DYNAMIC SIMULATION OF MANIPULATION OF CYLINDRICAL NANO PARTICLES WITH THE USE OF AFM BASED NANO ROBOT

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Abstract: With the extensive use of the Atomic Force Microscope as a tool for nano assembly and the inability to real time monitoring, the use of computer simulation to predict the process of nanoparticles displacement has become the focus of attention. In transferring cylindrical nanoparticles, three modes of sliding, rolling and spinning can be observed. In this research, by investigating the forces applied on a nanoparticle and considering the contact forces, a model has been presented that simulate dynamic of the process. An algorithm for predicting the movement of a nanoparticle on a substrate has been introduced. The results presented in this paper have been validated by comparing them with the simulation results. By using the presented model, the movement path can be predicted with regards to all the effective parameters, and a controlled displacement of a target nanoparticle can be implemented using the presented model.

Keywords: AFM nanorobot; Motion modes; Dynamic: Manipulation.

I. INTRODUCTION

With the growing use of AFM-based nanorobots, the precise displacement of nanoparticles using these instruments has become the focus of attention. Precise manipulation by means of an atomic microscope includes a variety of operations such as writing, touching, cutting and displacing in nano scale. By using the word manipulation in this article, we mean the exact displacement of nanoparticles. The displacement and movement of nanoparticle is initiated by the contact between AFM probe tip and nanoparticle as a result of the relative movement of probe and substrate. In this paper, the effective forces that are applied on the particle and probe from the moment of contact between them until the onset of movement have been dynamically modeled in 3-D format.

Due to the limitation that exists in simultaneously observing the displacement of nanoparticles, there is no image of the manipulation operation while it is in progress. The only medium between the macro and nano worlds is the produced forces. Therefore, in order to implement the process in a controlled and accurate manner and also to automate the process, it will be necessary to simulate the changes of forces during the manipulation. The goal of this article is to present a dynamic model which will be able to simulate the forces applied on the cantilever and make it possible to study the manner of process implementation.

In recent decades, the researchers have focused on the use of AFM microscopes for the transfer of nanoparticles. The first report on the displacement of spherical nanoparticles using the STM microscope was presented by Strasko [1]. Due to the limitations of the STM and its inability in moving non-conductive particles, the use of AFM in the manipulation process increased, and the subject of nanoparticle displacement using the AFM was introduced by Schafer [2]. Subsequent research works concentrated on the displacement of cylindrical particles (nanotubes) on various surfaces. Through the manipulation of nanotubes on surfaces, Fallow investigated their mechanical properties as well as the different modes of motion [3, 4]. In recent investigations, the movement of nanowires in different modes (e.g. rotating, rolling and sliding) has been studied experimentally [5, 6]. In the conducted research works, no model has been presented for the prediction of how the move is performed; and the transfer of particles has been accomplished through trial and error. So in continuation, several models are introduced for the precise performance of manipulation and the prediction of the displacement of nanoparticles. Gethold [7] introduced a nanomanipulator instrument for performing displacement operations on nanoparticles in a controlled way. For the first time, Sitti presented a dynamic model for the controlled manipulation of spherical nanoparticles [8].

In recent studies, 3D model for pushing cylindrical nanoparticles had been investigated [9]. All of observable modes of modes in cylindrical nanoparticles manipulation (sliding, rolling, and rotation) has been presented [10]. Possibility of determining critical time and force of manipulation process has been introduced [11]. Sensitivity analysis methods have been applied because of nonlinearity and complexity of governing equations.
In this paper, first, a 3-D kinematic model is formulated to obtain the accelerations and then the internal forces of the cantilever are modeled. In the next step, the equations of motion are expressed based on the Newton-Euler relations, and using the constant and variable parameters, dynamics is simulated.

