Account of capillary effects in the simulation of the atomic force microscope work

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Abstract

The aim of this study is to show that effect caused by the curvature of the surface under the action of the Laplace forces needs to be taken into account when materials are investigated by the Atomic force microscope (AFM). Indentation the probe of AFM into the fluid is considered. The equation of the boundary of fluid in the axisymmetric task is presented. It is analyzed different cone angle of the probe of the AFM and different scales. The contribution of effect caused by the curvature of the surface under the action of the Laplace forces is examined and it is found that the attenuation of surface curvature near the probe caused by the Laplace forces is occurred on the length 1 mm.

1 Introduction

There are many different methods and tools for studying the nanoworld. The important role belongs to the AFM. The AFM is used to obtain information about topology of material structure and about mechanical properties. The interaction forces, for example van der Waals force, electrostatic interaction, adhesion forces, capillary effects, need to be taken into account when we investigate material at nanoscale.

In this paper we examined the effects caused by the curvature of the surface under the action of the Laplace forces.

The Laplace law in total case is given as

$$\Delta p = \alpha \left(\frac{1}{r_1} + \frac{1}{r_2} \right),$$

where r_1 and r_2 – the principal surface curvatures, α – the surface tension, Δp – the pressure difference in neighboring phases, which are separated by a curved surface, or the capillary pressure.

In the simplest case of a spherical surface (bubble or drop of fluid in the weightless) both the principal radius of curvature r are equal and constant along the entire surface. In this case the Laplace law is given as:

$$\Delta p = \frac{2\alpha}{r}.$$

2 Equation of fluid boundary

The cylindrical system of coordinate and initial configuration is considered. The unit basis vectors of the coordinate axes in the cylindrical system of coordinate is denoted as $\mathbf{i}_r, \mathbf{i}_\theta, \mathbf{i}_z$

and properties of the unit basis vectors are known as

$$\frac{\partial \mathbf{i}_r}{\partial \theta} = \mathbf{i}_\theta,$$

$$\frac{\partial \mathbf{i}_\theta}{\partial \theta} = -\mathbf{i}_r.$$

The boundary between phases is modeled by a constant thickness thin membrane (Figure 1). The Level set method [2] is used.

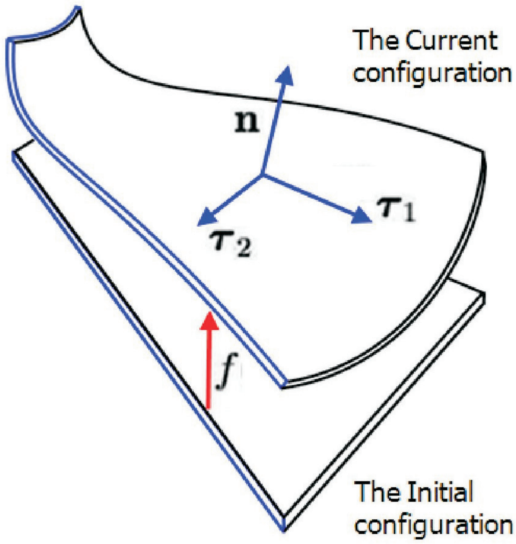

Figure 1: Modeling the thin membrane

Let us denote ξ - the curvature of the membrane.

$$\xi = f(r) + \gamma(r)z,$$

where $\gamma(r)$ – the parameter, which is responsible for the membrane thickness, $f(r)$ – the parameter, which is responsible for the movement of the membrane. The derivatives of this function is denoted as

$$\xi' = \frac{\partial \xi}{\partial r},$$

$$\xi'' = \frac{\partial^2 \xi}{\partial^2 r}.$$

Let us denote $\mathbf{x}$ – the position vector of membrane points

$$\mathbf{x} = r\mathbf{i}_r + \xi\mathbf{i}_z.$$

The gradient of deformation in the initial configuration in the cylindrical coordinates is given by

$$\text{Grad } \mathbf{x} = \mathbf{i}_r \otimes \mathbf{i}_r + \mathbf{i}_\theta \otimes \mathbf{i}_\theta + \gamma \mathbf{i}_z \otimes \mathbf{i}_z + \xi' \mathbf{i}_z \otimes \mathbf{i}_r. \quad (1)$$

