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Non-classic multiscale modeling of manipulation based on AFM, in aqueous and humid ambient

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ABSTRACT

To achieve a precise manipulation, it is important that an accurate model consisting the size effect and environmental conditions be employed. In this paper, the non-classical multiscale modeling is developed to investigate the manipulation in a vacuum, aqueous and humid ambient. The manipulation structure is considered into two parts as a macro-field (MF) and a nano-field (NF). The governing equations of the AFM components (consist of the cantilever and tip) in the MF are derived based on the modified couple stress theory. The material length scale parameter is used to study the size effect. The fluid flow in the MF is assumed as the Couette and Creeping flows. Moreover, the NF is modeled using the molecular dynamics. The Electro-Based (ELBA) model is considered to model the ambient condition in the NF. The nanoparticle in the different conditions is taken into account to study the manipulation. The results of the manipulation indicate that the predicted deflection of the non-classical model is less than the classical one. Comparison of the nanoparticle travelled distance on substrate shows that the manipulation in the submerged condition is close to the ideal manipulation. The results of humid condition illustrate that by increasing the relative humidity (RH) the manipulation force decreases. Furthermore, Root Mean Square (RMS) as a criterion of damage demonstrates that the submerged nanoparticle has the minimum damage, however, the minimum manipulation force occurs in superlative humid ambient.

1. Introduction

The manipulation is one of the AFM applications. Studying the behavior of nanoparticles during the manipulation process is considered by researchers [1]. The environmental conditions such as humidity are very effective in the precise manipulation. By considering different scales of Atomic Force Microscope (AFM), the modeling methods used in the studies can be classified into three categories: the continuum mechanics, the molecular dynamics and the multiscale model.

The origin of this type of sorting is that researchers have investigated the modeling of AFM behavior from two different aspects. The head of tip and nanoparticle section that is called nano field (NF) and the top of tip and cantilever is the macro field (MF). Its reason is that in many cases, nanoparticle and the head of tip that interacts with nanoparticle are considered in low dimension and using the governing equations stem from the continuum mechanics theory is not valid. Therefore methods like MD approach are in high consideration. Besides modeling of the whole structure with this method is impossible and multiscale approaches are therefore used as an interference for solving this problem.

According to this categorize, many studies have been done based on the continuum mechanics approach in this field. For the first time, the precise manipulation of gold nanoparticles on the Si/SiO2 substrate in a liquid environment using the tip of SFM was done by Resch et al [2]. The experiments were performed in deionized water and ethanol as an organic solution. Korayem et al. modeled the nanomanipulation of gold nanoparticle based on AFM in the liquid media and examine the effect of hydrodynamic and surface forces [3].

Recently, some attempts have been made to simulate the AFM applications such as imaging, scratching and nanomanipulation by the molecular dynamics approach. A theoretical non-contact atomic force microscope (nc-AFM) imaging of a C60 molecule adsorbed on the Si surface was investigated by Hobbs and Kantorovich [4]. Mahboobi et al. examined precise positioning of nanoclusters and investigated the material and manipulation strategy in final success [5]. In another study, Mahboobi et al. focused on MD simulation for analyzing metal clusters manipulation on double layer substrates [6]. Substrate geometry plays important role in the dynamics behavior of the manipulation. Mahboobi et al. modeled the manipulation of nanoclusters on stepped surfaces by considering five stepped surface forms and different combinations for particle and substrate [7]. The coarse-grained approach was used to

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overcome the computational limitation which limits system dimensions [8]. Using the Coarse-Grained Molecular Dynamics (CGMD), Korayem et al. modeled the manipulation of nanoclusters with a flexible AFM tip, and studied the effects of different parameters on the success of the nanomanipulation procedure [9].

The aforementioned studies are in the vacuum medium and ideal condition. With MD viewpoint, some studies have been done on the environmental effects such as capillary, hydration force, matter-water interface and etc. Choi et al. simulated an MD model of the water meniscus formed between an AFM tip and a surface that such a nanoscale meniscus is ubiquitous in AFM experiment. They examined how the meniscus structure changes as the distance between the tip and the surface changes [10]. Böcker et al. performed MD simulation of the mercury-water interface using flexible BJH water model [11]. Gulbinski et al. studied the influence of adsorbed water on measured AFM friction on molybdenum trioxide thin films [12]. The effects of water on the whole manipulation process were studied by using the SPC/E model based on molecular dynamics simulation [13].

A capped carbon nanotube (CNT) tip that may be used as an AFM probe for the measurement of hydration forces at the alumina-water interface was simulated by Argyris et al. [14]. The AFM tip was modeled as a rigid single-walled carbon nanotube by molecular dynamics method.

In recent decades, some approaches have been developed to investigate involving different atomistically problems in large material scale [15]. These efforts led to the creation of multiscale models such as Cauchy-Born rule [16,17], Virtual Atom Cluster (VAC) [18] and embedded statistical coupling method (ESCM) [15].

In manipulation field, Korayem et al. [19] proposed a Fixed Interfacial Multiscale Method (FIMM) as a concurrent multiscale model. This approach makes a direct link between the nano field atoms and macro field nodes by the local atomic volume displacements associated with every macro field node. Korayem et al. [20] used the FIMM to study the manipulation of metallic nanoparticles. They emphasized on the development of simulation times and length scales and solution of the invalidity problem of Continuum Mechanics (CM) approaches at small scales. In another study, Korayem et al. [21] used the FIMM by focusing on the hysteresis effects on the imaging and manipulation of nano-objects. In this study, some suggestions were presented for the prediction and improvement of undesirable errors in AFM operations.

