 CMC, vol.8, no.1, pp.17-21, 2008

A Modified Multiscale Model for Microcantilever Sensor

Yan Zhang[1] **and Shengping Shen**[1]

Abstract: In this paper, an existed model for adsorption-induced surface stress is modified with physical clarity, based on the equilibrium of force. In the proposed multiscale model, a four-atom system is used, instead of the existed three-atom system which did not consider the force equilibrium. By analyzing the force state of an atom, the thickness of the first layer atoms can be determined. Thus, the proposed model does not need to determine the layer-thickness by experiments or artificially. The results obtained from the proposed model agree very well with the experimental data. This paper is helpful to investigate the atomistic theory of the microcantilever sensor.

Keyword: Microcantilever, Multiscale model, adsorption-induced stress

1 Introduction

The microcantilever detection approach has attracted much attention as it can detect the biomolecules by measuring the deflection of the bending microcantilever (Shekhawat, Tark, Dravid, 2006). The bending of the microcantilever is induced by the adsorption of atoms on a single side of the microcantilever (Chen, Thundat, Wachter, Warmack, 1995). The origin of the nanoscale bending of the microcantilever is due to the change in surface stress induced by adsorption. The exact atomistic mechanism of adsorption-induced bending is still on the way. Recently, multiscale methods (Chen, *et al*., 2007; Ma, *et al*., 2006; Mebatsion, *et al*., 2006; Park, *et al*., 2006; Haasemann, *et al*., 2006; Hasebe, 2006; Kaczmarczyk, 2006; Li, *et al*., 2006; Dawson, *et al*., 2005; Kadowaki, Liu, 2005; Shen, Atluri, 2004b, c; Tewary, Read, 2004) have been extensively studied since its advantages over the continuum method and the molecular dynamics: it is more accurate than the continuum method, meanwhile it is computationally cheaper and more efficient than the molecular dynamics. By means of a multiscale method, Dareing and Thundat (2005) explained the deflection of the microcantilever in terms of the atomic potential energy and the elastic energy. They proposed a simulation model for adsorption-induced stresses based on the atomic interaction, in which the minimum of the total potential energy is used to define the relationship between the curvature of the microcantilever and the adsorption of the atoms. The total potential energy is the potential energy of a selected system, which consists of the atomic potential and the elastic bending potential.

In this paper, the model proposed in Dareing and Thundat (2005) is modified with physical clarity, based on the force equilibrium. In the proposed model, a four-atom system is used, instead of the three-atom system which is employed in the existed model. By analyzing the force state of an atom, the thickness of the first layer atoms can be determined. Thus, this model avoids to determine the layer-thickness by experiments or artificially. It is readily to find that the results from the proposed model agree very well with the experimental data. This paper is helpful for people to investigate the atomistic mechanism of the microcantilever detection.

2 The Modified Model

Similar to Dareing and Thundat (2005), the modified model is still based on the energy potential in the first layer of atoms attached to one surface of a microcantilever and the elastic potential in the microcantilever itself. Experiments show that the

[1] MOE Key Laboratory for Strength and Vibration, School of Aerospace, Xi'an Jiaotong University, Xi'an 710049, China

first atomic layer on the cantilever surface plays a dominate role in microcantilever deflection (Martinez, Augustyniak, Golovchenko, 1990; Schell-Scorokin, Tromp, 1990). In our modified model, atoms are located on the microcantilever surface as depicted in Fig. 1. The Lennard-Jones potential is employed to describe the interaction between atoms in the adsorbed film and the microcantilever:

$$w(r) = -\frac{A}{r^6} + \frac{B}{r^{12}} \tag{1}$$

where r is the distance between atoms. The distance b between two atoms in the beam is known for certain atoms. The distance a between the adsorbed film and the microcantilever, i.e. the layer-thickness, will be determined according to the force equilibrium of each atom in the film. However, in the existed model, the layer-thickness a was determined by experiments or artificially.