Now we can define the tangent vectors

$$\boldsymbol{\tau}_1 = \frac{(\text{Grad } \mathbf{x}) \ \mathbf{i}_r}{|(\text{Grad } \mathbf{x}) \ \mathbf{i}_r|} = \frac{1}{\sqrt{1+(\xi')^2}}\mathbf{i}_r + \frac{\xi'}{\sqrt{1+(\xi')^2}}\mathbf{i}_z \quad (2)$$

$$\boldsymbol{\tau}_2 = \mathbf{i}_\theta. \tag{3}$$

The surface unit tensor $\mathbf{I}_s$ is given by

$$\mathbf{I}_s = \boldsymbol{\tau}_1 \otimes \boldsymbol{\tau}_1 + \boldsymbol{\tau}_2 \otimes \boldsymbol{\tau}_2. \tag{4}$$

Using Eq.(2) and (3), we can write Eq.(4) as

$$\mathbf{I}_s = \frac{1}{1+(\xi')^2}\mathbf{i}_r \otimes \mathbf{i}_r + \mathbf{i}_\theta \otimes \mathbf{i}_\theta + \frac{(\xi')^2}{1+(\xi')^2}\mathbf{i}_\mathbf{z} \otimes \mathbf{i}_z + \frac{\xi'}{1+(\xi')^2}\left(\mathbf{i}_r \otimes \mathbf{i}_z + \mathbf{i}_z \otimes \mathbf{i}_r\right). \tag{5}$$

Let us move from initial configuration to current one. We can use next formula

$$J\mathrm{div}\mathbf{I}_s = \mathrm{Div}\left(J\mathbf{I}_s(\mathrm{Grad}\mathbf{x})^{-\mathrm{T}}\right). \tag{6}$$

We should find J - the third invariant and after that we can use Eq. (6).

$$J = \det\left(\mathrm{Grad}\mathbf{x}\right) = \gamma \tag{7}$$

We substitute Eq. (1), Eq. (5), Eq. (7) into the right hand side Eq. (6) and we obtain

$$\mathrm{Div}\left(J\mathbf{I}_s\left(\mathrm{Grad}\mathbf{x}\right)^{-\mathrm{T}}\right) = \gamma'\frac{1}{1+(\xi')^2}\mathbf{i}_r + \gamma\frac{\partial}{\partial r}\left(\frac{1}{1+(\xi')^2}\right)\mathbf{i}_r + \gamma'\frac{\xi'}{1+(\xi')^2}\mathbf{i}_z +$$
$$+\gamma\frac{\partial}{\partial r}\left(\frac{\xi'}{1+(\xi')^2}\right)\mathbf{i}_z + \frac{1}{r}\gamma\frac{1}{1+(\xi')^2}\mathbf{i}_r - \frac{1}{r}\gamma\mathbf{i}_r + \frac{1}{r}\gamma\frac{\xi'}{1+(\xi')^2}\mathbf{i}_z.$$

So divergence of the surface unit tensor is calculated as

$$\begin{aligned}\mathrm{div}\mathbf{I}_s &= \frac{\partial}{\partial r}\left(\frac{1}{1+(\xi')^2}\right)\mathbf{i}_r + \frac{\partial}{\partial r}\left(\frac{\xi'}{1+(\xi')^2}\right)\mathbf{i}_z - \frac{(\xi')^2}{r(1+(\xi')^2)}\mathbf{i}_r + \\ &+ \frac{\xi'}{r(1+(\xi')^2)}\mathbf{i}_z + \frac{\gamma'}{\gamma(1+(\xi')^2)}\mathbf{i}_r + \frac{\xi'\gamma'}{\gamma(1+(\xi')^2)}\mathbf{i}_z.\end{aligned} \tag{8}$$

We can write boundary conditions in total case as

$$\mathbf{T}\,\mathbf{n} = \mathbf{f} + \mathrm{div}(\alpha\mathbf{I}_s), \tag{9}$$

where $\mathbf{T}$ – the Cauchy stress tensor, $\mathbf{n}$ – the exterior unit normal, $\mathbf{f}$ – the external forces acting on the unit surface, α – the surface tension, $\mathbf{I}_s$ – the surface unit tensor. The equilibrium of fluid equation is given by

$$\mathrm{div}(\mathbf{T}) = \rho g, \tag{10}$$

where ρ – the density of fluid , g – the acceleration of free fall. We consider case without the external forces acting on fluid. In this case boundary condition Eq. (9) could be represented by

$$\mathbf{T}\,\mathbf{n} = \mathrm{div}(\alpha\mathbf{I}_s). \tag{11}$$

Now we can find scalar product Eq.(11) with the exterior unit normal

$$\mathbf{T}\,\mathbf{n}\cdot\mathbf{n} = \mathrm{div}(\alpha\mathbf{I}_s)\cdot\mathbf{n}. \tag{12}$$

