Virtual nano Reality Interface between an AFM and the Delta Haptic Device

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Abstract

Until today, manipulations [1] at the nanometric scale were achieved using Atomic Force Microscopy, which is not very intuitive to the user and require a high degree of training. Recently, some work has been done on haptic devices that would help give a better interface for nano-manipulations. Our aim is to provide a 3D Virtual-Reality interface capable of displaying simplified scenes for the user's convenience; it comes between the AFM and the Delta force-feedback device and allows user-friendly manipulation while minimising additional acquisition of data while in use.

[1]manipulation has been achieved, notably by the group at North Carolin University , see [**1**], [**3**], [**4**] and [**14**]

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CHAPTER 1

State of the Art

1. AFM

The AFM is constitued by a microlever which carries a pyramidal tip; an optical device allows measurements of vertical deflection of the lever.

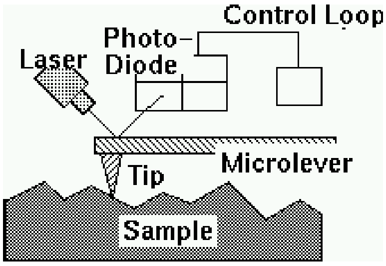


FIGURE 1. Principle of an AFM

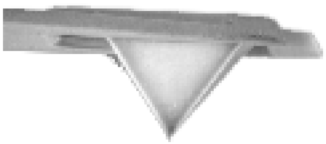


FIGURE 2. Example of an AFM tip

There are a number of different shapes of AFM tips (one can refer to `http://www.spmprobes.com` for further informations).

1.1. AFM operating modes. AFMs operate mainly in three different modes: *contact mode* , *non-contact mode* and *tapping mode.*

(1) Contact mode : the tip makes "physical" contact with the sample, and wanders over it so to maintain the *force* over the tip constant. Actually, this gives no information on the topography of the sample, but rather on the *forces* that apply on it; there is indeed a correlation between the topography and the forces it generate, but it night be important to keep this distinction in mind.
This mode is quite likely to damage the sample by friction; it can also be used for manipulation.
Also, the torsion of the microlever induces a lateral deflexion of the laser beam. Thus, using a four-quadrant photodiode, it is possible to measure both lateral and vertical deflexions of the lever, and this way to get information on the sample topography (actually, on the forces that influence the vertical behaviour of the tip) and on tip-surface friction forces on the same time.
(2) Non-contact mode : the tip has no physical contact with the sample. The *vibration amplitude* is maintained constant, which in fact gives "equi-gradient" surface. The resolution is not as good as in contact mode, but it is much less likely to damage the surface.
(3) Tapping mode : At each cycle, the tip lowers to the surface until it makes physical contact; amplitude is limited by repulsive interaction between surface and tip. With a constant scanning amplitude, it is possible to get informations about the sample topography.

1.2. AFM - surface interaction. When an AFM tip lowers to a surface, a snap in effect occurs. It is as if the surface was made of soap bubbles, that very suddenly begin to attract the tip. It is remarkable that even metals display this behaviour at nano-scale, though it is rather caracteristic of liquids in everyday world. This creates a hysteresis that leads to a distinction between the *topology* of the sample and the *forces* that take place on its surface.
In the same way, when leaving the surface, the AFM tip endures a snap out effect.

These effects are of *catastrophic* nature, which means that they occur extremely quickly, and that there is no telling when exactly they would

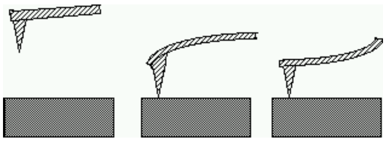


FIGURE 3. Snap-in effect; the snap-out effect would reverse the order of the images.

happen. However, it can be said that if the force gradient exceeds the lever stiffness coefficient, the snap effect occurs. As an illustration, a typical lever stiffness coefficiant is about 1 N/m.

In conclusion, we display some of the main potentials used to modelise contact interaction with surfaces. We can see that at long range, the potential tends to zero, while at very close range, it gets repulsive in an exponential manner. For the most advanced models, a region appears, where the potential is attractive.

