Path-Planning and Manipulation of Nanotubes Using Visual and Haptic Guidance

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***Abstract*—This paper presents a VR toolkit for path planning and manipulation of nanotube. The toolkit is capable of modeling the interactions between an AFM tip and carbon nanotubes on a substrate surface and generating optimum and safe manipulation paths. In addition, haptic guides were designed to help the user to follow the calculated paths, to avoid obstacles.**

I. INTRODUCTION

Carbon nanotubes (CNT) qualify for many applications, such as biomedical, optical and electronic fields. However, the most interesting property of nanotubes is their capability to be maneuvered to build complex nano devices. Such devices mainly include nano electronics or nano electromechanical systems (NEMS). The applications of nanotubes for NEMS require the operations of characterizing, placing, deforming, and/or connecting nanotubes [1]. Nano manipulation tasks are defined in a similar way as in macro-scale, such as positioning, assembling, pushing or pulling, etc [2].

Atomic Force Microscopy (AFM), introduced by Binnig, is a widely used imaging technique at nanoscale [3]. In AFM, a micro cantilever shaped probe with a sharp downward tip underneath is used to scan samples on substrate surface. The interaction forces (attractive and repulsive) between the tip and the substrate cause the free end of the probe to deflect. Through the measurement of the height field of the substrate, 3D topographic map of the sample and the substrate surface can be obtained. Using an AFM, it is also possible to manipulate nano-scale objects. For example, AFM is utilized for positioning particles [4] or carbon nanotubes [5] on a substrate by contact pushing or pulling operations. Fig. 1 shows the situation of a nanotube pushed by an AFM probe tip in a VR simulator [6].

II. VR FOR NANOTUBE MANIPULATION

Virtual reality (VR) technologies enable scientists to extend their eyes and hands into the nano world and also enable new types of exploration [2]. Taylor introduced virtual reality graphics and force feedback for touching the nano-world [7]. To our best knowledge, most previous researches on VR for nano-manipulation dedicate to manipulating nano particles. Nanotubes may be more difficult to manipulate than nano particles. Reasons mainly include our limited knowledge of nano mechanics, the deformation of nanotubes as compared to the rigidity of nano particles. Furthermore, the nature of AFM-based manipulation indicates that the scanning and manipulation are done in sequences using the same probe. Therefore, operators are blind during manipulation because they cannot see the real-time environment changing. This scan-manipulate-scan cycle makes nanotube manipulation a time-consuming, tedious and unintuitive task.

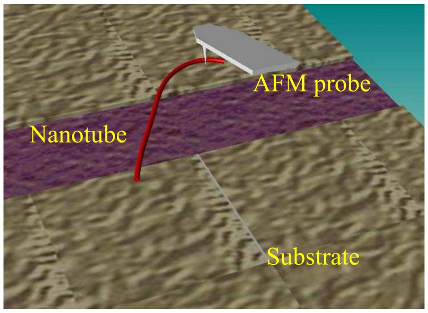


Fig. 1. AFM manipulation of nanotubes

In our previous research [6], a haptic VR simulator for training and prototyping of telemanipulation of nanotubes is proposed. In the following paper, our objective is to develop a virtual reality toolkit with visual and haptic feedback to assist the manipulation of nanotubes. The VR toolkit can be used to generate optimal and safe manipulation paths. The VR toolkit also provides virtual guides which permit the operator to perform tasks with higher confidence and accuracy. Similar topics of tele-manipulation at nano-micro scale have been addressed in [8] and [9]. However, they mainly focus on the manipulation of nano particles.

In the following sections, we describe a human-machine interface based on VR techniques for real-time telemanipulation with visual and haptic feedback. Different virtual guides are proposed for guidance and assistance during the nanotube manipulation tasks.

III. MECHANICS OF NANOTUBE MANIPULATION

A. *Physics of nano-manipulation*

Nano objects show different mechanics from macro sized objects. For example, adhesive surface forces dominate over inertial forces at nano-scale. In addition, there are non-contact forces such as Van der Waals, capillary, and electrostatic forces. There are three major categories of interaction forces in the physics of nano-manipulation: tip-nanotube, nanotube-substrate and tip-substrate interactions.

