Design of an Information Based Manufacturing framework for Nano Manipulation

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Abstract – This paper outlines the preliminary development of an information based manufacturing framework and a test bed for nano manipulation. This paper delineates the design of an information based manufacturing framework in the context of a virtual reality based simulation test-bed; creation of various modules in this framework is discussed including an analysis module which seeks to study the role of van der Waals forces during nano-manipulation tasks.

Index Term: nano-manipulation, Virtual Reality, Simulation

1 Introduction

This paper discusses the creation of an information based manufacturing framework (INBM) to support nano-manipulation activities. Nanotechnology has been the research of numerous research efforts in recent years; the development of new fabrication methods has contributed to this growing importance of this domain. However, many of these advances have yet to be realized because of problems and limitations associated with nano manipulation [8]. The field of nano manipulation is in its infancy and related physical and chemical phenomena are not completely understood; in this context, there is a need to develop innovative methods to help understand issues relating to nano manipulation and assembly. The proposed Nano-Manipulation Research Test-bed (NMRT, which is under development in the context of an INBM framework) would help study nano-manipulation techniques in a virtual environment before physical experiments need to be conducted. A simple example of this test would be to determine virtually if a specific kind of probe tip can be used to 'pull' or 'push' a nanoparticle from a given substrate..

INBM refers to the study of information modeling, simulation / visualization and exchange in a product / process design context across a variety of domains. The 3 major facets of INBM include modeling of information related to process design and planning (among others), the use of virtual reality based prototyping techniques to support analysis, visualization and simulation to aid in manufacturing, assembly and other process design activities and finally the design of collaborative

infrastructures to support the distributed exchange of information among product development or engineering partners [13].

In [2], a discussion of an augmented reality enhanced nanomanipultaion approach is outlined that provides force feedback and locally updates visual feedback based on a tip-substrate-object model. In [3], the use of an AFM for nanomanipulation using a haptic device is outlined. Taffazoli [4] introduced Johnson-Kendall-Roberts model to the contact problem of nanoparticle pushed by a probe. In [1], a discussion of control strategies for nanomanipulation systems s provided including control approaches are for autonomous or semi autonomous manipulation.

NMRT is based on the concept of expandability. This is made possible by designing an 'information oriented' or 'information intensive' model for a target set of nano-manipulation activities which maps in detail various attributes (such as forces, geometries etc.) related to a target nano-manipulation process [5]. For example, consider an existing information model for interaction of a probe tip with a spherical particle; a user can use an existing information model (pertaining to a specific manipulation scenario) to a modified or different configuration: for example, a scenario involving the presence of a second similar probe-tip to aid in the target nanomanipulation task. This would allow a quick turn around from analysis dealing with a single probe based manipulation task to multiple probe based manipulation.

For a target nano-manipulation process (for example, assembly of nano particles using an Atomic Force Microscope probe as a gripper), an information model can represent the core attributes influencing the target process. Influencing criteria including constraints, information inputs, and physical inputs can be modeled explicitly and used to drive a target analysis or simulation activity.

In the context of previous efforts, while other researchers have attempted to use visualization modules, the proposed approach is different in the following manner. We attempt to explore an information module driven manipulation strategy as opposed to [6] and [7] where direct or semi autonomous manipulation strategies are explored. This approach would help avoid the use of physical equipment while planning a manipulation strategy. Since our test-bed is information model driven, alternate manipulation strategies proposed from various sources and locations can be embedded in the test bed. Over a period of time, the NMRT will evolve into an information-rich environment that would allow users to test and combine different probe based nano-manipulation strategies. Figure 1 illustrates this concept of using information models to drive the simulation tasks.
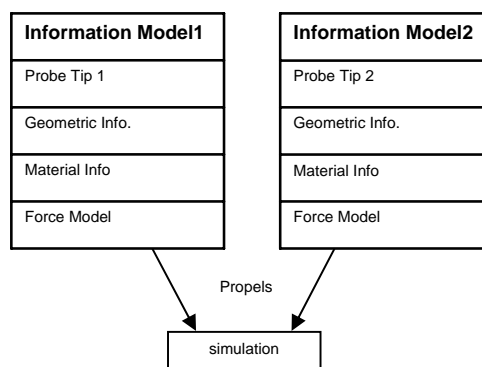

Fig. 1 Two Information models combine to propel a simulation

2 The INBM Framework

The overall INBM framework in shown in figure 2. It consists of a virtual worksite and a real worksite. The scope of this paper is restricted to discussions relating to the design of virtual components or worksite. The virtual environment has 3 components:
(a) the simulation / analysis module (b) the information model (c) the virtual reality sensors and haptic devices.

