



The Second Phase of Gold Nanoparticle Manipulation based on AFM in Different Liquid Environments

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Abstract

The use of gold metal in astronautics, electronics and medical sciences has led to it being considered. Therefore, structural studies and changes have been made to improve the properties or establish special atomic arrangements in nanoscience for this particular metal. Atomic force microscopy (AFM) is one of the most widely used tools for these purposes. Therefore, in this paper, the displacement of gold nanoparticles during manipulation using the atomic force microscopy, which is one of the objectives of the second phase, in the environmental conditions of water, plasma and methanol, has been investigated. For this purpose, the process is first modeled in two dimensions and the intermolecular forces of van der Waals, the double layer force and the hydration force are considered. Then, the displacement diagrams are drawn considering the forces between the molecule and the studied environments. Finally, according to the simulation results in different environments, the highest displacement of gold nanoparticles in the second phase of manipulation was in water and the lowest in plasma.

Keywords: Manipulation, Gold Nanoparticles, Atomic Force Microscope, Intermolecular Forces, Different Liquid Environments.

1. Introduction

Examining the geometrical and chemical structure of materials, improving the properties of nanostructures, studying biological cells and determining the mechanical properties of cells and nanoparticles are among the important factors of the atomic force microscope in the construction, medical, aerospace and electronics industries; Therefore, this tool has been widely used in various fields and during processes such as manipulation; Also, the importance of gold metal due to its electrical properties, conductivity and other things has caused attention to this metal in various industries; Therefore, during the manipulation process, the parameters affecting the gold nanoparticle in the first and second phases have been examined so that by fully understanding this metal in nano dimensions, its properties can be improved and used in the construction of nanostructures with atomic precision.

Taheri and Bathaee [1] analyzed the sensitivity of environmental parameters on rolling force and time using E-fast statistical method. Kreig et al. [2] have investigated the advantages and limitations of atomic force microscopy in determining the mechanical properties of complex biological particles. Korayem et al. [3] have investigated the roughness of the cancer cell

surface during the manipulation process using an atomic force microscope. Motaghi et al. [4] have simulated the first phase of gold nanoparticle manipulation. Taheri [5] has investigated the application of atomic force microscope in extracting the critical force and time of two-dimensional manipulation for gastric cancer tissue with different friction models of Coulomb, HK and LuGre.

In this research, manipulation of gold nanoparticles in different liquid environments and in the second phase has been modeled and simulated. Also, the surface of this nanoparticle was explored by atomic force microscope and the topographic images and the results were presented. The investigated environments include water, plasma and methanol. The reason for considering these environments is that the test conditions are close to the real biological conditions. Finally, the displacement rate in all three environments has been investigated in the second phase of manipulation. The modeling is done in two dimensions.

2. Methodology

In this section, intermolecular forces and their equations have been investigated first. Then, the equations of the second phase have been analyzed in

two dimensions.

2.1. Intermolecular Forces

The investigation of intermolecular forces in nano dimensions has been analyzed in this section, and the equations presented in this section have been used in the simulations of the second phase of gold nanoparticle manipulation.

2.1.1. Van der Waals force

$$F_{\text{vdw}}(D) = -\frac{H R_t}{6 D^2} \quad (1)$$

$$\begin{aligned} H_{\text{total}} &= H_{v=0} + H_{v>0} \\ &\approx \frac{3}{4} k T \left(\frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_1 + \varepsilon_3} \right) \left(\frac{\varepsilon_2 - \varepsilon_3}{\varepsilon_2 + \varepsilon_3} \right) \\ &+ \frac{3 h \nu_e}{8 \sqrt{2}} \frac{(n_1^2 - n_3^2)(n_2^2 - n_3^2)}{(n_1^2 + n_3^2)^{\frac{1}{2}}(n_2^2 + n_3^2)^{\frac{1}{2}} \left[(n_1^2 + n_3^2)^{\frac{1}{2}} + (n_2^2 + n_3^2)^{\frac{1}{2}} \right]} \\ &\approx \frac{3}{4} k T \left(\frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_1 + \varepsilon_3} \right) \left(\frac{\varepsilon_2 - \varepsilon_3}{\varepsilon_2 + \varepsilon_3} \right) \end{aligned} \quad (2)$$

2.1.2. Double layer electrostatic force

$$F_{\text{el}} = \frac{4 \pi R \sigma_S \sigma_T \lambda_D}{\varepsilon \varepsilon_0} e^{-D/\lambda_D} \quad (3)$$

