates in a non-resonant mode. The PeakForce Tapping oscillation is performed at frequencies well below the cantilever resonance, thus avoiding the filtering effect and dynamics of a resonating system. In PeakForce Tapping, we now have an oscillating system that combines the benefits of contact and TappingMode imaging: direct force control and avoidance of damaging lateral forces. The differences to a conventional force curve (and force volume imaging) are that the z-position is modulated by a sine wave and not a triangular one, thus avoiding unwanted resonances at the turnaround points. A triggering at the peak force and an algorithm to extract the force curves from even noisy backgrounds complete the package. Continuous force curves can now be executed at frequencies between 1kHz and 10kHz, which in turn enables imaging speeds that are comparable to TappingMode imaging. The general operation is illustrated in figure 9.
All the curves shown are experimental data obtained using a silicon probe approaching a silicon surface. The top curve represents tip trajectory as it approaches the sample. Depicted underneath are plots of deflection (or force) as a function of time and z-position, respectively. The latter being the more familiar representation. The dashed line is the zero force (no load) reference, established when tip is not interacting with the sample. As the tip approaches the sample surface, it will experience long-range van der Waals attraction until $\frac{dF}{dx} > k$, causing the cantilever to jump into contact with the sample. After contact, the short range repulsive forces dominate the interaction, leading to the peak point at the approaching curve. When the tip begins to unload it goes through an adhesion minimum, usually caused by capillary meniscus and finally becomes free.

PeakForce Tapping refers to the proprietary control method that uses the individual peak force points as triggering mechanisms to force the the z-piezo to retract. Its effectiveness can be seen from the force curves in the left column. The feedback algorithm recognized the local peak force even though the setpoint is below the baseline. Operating below the baseline allows operation at very low forces, which in turn is crucial for obtaining high-resolution data on soft samples. It is important to note for comparison purposes that all curves shown were obtained using a cantilever with a spring constant of 40N/m, as is commonly used in TappingMode operation. With a softer cantilever, the controlled interaction force can of course be much lower due to the higher force sensitivity. The typical repetition rate of 2kHz allows for imaging speed speeds that are comparable to TappingMode operation. An example of clearly resolved atomic steps on graphene is shown in figure 10.

ScanAsyst

ScanAsyst uses the previously described PeakForce Tapping mechanism, which decouples cantilever response from resonance dynamics, to automatically adjust all critical imaging parameters. Because the peak force feedback directly controls the interaction force, there is no distinction for peak force for soft or hard parts of the sample. Direct interaction force control enables the possibility of producing a uniformly optimized feedback loop for all the points of the inhomogeneous sample. Using a patent pending image correlation algorithm, feedback oscillation is detected and eliminated in a matter of milliseconds. A real-time feedback loop constantly monitors and adjusts the gain to keep the data quality within a predefined noise level (unlike manual gain adjustment where usually one gain is used for a whole image). ScanAsyst optimizes the gain according to current sample condition at different locations. The ScanAsyst algorithm also optimizes the set-point to the minimum force required to track sample surfaces, controls the scan rate, and can automatically lower the z limit if necessary. This results in extremely high-quality images without user adjustment of imaging parameters and without the normally problematic AFM user interfaces exhibiting numerous and often confusing parameters.

A basic ScanAsyst interface is shown in figure 11. The whole “Feedback” section is on “autopilot” and is constantly updated. In addition, ScanAsyst also sets the actual scan speed and the z-limits. The only task left for the user is the selection of the actual scan area, which can be achieved by either typing the appropriate values in the corresponding fields or by simply using the mouse and drawing a box inside the image acquired. If the flexibility of partial or fully manual operation is desired, the user can set the AutoControl field to individual and choose which parameters should be selected by the system and which by the human operator.

The underlying calculations enabling ScanAsyst happens on the fast FPGA chips implemented in Bruker controllers. One of the key parameters controlling the auto-optimization procedure is the “noise threshold” parameter. Noise threshold is determined by analyzing the high-frequency components of the AFM data and adjusting, for example, the feedback gains accordingly. The noise threshold is also automatically adjusted by the AFM itself after it has completed a full frame, with values typically ranging from 0.1 to 1. The reasoning behind this feature is that not all scans require the ultralow noise that Bruker AFMs are
Figure 11. Screen shot of the basic ScanAsyst interface. All feedback settings and the scan rate are automatically calculated by the AFM.

Figure 12. 80nm scan of C\textsubscript{18}H\textsubscript{38} alkane chains obtained in PeakForce Tapping. The inter-lamellar distance is only 2nm!