2. Nanotubes

Carbon Nanotubes (CNTs) are produced by electrical discharges between two carbon electrodes or by catalysis; their shape and size cannot be controlled directly. At the EPFL, we use the electric arcs method, which produces samples of higher quality.
The typical CNT has a diameter about 10 nm, and a length of more than 1 μm.

2.1. Behaviour of CNTs towards surface. CNTs are maintained on the surface mainly through capillary and Van Der Waals forces. Forces applied by the AFM tip are negligible, as well as gravity.

2.2. Behaviour of CNTs toward each other. CNTs attract each other through Van Der Waals forces; they arrange in fiber-like structures, thus creating large and robust paterns. Such a formation is displayed in figure 6

ANother interesting feature of CNTs is *Multi-Wall CNTs* (MWNTs): these are CNT put into other CNTs like a telescopic antenna. This has an incidence on their rigidity.

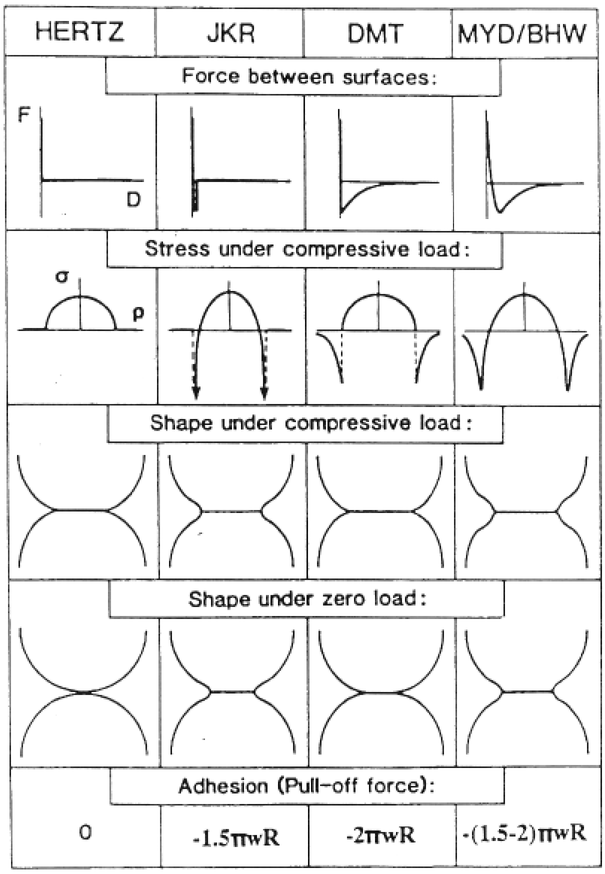


FIGURE 4. Some of the main potentials used to modelise contact, as presented in [**12**]

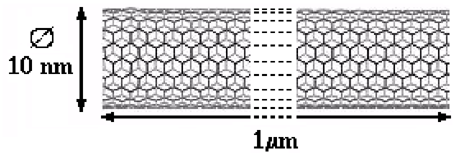


FIGURE 5. typical nanotube

2.3. Behaviour of CNTs toward AFM tips. The tip of the AFM is quite enormous compared with the CNTs: actually, the curve radius of the CNT is comparable with the curve radius of the extremity of the AFM tip (see [**2**]). Only the very extremity of the tip interacts with CNTs.

The force is attractive at long range, and becomes repulsive at closer range (See figure 4). Determining the exact range at which the potential becomes repulsive is quite far from a trivial

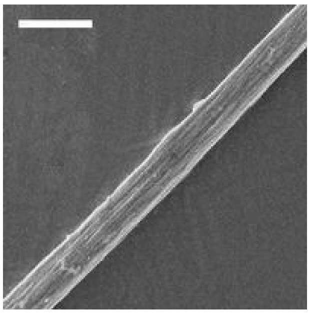


FIGURE 6. Nano-fiber constitued of CNTs

problem.
Like in the AFM - surface interaction, there is a snap in - snap out effect when the tip approaches a CNT, but this time, the effect occurs laterally (see figure 3, page 8).

At close range, one can consider nanotube-tip interaction similar to contact between solid bodies [1].

When pushed laterally, CNTs could translate (by sliding or rolling), rotate, bend or break (or any combination of those).