According to the Lennard-Jones potential (1), the force between two atoms can be obtained as

$$F(r) = -\frac{\partial w(r)}{\partial r} = -\frac{6A}{r^7} + \frac{12B}{r^{13}} \tag{2}$$

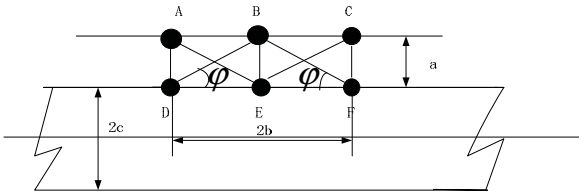

Figure 1: Atoms on the microcantilever surface

For the atom B, the force equilibrium along the direction BE can be written as

$$\mathbf{F}(r_{BD})\cos\varphi + \mathbf{F}(r_{BF})\cos\varphi + \mathbf{F}(r_{BE}) = 0 \tag{3}$$

Thus, by substituting Equation (2) into Equation (3), the thickness a of the adsorbed film (atomic monolayer) can be determined according to the following equation

$$2\left[-\frac{6A}{\left(\sqrt{a^2+b^2}\right)^7} + \frac{12B}{\left(\sqrt{a^2+b^2}\right)^{13}}\right]\frac{a}{\sqrt{a^2+b^2}} - \frac{6A}{a^7} + \frac{12B}{a^{13}} = 0 \tag{4}$$

where A and B are the Lennard-Jones constants.

To determine the deflection of the microcantilever, the energy transfer between the atomic energy and the bending energy should be considered (Ibach, 1997; Raiteri, Grattarola, Butt, Skladal, 2001), by minimizing the sum of the Lennard-Jones potential and the elastic energy in the microcantilever, similar to that in Dareing and Thundat (2005). The chemically homogeneousness of the surface of the microcantilever leads the uniform distribution of the adsorbate atoms over the surface. As indicated before, the second and higher layers of atoms play a minor role in deflecting the microcantilever. A representative unit of the microcantilever consists of four atoms, with the length b, which is the atomic space between two atoms, as shown in Fig. 2.

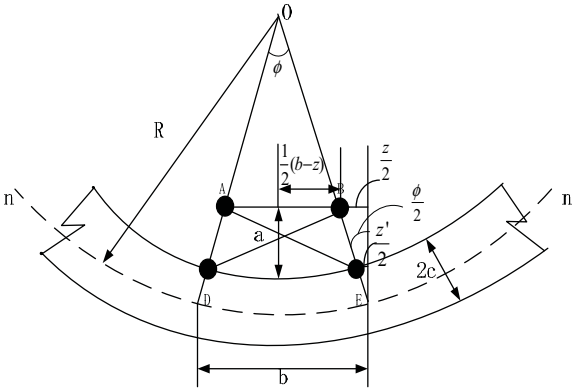

Figure 2: The deflected cantilever and the representative unit

The atomic potential of the representative unit, U_r, in terms of the beam curvature $1/R$ per the Lennard-Jones potential can be expressed as

$$\begin{aligned} U_r =& w(r_{AB}) + w(r_{AE}) + w(r_{BD}) \\ &+ \frac{1}{2}w(r_{AD}) + \frac{1}{2}w(r_{BE}) \\ =& 2\left(\frac{-A}{\left\{a^2+[b-(z+z')]^2\right\}^3}\right. \\ &\left. + \frac{B}{\left\{a^2+[b-(z+z')]^2\right\}^6}\right) \end{aligned} \tag{5}$$

$$-\frac{A}{(b-z)^6}+\frac{B}{(b-z)^{12}}-\frac{-A}{a^6}+\frac{B}{a^{12}}$$

where

$$z=\phi\,(a+c),\quad z'=\phi c,\quad \phi=b/R$$

According to the beam theory, the elastic bending potential, U_b, of the representative unit can be written as

$$U_b=\frac{1}{2}EI\left(\frac{1}{R}\right)^2 b \tag{6}$$

The equilibrium configuration is determined by minimizing the total potential energy