2.1.3. Hydration force

$$U = A e^{-X/\lambda_H} \quad (4)$$

2.2. Modeling of Nanomanipulation

Atomic force microscope is used as a tool for exploring the surface of materials and biological cells due to the lack of limitations in studying materials in different environments and other advantages. This tool extracts properties by making contact on two surfaces of particle-tip and particle-substrate, and exploring the surface of the desired nanoparticle. In this process, the application of force begins with the contact of the tip of the atomic force microscope with the nanoparticle, and

this process of increasing the force continues until the resistance forces are overcome and the movement begins. The time and force that start the movement are called critical time and force, respectively. The equations of this section are as follows:

$$F_y = K_y y_p \quad (5)$$

$$F_z = K_z z_p \quad (6)$$

$$M_\theta = K_\theta \times \theta \quad (7)$$

$$y_p = y_{\text{sub}} + (R_p - \delta_r) \sin \phi - H \sin \theta \quad (8)$$

$$z_p = y_{\text{sub}} + (R_p - \delta_r) \cos \phi + (R_p - \delta_s) - H \cos \theta \quad (9)$$

$$\sum F_y = m a_y = m \left(\frac{\ddot{y}_T + \ddot{y}_P}{2} \right) \quad (10)$$

$$\sum F_z = m a_z = m \left(\frac{\ddot{z}_T + \ddot{z}_P}{2} \right) \quad (11)$$

$$F_y = F_y + \frac{m}{2} H \dot{\theta}^2 \sin \theta \quad (12)$$

$$F_z = F_z - \frac{m}{2} H \dot{\theta}^2 \cos \theta \quad (13)$$

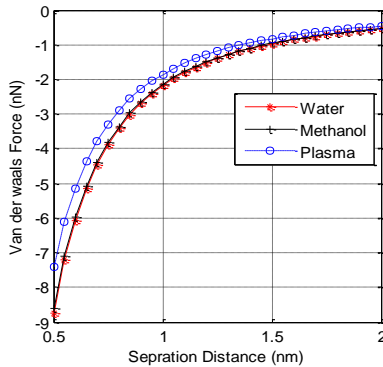
$$F_r = \sqrt{(F_y^2 + F_z^2)} \quad (14)$$

3. Discussion and Results

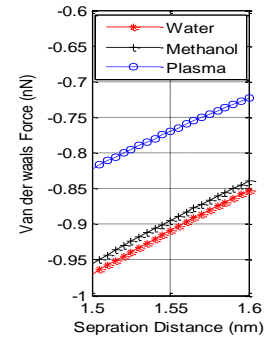
In this section, the intermolecular force has been compared and verified in different environments.

Figure 1 shows the graphs of changes in intermolecular forces during displacement in different environments.

In Figure 2, the graphs of force, acceleration, speed and finally displacement in plasma, water and methanol environments are drawn.