(1) Translating :
Translations of nanotubes can be divided into two categories:
- *sliding :* CNTs most of the time slide when pushed
- *Rolling :* Under certain circumstances (that remain to be clarified in the laboratory), CNTs roll.

Rolling would seem intuitive and close to the macroscopic world, but the exact behaviour is still to be understood (see [**1**] for instance). However, it is possible to say that unlike our macroscopic world, rolling requires more energy than sliding, and is not the priviliged behaviour. Rolling might occure when some specific features of the surface occure.

(2) Rotation : If pushed far from its center, a nano-tube can change its orientation.
(3) Bending : When maintained still by colloid particles, nanotubes react to stress by bending. They are extremelly elastic (permanent deformation is very unoikely to occur).
(4) Breaking : Despite of their strength, CNTs sometimes break when pushed. This event is catastrophic, in the sense that it happens suddenly and occurs in a very short time. It is not predictable (it is extremely difficult to predict whether a particular CNT will break, where it would, or under which stress the breaking is likely to occur).

2.4. Conclusion on CNTs. Some of CNT behaviours are still not very well-known. In addiction, it is difficule to know whether they are going to break, to roll or to translate (though on this point, statistical studies might give hints). However, the behaviour of nanotubes is fundamentally predictible (as pointed out in [**14**])

3. Nano-Manipulators

Several other groups are working on nano-scale manipulation, and some are specifically interested in force-feedback manipulation of CNTs.

3.1. North Carolina. The group at the University of North Carolina have developed a 6 Degree Of Freedom haptic device that controls an AFM. The impressive results are displayed in [**1**] and [**4**]. They have achieved the construction of a force-feedback device coupled to an AFM that allows the manipulation of objects at nano-scale. The computer also displays a three-dimensional scene that is supposely more intuitive than the usual two-dimensional false-colour displays used with AFMs (though for very flat samples, 2D is superior to 3D). However, what they call "Virtual Reality" is nothing more than simply the 3D rendering of the scene. There seems to be no actual calculation of a stylised world.

Virtual tools : This group has introduced an extremely interesting concept: the *virtual tool.* The virtual tool is a great step in abstraction of the tool for the user. It consists in programming

[1]However, experiences have occured, in which a CNT was bent and released several times (See [**1**] or [**3**]); in other circumstances, CNTs are subject to breaking. In these conditions, the approximation of non-deformable solids cannot be used.

typical manoeuvrs that will be exectuted automatically. For instance, the tip might execute a fast back and forth movement perpendiculary to its movement direction to push a CNT, thus creating a “virtual spoon”; the tip would then be displayed as a spoon to the user, who then has to care only about the simple movement of the virtual spoon, rather than the complex movement of the tip.

3.2. Tokyo. Another work of interest is the one done by the Institute of Industrial Science of University of Tokyo [**6**]: they have constructed a little 1 DOF force-feedback device, and also realised a real-time simulation of the forces that occur at the nanometric scale: non-contact forces (Van Der Walls, electrostatic and capillary) and contact (stiffness and damping on the sample). However, their work was aimed at surfaces covered with water layers; they did not work with nanotubes.

CHAPTER 2

Simple model of CNT-AFM interactions

Our aim is to produce an interface that would

(1) input data from the AFM and output both three-dimensionnal computer display and force feedback
(2) input data from the haptic device and output both display and commands to the AFM.

The interface has to compute a real-time simulation of the behaviour of the CNTs.

1. Accuracy of virtual-reality model

1.1. Dynamic model: blind man playing ice-hockey. At the macroscopic scale, as long as Newtonian force are involved, it is possible to compute impressive real-time simulations that fit the reality.
In our case, it is impossible. Some behaviours are of catastrophic nature, which means that they are both extremely fast and that it is very difficult to predict the time they occur with accuracy.
In addition, for certain circumstances, several behaviours can occur. This is typically the case of a nanotube being hit by an AFM tip: it could translate (sliding or rolling), rotate, bend or break.
As the AFM tip is used for both scanning and manipulating, it is impossible to have a continuous input of the sample situation. We are like a blind man playing ice-hockey, using his stick for both sensing the position of the puck and playing. The "sensing" is when the AFM is used in non-contact or tapping mode for scanning, and the "playing" is when the AFM is used in contact mode for manipulation.

