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Topical Perspectives

Comprehensive modelling and simulation of cylindrical nanoparticles manipulation by using a virtual reality environment

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ABSTRACT

With the expansion of nanotechnology, robots based on atomic force microscope (AFM) have been widely used as effective tools for displacing nanoparticles and constructing nanostructures. One of the most limiting factors in AFM-based manipulation procedures is the inability of simultaneously observing the controlled pushing and displacing of nanoparticles while performing the operation. To deal with this limitation, a virtual reality environment has been used in this paper for observing the manipulation operation. In the simulations performed in this paper, first, the images acquired by the atomic force microscope have been processed and the positions and dimensions of nanoparticles have been determined. Then, by dynamically modelling the transfer of nanoparticles and simulating the critical force-time diagrams, a controlled displacement of nanoparticles has been accomplished. The simulations have been further developed for the use of rectangular, V-shape and dagger-shape cantilevers. The established virtual reality environment has made it possible to simulate the manipulation of biological particles in a liquid medium.

1. Introduction

In the last decade, the displacing of nanoparticles and building of nanostructures by means of AFM-based robots has greatly attracted the attention of nanotechnology researchers. In this process, various nanoparticles (spherical, cylindrical, and biological) are pushed and displaced by the probe tip of the atomic force microscope in order to build the considered nanostructures. The major drawback of this method is the inability to simultaneously observe the operation during its implementation [1].

To improve the effectiveness of the AFM-based Nano robots, more attention has been paid to the computer modelling and simulation of the dynamics of a manipulation process for the displacement of spherical nanoparticles [2]. Onal et al. have investigated the optimal manipulation of spherical nanoparticles in a 2D space, by using a proper displacement velocity [3,4]. The manipulation of biological spherical nanoparticles has been modelled and simulated by Korayem et al. [5]. Hou has modelled the assembling process of nanotubes [6]. The dynamics of the 3D manipulation of cylindrical nanoparticles have been modelled by some researchers [7,8]. This paper has been developed and presents a comprehensive simulation environment by using image processing. The use of AFM image, made the simulation more feasible. Other works have focused on the effect of AFM cantilever shapes [9–11]. Some models for simulating the displacement of nanoparticles in liquid environments have been developed [12,13].

In order to solve the problem of simultaneous process observation, Lie et al. have proposed an added reality system [14]. Varol et al. have explored the use of a virtual reality tool kit for path planning in the displacement of spherical nanoparticles [15]. They have also presented a graphical interface to make the virtual reality environment practical [16]. Naebi et al. have investigated the issue of nanoparticles collision during a manipulation operation and the selection of the best path in order to minimize the moves of an atomic force microscope [17]. Using the method of image processing by means of Genetic Algorithm, a virtual reality software has been presented for the manipulation of spherical particles [18]. The virtual reality environment has been extended for simulating the displacement of cylindrical nanoparticles in the air medium and in the sliding and rolling motion modes [19]. The virtual reality environment presented in this paper has thoroughly considered all the motion modes, environmental conditions and cantilever geome-

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tries. The simulation environment has been improved to include two mediums (air and liquids), and for the liquids medium four different types of liquids, water, glycerine, ethylene and olive oil, could be selected. Moreover, in this simulation software, user can select the type of AFM cantilever as rectangular, dagger or V-shape. The transferring of nanoparticle images to a virtual reality environment has also been addressed in this paper.

Image processing by means of the Ant Colony Algorithm has been investigated in previous research works [20–22]. In this paper, for detecting the edges of particles, a modified version of the ant colony algorithm has been used after performing a pre-processing step on the acquired Nano-images. Then by using the morphological operators, the image processing steps have been completed, and the particles have been identified and numbered. The simulation software has been designed graphically and named CNMVR, C: Cylindrical, N: Nanoparticle, M: Manipulation, V: Virtual, R: Reality.

2. Comprehensive modelling of the manipulation of cylindrical nanoparticles

In this paper, the displacement of cylindrical nanoparticles in different mediums and by means of rectangular, V-shape and dagger cantilevers has been simulated for all kinds of motion modes (sliding, rolling and spinning). The manipulation dynamics presented in different papers in the literature have been thoroughly reviewed [7,8,11,13].

In this paper, the procedures for obtaining the governing dynamic equations have been ignored and in the modelling section, only the relevant reference has been cited. The first step in the manipulation modelling of nanoparticles is the presentation of the kinematic equations of motion. With the consideration of all the deformations produced in nanoparticle and cantilever, the general kinematic equations have been presented as follows [13]. The modelling of the manipulation of cylindrical particles in air is carried out in five steps. In the first step, the elastic deformation of the particle is not taken into consideration. In the second step, the elastic deformations produced between probe tip and particle and also between particle and substrate is incorporated into the relevant equations. Then, due to the application of a force, the cantilever experiences an upward movement, a rotation and a small deflection; which are considered in the third step. In the fourth step, the inward bending of the cantilever is considered in the computations. And finally in the fifth step, the motion kinematics of the nanoparticle with regards to the rotation of the nanotubes are taken into account.

$$\begin{aligned} X_p &= X_s + \left(R_p - \delta_t\right)\sin\varphi - H\sin\theta - 2\delta_D - \delta_{ST} + l\sin\lambda \\ Z_p &= Z_s + \left(R_p - \delta_t\right)\cos\varphi + \left(R_p - \delta_s\right) + H\cos\theta - 2H\sin^2\left(\frac{\gamma}{2}\right) \\ Y_p &= Y_s + 2H\sin(\gamma)\cos\left(\frac{\gamma}{2}\right) + 2L\sin^2\left(\frac{\lambda}{2}\right) \end{aligned} \tag{1}$$

In the above equations, X_p, Y_p and Z_p are the coordinates of the reference point, φ is the probe tip-particle contact angle (which is assumed as constant), λ is the nanoparticle rotation angle, R_p is the nanoparticle radius, l is the nanoparticle length, and H is the height of probe tip, δ_t, δ_s are the elastic deformations of substrate and particle, F_{st} and F_D are surface tension force and drag force, and δ_D, δ_{ST} are the deformations resulting from the surface tension force and drag force, respectively.

