Int. J. Nanosci. Nanotechnol., Vol. 11, No. 2, June 2015, pp.83-92

Effective Parameters in Contact Mechanic for Micro/nano Particle Manipulation Based on Atomic Force Microscopy

M. H. Korayem[1*], H.Khaksar[2], M. Taheri[2]

1. Robotic Research Laboratory, Center of Excellence in Experimental Solid Mechanics and Dynamics, School of Mechanical Engineering, Iran University of Science and Technology, Tehran, I. R. Iran
2. PhD student, School of Mechanical Engineering, Iran University of Science and Technology, Tehran, I. R. Iran

(*) Corresponding author: hkorayem@iust.ac.ir
(Received: 15 Oct 2014 and Accepted: 22 Feb. 2015

Abstract
The effect of geometry and material of the Micro/Nano particle on contact mechanic for manipulation was studied in this work based on atomic force microscopy. Hertz contact model simulation for EpH biological micro particle with spherical, cylindrical, and circular crowned roller shape was used to investigate the effect of geometry on contact simulation process in manipulation. Then, to validate the simulation results, they were compared to experimental ones. The results can be interpreted from two perspectives, first from the perspective of types of nanoparticles and second from the perspective of types of theories.To investigate the effect of the material of micro/nano particle in contact mechanic simulation process, spherical contact simulations of two EpH and C3T3 cells were compared with each other. EpH cells simulations with different geometries showed that the cylindrical shape estimation did not provide accurate response due to longer contact length. However, spherical and circular crowned roller estimations which had 19.6% and 15.6% difference from experimental results, respectively, had relatively accurate response. Therefore, selection of circular crowned roller geometry will produce more logical response. Also, the comparison of spherical contact simulation of EpH and C3T3 cells showed that C3T3 cell shows more indention depth under the same applied force.
***Keywords**: Contact Mechanic, Geometry, Hertz contact model, Micro/nano manipulatn.*

1. INRODUCTION

Many factors affect the investigation of contact mechanics and its application in the manipulation of biological particles. Some of these factors include the material and geometry of the biological particle, and the environment in which the manipulation process is implemented. One of the most effective tools in the manipulation of biological micro/nanoparticles is the atomic force microscope (AFM).

Falvo [1] was the first researcher who modeled the manipulation of nanoparticles. The shortcoming with the Falvo's model was that he did not consider the adhesion force in his modeling. Taffazzoli and Sitti [2] attempted to control the process of nanoparticles manipulation. In order to consider the adhesion force in their simulations, they used the JKR theory in simulating the mechanics of contact. Castillo et al. [3] investigated the manipulation of micro/nano biological samples via 2D and 3D methods.

Korayem et al. [4] modeled the nanomanipulation of spherical particles in liquid medium. In their modeling, they also considered the effect of the hydrodynamic forces. Then, they simulated the manipulation of gold particles with a 50 nm radius on a silicon substrate moving at 100 nm/s. In another part of their work, they studied the dynamic behaviors of particle and probe tip. Their results indicated that in liquid environments, the manipulation force and manipulation time needed for the sliding and rolling of nanoparticles increase by 3.5 to 6.5%, depending on the viscosity of the liquid medium.

The manipulation of nano-scale materials in cluster form has always faced numerous challenges. Hynninen et al. [5] explored these challenges and tried to find a solution to the existing drawbacks in the manipulation of cluster-shape materials on insulated surfaces. For this purpose, they investigated the manipulation of clustered gold particles on the surface of salt and demonstrated that, in some cases, the movement of gold clusters is restricted to certain crystallographic directions. These researchers maintained that such isentropism is due to the existing flaws on the substrate surface on which the clustered gold particle is moved.