- Tip-nanotube interactions: non-contact force models are considered in addition to the contact force models.
- Nanotube-substrate interactions: during the manipulation, the nanotube is in continuous contact with substrate surface. Therefore, contact and friction forces must be considered here.
- Tip-substrate interactions: both contact and non-contact models are used to calculate the interaction forces. Tip-substrate interaction in nano scale is particularly different from one's experience in macro scale.

B. *Tip-Substrate-nanotube Interaction Model*

Based on the tip-substrate-nanotube interaction model in [10], a simplified force model is introduced. Because the lateral direction stiffness of the tip is much higher than that of normal direction, we believe that the tilting of the probe tip is rather minute. Therefore, the tip is assumed to be vertical. Also, the tip is modeled with a cylinder since the taper angle of the tip is also very small. The force variables are labeled in a way similar to [10], such that the superscript can be: a = adhesive, f = frictional, or r = repulsive. The subscripts are a combination of two letters (t = tip, n = nanotube, s = substrate) that indicate the force between the two objects. For example, F^a_{ts} means the adhesive force between tip and substrate. Fig. 2 (a) shows the forces applied on the nanotube. According to the equilibrium condition of the nanotube both in horizontal and vertical direction, we have:

$$F^r_{nt} = F^f_{ns} + F^a_{nt} \tag{1}$$

$$F^r_{ns} = F^a_{ns} \tag{2}$$

The forces applied to the tip as shown in Fig. 2 (b) should be balanced by the normal force F_z, and the lateral force F_l from the cantilever. The equilibrium condition of the tip in the normal and lateral direction is

$$F_z = F^r_{ts} - F^a_{ts} \tag{3}$$

$$F_l = F^r_{tn} - F^a_{tn} + F^f_{ts} \tag{4}$$

According to Newton's third law, $F^r_{nt} = F^r_{tn}$ and $F^a_{nt} = F^a_{tn}$. The equation for the friction between the nanotube and substrate is:

$$F^f_{ns} = \mu_{ns} F^r_{ns} + \upsilon F^a_{ns} \tag{5}$$

where μ_{ns} is the is the sliding frictional coefficient between object and substrate surface and υ is the shear coefficient. The adhesive force between the tip and the substrate F^a_{ts} can be measured by using AFM in force calibration mode. The adhesive forces, such as F^a_{ts}, F^a_{tn} and F^a_{ns}, can be assumed to be proportional to the contact area [10]. Therefore, the adhesive force F^a_{nt} and F^a_{ns} can be estimated by relating tip-substrate contact area and the nanotube-substrate contact area.

$$F^a_{tn}/F^a_{ts} = A_{tn}/A_{ts} \tag{6}$$

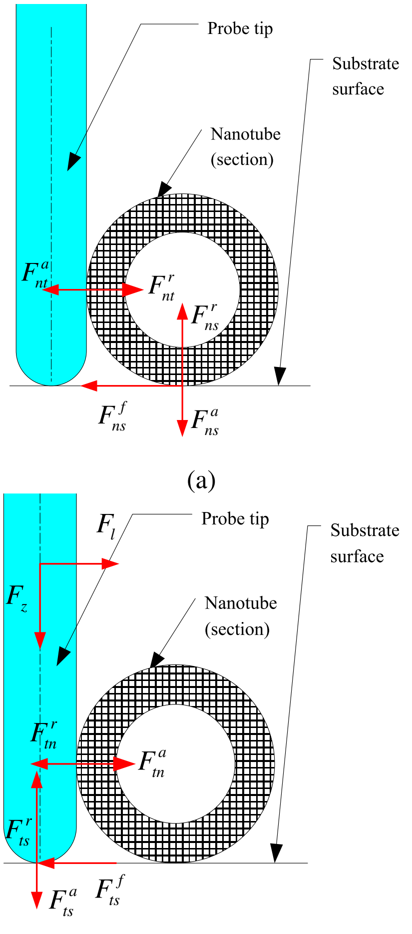


Fig. 2. Tip-Substrate-Nanotube interaction model

$$F^a_{ns}/F^a_{ts} = A_{ns}/A_{ts} \tag{7}$$

More details about the interaction model and implementation can be found in [6].

IV. PATH PLANNING AND VIRTUAL GUIDES

A. *Nanotube manipulation and assembly*

The purpose of nanotube manipulation is to form nano assembly and structure. Nanotubes should be maneuvered to specific positions, orientations and shapes. During the manipulation process, the nanotube should be kept away from any obstacles and other nanotubes. Accidental collisions between two nanotubes often cause adhesion between each other. Although the nanotubes could be separated, the separation operation generally leads to the drastic change of the form and orientation of nanotubes. It could take long time to separate the accidental adhesions and to recover the resulted changes. Therefore, collision between nanotubes should be carefully avoided.