The simulation / analysis module seeks to support the study of the inter atomic forces which come into play during nano assembly. Currently, the focus is on understanding Van der Waals forces (VDW) in the context of nano assembly. The typical modeling scenarios considered are discussed in section 2.1

The information model encapsulates specific attributes relating to the accomplishment of the simulation and physical activities. In the INBM framework, the information models are stored as Engineering Enterprise Modeling Language (eEML) models; the discussion of the eEML is beyond the scope of this paper [13, 14].

The immersion module's function is to enable users to interact with the virtual environment; these devices include a work wand and a haptic device along with motion trackers and eye wear. In a typical interaction session, a user would evaluate a nano-manipulation strategy in the virtual-site and then use the results from this segment of the module to drive the physical experiments; the simulation environment seeks to provide additional understanding of a target task so as to enable users to predict outcomes or evaluate alternate manipulate strategies.
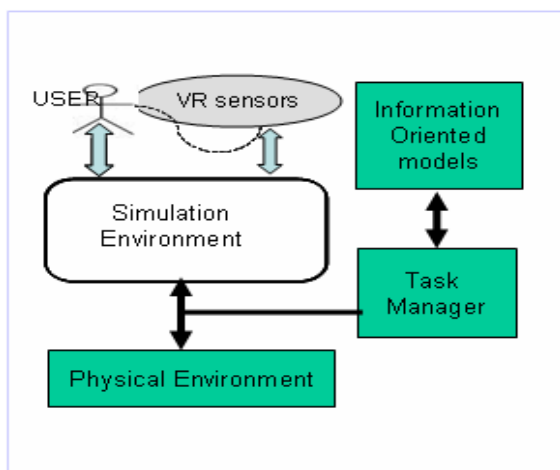

Fig. 2 The INBM Framework

The INBM framework is under implementation. Currently, the preliminary implementation of the simulation module has been completed. Other activities under progress include the interfacing of the information model with the simulation module and the development of a physical environment comprising of nano probes, sensors and actuators. The simulation module has been implemented using C++ Open Inventor graphical libraries (from TGS™ for graphics rendering).

2.1 Analysis Model for interaction of virtual probe tip with nano particle

This section discusses the information model that we have used for probe tip interaction with nano-particles. Presently, we have considered only spherical nano particles, but the expandable nature of the test-bed will enable accommodation for other geometries in the future.

In this preliminary research phase, only the van der Waals force interactions to model forces between the probe-tip, nano particle and substrate have been considered. Work in progress (WIP) and future plans include the study of other force components, such as electrostatic force and surface tension [9]. The probe-tip and nano-particle interaction that have been modeled resembles typical nano-manipulation scenario [10]. The net force (see figure 3) on the nano particle can be represented by:

$$F_{net} = F_{vdw\text{-}tip} - F_{vdw\text{-}subs} - F_{grav} + F_{control\text{-}tip} + F_{unknown} \qquad (1)$$

where $F_{vdw\text{-}tip}$ is the van der Waals force between the tip and particle, $F_{vdw\text{-}subs}$ is the van der Waals force between the particle and substrate, F_{grav} is the force of gravity on the particle and $F_{control\text{-}tip}$ is any other controlled force that the probe tip can use to pull out a particle. Example of a controlled force can be dielectrophoretic force as outlined in [8]. $F_{unknown}$ is any other known force component that can be added as needed in a manipulation strategy.