Figure 13. Screen shot of the expanded ScanAsyst interface. If desired, ScanAsyst allows flexibility for parameters to be adjusted manually.

capable of achieving (e.g., the Dimension\textsuperscript{®} Icon\textsuperscript{®} has a noise level of 30pm!). If a sample exhibits features hundreds of nanometers high, picometers of noise are simply not visible. It is, however, quite important to properly follow the often steep sample features without bringing the actual scan speed to a crawl. ScanAsyst consequently uses a more aggressive feedback gain for imaging. On flat samples like silicon wafers, a very low noise threshold is chosen by the auto-optimization routine, which results in less aggressive gain parameters to take full advantage of the ultra-low noise levels of the AFM. By selecting a discrete threshold we are asking the AFM to adjust feedback and imaging speed to get a certain result instead of manipulating the feedback loop trying to figure out what the actual result is!

The data that ScanAsyst produces is often better than what even a seasoned AFM expert can produce. More so, this data is often generated during the first time imaging a sample, is reproducible, and is independent of the skill of the AFM operator. The 80x80nm\textsuperscript{2} image of the alkane C\textsubscript{18}H\textsubscript{38} deposited on HOPG in figure 12 strikingly illustrates that point.

ScanAsyst does have an amazing amount of flexibility built-in that allows users to fully or partially control the PeakForce Tapping operation. An example of an expanded ScanAsyst user interface is shown in figure 13.

In this specific example, an advanced user elected to manually control all relevant feedback parameters, with the exception of the imaging speed. At the bottom of the dialog are two previously not mentioned parameters. “Peakforce Amplitude” refers to the actual z-excursion of the AFM tip during operation. The value is pre-set for the specific experiment selected, e.g., operation in air or fluids, but can be changed if desired. “Lift Height” refers to a value that is used to determine any background signals affecting the data (it is not related to the LiftMode feature, where the tip follows a previously scanned line). This becomes especially important for operation in fluids where small volume changes due to evaporation or fluctuations in temperature can have significant effects on AFM operation.
During ScanAsyst/PeakForce Tapping imaging the user can constantly monitor the integrity of operation by looking at the built-in force monitor shown in figure 14. Here the top graph depicts the familiar force versus z plot, whereas the bottom shows force versus time.

PeakForce Tapping also avoids another phenomena that plagues TappingMode. The cantilever amplitude in conventional TappingMode can change as a result of both long range and short range interactions. As a result, the height data represents the system response to a combination of interactions. PeakForce Tapping, on the other hand, only responds to short range interaction. The long range interactions (adhesive and electrostatic forces) are basically ignored for height control. Short range interactions are the key to high-resolution imaging. By consistently controlling the short range interaction forces, PeakForce Tapping enables image quality control with fewer artifacts linked to complication of the tip surface interactions and cantilever dynamics.

An example of a structure difficult to image in regular scan modes is shown in figure 15, which depicts a cross-section of a sample with very narrow trenches. This type of sample is very difficult to image in TappingMode because the geometry would cause the AFM to “stick” to the sidewalls, thus damping the tapping vibration and preventing the tip from reaching the bottom of the trench. A researcher using TappingMode would likely conclude that the trenches do not have flat bottoms or that they are significantly shallower than shown. Peak Force Tapping is insensitive to the effects that geometries like this have on a resonating system and therefore has no difficulty reaching the bottom of the trench.

Another type of sample where PeakForce Tapping solves problems commonly encountered in TappingMode are nested structures with steep and often high topographies. As one can clearly see in figure 16, the PeakForce Tapping image on the left is flawless, whereas the TappingMode image on the right shows streaking and some tip parachuting. This is again a direct effect of not operating at resonance, which enables direct force control and thus not being affected by the Q-factor of the cantilever.

Examples for operation in changing environments include heating and cooling experiments and scanning in fluids. Heating and cooling can be useful for learning about dynamics in melting and crystallization experiments. Imaging in fluids is a common and necessary operating mode for an AFM. Besides the obvious benefit of being able to study a sample under low force due to the lack of

Figure 14. Real-time shot of the force-monitor during imaging with ScanAsyst. This allows the user to constantly monitor the integrity of the imaging process.