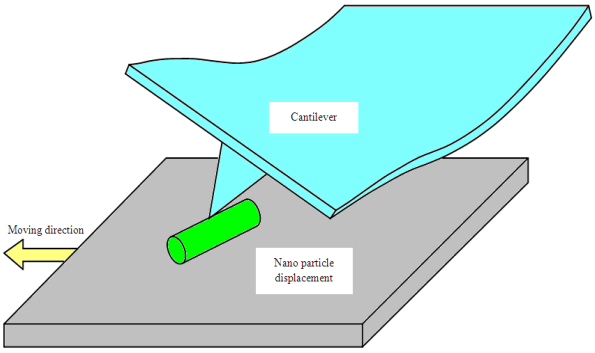


Fig.1. Pushing process of cylindrical nano particles by the means of AFM nano robot

II. DETAILS EXPERIMENTAL

In cylindrical nanoparticles manipulation modeling divided into 2 parts. In the first part, 3D cantilever dynamics has been considered and in the second, motion modes have been investigated. In general, model of 3D manipulation contains 25 equations. In sliding state, operation continued until getting to the target point whereas in spinning mode after specified distances cantilever passed along the particle and particle stop moving. Manipulation equations included 25 coupled equations which represent system dynamics from first contact to reaching target point or separation of probe and particle. The kinematic equations have been introduced in previous works [9]. In these equations a_a, a_y, a_z are accelerations of probe tip, $\ddot{\theta}, \ddot{\gamma}$ are angular accelerations, H, is height of probe tip and θ, γ are torsional and bending deformations of probe. Kinematic relations are introduced here as the first step:

$$a_x = -H\ddot{\theta}\cos\theta + H\dot{\theta}^2\sin\theta \quad (1)$$

$$a_z = -H\ddot{\theta}\sin\theta - H\dot{\theta}^2\cos\theta - 2H\ddot{\gamma}\sin(\frac{\gamma}{2})\cos(\frac{\gamma}{2}) \quad (2)$$
$$- H\dot{\gamma}^2\cos^2(\frac{\gamma}{2}) + H\dot{\gamma}^2\sin^2(\frac{\gamma}{2})$$

$$a_y = H\ddot{\gamma}\cos^2(\frac{\gamma}{2}) - H\ddot{\gamma}\sin^2(\frac{\gamma}{2}) - 2H\dot{\gamma}^2\sin(\frac{\gamma}{2})\cos(\frac{\gamma}{2}) \quad (3)$$

$$\ddot{\theta} = \dot{\theta}^2\tan\theta \quad (4)$$

$$\ddot{\gamma} = 2\dot{\gamma}^2\frac{\sin(\frac{\gamma}{2})\cos(\frac{\gamma}{2})}{\cos^2(\frac{\gamma}{2}) - \sin^2(\frac{\gamma}{2})} \quad (5)$$

Deformations of cantilever causes internal forces that introduced by equation 6 in similar way. In this equation F_x, F_y, F_z are internal forces, $K_X, K_Y, K_Z, K_{\theta_Y}, K_{\theta_X}$ are spring constants, H, is height of probe tip, $\varepsilon_X, \varepsilon_Y, \varepsilon_Z$ are deformations, and θ_X, θ_Y are angular deformations. In the equations, the spring constants are used according to the models represented in the previous researches. It should be noted that this spring constants are different for V-shape and rectangular cantilever [9].

$$\begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix} = \begin{bmatrix} K_X & 0 & 0 & 0 & \frac{K_{\theta_Y}}{H} \\ 0 & K_Y & 0 & \frac{K_{\theta_X}}{H} & 0 \\ 0 & 0 & K_Z & 0 & 0 \end{bmatrix} \times \begin{bmatrix} \varepsilon_X \\ \varepsilon_Y \\ \varepsilon_Z \\ \theta_X \\ \theta_Y \end{bmatrix} \quad (6)$$

