Virtual Reality approach for nanoparticles tracking using simulated forces

Pavel G. Ikonomov and Muralidhar K. Ghantasala*

Department of Industrial and Manufacturing Engineering, pavel.ikonomov@wmich.edu
* Department of Mechanical and Aeronautical Engineering, m.ghantasala@wmich.edu
Western Michigan University, Parkview Campus, Kalamazoo, MI 49008

ABSTRACT

In this paper we propose a Virtual Reality (VR) approach to track the nanoparticle movement using simulated forces. As a first step in this direction we have considered the representation of the interaction between nanoparticles and Atomic Force Microscope (AFM) tip. This involved the computation of both long and short-range forces. In particular, the forces considered in the simulation include Van der Waals, adhesive, capillary, gravitational, electrostatic, and frictional forces. These forces were calculated using standard equations with MatLab and are provided as input to the VR software (EONReality) for the representation of the direction of the particle movement. The VR visualization and control of the magnitude and direction of these forces is demonstrated.

Keywords: Virtual Reality, nanoparticles, simulation of forces, AFM

1. INTRODUCTION

The manipulation and assembly of nanoparticles has recently been identified as one of the important aspects of nanomanufacturing. This kind of controlled manipulation of nanoparticles could help in monitoring protein functions in living cells in real time [1]. Though a number of research groups have been working on the simulation of different forces, so far the literature is scarce with the respect to their representation and control in a practical environment. Different forces are experienced by the nanoparticle during its movement stimulated by an atomic force microscope (AFM) tip. Though the concept of tele-nanorobotics was suggested in 1998 [2], the modeling and estimation of a number of possible forces between the tip and particle and the particle and substrate were published a couple of years later [3, 4]. The forces that were identified to contribute significantly in the determination of the particle movement on a given surface are classified as contact and non-contact forces. The non-contact forces were mainly the Van der Waal's, adhesive, gravitational and electrostatic forces, the sum of which represents the total non-contact force involved in the concerned nanoparticle movement/manipulation. The friction forces, repulsive contact forces and capillary forces are the main contact forces identified in this process. [4, 5]

Some of the results obtained in the modeling of these forces were verified experimentally too. Further, Sitti et al. [6] recently reported the results of their investigations in modeling the dynamic modes of nanoparticle motion considering different friction models and relevant adhesion forces.

One of the major challenges with the modeling and manipulation of nanoparticles is the visualization of the real time processes. This is conventionally achieved through using 2D-plots (for example using MatLab, Excel etc.), which are not capable of representing the interaction between different forces dynamically, as required in the present situation. In this context, Virtual Reality simulation is the best approach not only to represent the forces but also to visualize their real time effects. In addition, VR techniques would also allow the controlled manipulation of the particles. Realizing the potential of the VR techniques in the simulation and visualization of nanoparticle motion and manipulation, in this work we considered the representation of the interaction between nanoparticles and Atomic Force Microscope (AFM) tip. An interesting aspect of the present work is that it goes a step further compared to the existing VR visualization techniques (used with nanoparticle motion), in terms of representing the force vectors in a real time domain. The computation of both long and short-range forces was carried out using MatLab. These forces were provided to the Virtual Reality software (EONReality) for their representation and also particle movement.

2. VIRTUAL REALITY SIMULATION

The simulation of the movement of the nanoparticles by proposed Virtual Reality methods is different from other simulation techniques in the representation of force vectors, which ultimately cause the movement in a resultant direction. The small size of these nanoparticles poses the major limitation on using a wide cross-section of simulation techniques that are available currently. The use of VR techniques is advantageous in the present

context, as this method can easily be scaled for visualization at the macro level human perception, while providing the adequate representation of all relevant nano-phenomena. Further, the VR model not only represents the particles for visualization and control, but also allows building of the simulation of the assembly of the particles into different small structures. The forces between the particle, tip and substrate can be represented using mathematical models [2]. This is followed by incorporating movement control strategies into the algorithm. It is obvious that those models and algorithms will be imperfect, the refinement of which will involve the development of a feedback system that uses the real events. Once the real particles are assembled together, we can observe them, determine the relative positions and can potentially provide a feedback to the Virtual Reality model. That will update the simulation model and control algorithm which in turn increases the precision.

3. METHODOLOGY

The first part of this work is mainly related to the identification of important relevant forces and their interactions to provide a resultant force in a given direction. This is mainly carried out based on the experience built by different research groups working around the world, especially related to the nanoparticle dynamics. This method considers both static and dynamic forces in the simulation and provides the visual representation of these forces through the VR simulation in the second part. The magnitude and direction of individual forces and the resultant direction of the motion were represented using the Virtual Reality method.