To manipulate a nanotube to a specific position and shape, two steps of manipulation have to be executed. The first step is a preparation, in which a nanotube is moved from its initial position roughly to the final target location. The second step is finalization. In this step, the nanotube is finely adjusted towards the final target position and shape.

B. Requirements

The manipulation and assembly of nanotubes are described in the previous subsection. In this subsection, requirements about path-planning and virtual guides are discussed.

For the preparation stage:

- A path-planning tool, which is required to generate safe and free-of-collision manipulation paths.
- A soft virtual guide should be provided to help the operator to follow the path.

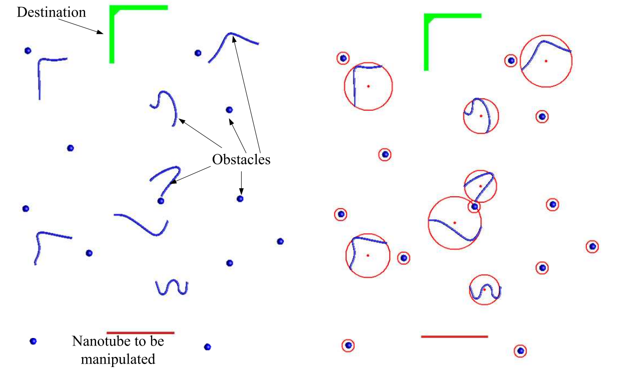
For the finalization stage of manipulation, obstacle avoidance virtual guide should be provided. It is used to prevent the AFM tip from accidentally colliding into obstacles or other nanotubes.

C. Path planning and the virtual guide of path-following

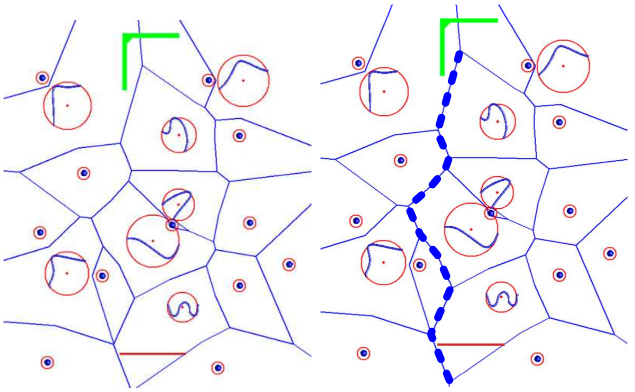
The purpose of path-planning is to generate a set of paths while respecting maximization of the distance from obstacles in order to avoid collision or attraction forces due to micro-physics [8]. Most previous researches on path planning for nano-manipulation focus on the manipulation of nano particles. Although these methods are capable to obtain optimum paths suitable for nano particles, those paths are not safe enough to guarantee zero collision during the manipulation. Firstly, this is because nanotubes occupy much bigger volumes than nano particles. In addition, deformations and movement of nanotubes along the manipulation trajectories also increase the chance of collision. A two-step strategy is introduced. In the first step, a potential field method [11] is used to generate a path for the AFM tip. Then, in the second step, the virtual nanotube is simulated to move along the path to detect any potential collision.

1) Graph construction: For the nanotube manipulation task, obstacles include other nanotubes and dusts on the substrate. Firstly, smallest enclosing circles of the nanotubes and dusts are found out. The circles are the boundaries which the manipulated nanotube should not cross. A graph that represents all possible trajectory paths is then generated with Apollonius Voronoi diagram. The Apollonius diagram is also known as the additively weighted Voronoi diagram, which can be thought of as the generalized Voronoi diagram of a set of disks under the Euclidean metric. In this research, the Apollonius Voronoi graph is constructed with CGAL [12].

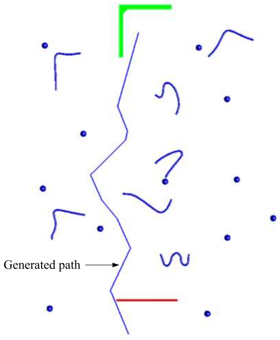
2) Optimal path generation : With the Apollonius Voronoi diagram, a search algorithm is used to find the optimal path. The A^* algorithm is chosen for this task [13]. The shortest path from the initial node to the final node is found by searching the edges of the Apollonius Voronoi diagram.