Actually, we are not completely blind when the AFM is in contact mode, as this mode provides information on lateral forces (see sec. 1.1, page 7): it is therefore possible to have a general idea of what is going on at the nanoscopic scale (for instance, we could know that the CNT is stuck on the surface if we encounter resistance, and that it has just broken if all resistance suddenly ceases).

2. Definition of a possible model

Our aim being to manipulate CNTs, we can limit our model to a kinematic approach (we will not bother abour calculating the *forces*, such as friction).
We might as well neglict detailed features of the surface of the nanotube, such as bumps, and suppose CNTs perfect cylinders.

2.1. main behaviours and their parameters. Though the behaviour of CNTs cannot be predicted with certainty, we can point four main possibilities: due to a touch, CNTs might move, rotate, bend or break. Each of these behaviours can be caracterised by parameters:

(1) translation : movement direction
(2) rotation : pivot point, contact point, rotation angle (contact point displacement)
(3) bending : in a first approach, bending point, bending angle; in a second approach, position of several points along the CNT to fully describe the deformation.
(4) breaking : rupture point

As we will see,thanks to our strong approximations, we will be able to compute these elements.

2.2. translation. CNT translations divide in two categories: *sliding* and *rolling*. Unlike our macroscopic world, it is more difficul for CNTs to roll than to slide. For a first approximation, we will assume that all translations are simple slidings.
Under the assumptions that the tip stay stuck on the CNT (which is correct, as can be verified in [**2**]), the movement of the CNT is extremely simple: it follows the AFM tip. Computing the

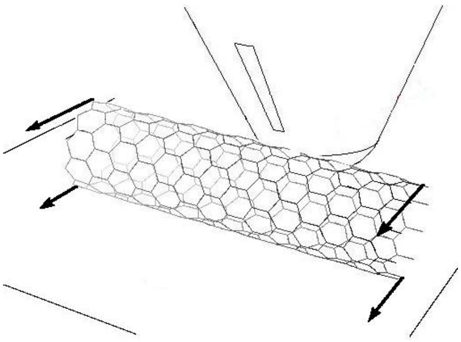


FIGURE 1. AFM tip pushing a CNT, causing it to slide.

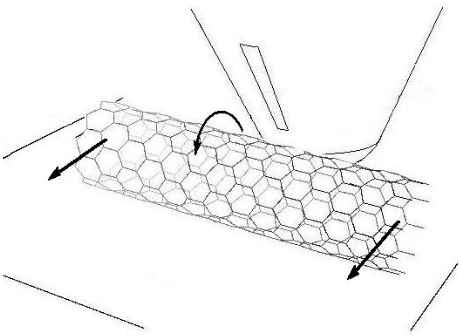


FIGURE 2. AFM tip pushing a CNT, causing it to roll.

new position of the CNT would consist in translating its position in the same direction and magnitude as the tip moved.

To ensure the AFM will not rotate (see section 2.3), a back and forth movement might be added to the linear movement of the AFM tip; thus, a "virtual" spoon-like tip would be obtained (see [**4**] for more details on "virtual nanotools")

2.3. Rotation. We will assume uniform friction on the surface where the CNT lies, and that the CNT stays stuck on the AFM tip. Rotation of a CNT might occur when the push is given far from its center. Under the assumption of uniform friction, we can calculate the pivot point by minimising the energy of friction [**14**].

Let be L the length of the CNT, x_0 the position of the pivot point and x_1 the position of the tip (push point); we then have

$$x'_0 = x'_1 - \sqrt{(x'_1)^2 - \frac{1}{2}(2x'_1 - 1)}$$

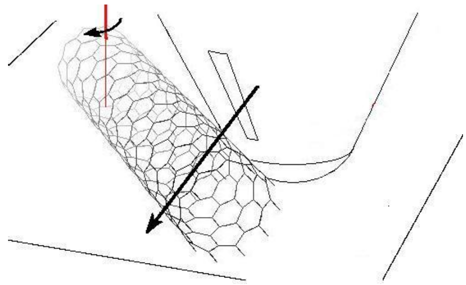


FIGURE 3. AFM tip rotating a CNT

where $x'_0 = x_0/L$ and $x'_1 = x_1/L$. See [**14**], and for a demonstration, see section 1, page 19 of this document.