An important part of the manipulation investigation is the study of the mechanics of contact between an AFM cantilever's probe tip and the target micro/nanoparticle and also between the micro/nanoparticle and the substrate. So, Korayem et al. [6] studied the application of the JKR contact model in the nanomanipulation of biological cells in the air and liquid environments. The obtained results were ultimately compared with the results obtained from the manipulation of gold nanoparticles in similar conditions and with the theoretical and experimental results pertaining to the embryonic cells of mice. The comparison showed that less force is needed in DNA to create the same deformation than gold, which is due to the difference in the elasticity modulus values of these particles. They also confirmed this finding by means of sensitivity analysis. Also, the contact area of DNA was larger than that of the gold nanoparticle. Lin et al. [7] investigated the nanomechanics of polymer jells and biological tissues by using the amount of indentation in the nano unit and determined the mechanical properties of these materials. In this article, they used the Hertz contact theories (without the consideration of adhesion), the JKR contact theory (with the consideration of adhesion), contact-based numerical theories such as the methods of Crick and Yin, the method of Jaasma et al. and the data processing techniques for the calculation of the modulus of elasticity. Then, by testing the laboratory samples by the atomic force microscope, the existing limitations in various theories were revealed. Finally, the Lin's group concluded that in the application of contact mechanics for soft materials, the most important point is the use of theories that take large deformations into consideration.

Chaudhury et al. [8] explored the adhesion force between a cylindrical lens and a flat plate and presented an experimental protocol for the estimation of adhesion energy in soft materials by using the contact of a cylinder with a flat surface.

Daeinabi & Korayem [9] employed the contact nanomechanics models to investigate the indentation depth of spherical nanoparticles in AFM-based manipulations. They first performed a kinematic analysis of the indentation depths resulting from the contact of nanoparticle with the cantilever and with the substrate. In another part of their work, they analyzed these indentation depths by using the models of contact nanomechanics. In the last part of their work, these researchers employed the models of contact nanomechanics to simulate the indentation depth and the contact radius of nanoparticle due to the contact with the cantilever and the substrate.

Ikai et al. [10] used the contact models of Tatara and Hertz to model the proteins under pressure. In order to apply these two models, they considered the geometry of the protein as a sphere, and compared the results of their work with experimental results. They realized that the contact models of Tatara and Hertz agree with the experimental results of the protein particle by about 50% and 10%, respectively.

Considering the research history on the subject of contact mechanics in the manipulation of micro/nanoparticles by the AFM, it can be observed that most of these activities have only involved the simple spherical particles. Therefore, this paper has attempted to investigate the cylindrical and circular crowned roller contact models. First, the spherical contact model of Hertz is introduced. Next, for a more thorough investigation of the effect of geometry on the manipulation process, two cylindrical and circular crowned roller contact models are described. Then, the changes of indentation depth with force are simulated for the three geometries of sphere, cylinder and circular crowned roller shaped particles and the obtained results are compared with the available experimental results. Finally, to better explore the effect of material properties on the mechanics of contact during the manipulation, the spherical contacts of two biological cells (EPH and C3T3) are simulated.

2. Spherical, cylindrical and circular crowned roller contact models of Hertz

The first activities on the subject of contact mechanics belong to Hertz [11]. The Hertz contact model expresses the mechanics of contact between a sphere and a flat surface in elastic form.

2.1. Spherical contact model of Hertz

The Hertz contact model can be used for the simulation of contact mechanics when large magnitude forces and low adhesion are involved. So, this contact model doesn't always provide the right answer in all the cases. However, since in this paper, a fairly large force is applied to a biological microparticle that has a low adhesion [12], the contact model of Hertz can be used (Figure. 1).

In this model, the relationship between contact radius and loading force for the spherical geometry has been given by Eq. 1.

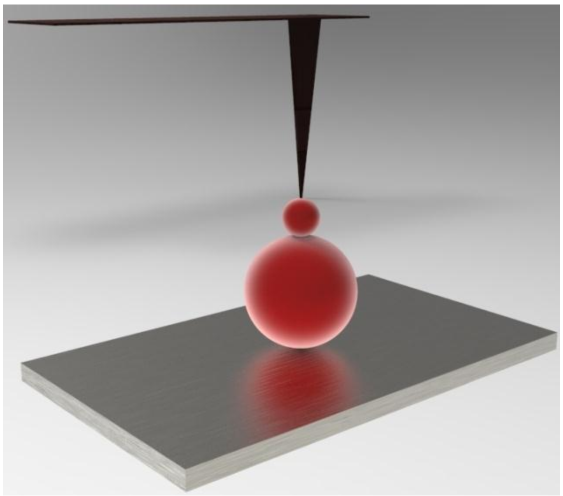


Figure 1. *Spherical contact*

$$a_{Hertz} = \left(\frac{RP}{K}\right)^{1/3} \tag{1}$$

This theory also expresses the relationship between indentation depth and contact radius as Eq. 2.

$$\delta_{Hertz} = \frac{a_{Hertz}^2}{R} \tag{2}$$

In Equation (2), $a^{\backslash}_{Hertz}$ is the contact radius.