(a) Initial situation (b) Minimal enclosing circles for obstacles



(c) Apollonius Voronoi diagram (d) Path searching



(e)

Fig. 3. Optimal path generation

Fig. 3(a) shows the initial situation of a nanotube manipulation task. The L shape in the top is the destination of this manipulation and a straight tube is to be pushed there. On the substrate, there are dusts and other nanotubes, which should be avoided during the manipulation. Fig. 3(b) shows the enclosing circles and Fig. 3(c) shows the obtained Apollonius voronoi graph. Fig. 3(d) shows the optimal path generated with the A^* searching algorithm. Fig. 3(e) shows the path as the final result.

3) Nanotube deformation simulation: In the simulation, the AFM tip first pushes the nanotube into a U shape, then the AFM tip moves along the path at a constant speed. If any collision is detected, the path should be modified and the simulation is restarted. The procedure is repeated till no collision happens any more. The simulation of nanotubes deformation is based on Tserpes and Papanikos's method [14] which treats nanotubes as solid beams at a global level. In this research, deformation of nanotubes is simulated based on

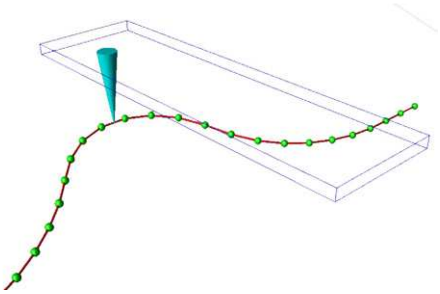


Fig. 4. Nanotube model for deformation and collision detection

beam theory in order to achieve real-time updating rate. It is assumed that the bending stiffness, *EI*, of a nanotube is given by the classic formula:

$$EI = E\frac{\pi}{4}\left[\left(R+\frac{h}{2}\right)^4 - \left(R-\frac{h}{2}\right)^4\right] \tag{8}$$

where *E* is Young's module, *R* is the radius of nanotube and *h* is the wall thickness of nanotube. Based on beam theory, nanotube is modeled with a mass-spring system. Particles are connected by linear springs and torsion springs. The length and deflection angle of the *i*-th element are denoted as l_i and γ_i, respectively. The force applied with the tip is *F* and the friction forces applied on each element is F_i^f. The moment caused is *M*. For each element, we have

$$M = F\sum_{i=1}^{n} l_i + \sum_{i=1}^{n} F_i^f l_i \tag{9}$$

$$M = k_i \cdot \gamma_i \Rightarrow \gamma_i = M/k_i \tag{10}$$

where the torsion spring stiffness is

$$k_i = \frac{2EI}{l_i^2} \tag{11}$$

The skeletal model of nanotube for deformation and collision detection is shown in Fig. 4. Once the path is verified, the path planning module transmits the optimal trajectory to the visual and haptic rendering modules. The optimized path is rendered as a virtual curve which connects the initial location and destination location. For the haptic rendering, the virtual guide is rendered as a viscoelastic connection between the virtual AFM tip and the optimal path. The values of stiffness *K* and viscosity *B* should be selected appropriately in order to avoid unstable haptic feedback [15]. Fig. 5 shows a nanotube is manipulated along the path.

D. Virtual guides for safe manipulation

During manipulation tasks, the AFM tip can accidentally collide with dusts or other nanotubes which are already present in the configuration of assembly. These accidental collisions can greatly disturb the manipulation operations. The solution is to use repulsive potential fields as obstacle avoidance virtual guides which are implemented in the master's haptic controller (Virtuose). Virtual repulsive forces are generated around obstacles from potential fields when the AFM tip enters into