Therefore, amongst the four parameters needed to describe the rotation (the two extremal points of the CNT, the pivot point and the tip position), one is known (the tip position), and the three other can be calculated, and thus real-time computed (providing that we know the initial position of the extremity of the CNT; this information would be provided by prior scans).

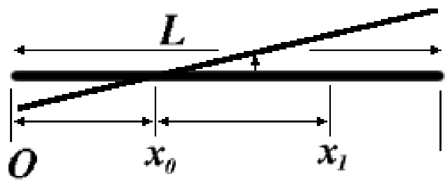


FIGURE 4. Schema of the situation discribed in the equation

2.4. Bending. Bending is far less simple that the two previous motions. To bend to CNT, one need "anchor points", generally colloid particles that "stick" certain point of the CNT; pushing a part of the CNT causes it to deform (see [**3**] or [**1**]).

One can distinct two categories of bendings: bendings with both CNT extremities stuck (rubber-like bending) or bending with one extremity free.

In the case of "free extremity bending", it is difficult to predict the position of the curving point. In a first approximation, we might consider the nearest anchor point to be the curving point.

In the case of "bound bending", we would naturally consider the AFM contact point to be the curving point.

2.5. Breaking. CNTs are extremely strong; thus, breaking of nanotubes is rare. We could suppose that the CNT breacks near the AFM contact point. However, we should strongly recommand a new scan to be performed if the CNT should break.

2.6. Recognition of the motion by the computer. To chose amongst the previour models, the computer could use the input provided by AFM cantilever deflexion. Calibration should be made (i.e. typical forces for each behaviour should be acquired). It is possible to assume that the typical behaviours of nanotubes have recognisable "signatures"; in [**14**], we can see caracteristic signatures that allow to distinguish between sliding translations and rolling translations. Using the continuous lateral force input, the computer could perform real-time update of the situation. It should also be capable of predicting significant divergence between the model and reality, that would trigger a scan.

CHAPTER 3

Implementation

1. Features

The module developped at the VRAI group recieves datas from the microscope in input , and returns the computed position of the nanotube.

input signals : To perform its task, the module needs to know the initial position of the CNT. Aditionally, the module recieves a continuous flow of informations about the AFM tip position and lateral force.

output signals : The module returns the real-time estimated state of the CNT. The term "state" here sould be understood as

- if no deformation occured: position of the CNT and position of the tip.
- in the bending case: position, curving point and deformation angle.
- in the breaking case: position of both sub-CNTs.

2. Input Signals

2.1. CNT Position. The position of the CNT has to be acquired by prior AFM scanning, and computed by a detection algorithm. To consider the postion of the AFM known, we need three informations: the 2D position of both extremities of the CNT (4 real numbers) and the CNT diameter.
The CNT diameter is a constant parameter (for each CNT; it changes from CNT to CNT); the positions of the ends of the CNT will provide initials conditions for our algorithm.

2.2. AFM Tip position. This information will have to be real-time updated. It allows calculation of CNT state without performing aditionnal scans, as the tip position repercutes on the CNT.

2.3. AFM Lateral Force. The lateral force ploted versus time displays caracteristic features for each of the typical behaviours we isolated. Therefore, a real-time analysis of the input allows the computer to decide which simple model is closer to what happens in reality at the end of the tip.

3. Implementation

Four classes were written in C++:

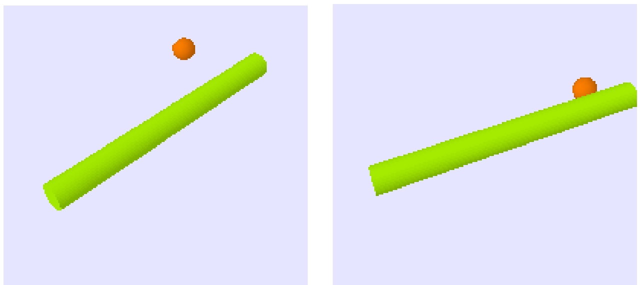
(1) `PhysTip` : Describes the position and radius of the end of the AFM tip; remembers the position of the previous step as well.
(2) `PhysCNanoTube` : Describes the position of the CNT. Decides which movement would occure inthe event of a contact with the AFM tip.
(3) `PhysWorld` : Contains one CNT and one AFM tip. Allows to move the AFM tip. Tests wether there is contact between the CNT and the AFM tip.
(4) `ContactException` : Message sent when the AFM comes in contact with the CNT, which triggers the update of the CNT position.