Continuum mechanics theories are used for the modeling of the MF in multiscale methods. Experiments show that the size effect plays an important role in the micro/nano scale [22,23] which the classical continuum mechanics theory cannot predict this effect, however, non-classical continuum mechanics theories like the couple stress, non-local, and strain gradient theories can take the size effect into account by applying the material length scale parameter. The classical couple stress elasticity theory was presented by Toupin [24] and Mindlin and Tiersten [25]. Yang et al. [26] introduced the modified couple stress theory in which use a parameter as the material length scale parameter. Yin et al. [27] and Jomehzadeh et al. [28] have investigated the size effects in the free vibrations of Kirchhoff model micro-plates based on the modified couple stress theory. The natural frequencies of micro-plates with various boundary conditions have been analyzed in the presence of the length scale parameter. They demonstrated that the size effect causes the plate frequency to increase. Since the scale is micro in the structural components AFM, The dynamic investigation of the AFM cantilever was studied based on modified couple stress theory [29,30]. In manipulation field, Korayem and Homayooni [31] investigated the manipulation behavior of the AFM by focusing on the multiscale method as a combination of large-scale equations with MD equations based on the modified couple stress theory.

The previous studies have not covered the modeling of the precise nanomanipulation in the liquid medium based on a non-classical theory. In this paper, a non-classical multiscale model of the manipulation in aqueous and wet media has been presented using the modified couple stress theory. For this purpose, the MF governing equations of the cantilever and tip are derived based on the modified couple stress theory. The MF drag force is modeled using creeping and Couette flow assumptions [32]. The electrostatics-based (ELBA) [33] as a coarse-grained model has been used to investigate the water and humidity effect in the NF. The multiscale algorithm is utilized to combine the equations of the MF with the NF, and finally, the manipulation process is modeled.

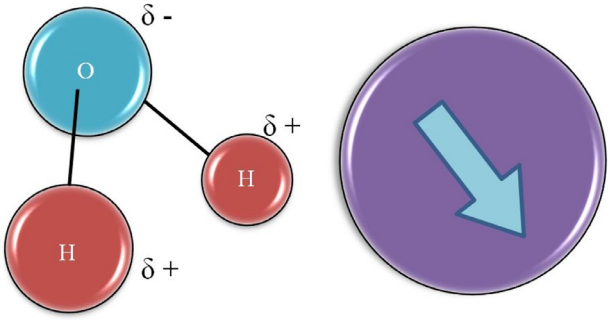

Fig. 1. Coarse-grained water site represents a single water molecule.

2. ELBA water model

The ELBA [33] force field is a model that is extended with the concentration on electrostatics properties. This model is adequate for the modeling of dipole molecules. Therefore, it's an appropriate choice for the water molecules. Fig. 1 shows the schematics of the ELBA equivalent coarse-grained atom model and an atomistic water molecule.

Based on this model, the total potential energy U_{ij} for a pair of water particles i and j can be expressed as

$$U_{ij} = U_{LJ} + U_{dip.} \tag{1}$$

where U_{LJ} and $U_{dip.}$ are the Lennard–Jones and the dipole-dipole terms, respectively. Eq. (2) present U_{LJ}

$$U_{LJ} = 4\varepsilon\left[\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] + \left[6\left(\frac{\sigma}{r_c}\right)^{12} - 3\left(\frac{\sigma}{r_c}\right)^{6}\right]\left(\frac{r_{ij}}{r_c}\right)^{2} - 7\left(\frac{\sigma}{r_c}\right)^{12} + 4\left(\frac{\sigma}{r_c}\right)^{6}\right] \tag{2}$$

where r_{ij} is the interparticle distance of pair i and j coarse-grained molecules, r_c is the cutoff radius, ε and σ are standard Lennard-Jones parameters.

By considering r_s and r_c as the switching and cutoff radius respectively, $U_{dip.}$ can be defined as Eq. (3)

$$U_{dip.} = \frac{1}{4\pi\varepsilon_0}\left[\frac{\mu_j.\mu_i}{r_{ij}^3} - \frac{3(\mu_i.r_{ij})(\mu_j.r_{ij})}{r_{ij}^5}\right]s_{ij}$$

$$s_{ij} = \begin{cases} 1 & if \quad r_{ij} < r_s \\ \frac{(r_c - r_{ij})^2(r_c + 2r_{ij} - 3r_s)}{(r_c - r_s)^3} & if \quad r_c < r_{ij} < r_c \end{cases} \tag{3}$$

in which ε_0 is the electric permittivity of vacuum, r_{ij} is the interparticle distance, μ_i,μ_j are dipole moment vectors of sites i and j, also s_{ij} is a cubic switching function that acting between a r_s and r_c.

3. Macro field model

Fig. 2 illustrates the geometrical parameters including L_b, w_b, L_p and L_t that are the cantilever length, the cantilever width, length of piezoelectric patch and length of the tip, respectively. According to the coordinate system shown in Fig. 1, the displacement field is assumed as:

$$u_1(x_1, x_2, x_3, t) = u_0(x_1, x_2, t) + x_3\psi_1(x_1, x_2, t)$$