First section of curve in the figure 2 is determined by entering kinematic equations and internal forces at kinetic equations of cantilever as shown in figure1 [9]. In the given dynamics equations (equations 7 to11) the external forces that enter to tip of probe from environment are included F_X, F_Y, F_Z and $F_x, F_y, F_z, M_{\theta_X}, M_{\theta_Y}, W, V$ are internal forces andθ is torsion angle, γ is bending angle and FT is the pushing force, a_x, a_y, a_z are accelerations based on kinematic relations, I, is moment of inertia and m is the mass of cantilever.

$$F_Z = \left(\frac{I\ddot{\theta} + M_{\theta_X}}{H}\right)\sin\theta - ma_x\sin\theta\cos\theta \quad (7)$$
$$- F_x\sin\theta\cos\theta + F_z\cos^2\theta + ma_z\cos^2\theta + W\sin\gamma\cos^2\theta$$

$$F_Y = \left(\frac{I\ddot{\gamma} + M_{\theta_Y}}{H}\right)\cos\gamma - F_z\sin\gamma\cos\gamma \quad (8)$$
$$- V\sin\theta\cos\gamma\sin\gamma - ma_z\cos\gamma\sin\gamma - ma_y\sin^2\gamma + F_y\sin^2\gamma$$

$$V = \frac{1}{\sin\theta}(F_Z - F_z - w\sin\gamma - ma_z) \quad (9)$$

$$w = \frac{1}{\sin\gamma}(F_Z - F_z - v\sin\theta - ma_z) \quad (10)$$

$$F_X = ma_x + F_x + V\cos\theta \quad (11)$$

The obtained dynamics equations caused deformation at contact point of particle and probe and contact point of particle and surface. The deformed surfaces are identified based on equation 12 to 15 [10]. In the given equation F is compressive force on the surface,ω is adhesive energy of the surface, K is equivalent elasticity modulus, R' is equivalent radius equation, R is radius of nanoparticle and L is length of it, A_t, δ_t are area and depth of deformed surface at contact point of nanoparticle and probe respectively and A_s, δ_s are deformed area and depth at contact point of nanoparticle and substrate.

$$A_t^3 = \frac{3R'}{4K}\left(F + 3\omega\pi R' + \sqrt{6\omega\pi R'F + (3\omega\pi R')^2}\right) \quad (12)$$

$$\delta_t = \frac{A_t^2}{R'} - \frac{2}{3}\sqrt{\frac{3\pi\,\omega\,A_t}{K}} \quad (13)$$

$$P = \frac{3\pi K A_s^2 L}{8R} - \sqrt{6\pi w K A_s L^2} \quad (14)$$

$$\delta_s = \frac{3\pi A_s^2}{8R}L - \sqrt{\frac{6\pi\,L^2\,\omega\,A_s}{K}} \quad (15)$$

After determining deformed surface and dynamic forces in previous steps and using simulation of motion modes, simulation of dynamics modes has been introduced. In the relations F^*_S is critical force of sliding, F^*_R is critical force of rolling, F^*_{SP} is critical force of spinning which are function of angle

between forces , ψ contact angle of probe and particle , ϕ the contact surface parameters μ , τ , contact surfaces As and At , radius of particle R and length of it L, point of probe and particle contact X, τ_s adhesive surface constant in sliding , and adhesive surface constant in spinning . The angle between forces FY and FZ is showed by angel ψ_1 and angle between ψ_1 and f_{T_t} is also demonstrated by parameter ε ($\varepsilon = \psi_1 - \phi - 90$).