The forces between the particle and tip and particle and substrate were the two important categories considered in our modeling, as discussed by Sitti et al and others [3, 4]. Van der Waal's forces, capillary forces and electrostatic forces, gravitational forces, repulsive contact forces, adhesive forces, and friction forces are the most important of all the existing forces that can potentially influence the direction of the nanoparticle motion. In this case, the acting force vector of AFM cantilever tip is assumed to pass through the body of the nanoparticles, not necessarily it's center, unlike the other simulation techniques [2]. Further, we assumed that the acting vector produces a force against the sum of all the internal forces of the nanoparticles, as depicted in Figure 1. In the figure the forces are represented following a simple convention. The first letter of the subscript refers to the type of force (example f – friction, e- electrostatic, c-capillary, a-adhesive, and v-Van der Waal's), while the second subscript

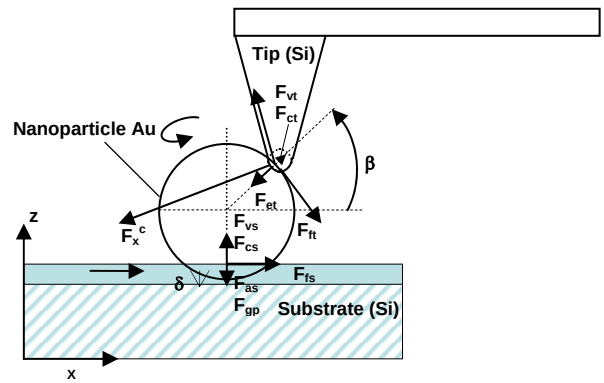

Figure 1. Schematic representation of forces with their directions

represented with letters t, s, and p (t-tip to particle, s –substrate and particle, and p- force exerted on the particle). In this figure the forces F_x^c is the driving force from the tip. b is the angle between the driving force vector F_x^c and the horizontal substrate plane. F_{fs} and F_{ft} represents the friction forces. F_{as} is the adhesive force.

This model is developed assuming an AFM tip made of silicon with gold being the material of the nanoparticle (spherical). The substrate in this case is single crystal silicon. In this model, we have considered the Van der Wall's forces between the particle and tip and particle and the substrate (F_{vt} and F_{vs}) separately and calculated the respective values.

Assuming the nanoparticle manipulation to be carried out in a laboratory environment, the presence of a thin water layer (from the water vapor with in the environment) on the substrate necessitates the consideration of capillary forces. Determination of the capillary forces between particle-substrate (F_{cs}) and tip-particle (F_{ct}) was done in a similar way as Van der Waal's forces. The fundamental equations used in the computation of the above two forces (Van der Waal's and capillary) were derived from the literature [4].

Considering a semiconducting substrate (silicon, non-grounded) requires the determination of electrostatic forces, which might arise due to local charging or charge trapping occurring at different stages of particle movement with respect to the tip. This depends on the materials selected for the particle and substrate as explained by Sitti et al [4]. The electrostatic force (F_{et}) calculated between the tip and particle is represented in the VR simulation.

The gravitational forces though appear to be relatively smaller when compared with the capillary forces these forces acting on the particle were considered in this model and simulated. As these are

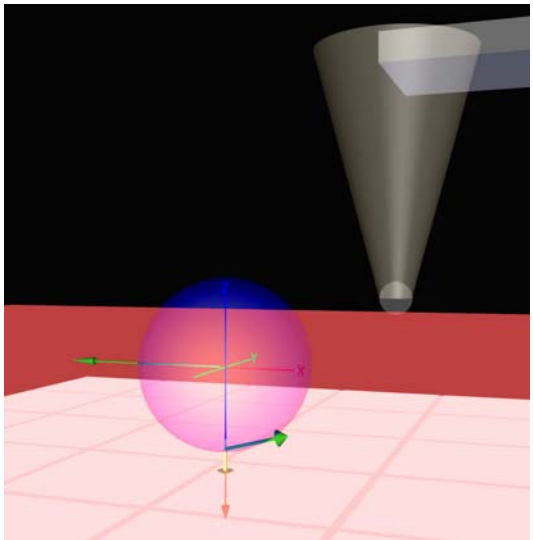

Figure 2. VR illustration of forces before the tip come in contact with the particle

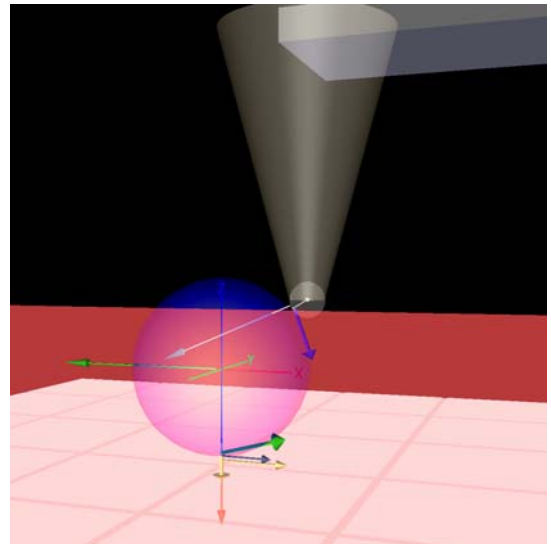

Figure 3. VR illustration of forces during tip to particle contact

primarily mass dependent, it may influence the overall resulting forces in different situations. Hence, the gravitational force acting on the particle (F_{gp}) is calculated and represented.