With the kinematic model specified, the cantilever model is presented for the purpose of modelling the internal forces. The provided model, which depends on cantilever shape, is obtained for different cantilevers with regards to Eq. (2) and Table 1.

$$\begin{bmatrix} F_X^c \\ F_Y^c \\ F_Z^c \end{bmatrix} = \begin{bmatrix} K_X & 0 & 0 & 0 & \dfrac{K_{\theta y}}{L_{tip}^2} \\ 0 & K_Y & 0 & \dfrac{K_{\theta x}}{L_{tip}^2} & 0 \\ 0 & 0 & K_Z & 0 & 0 \end{bmatrix} \times \begin{bmatrix} \varepsilon_X \\ \varepsilon_Y \\ \varepsilon_Z \\ \theta_X \\ \theta_Y \end{bmatrix} \tag{2}$$

In Table 1, L_{top} is the length of the triangular section, and θ_I and θ_{II} denote the deflections at the ends of Sections I and II of the V-shaped cantilever, respectively. The other parameters have been presented in detail by Korayem et al. [11].

Korayem and Hoshiar have used the JKR contact model for modelling the elastic deformation and adhesion of nanoparticles [7,8]. The JKR contact model has been provided for two contact cases. The first case, involving the contact between probe tip and particle, is considered as a contact between two spheres; and the second case, the contact between particle and substrate, is considered as a contact between two cylinders. The comprehensive equations of motion dynamics (Eqs. (3)–(7)) have been subsequently provided. By solving these equations, the dynamic forces involved in a manipulation can be simulated.

$$F_Z = \left(\frac{I\ddot{\theta} + M_{\theta_X}}{H}\right)\sin\theta - ma_x\sin\theta\cos\theta - F_x\sin\theta\cos\theta + F_z\cos^2\theta$$
$$+ma_z\cos^2\theta + W\sin\gamma\cos^2\theta \tag{3}$$

$$F_Y = \left(\frac{I\ddot{\gamma} + M_{\theta_Y}}{H}\right)\cos\gamma - F_z\sin\gamma\cos\gamma - V\sin\theta\cos\gamma\sin\gamma - ma_z\cos\gamma\sin\gamma$$
$$-ma_y\sin^2\gamma + F_y\sin^2\gamma \tag{4}$$

$$V = \frac{1}{\sin\theta}\left(F_Z - F_z - w\sin\gamma - ma_z\right) \tag{5}$$

$$w = \frac{1}{\sin\gamma}\left(F_Z - F_z - v\sin\theta - ma_z\right) \tag{6}$$

$$F_X = ma_x + F_x + V\cos\theta \tag{7}$$

In the above equations, F_X, F_Y and F_Z denote the external forces acting on the probe tip, and F_x, F_y, F_z, M_{θ_x}, M_{θ_y}, W and V are the internal forces and moments. θ is the rotation angle, γ is the bending angle, and F_T is the resultant force. a_x, a_y and a_z are the accelerations based on the kinematic equations, I is the moment of inertia and m is the cantilever mass. In this work, all the motion modes (sliding, rolling and spinning) have been simulated [7,8] (Eqs. (8)–(11)).

$$F^*Sl_1 = \frac{\tau_T A_T}{\cos\varepsilon + \mu_T\cos\varepsilon}\ \text{Sliding} \tag{8}$$

$$F^*S = \frac{\tau_S A_S}{\sin\psi_1 - \mu_S\cos\psi_1}\ \text{Sliding} \tag{9}$$

$$F^*R = \frac{\tau_{rS}A_S + \tau_{rT}A_T}{R_P(\cos\varepsilon + \sin\psi_1) - \mu_{rS}\cos\psi_1 + \mu_{rT}\sin\varepsilon}\ \text{Rolling} \tag{10}$$

$$F^*SP = \frac{\tau_{rS}A_S + \tau_{rT}A_T}{\sin\psi_1\left(\frac{2X-L_p}{3}\right) + R\sin\psi_1\cot\psi_3 - \mu_{rS}\cos\psi_1 + \mu_{rT}\sin\varepsilon}\ \text{Spinning} \tag{11}$$

In the above equations, F^*, $F^*_{sl}2$, F^*_R, F^*_S, $F^*_{sl}1$ and F^*_{SP} are functions of the angle between forces ψ, probe-particle contact angle ϕ, surface contact parameters μ and τ, contact areas As and AT, particle radius RP, particle length LP, and the location of contact between particle and probe X. The angle between forces FY and FZ has been indicated by angle ψ_2. Also, the angle between F_{T_1} and f_{T_1} has been designated by ε. Ultimately, by simultaneously solving