For a particular case, consider Fig. 1. Suppose, the "force model" used inside "information model 1" is for a spherical probe tip interacting with spherical nano particle on an infinite flat plane and there is no controlled force (see figure 3) from the tip.
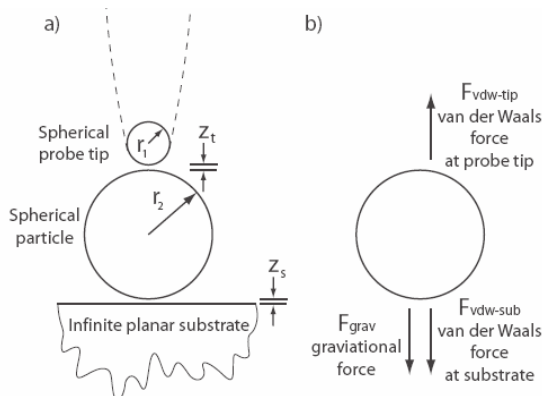

Fig. 3 Free Body Diagram of the Probe Tip and Nanoparticle, showing typical forces.

The forces can be calculated as close range van der Waals interaction between 2 spheres as presented by [12] :

$$F_{vdw-tip} = \frac{32Ar_1^3 r_2^3(z_t + r_1 + r_2)}{3z_t^2(z_t + 2r_1)^2(z_t + 2r_2)^2(z_t + 2(r_1 + r_2))} \quad (2)$$

Van der Waals forces between a sphere and a surface [8] can be caculated as:

$$F_{vdw-sub} = \frac{2Ar_2^3}{3z_s^2(z_s + 2r_2)^2} \quad (3)$$

earths's gravitational attraction:

$$F_{grav} = \frac{4}{3}\pi r_2^3 \rho g \quad (4)$$

where, A – Hamaker constant, ρ – typical density of nano particle and g – acceleration due to gravity. Figure 4 shows a screenshot of a simulation of this configuration, which is discussed in the next section.

2.2 Simulation and Analysis Modules

The simulation module has an analysis component that uses the force information and integrates it to generate a system state in real-time. The force integration module of the NMRT works in the following manner:

First, the positions and orientations of all geometries in the system are calculated at differential time; subsequently, surface forces are calculated using this system state (positions and orientations) at each differential time instance, to generate a new system state.
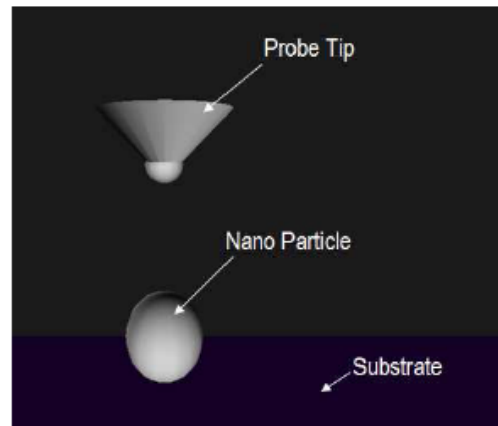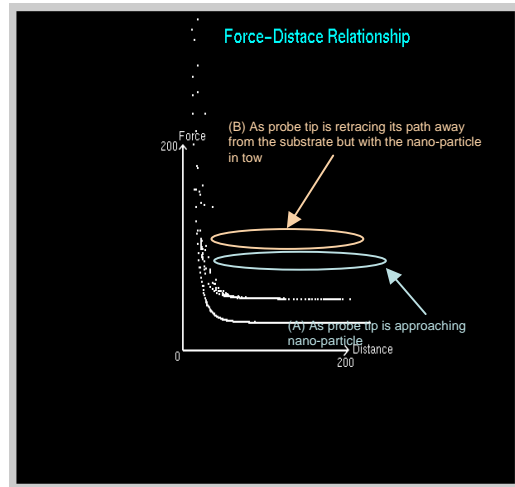

Fig. 4a Screen view of the simulation module

Figure 4b: Screen view of graphical display in simulation module for nanomanipulation

The simulation environment shows (in real-time) the interaction of a probe tip with spherical nanoparticle on a substrate surface. A screen shot from the simulation module in shown in figure 4.

Figure 4b shows the screen view of the graphs displayed in the simulation module related to the nanomanipulation tasks illustrated in figure 4a. When the probe approaches the particle, the Attractive Force (on Y-axis) increases as the distance between particle and probe-tip decreases (this is indicated by A in figure 4b); As the probe pulls away from the substrate, the nano particle comes along with the probe tip (this is shown as B in figure 4b)

This simulation module and visualization environment was developed in C++ using Open Inventor graphical library supplied by TGS™ for graphics rendering.