a) Van der Waals force



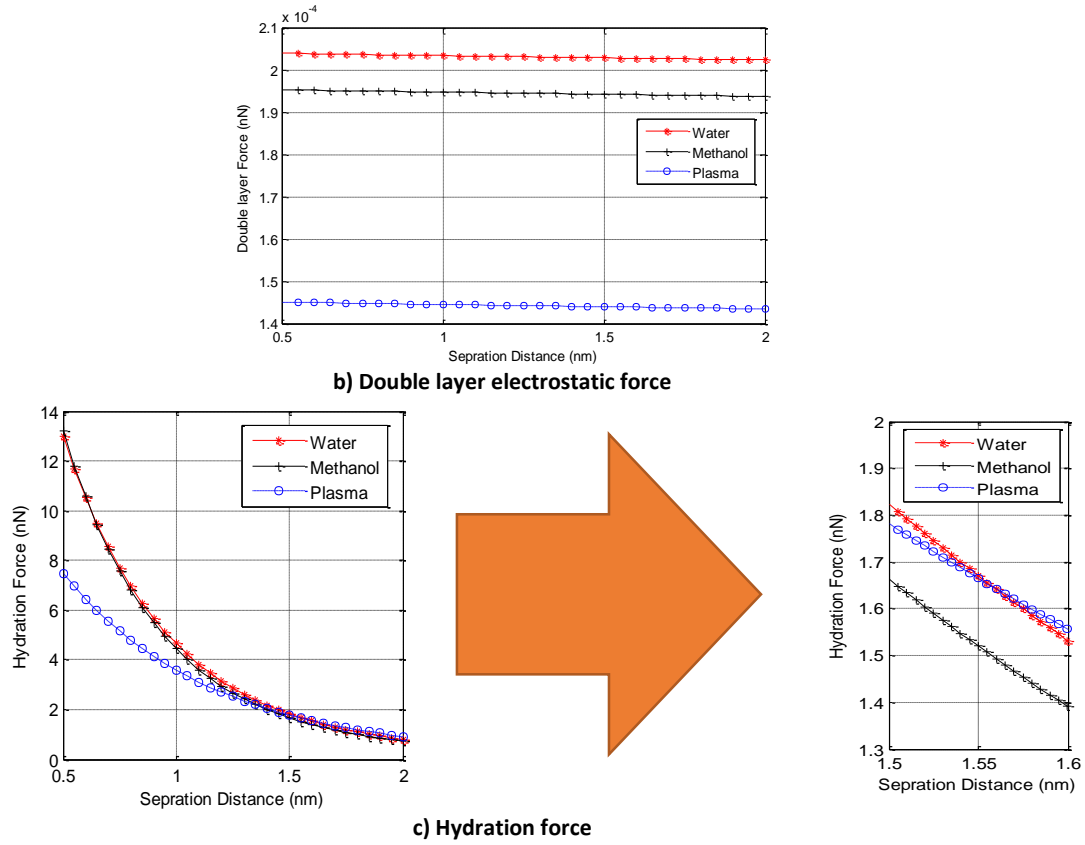
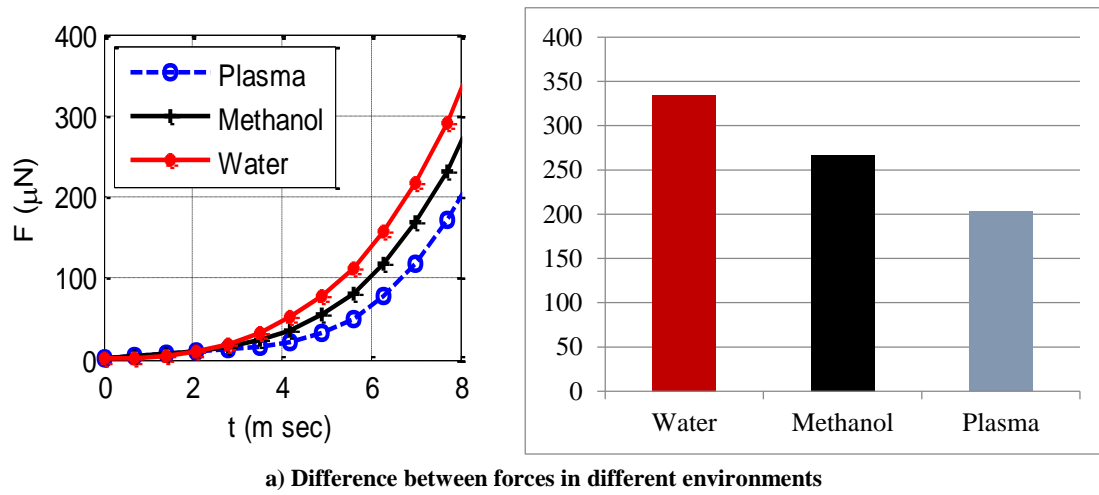


Figure 1. Diagram of intermolecular forces - separation distance in different environments