$$U=U_r+U_b$$

Thus, we have

$$\frac{dU}{d\,(c/R)}=0 \tag{7}$$

The above equation can be rewritten as

$$\begin{aligned}&\frac{EIb}{c^2}\frac{c}{R}+\frac{-6Ab\left(1+\frac{a}{c}\right)}{\left[b-b\left(1+\frac{a}{c}\right)\frac{c}{R}\right]^7}+\frac{-12Bb\left(1+\frac{a}{c}\right)}{\left[b-b\left(1+\frac{a}{c}\right)\frac{c}{R}\right]^{13}}\\&+\frac{6A\left[-b^2\left(2+\frac{a}{c}\right)+\frac{1}{2}b^2\left(2+\frac{a}{c}\right)^2\frac{c}{R}\right]}{\left[a^2+b^2-b^2\left(2+\frac{a}{c}\right)\frac{c}{R}+\frac{1}{4}b^2\left(2+\frac{a}{c}\right)^2\left(\frac{c}{R}\right)^2\right]^4}\\&-\frac{12B\left[-b^2\left(2+\frac{a}{c}\right)+\frac{1}{2}b^2\left(2+\frac{a}{c}\right)^2\frac{c}{R}\right]}{\left[a^2+b^2-b^2\left(2+\frac{a}{c}\right)\frac{c}{R}+\frac{1}{4}b^2\left(2+\frac{a}{c}\right)^2\left(\frac{c}{R}\right)^2\right]^7}\\&=0\end{aligned}$$

By solving the above equation, we can obtain c/R, which defines the curvature of the microcantilever beam. Then, the transverse deflection of the end of the cantilever can be determined by

$$W=R\,(1-\cos\theta) \tag{8}$$

where $\theta=\frac{l}{R}$ with l the length of the cantilevel.

Now, we turn to illustrate why the microcantilever can be used as a sensor. The effects of the magnitude of the two Lennard-Jones constants A and B on the beam curvature, c/R, can be used to evaluate the type of the adsorbates attached to the cantilever surface, since the physical property of the adsorbates is determined by the parameters A and B. This is the mechanism of the microcantilever sensor.

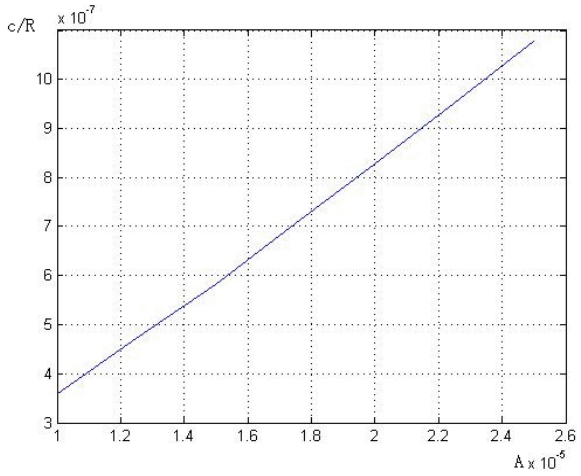

Figure 3: The effect of constant A on the beam curvature, B=1.0Jm$^{12}\times10^{134}$

Consider a typical microcantilever beam of 200μm length, with the cross section 30μm$\times$1μm. The Young's modulus is taken to be 1.79$\times10^{11}$Pa. The distance between two atoms on the surface is b=0.5nm. Figs. 3 and 4 show the influences of the Lennard-Jones constants A and B on the curvature, respectively. From these figures, it can be concluded that the beam curvature increases with the parameter A while it reduces with increases in the parameter B. This is physically reasonable since the parameter A represents the attractive effects and the parameter B represents the repulsive effects.

3 Validation of the Model

This modified model is validated by comparing the simulated results with the experimental data in Dareing and Thundat (2005). In that experiment, mercury vapor was adsorbed on the cantilever surface, which has 40-nm-thick layer of gold. The V-shaped cantilever is with 200μm length, 40μm width per leg, and 0.7μm thickness. The microcantilever is completely covered with a monolayer of mercury, the deflection of the beam is about W=300μm.

