Application of Contact Mechanics Models in Manipulation of Biological Cells

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Abstract

Contact mechanics is the study of the deformation of solids that touch each other at one or more points. The physical and mathematical formulation of the subject is built upon the mechanics of materials and continuum mechanics and focuses on computations involving elastic, viscoelastic, and plastic bodies in static or dynamic contact. Contact mechanics provides necessary information for the safe and energy efficient design of technical systems. During nano-manipulation process, contact forces cause indentation in contact area between nano-particle and tip/substrate which is considerable at nano-scale and affects the nano-manipulation process. Several nano-contact mechanics models such as Hertz, DMT, JKRS, BCP, MD, COS, PT, and Sun have been applied as the continuum mechanics approaches at nano-scale. Manipulation of nano-scale biological particles such as cells and proteins are so important but have not been studied properly till now. These particles have different mechanical properties so their manipulation and equations are more complicated and contact mechanics models should be modified for biological particle and its environment. In this article different nano-contact mechanics models have been simulated and compared for biological condition. These simulations and comparisons resulted in choosing Tatara as the most proper model. Since biological cells have large deformation and this model can conveniently be used.

Key words: Nano-contact mechanics, Cell manipulation, Tatara model

1. Introduction

Living cells are inherently mechanical. Through various biochemical and biomechanical mechanisms they are able to respond to their three-dimensional mechanical environments and alter their mechanical properties such as Young's Modulus or viscoelasticity and even produce distinct mechanical forces during biological processes such as contraction, migration and division. To estimate mechanical properties of biological cells different contact mechanics models have been used. Some of contact mechanics models have been used to detect mechanical response of living cells subjected to transient and dynamic loads. They are also applicable to measure membrane proteins force. In a detailed consideration of the compressive mechanics of microscopic single spherical particles, the effect of large strains, which was not incorporated in the original Hertz theory, needs to be included. In particular, for these soft organic materials, the low-strain limitation of the Hertz analysis may easily be exceeded in many applications. In the case of an elastic sphere undergoing a large deformation, experimental and theoretical work are done. In experimental and theoretical study of the mechanical response of microscopic particles, the theoretical predictions of various models for the dependence of the reaction force on the compressive deformation of a spherical particle was confirmed. At values of the dimensionless approach [(compressive displacement)(initial particle diameter)] up to 10%, the classical Hertz theory was found to be in good agreement with experimental results and confirms that the load is a function of the approach to the power 32 . At larger deformations (dimensionless approaches in the cases 10 - 37%), a numerical implementation of Tatara's large deformation model for the compression of an elastomeric sphere gives good agreement with experimental results. Some review about recent progress of molecular level studies on the rigidity of surface immobilized as well as membrane bound proteins embedded in the lipid bilayer was done by Atsushi Iaki et al. Immobilization of protein molecules on a solid surface through covalent crosslinkers on one side and to the probe of the atomic force microscope on the other enabled us to pull or push a single protein molecule to specified directions. In their work two different contact mechanics models were compared (Hertz and Tatara). Results show that Tatara model is more accurate and compatible with experimental data.

In this article dynamic behavior of cantilever will be simulated. Different contact mechanics models will be compared for biological cell in vacuum environment and the most appropriate one will be chosen.

2. Research Methodology

Contact models

In this section, the theoretical, semi empirical, and empirical nano-contact mechanics models at nanoscale are introduced. In addition, the major assumptions and limitations inherent to each model are investigated (Table-1). Then, equations and parameters are extracted and work of adhesion force in nano-contact mechanics models is compared.

Model	Assumptions	Limitations
Hertz	Dose not consider the surface forces in contact $\omega \rightarrow 0$	If surface forces presents, this model in not appropriate for low loads
DMT	Considers a long-ranged surface force which acts outside the radius of the circle of contact, but contact geometry is similar to Hertzian	Applies to rigid systems with low λ, low adhesion and small radii of curvature, but may underestimate the true contact area

JKRS	Considers a short-ranged surface force which acts inside the radius of the circle of contact. also contact geometry allows to deform	It applies to high λ systems,high adhesion and large radii of curvature, but may underestimate loading
BCP	Considers a long-ranged surface force which acts outside the radius of the circle of contact. Hertzian functional dependence for geometry	Due to Hertzian function for geometry may underestimate pull-off force. It applies to actual adhesion systems with moderate λ
MD	Considers the Dugdale (a step function) potential to describe attractive forces	Has analytical solution, but parametric equations. It applies to all systems with all values of λ
COS	Considers the contact radius at zero applied force	Presents for enhancing the tractability of the MD model by developing an empirical approximation of the relationship between contact radius and applied force
PT	The COS and PT equations provide the means to effectively apply the MD model to experimental data but they have more rapid calculations than the MD analytical model	Presents a force indentation relationship that deviates from the MD model by 1% or less
SUN	Considers surface forces	Presents adhesive contact model for hyperboloid (blunted conical) indenters
Tatara	invokes a non-linear elastic response and a large-deformation formulation	The influence of adhesion and the effects of interfacial friction are not considered.