The effective modulus of elasticity is obtained from Eq. 3.

$$\frac{1}{K} = \frac{m_t}{2}\left(\frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2}\right) \tag{3}$$

In relation (3), E_1 and E_2 are the Young's modulus values and υ_1 and υ_2 are the Poison's ratios of the two surfaces in contact, m_t is a parameter associated with the shape of the AFM probe tip.

2-2- Cylindrical contact model of Hertz

As was previously stated, the original theory of Hertz only considers the contact between a sphere and a flat surface;

however, the investigation of contact mechanics involves more complex geometries.

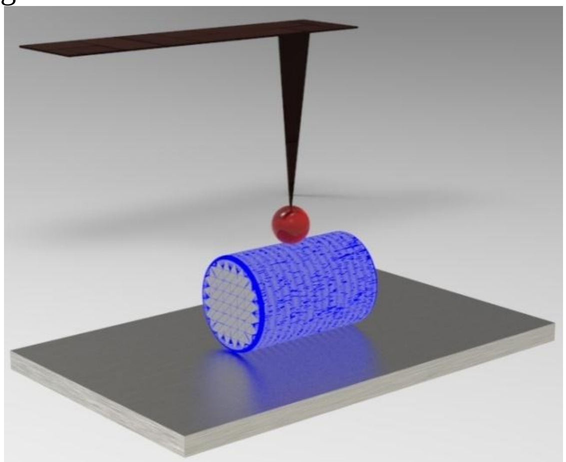


Figure 2. *Cylindrical contact*

Thus, the researchers have tried to develop this theory for objects with other geometries as well. The line contact is in fact an outcome of these activities. The line contact relations express the mechanics of contact between a cylinder and a flat surface (Figure 2). In the development of the Hertz contact model to the line contact model, the relationships between contact radius and force and between indentation depth and force are expressed by Equations (4) through (6) [13].

$$a_{Hertz} = \frac{4PR}{\pi K} \tag{4}$$

$$\delta_{Hertz} = \frac{a_{Hertz}^{2}}{2R}\left\{2\ln\left(4R/a_{Hertz}\right)-1\right\} \tag{5}$$

$$\delta_{Hertz} = \frac{P}{L\pi\pi}\left\{\ln\frac{4LR\pi K}{P}-1\right\} \tag{6}$$

In Equations (4), (5) and (6), R is the radius of cylinder and L is the length of cylinder.

2-3- Circular crowned roller contact model of Hertz

By using the spherical and cylindrical contact models of Hertz, the relations expressing the contact mechanics of circular crowned roller shaped particles can be derived (Figure 3). This can be done by dividing the circular crowned roller into one cylindrical section and two spherical sections [14] and applying the Hertz theory to this geometry.

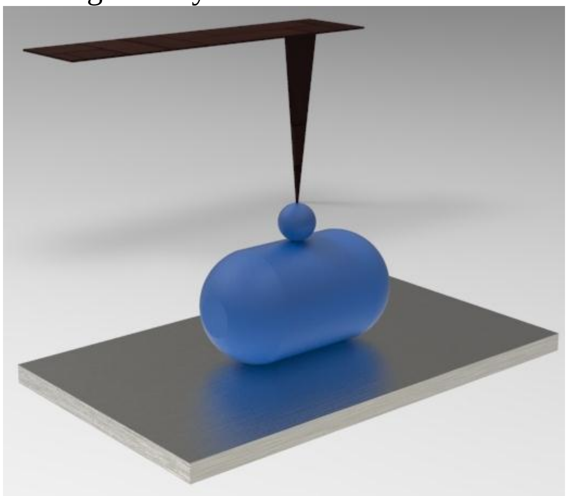


Figure3. *Circular crowned roller contact*

Based on the Hertz theory, the force exerted on the spherical section can be calculated from relation (7) [11].

$$P_s = \pi\kappa K[\frac{2\varepsilon R}{9}(\frac{\delta_s}{\zeta})^3]^{\frac{1}{2}} \tag{7}$$

In the above relation, κ, ζ and ε are the elliptical integral constants, which can be numerically obtained by Equations (8) through (10) [15].