For mercury, A=2.8377 $\times10^{77}$Jm^6, B=

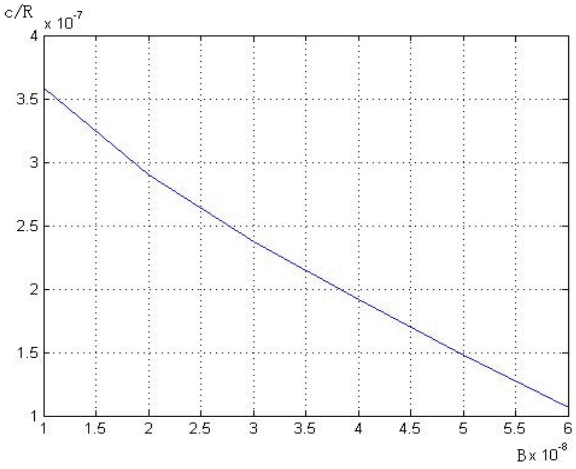

Figure 4: The effect of constant B on the beam curvature, A=1.0Jm$^6\times 10^{77}$

1.943×10^{134}Jm^{12}. The Lennard-Jones constants between gold and mercury are assumed to be the same as mercury-mercury. The Young's modulus is 1.79×10^{11}Pa, and b=0.4nm.

From the modified model proposed in this paper, the beam curvature can be determined as c/R=4.9671×10^6. The corresponding tip deflection of the cantilever is W=284nm, which agrees very well with the experimental result. Compared with the predicted result (W=269nm) in Dareing and Thundat (2005), this result is closer to the measured deflection data.

4 Conclusions

We modified the model proposed by Dareing and Thundat (2005) for adsorption-induced stress due to molecular adsorption on a microcantilever surface, with physical clarity, based on the force equilibrium. The modified model consists of four atoms, which is more reasonable than the three-atom system employed in the existed model. This model determines the thickness of the monolayer by analyzing the force equilibrium of an atom, unlike in the existed model, where the layer-thickness is determined by experiments or artificially. The result from the proposed model in this paper agrees better with the experimental data than that from the existed model. This paper sheds light on the atomistic mechanism of the micro-cantilever sensor. By combining with the multi-scale method in Shen and Atluri (2005, 2004a), the more accurate mechanism and more complex molecular adsorption of the microcantilever sensor can be explored. Also, some other multiscale methods (Liu, *et al*., 2007; Wallstedt, Guilkey, 2007; Ma, *et al*., 2005; Chung, *et al*., 2004) can be applied to investigate this problem.

Acknowledgement: We gratefully acknowledge the supports by the NSFC under Grant No. 10672130, the 973 Program under Grant No. 2007CB707702, and the Ministry of Education, China under Grant No. NCET-05-0827.

Refferences

Chen, G.Y.; Thundat, T.; Wachter, E.A.; Warmack, R.J. (1995): Adsorption-induced surface stress and its effects on resonance frequency of microcantilevers. *Journal of Applied Physics* 77: 3618-3622.

Chen, S.; Liu, Y.; Khoo, B., Fan, X.; Fan, J. (2007): Mesoscopic simulation of binary immiscible fluids flow in a square microchannel with hydrophobic surfaces. *CMES: Computer Modeling in Engineering & Sciences* 19: 181-196.

Chung, P.W.; Namburu, R.R.; Henz, B.J. (2004): A lattice statics-based tangent-stiffness finite element method. *CMES: Computer Modeling in Engineering & Sciences* 5: 45-62.

Dareing, D.W.; Thundat, T. (2005): Simulation of Adsorption-induced Stress of a Microcantilever Sensor. *Journal of Applied Physics* 97: 043526.

Dawson, P.R.; Boyce, D.E.; Rogge, R. (2005): Issues in modeling heterogeneous deformations in polycrystalline metals using multiscale approaches. *CMES: Computer Modeling in Engineering & Sciences* 10: 123-141.

Haasemann, G.; Kaestner, M.; Ulbricht, V. (2006): Multi-scale modelling and simulation of textile reinforced materials. *CMC: Computers Materials & Continua* 3: 131-145.

Hasebe, T. (2006): Multiscale crystal plasticity modeling based on field theory. *CMES: Computer Modeling in Engineering & Sciences* 11: 145-155.

