Molecular mechanics modelling and simulation of the adsorption-induced surface stress in micro-nano-cantilever sensors

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Abstract. Micro-nano-cantilevers have the exclusive potential to be an extremely sensitive sensor for chemical and biological detections. The mechanism of the sensor is that the adsorption-induced surface stresses cause the cantilever to bend, which can be measured by electronic or optical methods. In this paper, molecular mechanics method and theoretical energy minimization method are developed to study this bending behaviour. Molecular mechanics simulations were carried out on a homoepitaxy copper nano-cantilever to investigate the dependence of adsorption-induced surface stress on adatom concentration. Non-even pattern of development of adsorption-induced surface stress as adatom concentration increases was observed in the present atomistic simulations. To study the bending of micro-cantilever induced by adsorption, e.g. mercury adsorption on gold-coated cantilevers, the total energy consisting of atomic interaction energy of elastic bending energy is minimized. The Lennard–Jones model is employed to represent the interaction between mercury and gold atoms. Based on Dareinga’s model, we developed a model with more atoms and considered the periodic boundary conditions. Calculated deflections with the proposed new model agree better with measured deflection data. This discussion can contribute to our knowledge base about mechanisms of surface stress and micro-nano-cantilever bio-sensor.

1. Introduction

Micro-nano-cantilevers are widely used as sensors to detect the biological and chemical processes [1, 2, 3 and 4]. The change of surface stress due to the interactions between coating molecules (receptor) and target molecules (ligand) can bend the cantilever, which can be measured with the optical or other experimental methods. The molecular mechanism of this adsorption-induces surface stress is not fully understood.

Begley et al [5] presented a general mechanics framework to describe the interaction of molecular groups adsorbed on the deformable thin films. The framework is applicable to many interactions, even to living cells. There are some parameters are to be decided. Dareing et al [6] proposed a model for adsorption-induced surface stress based on atomic or molecular interaction. In his model, to study the bending of micro-cantilever induced by adsorption, e.g. mercury adsorption on gold-coated cantilevers, the total energy consisting of atomic interaction energy of elastic bending energy is minimized. This is a very good model which can agree well with results of experiments. However, the model seems a
little coarse because there are only three atoms considered and the interactions between these atoms and the neighboring atoms are ignored.

The aim of our research is to study the adsorption-induced stress and bending from molecular mechanics. Molecular mechanics method and theoretical energy minimization method are developed to study this bending behavior. Molecular mechanics simulations were carried out on a homoepitaxy copper nano-cantilever to investigate the dependence of adsorption-induced surface stress on adatom concentration. Non-even pattern of development of adsorption-induced surface stress as adatom concentration increases was observed in the present atomistic simulations. The Lennard–Jones model is employed to represent the interaction between mercury and gold atoms to do the energy minimization. Based on Darenga’s model, we developed a model with more atoms and considered the periodic boundary conditions.

2. Molecular mechanics modelling of adsorption to nano-cantilever

To do the molecular mechanics simulation of adsorption to nano-cantilever, embedded-atom-method (EAM) potential [7, 8] is employed to represent the interactions between copper atoms. The atomistic model is shown in Figure 1.

![Illustration of induced bending from a change in surface stress caused by depositing adatoms on one side of a nano-cantilever](image1)

**Figure 1.** Illustration of induced bending from a change in surface stress caused by depositing adatoms on one side of a nano-cantilever

![The plot of maximum adsorption-induced deflection of the nano-cantilever versus adatom concentration](image2)

**Figure 2.** The plot of maximum adsorption-induced deflection of the nano-cantilever versus adatom concentration

The positions of the atoms at the left end of the cantilever are fixed. The adsorption process is implemented by depositing adatoms step-by-step. During each step, the atoms can move to minimize the total potential energy. The energy is transferred between surfaced free energy and elastic energy
associated with structural bending of the cantilever. In our present simple case, the receptor atoms and ligand atoms are the same type. In fact, such simulations can be done with different types of atoms. The cantilever will bend with the depositing adatoms. It is evident that such bending is not the result of gravity of the adatoms, which is not ignored in this model. The bending comes from the change of surface stress due to depositing adatoms. The plot of maximum adsorption-induced deflection of the nano-cantilever versus adatom concentration is shown in Figure 2.

In Figure 2, the adatom concentration is defined as the ratio of the numbers of the depositing atoms to the numbers of one layer ideal copper atoms. When the concentration equals to 1.0, it means that the total system is again a cantilever without adatoms, so the deflection again equals to zero.