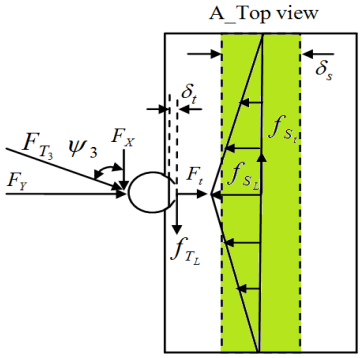


Fig.2. modeling of Pushing Forces during manipulation

$$F^*_S = \frac{\tau_s A_s}{\sin\psi_1 - \mu_S \cos\psi_1} \quad (16)$$

$$F^*_R = \frac{\tau_{rs} As + \tau_{rt} A_t}{R(\cos\varepsilon + \sin\psi_1) - \mu_{rs}\cos\psi_1 + \mu_{rt}\sin\varepsilon} \quad (17)$$

$$F^*_{SP} = \frac{\tau_{rs} A_s + \tau_{rT} A_t}{\cos\psi_1(\frac{4X-2L}{3}) + R\sin\psi_1\cot\psi_3 - \mu_{rs}\cos\psi_1 + \mu_{rt}\sin\varepsilon} \quad (18)$$

When sliding mode occurs the particle goes on its moving on the path until reaches target point. In case of spinning mode, the particle and probe separated from each other after some distance that make second critical time. It is shown in figure1 and determined according to relation19 to 21(it is necessary to noted that equation 6 actually included 5 equations that represented as matrix and given relations totally creating 25 equations). In the given relations is the maximum spinning angel, Ti is second critical time, is the velocity of reference surface, L is length of nanoparticle, and X1 is the contact point of probe and particle [11].

$$\theta_{ult} = \frac{Ti \times V_{sub}}{L - \left(x_1' + \sqrt{x_1' - \frac{1}{2}(2x_1' - 1)}\right)} \quad (19)$$

$$S_2 = D - D\cos(\theta_{ult}) \quad (20)$$

$$S_1 = L - x_1 \quad (21)$$

III. SIMULATION OF MANIPULATION PROCESS

In this section a simulation for manipulation process is presented. At this point, by knowing the dynamic motion modes, the manner of movement of cylindrical particles is explored, and the critical force and time, which are the main parameters of the manipulation operations, are obtained. First, the presented simulation algorithm is divided into three parts. The kinematics of motion is specified in the first part; the cantilever dynamics and the dynamic motion modes are obtained in the second part; and in the third part, the critical time and force are determined.

As a first step, the kinematics of movement is obtained by using the presented relations, and the kinematics is then used to determine the dynamic forces. By solving the presented equations for each time interval, the force-time diagrams are obtained. By using the simulation constants in these equations, the rolling, sliding and rotating motion modes are simulated. Next, the motion mode of operation (rolling, sliding, and rotating mode) is specified with regards to the conditions of the experiment and the time of operation. Then by knowing the dynamic mode of motion, the critical time and force of manipulation are investigated. There are 2 cases possible at this juncture, which will be explored in the third step.

With motion modes determined, the algorithm takes two routes in the third step. In the first case, the manipulation in the sliding or rolling mode, which is a one-dimensional operation, is simulated. Similar to the manipulation of spherical particles, in the case of cylindrical particles also, only one critical time and force has been used in the simulations related to the sliding and rolling modes. To obtain this critical time and force, the combination of cantilever dynamics and dynamic modes has been used.

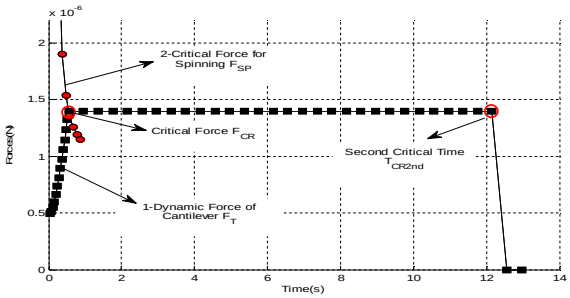


Fig.3. simulation of effective forces during process

CONCLUSIONS

As it is presented in the modeling part 25 effective forces has been modeled and based on this modeling the below results has been introduced:

1. Based on particle size and environmental parameters different motion modes have been observed.
2. For particle with higher length the spinning mode was the dominate mode as it is presented in Fig. 3
3. In spinning mode 2 separateparts has been observed. First, dislodge of particle and start of movement on substrate and then dislodge of probe which has been shown in Fig. 3.

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