Figure 15. 160nm linescan of steep trenches. The flat bottom indicates that the probe reached all the way.
usually high capillary forces, a lot of studies simply require the sample being immersed in fluids. Examples include the study of biological specimens under physiological relevant conditions or the examination of electrochemical phenomena for corrosion or battery research, to name just a few. It is often interesting or necessary to image samples under fluid or at temperatures above or below room temperature. ScanAsyst-PeakForce Tapping works well in these environments with several benefits over TappingMode. For one, it is not necessary to tune the cantilever at all, as the cantilever is operated at a fixed frequency. Consequently there is no re-tuning required when the temperature is changed or when changing from air to fluid operation. In TappingMode on the other hand, a temperature change causes changes in resonant frequency and Q of the cantilever, making it imperative that the drive amplitude and frequency are adjusted whenever the temperature is changed significantly. With PeakForce Tapping, the system is not being driven at the cantilever resonance, so it is not sensitive to changes in probe resonant frequency and Q. Any background changes caused by temperature or fluid level fluctuations that can influence operation are subtracted in real-time by the ScanAsyst software, allowing imaging forces as low as a few tens of pico-newtons. An example of a high-resolution image in buffer solution is shown in figure 17. One can clearly see the square origami DNA assemblies, the connection points on each corner, and the single DNA strand building blocks. An example of ScanAsyst operation at different temperatures is shown in figure 16.
temperatures is given in figure 18. The 500x500nm² images of C₆₀H₁₂₂ alkane with a lamella spacing of 7.5nm were obtained at room temperature and 70°C, respectively. At the elevated temperature, the alkane chains are able to slide into a more favorable energetic lower arrangement dictated by the underlying graphite substrate.

One of the strong points about ScanAsyst is that force curves are indeed available to the user to extract additional material specific information if desired. Using the High-Speed Data Capture (HSDC) functionality of the NanoScope® V Controller, a researcher can gather thousands of force-distance curves in one shot without interrupting the imaging process. The resulting force-curves can be extracted, correlated to the sample topography, and analyzed using NanoScope analysis or custom software. Bruker uses the capability of obtaining multiple force-distance curves at each image location in its PeakForce QNM™ package, which performs nanomechanical analysis in real-time. Figure 19 shows the resulting curves from a HSDC of 100ms on the top, and one selected curve on the bottom.

ScanAsyst and PeakForce Tapping have changed the landscape for AFM operation of basic imaging and nanomechanical analysis but this is far from the end. A
variety of modes, traditionally carried out in contact mode operation, can greatly benefit from combination with PeakForce Tapping. Electrical modes such as Scanning Capacitance Microscopy (SCM) or Tunneling AFM (TUNA) are two that would get a performance boost by reducing the lateral components stemming from imaging in contact mode. An example of a TUNA image obtained by combining the ScanAsyst/PeakForce Tapping is shown in figure 20. A scan of carbon nanotubes clearly shows the sample topography on the left and the current map on the right, highlighting the electrical connectivity of the nanotubes. This data is not obtainable using the traditional TUNA-contact mode combination due to excessive lateral tip-sample forces.

Conclusions
Tapping has long dominated the world of AFM. Its main advantage has been the lack of lateral forces that are inherent to contact imaging. At the same time, it has hindered the advancement of atomic force microscopy in some ways, due to the inherently complex nature of operation that has prevented automation of the adjustment of the feedback loop, arguably the most critical step. This application note shows that not only can PeakForce Tapping generate data that is equal and often better than TappingMode images, but that this data can be obtained reliably by a new user using ScanAsyst without sacrificing full flexibility for experienced researchers.
Appendix

Another way to look at the fact that we are not measuring a force but rather a derivative is shown here. Following Newton’s second law, the motion of the cantilever can be described as:

$$\frac{d^2 m_e}{dx^2} = -k_0 x + F_{ext} = -k_e x \quad \text{with} \quad k_e = k_0 - \frac{\partial F_{ext}}{\partial x}$$

with $k_e$ known as the effective spring constant. Thus, the effective resonance frequency becomes:

$$\omega_e = \sqrt{\frac{1}{m_e \left( k_0 - \frac{\partial F_{ext}}{\partial x} \right)}}$$

As the effective resonance frequency is the parameter the feedback signal is based upon, the force derivative, and not the force itself, is the crucial parameter here.

It may be beneficial to get an idea of the actual energy stored in the cantilever. Again Hooke’s law lets us calculate the elastic potential energy $E_p$ for a cantilever. Using a typical spring constant for a TESP lever of 40N/m and 10nm vibration amplitude, we get $E_p = \frac{1}{2} k z^2 = 2 \times 10^{-15} \text{[Joule]} = 12.5 \text{[keV]}$.

At 10% reduction in amplitude, the set-point results in a necessary energy dissipation of $0.1 \times 12.5 \text{ keV} = 1.3 \text{ keV}$. That number may look high, but one has to consider that the energy is dissipated over a large area when entering the contamination layer (see the literature for additional calculations).8-10

References

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