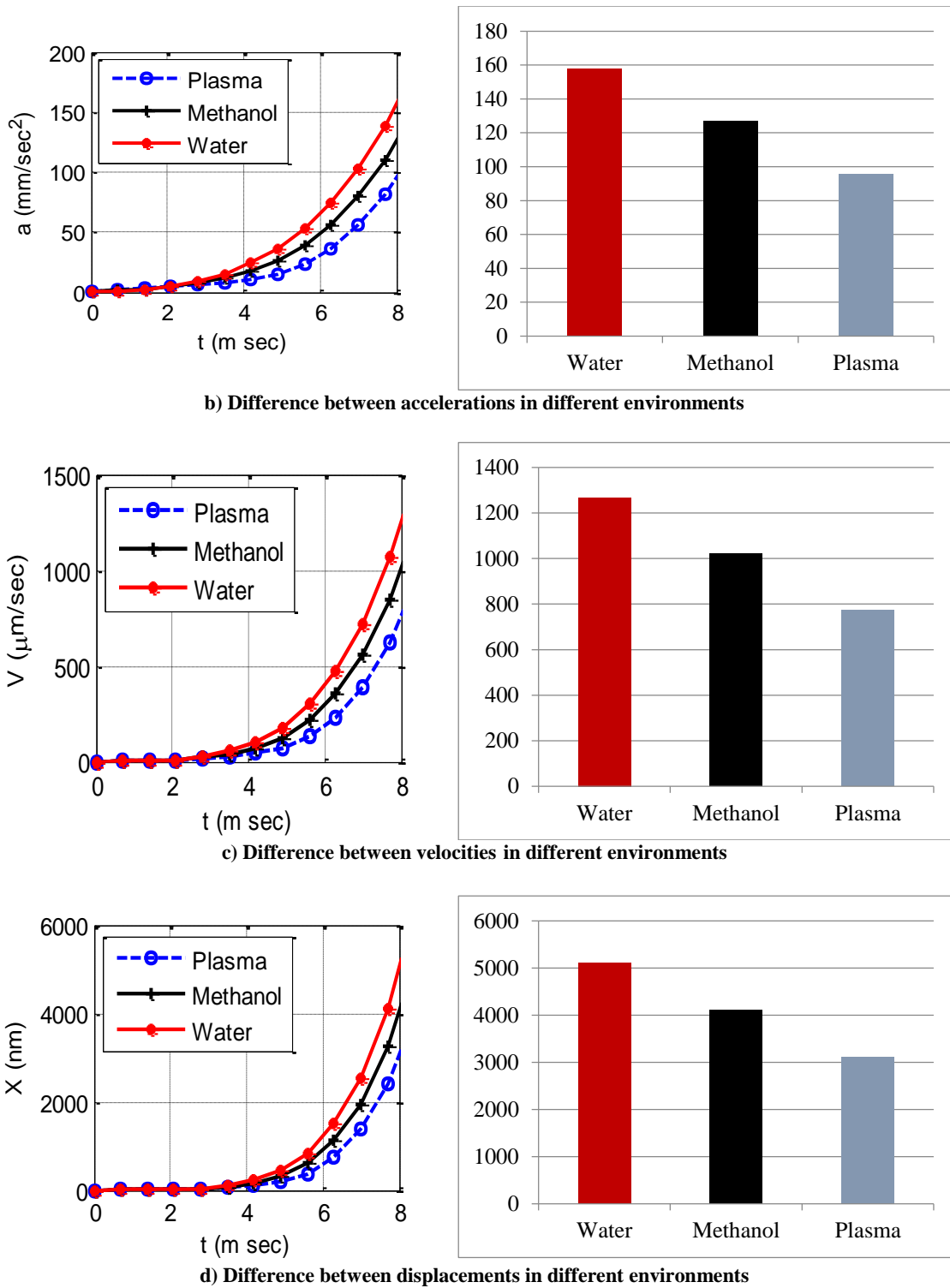


Figure 2. The results of the second phase of nanomanipulation of different environments

4. Conclusions

Considering the importance of gold metal in making electronic chips, aerospace industries, diagnosis of some diseases and in various laser-based sciences, researchers are interested in investigating the structure of this metal; Therefore, various processes have been carried out on gold nanoparticles to understand their atomic structure, improve their mechanical properties and other purposes. Considering the wide application of atomic force microscope in the study of particles in nano dimensions and during the process of nanomanipulation, therefore, this process has been used in this article to examine gold nanoparticles. Manipulation of nanoparticles takes place in two phases. In the first phase, by overcoming the resistant forces, the critical force and time are calculated, and the process continues in the second phase, with different goals, moving and exploring the surface by atomic force microscope; Therefore, in this article, in order to model the process, the equations of motion are considered in two-dimensional form, and the intermolecular, van der Waals, hydration and electrostatic double-layer forces are also analyzed. Considering that there are no limitations to working with the atomic force microscope in different environments, the amount of displacement in the second phase of manipulation has been investigated in water, plasma and methanol environments. The trend of changes in intermolecular forces with increasing

displacement has been investigated. Finally, the graphs of force, acceleration, velocity and displacement of gold nanoparticle in different environments and according to the changes of intermolecular forces have been drawn. The results indicate the highest amount of displacement in the water environment and the lowest amount in the plasma environment; also, with the increase in displacement, Van der Waals force has increased and other intermolecular forces have decreased.

5. References

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