2.3 Other components of the framework

Apart from the simulation / analysis module, a representation module has also been designed primarily to allow study of virtual reality based representation of objects and particles that are of direct relevance to the research topics outlined in this paper. One of the current approaches being studied is the use of carbon nano tubes (CNTs) as alternate probe tips; these CNTs are grown physically on the probe tips of Atomic Force Microscopes (AFMs); physical experiments are underway to study possible nano assembly approaches. Many researchers have proposed the potential of carbon nano tubes as a robust probe tip [11]. A key issue that needs to be investigated is the representation of the carbon nanotubes for simulation purposes within the INBM framework. A discussion of these issues follows.

One of the tasks in including a CNT based probe tip in NMRT is the graphical representation of a Single Walled Carbon Nanotube (SWCNT) or simply, a nanotube. Design of the graphical nanotube component has to accommodate for the changes in structure guided by the underlying information model. There are other graphical representation techniques such as the Protein DataBase (PDB) models for representing the carbon nanotubes. These techniques are useful and widely accepted for representing molecular structures; however, it is not possible to add a real-time system (component) that changes and manipulates the structure based on a information model that 'drives' it. In the proposed approach, such a drawback is overcome by use of such an information centric approach.

A brief description of representational approaches proposed to facilitate the simulation of nanotubes aided manipulation tasks follows. The Molecular structure of a carbon nanotube consists of a two dimensional graphitic lattice (figure 8) that is rolled to form a cylinder. Graphical modeling approach for SWCNTs is based on aforementioned graphitic basis. The proposed data structure contains basic information about a carbon atom, and its inter-atomic properties such as bond lengths, bond angles and number of unpaired electrons. (Figure 6)
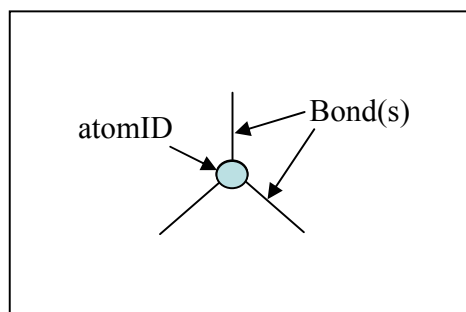

Fig. 6: Graphical Representation of class Atom

This atom acts as information / data source for representing a single carbon atom for modeling the nanotube. The 'Atom' can then be repeated in a 2D hexagonal array to form graphitic atomic basis for any carbon nanotube. The 'Atom' in this hexagonal array can gather information about all its neighbors using the bond vectors. Bond Vectors are used in the class called "Bond"(Figure 7). A "Bond" represents a single chemical bond. It has information about its location and direction in the overall

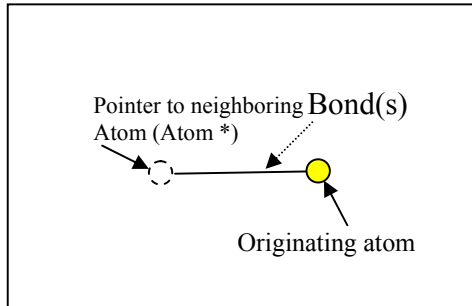structure it also has information about the Atom on the other side of it.

Figure 7: Graphical Representation of class Bond

This information is assumed to be sufficient to build the graphitic basis for nanotube generation.

2.3.1 Representation of Nanotubes

The task of building a nanotube from the graphitic basis formulated above involves bending each bond angle away from XY plane. This will cause the sheet to roll into a cylinder and form a nanotube. We start with calculating the number of atoms required to form the circular cross section using diameter of the tube. Subsequently, bonds across each atom falling on the axis of the tube are then bent accordingly to achieve the cylindrical shape.
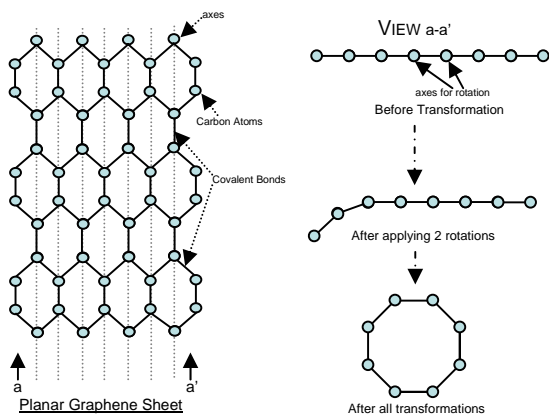