The cantilever induces motion to the nanoparticle; the resulting motion of the particle depends on direction of the driving force and the sum of the contact and non-contact forces described earlier. The direction of the nanoparticle movement is mainly dependent on the point of contact with the tip and the direction and magnitude of the applied force. In order to track the motion of the particle in desired course the cantilever drive force direction and magnitude are controlled. This process can be repeated with different particles until the desired structure is assembled. If the cantilever is not controlled, the particle will move in the direction of the resultant vector till it loses the contact with the cantilever and stops.

The magnitude and direction of the contact and non-contact forces are calculated in MatLab and changes are dynamically updated through interface to VR simulation. Typical force values obtained for capillary, adhesive and friction forces were in the micro Newton range, whereas the Van der Waal's, electrostatic, and gravitational forces were found to be in the nano to Pico Newton range. As different forces between the particle and substrate and particle and tip are active in different situations (when the particle is in contact or out of contact with the tip), it is difficult to provide the magnitudes of all these forces here in detail. The obtained values which were input to the VR simulation provided a dynamic representation in real or near-real time with only the active forces altered.

In terms of contact forces, this simulation takes into account the adhesion and friction forces. In the determination of the adhesive forces, two contacts viz., particle and tip and particle and substrate are to be considered. However, as mentioned in [4], the contact between the particle and tip is relatively smaller compared to the contact area between the particle and substrate. Hence, the adhesive force was estimated in terms of the contact pressure calculated using the standard relations. [4, 7]

From contact mechanics, it is well known that during the movement of a particle on given substrate, the friction forces play an important role. During the manipulation of the nanoparticle using an AFM tip, same analogy can be applied. Hence, in this case, we have considered the friction forces between the tip and particle and particle and substrate.

Following this analysis using relevant equations, a mathematical model is developed using MatLab. The forces calculated indicated that the magnitudes of capillary, adhesive and friction forces are the most dominant among all of them.

4. RESULTS AND DISCUSSION

VR techniques primarily simulate the motion of the particle caused by the driving cantilever tip and show the force vectors with their direction and magnitude. One of the interesting features of this simulation is that different force vectors are shown as soon as they become active. For example, the frictional force vector between the tip and particle will be absent as long as there is no contact between them.

The Virtual Simulation of the particle and the substrate at situations before and after a contact was established between the tip and particle are shown in Figures 2 and 3. Figure 2 shows forces acting before the tip touches the particle: driving (F_x^c), Van der Wall's (F_{vs}) capillary (F_{cs}), gravitational (F_{gp}), and adhesive (F_{as}). Figure 3 shows additional forces in action when the tip touches the particle: Van der Wall's between the particle and tip (F_{vt}), electrostatic (F_{et}), capillary forces (F_{ct}), and friction forces F_{fs} and F_{ft}

The implemented VR system differs from those already reported in the literature in its capabilities to visualize not only the geometry of the particle, substrate and cantilever but also the acting force vectors. More importantly, it gives us a tool to control, track and automate the manipulation and assembly of nanoparticles by using force vectors (with direction and magnitude) eliminating the uncertainties in determining the position and direction of the nanoparticle motion.

5. CONCLUSION

In summary, this work presents a Virtual Reality tool to manipulate nanoparticles in three-dimensional space by imputing different forces (among the nanoparticles, substrate, and AFM tip) calculated for a set of experimental conditions from MATLAB. The resultant interaction among tip, particle and substrate surface generates momentum in a direction that is predicted by this simulation. The work is in progress further to elucidate the contribution of all the above mentioned forces in the real time VR system which can be used to control the motion and/or assembly of nanoparticles in the experimental condition.

REFERENCES

[1] Qiling Tang, et al, Protein delivery with Nanoscale precision, Nanotechnology, VOL. 16, 2005, pp. 1062-1068

[2] Metin Sitti and Hideki Hashimoto, Tele-Nanorobotics Using Atomic Force Microscope, Proceedings IEEE/RSJ, intl. Conference on Intelligent Robots and Systems, Victoria, Canada, 1998, pp. 1739-46.

[3] B. Cappella and G. Dietler, Force-distance curves by AFM, Surface Science Reports 34, 1999, pp. 1-104.

[4] Metin Sitti and Hideki Hashimoto, Controlled Pushing of Nanoparticles : Modeling and Experiments, IEEE Transact. Of Mechatrionics, V5, N2, June 2000

[5] Deok-Ho Kim*, Jungyul Park*, Byungkyu Kim* and Kyunghwan Kim**Modeling and Simulation of Nanorobotic Manipulation with an AFM probe, ICCAS 2002, October 16-19, Muju Resort, Jeonbuk, Korea

[6] Afshin Tafazzoli and Metin Sitti,Dynamic Behavior and Simulation of Nanoparticles Sliding During Nanoprobe-based positioning, IMECE 2004-62470, Ananheim, CA, 2004. pp.1-7.

[7] C. Juvinall and K.M. Marshek R., Fundamentals of Machine component Design, Fourth edition, John Wiley and sons, 2006;