To visualise the output of the program, we use the SAI library: `PhysWorld` inheritates from SAI `CWorld`; `PhysTip` and `PhysCNanoTube` inheritate from SAI `CSolid`.

Here are a few snapshots of the viewport:

(a) Translation 1 (b) Translation 2

FIGURE 1. Screenshot: translation of a nanotube



(a) Rotation 1 (b) Rotation 2

FIGURE 2. Screenshot: rotation of a nanotube

4. Testing

The CNT simulator was tested using two computers. The simulation was executed on one of the computers, while the second was connected to the Delta Haptic Device. The computers communicated *via* two UDP [1] sockets, one to send datas from the simulator to the controler, and the other to send datas from the controler to the simulator.
The controler sent datas to the simulator to update the tip position; the other way, the simulator returned an elementary force to the controler to ease its use. In particular, it featured a force when the tip came into contact with the CNT, and a force that avoided the tip to come through the surface on which the CNT laid.

[1] User Datagram Protocole, a simple and fast communication protocole

CHAPTER 4

Future issues

1. Improvement of the model

The model used here (model of translation - rotation - bending - breaking) will have to be completed; we did not implement bending and rotating yet. Also, researches would have to be performed to caracterise the lateral force signatures of each of the possible movements (as said in section 2.6).
It is also possible to refine the model, by adding distinction between translation by rolling or translation by slipping, for instance (see section 2.2 or [**9**]).
Note that the system that has been built could itself help for this research.

2. Improvement of the interface

The interface could benefit of several improvements: the concept of "virtual tools" (as described in section 2.2 and [**4**]) could be implemented. Also, it might be interesting to see wether it is possible to run a fully virtual simulation, in which the forces would not come from a real AFM-sample interaction, but rather from the model itself, thus extending to three (or six) dimensions what the Tokyo team has achieved in one dimension (see [**6**]).

CHAPTER 5

Appendix

1. Verification of the law on rotation centers

assumptions : let the nanotube be a simple cylinder; let the friction be uniforme and dynamic (*vs* static); let there be an uniforme push in x_0;
Let us assume that we do not accelerate the nanotube; therefore, the first law of Newton is $F = ma = 0$; we have an uniforme rotation: $\omega = const$

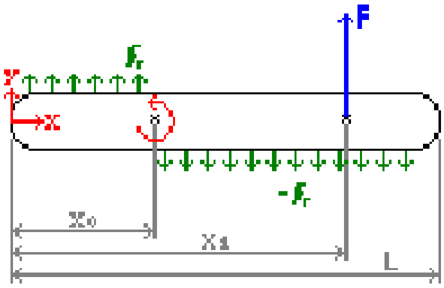


FIGURE 1. repartition of forces on a nanotube

1.1. First law of Newton.

z axis : The resolution of the equation in z axis is trivial.

y axis : we have

$$\int_0^{x_0} f_r dx - \int_{x_0}^{L} f_r dx + F = 0 \text{ (no acceleration)}$$

$$x_0 f_r - (L - x_0) f_r + F = 0$$

$$2x_0 f_r - L f_r + F = 0$$

$$f_r = \frac{-F}{2x_0 - L} = \frac{F}{L - 2x_0}$$

1.2. Inertia momentum.

assumptions : Let us assume that the tube radius is far smaller than its length ($R \ll L$) and that the masse is neglectible (which is justified as the nanotube is only a network of atoms).

$$I_\Delta = \frac{1}{2} m R^2$$

$$I_{\Delta'} = I_\Delta + (\Delta\Delta')^2 m$$

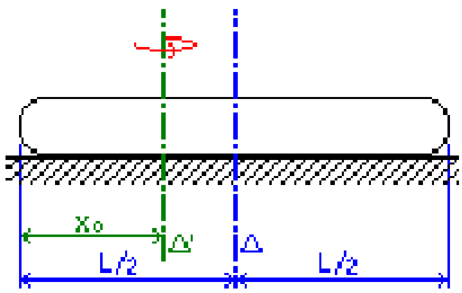


FIGURE 2. rotation axe of the nanotube

1.3. Kinetic energy :

We will consider only pure rotation (no translation) and we asume the angular speed (ω) to be less than one radian per second..