$$\zeta = \int_0^{\frac{\pi}{2}}[1-(1-\tfrac{1}{k^2})\sin^2\varphi]^{-1/2}d\phi \tag{8}$$

$$\varepsilon = \int_0^{\frac{\pi}{2}}[1-(1-\tfrac{1}{k^2})\sin^2\varphi]^{1/2}d\phi \tag{9}$$

$$\kappa = \sqrt{\frac{2\zeta-\varepsilon}{\varepsilon}} \tag{10}$$

Also, δ_S is the indentation depth in the spherical geometry, which was mentioned in the previous sections. Now, considering the estimated force for the spherical sections, the force exerted on the cylindrical section can be determined from relation (11).

$$P_c = P - 2P_s \tag{11}$$

In view of the relations given for calculating the forces applied on each section, and by using the relations expressed for determining the indentation depth in the spherical and cylindrical models of Hertz, the maximum amount of indentation depth in the circular crowned roller can be estimated based on the fact that the maximum indentation depth in this geometry occurs in the cylindrical section. Finally Equation (12) expresses the relationship between indentation depth and loading force for the circular crowned roller geometry.

$$\delta_{Hertz} = \frac{P - 2(\pi\kappa K[\frac{2\varepsilon R}{9}(\frac{\delta_c}{\zeta})^3]^{\frac{1}{2}})}{L\pi K}\left\{\ln\frac{4LR\pi K}{P - 2(\pi\kappa K[\frac{2\varepsilon R}{9}(\frac{\delta_c}{\zeta})^3]^{\frac{1}{2}})} - 1\right\} \quad (12)$$

In Equations (12), R is the radius of spherical and cylindrical part of circular crowned roller geometry and L is the length of cylindrical part of circular crowned roller geometry.

3- Biological cells under investigation

The biological cells selected for the simulation of contact mechanics in this investigation are the EpH and C3T3 cells. Girot et al. [12] employed the atomic force bio-microscope, which is a type of hybrid atomic force microscope, to obtain the biological characteristics of the EpH cell.

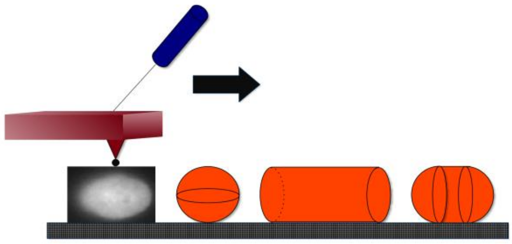
The EpH cell is considered as a soft material. The elasticity modulus of this cell is about 28 kPa and its Poisson's ratio is roughly 0.5.

In order to determine the indentation depth and to investigate the contact mechanics of the EpH cell, Girot et al. considered this cell as a spherical cell with a radius of 5 µm. Their experimental results indicated that this cell behaves elastically under a load of up to 0.15 µN. In this investigation, they chose a silicon type substrate.

Sirghi [16] used the atomic force microscope to obtain the characteristics of the C3T3 cell. He computed the elasticity modulus of this cell as 1.83 kPa and its Poisson's ratio as 0.5.

4- Simulation of the Hertz contact theory

In this section of the paper, the contact theory of Hertz is simulated for the spherical, cylindrical and the circular crowned roller geometries. Figure 4 illustrates the estimated geometries for the simulation of the EpH cell.



(b) (c) (d)

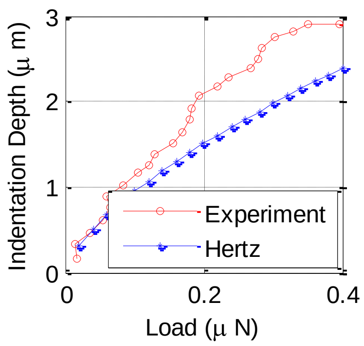
(a [12])

Figure 4. *Approximation geometries for simulation*

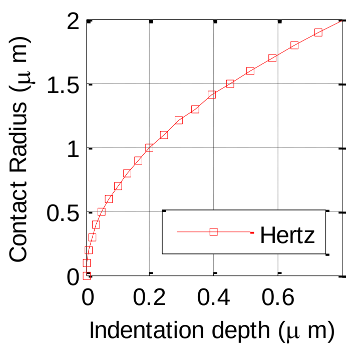
Figure 4(a) shows the real image of the biological cell. Fig. 4(b) approximates the biological cell as a sphere with a 5µm radius approximates. Fig. 4(c) approximates the biological cell as a cylinder with a 5µm radius and a 10µm length and. Fig 4(d) shows the approximation of the biological cell in the form of a circular crowned roller that has two spherical sections with a radius of 5 µm and a cylinder section with the length of 1 µm.