Fig. 8: Conceptual Approach to convert Planar Graphitic sheet into a Nanotube

Figures 9 a, b provide screen views of the final renderings of the CNT representations within the simulation module based on the approach described earlier in this section.
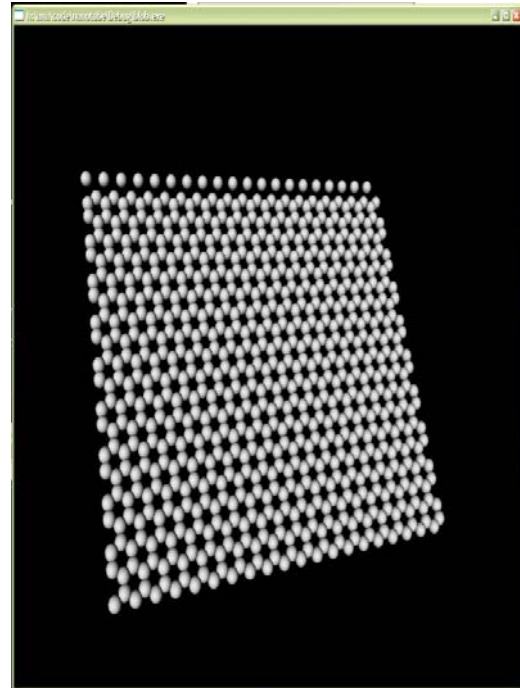

Fig. 9 a: Initial stage in the representation of a CNT: a 2 Dimensional grapheme sheet (shown here) is used as the basis for the creation and manipulation of a CNT
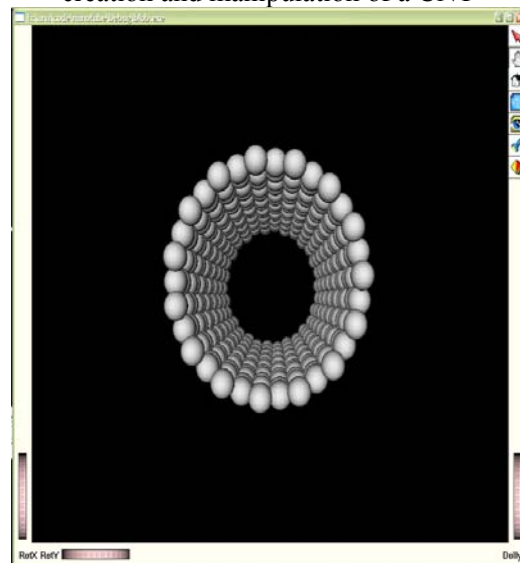
Fig. 9 b: Screen view of the renderings of various stages of Nano-Tube visualization.

Once this nano-tube model is constructed, the graphical and force modeling information can be embedded into the information module and imported into NMRT. Subsequently, the user can use this new probe information model to study other nano-manipulation strategies of interest.

The simulations and visualization discussed in this paper were developed in C++ using Open Inventor graphical library supplied by TGS™ for graphics rendering.

4 CONCLUSION

In this paper, the preliminary design and implementation of modules related to the NMRT are described. The first focus of this paper was a discussion of the force model dealing with van der Waals force interactions between the probe-tip, nano particle and substrate force and surface tension [12]. The probe-tip and nano-particle interaction that have been modeled resembles a typical non contact mode nano-manipulation scenario.

The second thrust discussed in this paper is on the graphical representation issues that need to be addressed relevant to use of nanotubes as manipulators themselves. The simulation and representation modules and visualization environment was developed in C++ using Open Inventor graphical library supplied by TGS™ for graphics rendering. Current work is focusing on additional modeling of interactive forces which come into play and developing additional test bed modules which will allow users to manipulate nano particles using haptic and other sensors.

Acknowledgement

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