$$K = \frac{1}{2} I_{\Delta'} \omega^2 = \frac{1}{2}\left(\frac{L}{2} - x_0\right)^2 m\omega^2 \simeq 0$$

1.4. Work :

(1)

$$W = \int_0^{2\pi}\int_0^{x_0} f_r x\theta dx d\theta - \int_0^{2\pi}\int_{x_0}^{L} f_r x\theta d\theta + \int_0^{2\pi} F x_1 \theta d\theta$$

as we have $\theta = \omega t$ and $d\theta = \omega dt$,

(2)

$$W = \int_0^{\Delta t} \frac{x_0^2}{2} f_r \omega^2 t dt - \int_0^{\Delta t} \frac{(L^2 - x_0^2)}{2} f_r \omega^2 t dt + \int_0^{\Delta t} F x_1 \omega^2 t dt$$

Let us assume now that the time taken to do a complete revolution is Δt; then $\omega \Delta t = 2\pi$ and

$$W = \pi^2 x_0^2 f_r - \pi^2 (L^2 - x_0^2) f_r + 2\pi^2 x_1 F$$

1.5. Energy conservation :

$$K = W \Leftrightarrow W \simeq 0$$

Using the first law of Newton, we know that $f_r = \frac{F}{L - 2x_0}$

$$x_0^2 - (L^2 - x_0^2) + 2x_1(L - 2x_0) = 0$$

$$x_0^2 - 2x_1 x_0 = \frac{1}{2}L^2 - x_1 L$$

The solution of this equation is

$$x_0 = x_1 \pm \sqrt{x_1^2 - \frac{1}{2}(2x_1 L - L^2)}$$

The solution that takes a + comes outside of the CNT, which is physically meaningless.

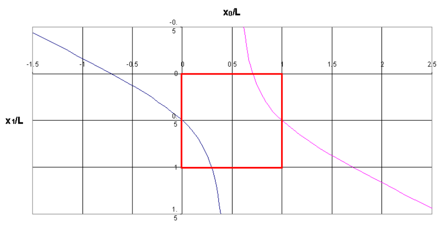


FIGURE 3. Position of the center of rotation function of the contact point

Therefore, we only keep

$$x_0 = x_1 - \sqrt{x_1^2 - \frac{1}{2}(2x_1 L - L^2)}$$

Q.E.D.

2. e-mail from Russel M. Taylor II

(...)

Hopefully, the papers at `http://www.cs.unc.edu/Research/nano/publications/papers/3DI_reprint.pdf` and the 1993 SIGGRAPH paper (reference on our publication page at `http://www.cs.unc.edu/Research/nano/publications/index.html`) will answer similar questions; I'll try to answer the ones below. There is also a copy of my dissertation online at that page, which should provide all the gory details.

At 05:50 AM 8/3/2001, you wrote:
Greetings,
I have read several of your articles, but I don't completely understand how you refresh the display of the 3D scene; does the nanoManipulator stop at regular inervals to perfom additional scans ? What criteria trigers new scanning ? And what is the exact definition of a "mini-experiment"?

The AFM continues scanning over and over again untill the user enters "touch" mode to feel or modify the surface. After a touch/modification, the system goes back to scanning continuously again.

A "mini-experiment" is attempting a single, simple action and observing the results. Example include: pushing on a nanotube to see if it will push or roll, pushing the tip into the top of an Adenovirus to see if it will smash or burst, pushing a strand of DNA to see if it will move or break.

Another question: if I understood your articles weel, between two scans, the nanoManipulator provides haptic information to the user; where does this information come from ?

The AFM tip is moved to follow the motions of the user's hand across the surface; the information about the surface height as it moves around is used to provide a haptic surface that the user can feel.

(...)

3. Aknowlegements

We are grateful to our patient and competant micro-engineering assistants, S. Grange and F. Conti; to the physicists, A.J.Kulik and A. Kis, who helped us catch up a little bit with the nanoscale world; R.M.Taylor, for his accurate and quick answers; and all the people who wrote the software we used, notably LaTeX and Linux.

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