4-1- Simulating the spherical contact model of Hertz

Fig. 5(a) shows the simulation of the indentation depth versus the force applied on the sphere-shaped biological microparticle. By comparing Fig. 5 with the experimental results of the EpH cell, it can be concluded that the approximation of a spherical geometry for the EpH cell can provide a fairly accurate estimation. The almost linear slope of the diagram indicates that with the gradual increase of force, the indentation depth of the EpH cell into the silicon substrate increases. Also, Fig. 5(b) shows the diagram of contact radius changes with the indentation depth in the spherical contact model of Hertz for the EpH cell. As the figure illustrates, with the increase of the indentation depth, the contact radius increases by a power of 2, which agrees with the Hertz equation. This simulation results shows that with the increase of the load, indentation depth and contact radius increases.



a. Indentation depth versus the force



b. Contact radius versus the indentation depth

Figure 5. *Simulation of spherical contact (EpH cell)*

4-2- Simulating the cylindrical contact model of Hertz

In this section, the simulation of cylindrical contact has been carried out. As Figure 6 (a) shows, the indentation depth resulting from the penetration of a cylindrical EpH cell into a silicon substrate is about 1/3 of the indentation depth in the spherical contact model. Actually, due to the existence of length in cylindrical approximation and the distribution of force along the length of the cylinder, the indentation depth diminishes significantly in this case. Therefore, considering the results pertaining to the laboratory sample, it can be realized that the approximation of the EpH cell as a cylinder is not correct. Also, Figure 6(b) illustrates the changes of contact radius with indentation depth in the Hertz contact model for the cylindrical EpH nanoparticles. This diagram indicates that the contact area increases in this case relative to the spherical contact model. Finally, the cylindrical contact models developed in this article indicate that under the application of the same force, the cylindrical shaped nanoparticles undergo less indentation depth and contact radius than spherical nanoparticles.

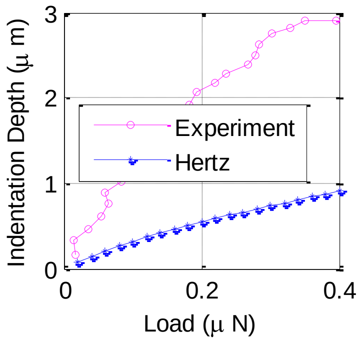
4-3- Simulating the contact model of Hertz for circular crowned rollers

As was stated before, by dividing a circular crowned roller into two spherical and one cylindrical sections and calculating the force exerted on each section, the maximum indentation depth can be determined. Fig. 7(a) shows the simulation of the indentation depth versus the force exerted on an EpH cell shaped as a circular crowned roller.

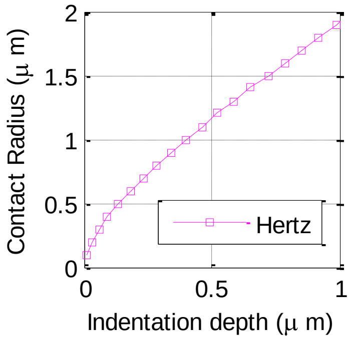
By comparing this diagram with the experimental results, it can be concluded that approximating the geometry of an EpH cell as a circular crowned roller with a small length for the cylindrical section, is a fairly accurate approximation. In comparison with the spherical geometry approximation, it can be observed that the slope of the diagram is not linear any longer; but nevertheless, like the spherical and cylindrical geometries, the indentation depth of the biological sample into the silicon substrate increases with the increase of the applied force. Also, Figure 7(b) shows the changes of contact radius with indentation depth in the Hertz contact model for the EpH nanoparticles with circular crowned roller shapes.

5- Error analysis

In this section, in view of Figs. 5, 6 and 7, the amount of error is analyzed in the force-displacement diagrams related to the spherical, cylindrical and the circular crowned roller contact geometries.