Table-1: Comparison of the theoretical, semi-empirical, and empirical nano-contact mechanics models

Hertz theory model

As mentioned in Table-1, the Hertz theory model does not consider the surface forces and adhesion in contact. If surface forces present, this model does not appropriate for low loads. However, during nano manipulation, it may be low loads and high surface forces; for these reasons, this model cannot be applied to all systems. The relationship between applied load and indentation depth (d) on the tip–particle and particle–substrate is given by the following equations:

$$F = Ka\delta \quad (1)$$

$$\delta = \frac{a^2}{\tilde{R}} \quad (2)$$

Contact-radius (a) and adhesion force (Fad) are obtained as follows:

$$a^3 = \frac{\tilde{R}}{K}F \quad (3)$$

$$F_{ad}=0 \quad (4)$$

DMT theory model

The DMT theory model attempts to rectify limitation in the Hertz theory by increasing surface forces. On the other hand, the DMT model is the Hertz model with an offset due to surface forces. It considers a long-ranged surface force which acts outside the contact area but contact geometry is similar to the Hertz model. The equations are derived as:

$$F = Ka\delta - 2\omega\tilde{R} \qquad (5)$$

$$\delta = \frac{a^2}{\tilde{R}} \qquad (6)$$

Contact-radius (a) and adhesion force (Fad) are obtained as follows:

$$a^3 = \frac{\tilde{R}}{K}\left(F + 2\pi\omega\tilde{R}\right) \qquad (7)$$

$$F_{ad} = 2\pi\omega\tilde{R} \qquad (8)$$

JKR theory model

The JKRS theory model considers a short-ranged surface force which acts inside the contact area. The tip–particle geometry is not constrained to remain the Hertz model. Therefore, it applies to high adhesion systems with high λ that have large radii of curvature and low stiffness. Due to considering surface forces, may underestimate loading. During unloading, a connective neck is formed between the tip and nano particle, and contact is ruptured at negative loads. This causes adhesion hysteresis. The equations are:

$$F = \frac{Ka^3}{\tilde{R}} - \sqrt{6\pi\omega K a^3} \qquad (10)$$

$$\delta = \frac{a^2}{\tilde{R}} - \frac{2}{3}\sqrt{\frac{6\pi\omega a}{K}} \qquad (11)$$

Contact-radius (a) and adhesion force (Fad) are obtained as follows:

$$a^3 = \frac{\tilde{R}}{K}\left(F + 3\pi\omega\tilde{R} + \left(6\pi\omega\tilde{R}F + \left(3\pi\omega\tilde{R}\right)^2\right)^{\frac{1}{2}}\right) \qquad (12)$$

$$F_{ad} = (6\pi\omega K a^3)^{\frac{1}{2}} \qquad (13)$$

MD theory model

The MD theory model is more complex and more accurate than the other nano-contact mechanics models up to now. This model does not have to assume a particular limit for the materials properties. Hence, the MD model applies to all systems; so that, the other contact-mechanics models are special cases of this model. The equations are:

$$F = \frac{Ka^3}{\tilde{R}} - \lambda a^2\left(\frac{\pi\omega K^2}{\tilde{R}}\right)^{\frac{1}{3}}\left[\sqrt{m^2-1} + m^2 arctan\sqrt{m^2-1}\right] \qquad (14)$$

$$\delta = \frac{a^2}{\tilde{R}} - \frac{4\lambda a}{3}\left(\frac{\pi\omega}{\tilde{R}K}\right)^{\frac{1}{3}}\sqrt{m^2-1} \qquad (15)$$