Non-even pattern of development of adsorption-induced surface stress as adatom concentration increases was observed in the present atomistic simulations. In low coverage regime where interactions between neighboring adatoms are negligible and the surface stress mainly originates from the local interactions of each adatom with the underlying surface atoms in the neighborhood, a negative adsorption-induced surface stress develops and changes linearly associated with adatom concentration. This trend could extend to full monolayer coverage if the interactions between neighboring adatoms were discarded in the atomistic simulations. In the medium coverage regime where the neighboring adatoms come into interaction with each other and dominates the contribution of adsorption-induced surface stress, the negative adsorption-induced inverses into a positive one and increase sharply to a maximum at the adatom concentration of half monolayer. In the large coverage regime, the tensile stress between neighboring adatoms drops as their separations reduce. This adsorption-induced tensile stress is also counteracted by the continuing negative contribution of local adatom-substrate interactions, and the nano-cantilever eventually arrive back at the state with equally stressed double surfaces.

3. Theoretical energy minimization of adsorption to micro-cantilever

In the last section, we did not use any continuum mechanics assumptions or theories. However, the usage of full atomistic simulation is very limited. Due the restriction of computer power, atomistic simulation of cantilever with micro-meters is out of range.

![Figure 3. The arrangement of atoms on micro-cantilever surface](image)
Our present work is developed on the base of Dareing and Thundat’s work [6]. We continue to use the assumption that the first atomic layer on the beam’s surface plays a dominate role in micro-cantilever deflections. Here, we consider more atoms. The arrangement of atoms on micro-cantilever surface is shown in Figure 3.

Lennard-Jones potential formula is used to represent the interactions between the atoms in the attached film. The strain energy of the bended cantilever is described by classic elastic mechanics. The equilibrium configuration of the cantilever is determined by minimizing the total energy. As shown in Figure 3, we consider atomic interaction potential of seven pairs, which are (1-2), (2-3), (1-3), (2-4), (3-5), (2-6) and (3-7). The simulation cell length of 2d of the beam is considered. The periodic boundary condition is implemented by accounting for the same ratio of the energy between atom 2 and atom 6, as well as atom 2 and atom 7, though atom 6 and atom 7 are outside the simulation cell.

The movements of neighboring adatoms are the same as \( z \). \( T \) is the curvature of the micro-cantilever. The deflection of the beam is

\[
\delta = \left( \frac{c}{T} \right) \left[ 1 - \cos \left( \frac{LT}{c} \right) \right],
\]

where \( T = \frac{c}{R} \), and \( z = \frac{b}{R} (c + a) \).

We define some parameters as

\[
p_1 = \frac{EI}{2c}, \quad p_2 = \frac{A}{b^2}, \quad p_3 = \frac{B}{b^2}, \quad p_4 = 1 + \frac{a}{c}, \quad p_5 = \frac{a}{b}, \quad p_6 = \frac{d}{b} \quad \text{and} \quad p_7 = \frac{1}{2} \left( 1 + \frac{a}{c} \right) \frac{d}{b}.
\]

The classic elastic bending energy is

\[
U_s = \frac{1}{2} EI \left( \frac{1}{R} \right)^2 b = EI \left( \frac{1}{R} \right)^2 b = E\frac{b}{2c^2} T^2 = bp_T^2.
\]

The atomic potential \( U_s = U_{12} + U_{23} + U_{13} + U_{24} + U_{35} + U_{26} + U_{37} \)

For equilibrium, the total energy is minimized.

\[
\frac{dU_s}{dT} = \frac{dU_s}{d\delta}.
\]

Solving this equation, we can obtain

\[
T = \frac{c}{R} = 5.87 \times 10^{-6} \quad \text{and} \quad \delta = 3.35 \times 10^{-7} m = 335 \text{nm}
\]

Here we use the same parameters as Ref [6]. The result of 335nm agrees better with the experimental output than Dareing’s original model. We contribute it to more atoms considered and the periodic boundary condition.

4. Concluding remarks

The sensing mechanism of such kinds of micro-nano-cantilever sensors are a very important topic to study. In this paper, we presented some primitive numerical simulation results to investigate the relationship of the deflection with the concentration of ligands. Here we study simple materials like metal atoms. This modeling and simulation method can be extended to complex molecular systems, such as biological and chemical molecules. An array of such cantilevers can be used as a selective chemical multi-sensor for the recognition of special chemical materials, like DNA, proteins. Atomistic simulation can give detailed information about the origin of surface stress. Classic continuum mechanics can extend the simulation cell to micrometers scale or larger.
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