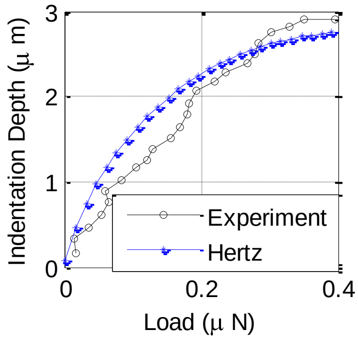
a. Indentation depth versus the force



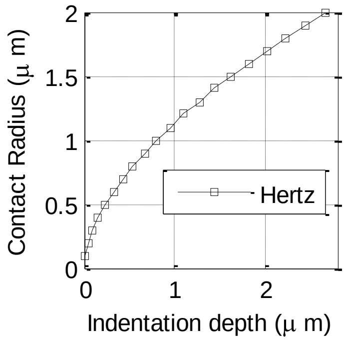
b. Contact radius versus the indentation depth

Figure 6. *Simulation of cylindrical contact (EpH cell)*

Figure 8(a) shows the comparison of the spherical, cylindrical and the circular crowned roller geometries along with the experimental results. Also, Figure. 8(b) illustrates the diagram of error versus force for the spherical geometry. According to this diagram, the highest possible error between the spherical approximation and the experimental results is 27.4%, which is produced at a force of 0.3 nN. Figure. 8(c) shows the diagram of error versus force for the cylindrical geometry. The largest error for this geometry is 73.43%, which is produced at a force of 0.2 nN. The diagram of error versus force for the circular crowned roller geometry has been sketched in Figure 8(d). The slope and the behavior of this diagram are very different from those of the last two diagrams. The largest error in this section is 43.16%, which is produced at a 0.05 nN force.



a. Indentation depth versus the force

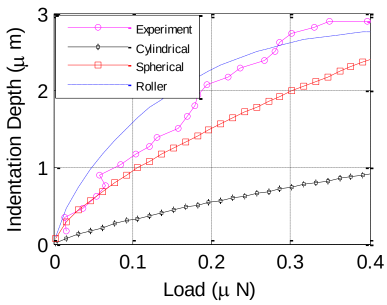


b. Contact radius versus the indentation depth

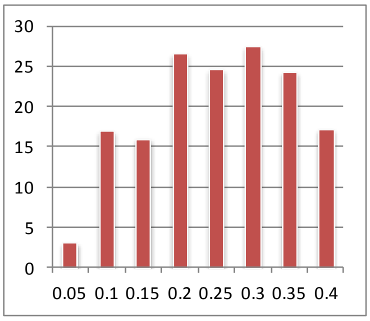
Figure 7. *Simulation of circular crowned roller contact (EpH cell)*

6- Comparing the spherical contact simulations of the EpH and the C3T3 cells

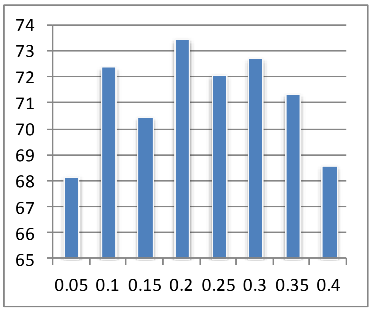
Figure 9(a) shows different simulations of indentation depth versus force for two spherical cells of EpH and C3T3, based on the Hertz contact theory. As is indicated by the figure, for the same applied force, the C3T3 cell undergoes a much larger deformation. This considerable discrepancy can be attributed to the difference that exists between the mechanical properties of the two biological cells. This figure indicates the significant influence of the modulus of elasticity and Poisson's ratio on the simulation of the manipulation process. Figure 9(b) illustrates the diagrams of contact radius versus indentation depth for the two EpH and C3T3 cells in the spherical geometry model. In view of the Hertz theory, the contact radius values obtained in both types of cells are very close to each other.