Contact-radius (a) and adhesion force (Fad) are obtained as follows:

$$1 = \frac{\lambda a^2}{2}\left(\frac{K}{\pi\tilde{R}^2\omega}\right)^{\frac{2}{3}} \times \left[\sqrt{m^2-1} + (m^2-2)arctan\sqrt{m^2-1}\right] + \frac{4\lambda a^2}{3}\left(\frac{K}{\pi\tilde{R}^2\omega}\right)^{\frac{1}{3}} \times \left[1 - m + \sqrt{m^2-1}\,arctan\sqrt{m^2-1}\right] \qquad (16)$$

$$F_{ad} = \lambda a^2 \left(\frac{\pi\omega K^2}{\tilde{R}}\right)^{\frac{1}{3}} \times \left[\sqrt{m^2-1} + m^2 arctan\sqrt{m^2-1}\right] \tag{17}$$

Tatara theory model

Tatara model is the modified Hertz model which is applicable for large deformation. As mentioned in Table-1 this model does not consider adhesion force. The equations are as follows:

$$F = aI_H^{3/2} + \left(\frac{3a^2}{2a_c}\right) I_H^2 + \left(\frac{15a^3}{8a_c^2}\right) I_H^{5/2} \tag{18}$$

Where:

$$a_c = \frac{4\pi Y_1 R_1}{(1+\nu_1)(3-2\nu_1)} \tag{19}$$

Where I is the displacement occurs during indentation.

Other models are empirical and there is no need to mention their equations here.

3. Results and Analysis

In this section the result of contact theories modeling will be shown in different diagrams.

As shown in fig-2 Tatara model has the most accurate value of the force between contact models. Other models underestimated the applied load and their diagrams are approximately linear which shows lower accuracy than Tatara theory. Models such as JKR and DMT which consider adhesion forces, cannot determine applied load exactly. In Fig-2 the relation between contact radius and cantilever base position is demonstrated which shows that JKR model and Hertz model predict the largest and the smallest contact area respectively, because JKR considers adhesion force and this consideration results in larger contact area determination. In Fig-4 the relation between load and cantilever base position for different young modules is shown. As the young module decreases the applied force will be reduced to zero which means for particles with small young module even small applied loads will result in large deformations. In contrast as shown in fig-5, increasing the young module will result in decreasing contact radius, which shows that for the samples such as cells which have small young modules, small vertical deformations will cause large contact area.