Look at the left hand side Eq.(12), we can write it as

$$\mathbf{T}\,\mathbf{n}\cdot\mathbf{n} = -p\,\mathbf{I}\,\mathbf{n}\cdot\mathbf{n} = -p, \tag{13}$$

where $\mathbf{I}$ – the unit tensor, p – the pressure. The exterior unit normal is defined as

$$\mathbf{n} = -\frac{\xi'}{\sqrt{1+(\xi')^2}}\mathbf{i}_r + \frac{1}{\sqrt{1+(\xi')^2}}\mathbf{i}_z.$$

Now we can find the right hand side Eq. (12)

$$\mathrm{div}\mathbf{I}_s\cdot\mathbf{n} = -\frac{\xi'}{\sqrt{1+(\xi')^2}}\frac{\partial}{\partial r}\left(\frac{1}{1+(\xi')^2}\right)+\frac{1}{\sqrt{1+(\xi')^2}}\frac{\partial}{\partial r}\left(\frac{\xi'}{1+(\xi')^2}\right)+\frac{\xi'}{r(1+(\xi')^2)} \quad (14)$$

We simplify Eq. (14) and the final form is

$$\mathrm{div}(\alpha\mathbf{I}_s)\cdot\mathbf{n} = \frac{\alpha}{\sqrt{1+(\xi')^2}}\left(\frac{\xi''}{1+(\xi')^2}+\frac{\xi'}{r}\right). \quad (15)$$

Using Eq. (13) and Eq. (15), pressure is found

$$p = -\frac{\alpha}{\sqrt{1+(\xi')^2}}\left(\frac{\xi''}{1+(\xi)^2}+\frac{\xi'}{r}\right). \quad (16)$$

Verification of formula. The boundary of the top half of drop is given by

$$\xi|_{z=0} = \sqrt{R^2-r^2}.$$

The derivatives of this function is denoted as

$$\xi'\big|_{z=0} = -\frac{r}{\sqrt{R^2-r^2}}, \quad (17)$$

$$\xi''\big|_{z=0} = -\frac{R^2}{(R^2-r^2)^{1.5}}. \quad (18)$$

Using Eq. (17) and Eq. (18), we can write Eq. (16) as

$$p = \frac{2\alpha}{R}. \quad (19)$$

Thus, we have the familiar Laplace formula. So Eq. (16) is true.

Consequence. The boundary conditions is considered

$$\gamma = \sqrt{1+(\xi')^2}\Big|_{z=0}. \quad (20)$$

$$\frac{\gamma'}{\gamma} = \frac{\xi'\xi''}{1+(\xi')^2}\Big|_{z=0}. \quad (21)$$

We can find scalar product $\mathrm{div}\mathbf{I}_s$ with $\boldsymbol{\tau}_1$, using Eq. (2) and Eq. (8)

$$\mathrm{div}\mathbf{I}_s\cdot\boldsymbol{\tau}_1 = -\frac{\xi'\xi''}{\sqrt{1+(\xi')^2}(1+(\xi')^2)}+\frac{\gamma'}{\gamma\sqrt{1+(\xi')^2}}.$$

Using Eq. (20) and Eq. (21), one can be write

$$\mathrm{div}\mathbf{I}_s\cdot\boldsymbol{\tau}_1 = 0.$$

Similarly we can find scalar product $\mathrm{div}\mathbf{I}_s$ with $\boldsymbol{\tau}_2$

$$\mathrm{div}\mathbf{I}_s\cdot\boldsymbol{\tau}_2 = 0.$$

So, at the boundary between phases does not appear additional shear strength.

3 Solution

Introduction of the conical probe into the water at the temperature 20^0 C is considered as an example. The density of fluid is $\rho = 998$ kg/m^2. The acceleration of free fall is $g = 9.8$ m/s^2. The pressure acting on fluid is $p = -\rho g \xi$. The surface tension is $\alpha = 72.8 * 10^{-3}$ N/m. The wetting angle is 8^0, for example.

Equation of the boundary of fluid in the axisymmetric task is given by

$$\xi'' = -(1 + (\xi')^2)\left(\frac{-\rho g \xi}{\alpha}\sqrt{1 + (\xi')^2} + \frac{\xi'}{r}\right). \tag{22}$$

Eq. (22) is solved numerically with respect to ξ. Figure 2 shows the change in the geometry of fluid surface by the Laplace forces, where the cone angle of the probe is 20^0.