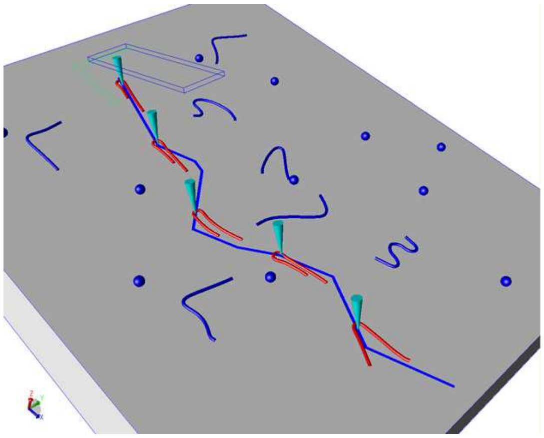


Fig. 5. Manipulation of nanotubes along the path

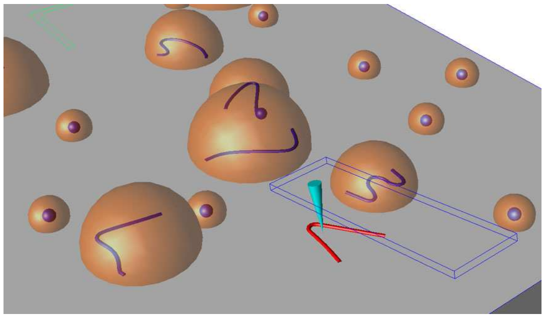


Fig. 6. Virtual guides for safe manipulation

a specific threshold. For the dust obstacles, the geometrical representation of the threshold of the potential field is a spherical bulb with the dust as its center. While for nanotubes, the threshold of the potential field can be represented as bulbs formed by the minimal enclosing circles of nanotubes. The formula of the potential field can be expressed as the following:

$$P(d) = \begin{cases} \frac{1}{2}\lambda(\frac{1}{d} - \frac{1}{d_0}) & d \leq d_0 \\ 0 & d > d_0 \end{cases} \tag{12}$$

where

- d : is the penetration distance ;
- d_0 : is a positive constant which represents the action distance of the potential ;
- λ : is a position scaling factor.

The repulsive force is defined as the negative gradient of potential function:

$$\overrightarrow{F}(d) = -\nabla P(d) \tag{13}$$

where ∇ represents the gradient operator. Fig. 6 shows the geometric representation of the virtual guides for safety.

V. IMPLEMENTATION

The VR toolkit has been developed in C/C++ using HOOPS for graphics rendering [16]. The VR toolkit utilizes a Virtuose

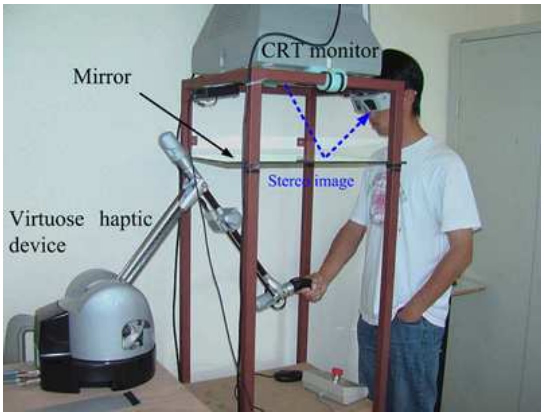


Fig. 7. Hardware setup

6DOF device from Haption [17] for controlling the tip position of an AFM and for reflecting interaction forces back to a user. Besides the haptic feedback, an stereoscopic immersive visual display, similar to [18], is provided to obtain the better depth cue and eye-hand coordination.

The system is illustrated in Fig. 7. The stereoscopic display image is reflected by a horizontal mirror to the operator. The visual coordinate system is coincident with the haptic device coordinate system. LCD shutter glasses are used to provide a stereoscopic display with a refresh rate at 150 Hz. After proper calibration, the virtual AFM tip and operator's hand remain co-registered from the viewpoint of the operator. The visual display is designed in a way similar to the microscopic view field. We expect that this metaphoric similarity is helpful for the operator.

VI. Conclusion and future work

This article described a haptic VR toolkit for manipulation of nanotubes. With both haptic feedback and virtual guides provided by the toolkit, it is expected that operators could concentrate more on the useful part of operational gesture and hence nanotube manipulation would be conducted more intuitively, safely and quickly. Although our first users have expressed satisfaction with this VR toolkit after trials, quantitative evaluation and test must be conducted in the near future. The manipulation is optimal in terms of the shortest distance, however, zero-collision between the manipulated tube and the obstacles can not be guaranteed and follow-up rehearsal simulations are used to identify any potential collisions. More intelligent path planning algorithms should be developed to generate collision-free path for nanotube manipulation. In addition, new interaction techniques and metaphors specific for nanotube manipulation are to be developed and tested in this VR benchmark in the future.

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