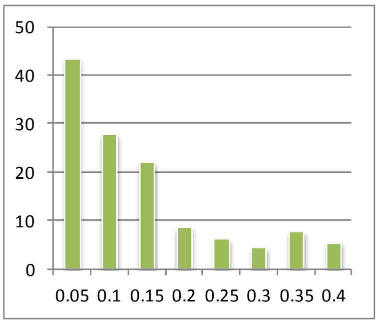
a. comparison of the spherical, cylindrical and the circular crowned roller geometries along with the experimental results



b. Error versus force for the spherical geometry



C- Error versus force for the cylindrical geometry



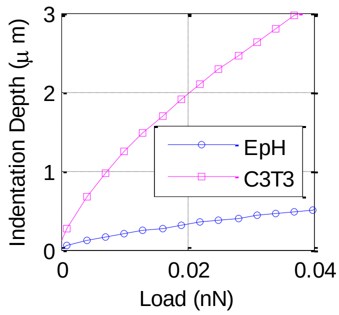
d. Error versus force for the circular crowned roller geometry

Figure 8. *Error versus force diagrams*

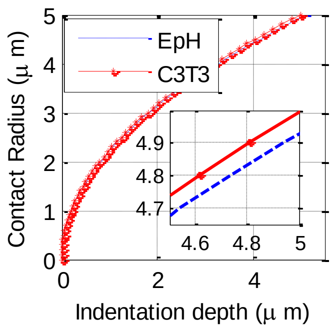
7- CONCLUSION

Various laboratory instruments exist for performing the manipulation process in laboratory settings. One of the most effective tools is the atomic force microscope. The simulation of the manipulation process makes it possible to study the behavior of the biological sample instantaneously. The atomic force microscope is a unique tool for measuring the reaction forces and it also enables the investigation of the inter-molecular and intra-molecular forces.

In order for the micro/nanoparticle to start moving, the applied force by the AFM cantilever probe tip must reach a certain magnitude to overcome both the frictional forces and the adhesion forces. This threshold force is called the *critical force*. Following the exertion of the critical force on the biological sample, the particle starts to move; and this movement continues for a specified duration. Hence, in the biomanipulation process, the mechanics of contact plays a key role in simulating the manipulation of micro/nanoparticles.



a. Indentation depth versus the forc



b. Contact radius versus the indentation depth

Figure 9. *Simulation of spherical contact for two spherical cells of EpH and C3T3*

In biomanipulation, mechanics of contact comes into play in two places; once in the contact between cantilever probe tip and sample and once in the contact between sample and substrate. Therefore, with regards to the type and geometry of biological micro/nanoparticles, the complete understanding and identification of contact mechanics and contact forces is a major priority in the investigation of the process. In this paper, the effects of different contact geometries including the spherical, cylindrical and circular crowned roller geometries as well as the impact of material type on the mechanics of contact, as applied in the manipulation process, have been investigated. The contact model selected for this research is the contact model of Hertz. This model provides the right solution only in the cases in which the force exerted on the sample is large and the sample itself has a low adhesion force. Therefore, considering the chosen magnitude of applied force in this article and the properties of the EpH and C3T3 cells, this theory was used for the simulation of manipulation.

An important innovation of this paper is the use of cylindrical and circular crowned roller geometries for the manipulation process.

The performed simulations show the effects of geometry and properties of biological cells in the biomanipulation process. The performed simulations for the biomanipulation of the EpH cell with different geometries indicated that the spherical and circular crowned roller type geometries, compared to the cylindrical geometry, yield results that are closer to reality. In the cylindrical geometry, due to the existence of force along the length of the particle, a smaller indentation depth is produced; however in the circular crowned roller type geometry, the indentation depth increases due to the reduction of the cylindrical section. In the comparison of the results of different geometries with the experimental findings, it was concluded that the results of the spherical, cylindrical and the circular crowned roller type geometries, in their average values, agree with the experimental results by 80.4%, 28.87% and 84.4%, respectively. Thus, by choosing the circular crowned roller type geometry for the simulation of the EpH cell, a more logical and realistic response will be obtained.

The comparison between the simulations of the EpH and C3T3 cells demonstrated that under the application of the same force, the C3T3 cell, because of different mechanical properties (i.e., elasticity modulus and Poisson’s ratio) than those of the EpH cell, displays a much larger indentation depth. This simulation can also point out the fact that the force needed for the manipulation of the C3T3 cell should be less than that needed for the manipulation of the EpH cell.

The final conclusion is that choosing the correct geometry in the investigation of the micro/nanoparticles manipulation is very essential. Therefore, following the proper identification and selection of the correct shape for the biological micro/nanoparticles, different contact models should be extended and adapted to these particles in consideration of their characteristics, and the manipulation process should be ultimately investigated through accurate simulations.

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