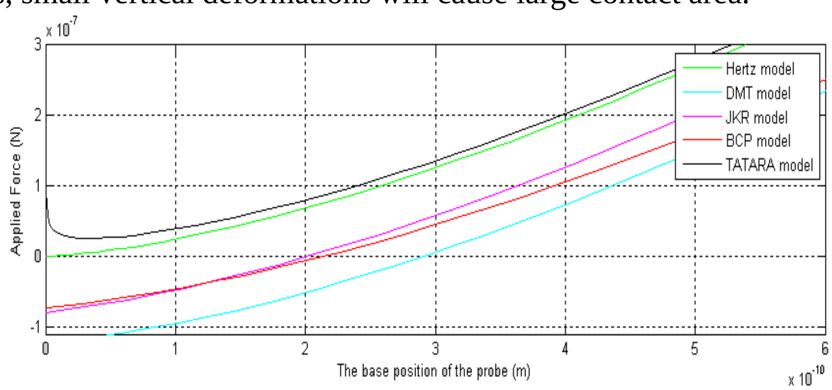

Fig-2: Applied force vs. the base position of the probe for contact models

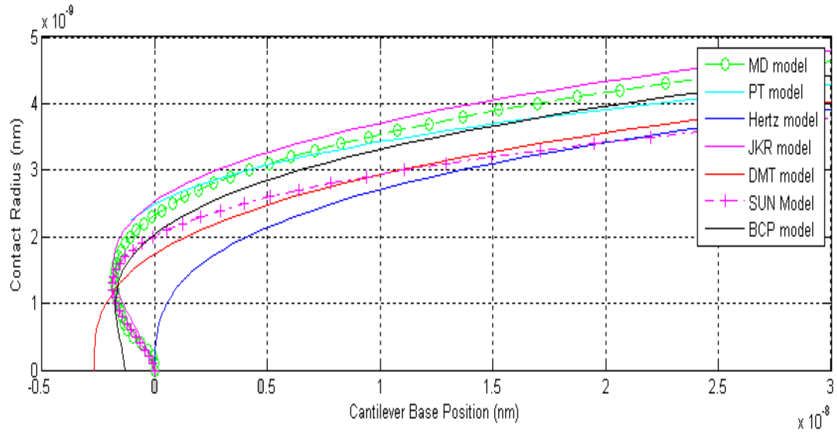

Fig-3: Contact radius vs. Cantilever base position for contact models

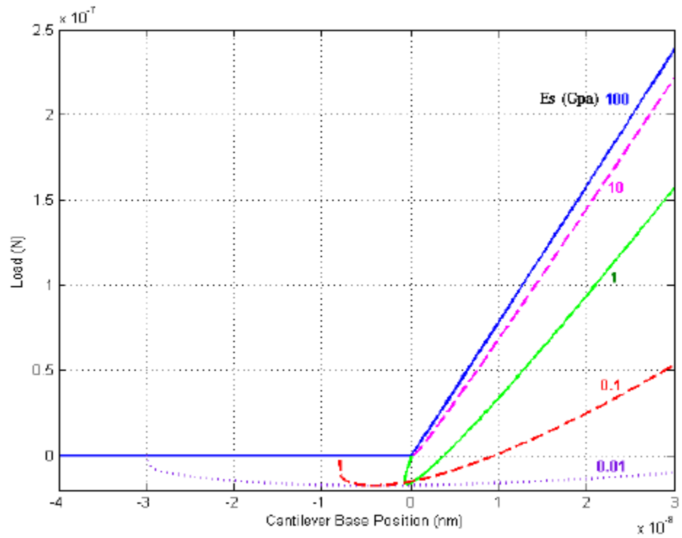

Fig-4: Load vs. Cantilever base position for different young modules

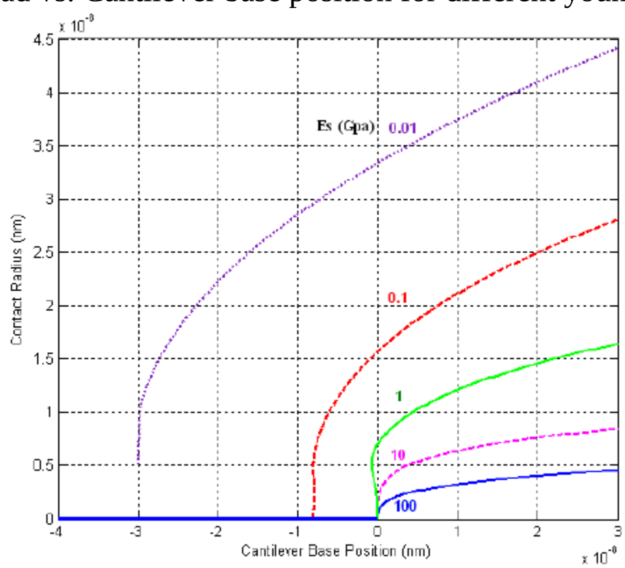

Fig-5: Contact radius vs. Cantilever base position for different young modules

4. Conclusions

In this paper different kinds of contact mechanics models were introduced and their limitations and considerations were studied. Using their relations and equations, a Matlab program was established which shows relations between deformation, force and contact radius in diagrams. Studying these results show that small deformation models are not appropriate for biological cells because their young module is so low (about Kpa) and this property will result in large deformation even when applied load is so small. On the other hand cell dimensions are about micrometer. In this scale adhesion forces can be omitted so there is no need to use the theories such as JKR or DMT which consider adhesion forces. Since Tatara model is a large deformation theory and does not use adhesion forces in its formulation, it can be more useful and accurate.

References

Chu Y. S., Dofour S.,(2006), *Johnson-Kendall-Roberts theory applied to living cells*

Daeinabi K., Korayem M. H.,(2010),*Mechanics models during nano-manipulation based on atomic force microscopy*

Hyun, S., and M.O. Robbins, (2007), *Elastic contact between rough surfaces: Effect of roughness at large and small wavelengths*

Ikai A., Afarin R.,(2005),*Force measurements for protein membrane manipulation*

Ikai A., Afarin R., Sekiguchi H., (2007), *Pulling an pushing protein molecules by AFM*

Lim C.T., Zhou E.H., Quek S.T.,(2004), *Mechanical models for living cells*

Liu K. K., Williams D. R., Briscoe B. J., (1997), *A large deformation of a single micro-elastomeric sphere*

Sburlati R.,(2008), *Adhesive elastic contact between a symmetric indenter and an elastic film*

Serges-Nolten I., Van Der Werf K., Van Raaij M., Subramaniam V., (2007), *Quantitative Characterization of Protein Nanostructures Using Atomic Force Microscopy*

Tatara Y.,(1991), *On compression of rubber elastic sphere overa large range of displacements*

Vogler E. A.,(2006),*A thermodynamic model of short-term cell adhesion in vitro*

Zavaraise G., Paggi M.,(2006), *On the resolution dependence of micro mechanical contact models*