Ibach, H. (1997): The role of surface stress in reconstruction, epitaxial growth and stabilization of mesoscopic structures. *Surface Science Reports* 29: 193-263.

Kaczmarczyk, L. (2006): Enforcing boundary conditions in micro-macro transition for second order continuum. *CMC: Computers Materials & Continua* 4: 55-62.

Kadowaki, H.; Liu, W.K. (2005): A multiscale approach for the micropolar continuum model. *CMES: Computer Modeling in Engineering & Sciences* 7: 269-282.

Li, D.; Saheli, G.; Khaleel, M.; Garmestani, H. (2006): Microstructure optimization in fuel cell electrodes using materials design. *CMC: Computers Materials & Continua* 4: 31-42.

Liu, Y.; Zhang, X.; Sze, K.Y.; Wang, M. (2007): Smoothed molecular dynamics for large step time integration. *CMES: Computer Modeling in Engineering & Sciences* 20(3): 177-191.

Ma, J.; Liu, Y.; Lu, H.; Komanduri, R. (2006): Multiscale simulation of nanoindentation using the generalized interpolation material point (GIMP) method, dislocation dynamics (DD) and molecular dynamics (MD). *CMES: Computer Modeling in Engineering & Sciences* 16: 41-55.

Ma, J.; Lu, H.; Wang, B.; Roy, S.; Hornung, R.; Wissink, A.; Komanduri, R. (2005): Multiscale simulations using generalized interpolation material point (GIMP) method and SAMRAI parallel processing. *CMES: Computer Modeling in Engineering & Sciences* 8: 135-152.

Martinez, R.; Augustyniak, W.M.; Golovchenko, J.A. (1990): Direct Measurement of crystal surface stress. *Physical Review Letters* 64: 1035-1038.

Mebatsion, H.K.; Verboven, P.; Ho, Q.; Mendoza, F.; Verlinden, B.E.; Nguyen, T.A.; Nicolai, B.M. (2006): Modelling fruit microstructure using novel ellipse tessellation algorithm. *CMES: Computer Modeling in Engineering & Sciences* 14: 1-14.

Park, J.Y.; Cho, Y.S.; Kim, S.Y.; Jun, S.; Im, S.A. (2006): Quasicontinuum method for deformations of carbon nanotubes. *CMES: Computer Modeling in Engineering & Sciences* 11: 61-72.

Raiteri, R.; Grattarola, M.; Butt, H.; Skladal, P. (2001): Micromechanical cantilever-based biosensors. *Sensors and Actuators* 79: 115-126.

Schell-Scorokin, A.J.; Tromp, R.M. (1990): Mechanical stress in (sub)monolayer epitaxial films. *Physical Review Letters* 64: 1039-1042.

Shekhawat, G.; Tark, S.; Dravid, V.P. (2006): MOSFET-Embedded Microcantilevers for Measuring Deflection in Biomolecular Sensors. *Science* 311: 1592-1595.

Shen, S.; Atluri, S.N. (2004a): Multiscale simulation based on the meshless local Petrov-Galerkin (MLPG) method. *CMES: Computer Modeling in Engineering & Sciences* 5: 235-255.

Shen, S.; Atluri, S.N. (2004b): Atomic-level stress calculation and continuum-molecular system equivalence. *CMES: Computer Modeling in Engineering & Sciences* 6: 91-104.

Shen, S.; Atluri, S.N. (2004c): Computational nano-mechanics and multi-scale simulation. *CMC: Computers Materials & Continua* 1: 59-90.

Shen, S.; Atluri, S.N. (2005): A tangent stiffness MLPG method for atom/continuum multiscale simulation. *CMES: Computer Modeling in Engineering & Sciences* 7: 49-67.

Tewary, V.K.; Read, D.T. (2004): Integrated Green's function molecular dynamics method for multiscale modeling of nanostructures: Application to Au nanoisland in Cu. *CMES: Computer Modeling in Engineering & Sciences* 6: 359-371.

Wallstedt, P.C.; Guilkey, J.E. (2007): Improved velocity projection for the material point method. *CMES: Computer Modeling in Engineering & Sciences* 19(3): 223-232.