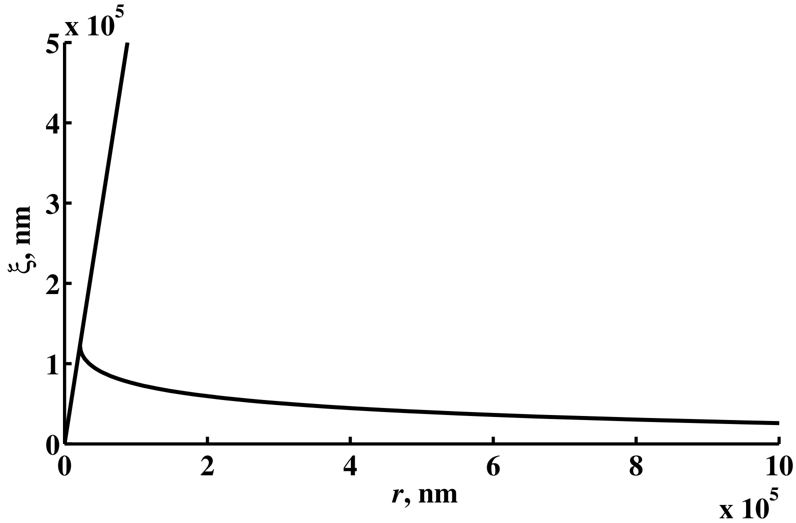

Figure 2: The change in the geometry of fluid surface at the nanolevel

Table 5 compares the depth of probe indentation and the height of fluid lifting.

Depth of probe indentation (m)	Height of fluid lifting (m)
$-1.53 \cdot 10^{-4}$	$4.15 \cdot 10^{-4}$
$7.76 \cdot 10^{-6}$	$6.45 \cdot 10^{-5}$
$3.08 \cdot 10^{-6}$	$8.75 \cdot 10^{-6}$
$5.38 \cdot 10^{-7}$	$1.11 \cdot 10^{-6}$
$7.68 \cdot 10^{-8}$	$1.34 \cdot 10^{-7}$
$9.88 \cdot 10^{-9}$	$1.56 \cdot 10^{-8}$
$1.17 \cdot 10^{-9}$	$1.74 \cdot 10^{-9}$

Table 5: The depth of probe indentation and corresponding the height of fluid lifting

The obtained solution shows that the indentation of a probe into the fluid at 10.7 nm is the cause of rising of fluid to a height of 20.2 μm. Thus, effect caused by the curvature of the surface under the action of the Laplace forces needs to be taken into account.

Surface profiles were calculated for different scales and cone angle of a probe. It is found that changing the geometry of the fluid surface caused by the Laplace forces is occurred on the length 1 mm. Figure 3 shows the attenuation of surface curvature near the probe on a nanolevel.

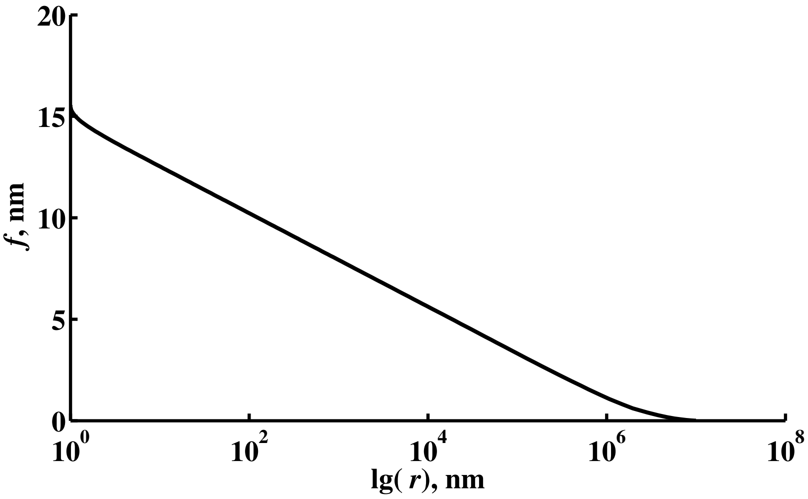

Figure 3: The attenuation of surface curvature near the probe caused by the Laplace forces

4 Conclusions

It is built model which is taken into account effect caused by the curvature of the surface under the action of the Laplace forces. Surface profiles were calculated for different scales.The calculations shows that changing the geometry of the fluid surface caused by the Laplace forces is occurred on the length 1 mm.

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