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# Deformation of PDMS membrane and microcantilever by a water droplet: Comparison between Mooney–Rivlin and linear elastic constitutive models

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ABSTRACT

In this paper, we studied the role of vertical component of surface tension of a water droplet on the deformation of membranes and microcantilevers (MCLs) widely used in lab-on-a-chip and micro- and nano-electromechanical system (MEMS/NEMS). Firstly, a membrane made of a rubber-like material, poly(dimethylsiloxane) (PDMS), was considered. The deformation was investigated using the Mooney–Rivlin (MR) model and the linear elastic constitutive relation, respectively. By comparison between the numerical solutions with two different models, we found that the simple linear elastic model is accurate enough to describe such kind of problem, which would be quite convenient for engineering applications. Furthermore, based on small-deflection beam theory, the effect of a liquid droplet on the deflection of a MCL was also studied. The free-end deflection of the MCL was investigated by considering different cases like a cylindrical droplet, a spherical droplet centered on the MCL and a spherical droplet arbitrarily positioned on the MCL. Numerical simulations demonstrated that the deflection might not be neglected, and showed good agreement with our theoretical analyses.



## 1. Introduction

Since poly(dimethylsiloxane) (PDMS) has many advantages, e.g., (1) good biocompatibility; (2) nontoxic and optically transparent; (3) easily fabricated, it has been widely used in lab-on-a-chip [1–6] and some microfluidic devices [7–13], etc.

Up to now, researchers have made many experiments about the mechanical properties of PDMS. Lötters et al. [14] first used PDMS PS851 from ABCR to measure the shear modulus and further studied relationship versus frequency and temperature. Armani et al. [15] utilized PDMS from Dow Corning to measure the Young's modulus with different mixing volume ratios of the curing agent and the polymer. Huang and Anand [16] carried out experiments on traditional macroscale specimens and thin-film specimens of PDMS with three varying ratios of monomer and curing agent to study the nonlinear mechanical behavior of PDMS material. Recently, Schneider and co-workers [17] have studied the mechanical properties of PDMS (weight ratio: 10:1) with different thinner concentrations (the thinner was added in order to get a lower viscosity) and the elastic modulus for Sylgard 184 without adding thinner against temperature and strain rate, respectively.

As a matter of fact, PDMS is a kind of rubber-like material with nearly or purely incompressible property. As a common knowledge, one of the most widely used models for such a material is the Mooney–Rivlin (MR) constitutive model. Mooney [18] and Rivlin and Saunders [19] developed the first hyperelastic models. Many other hyperelastic models have since been developed. Hyperelastic models can be classified as [20]:

(1) Phenomenological descriptions of observed behavior
- Polynomial model: Subject to the regularity assumption that strain energy function $W$ is continuously differentiable several times with respect to three strain invariants $I_1$, $I_2$ and $I_3$, the strain energy function is assumed to be an polynomial form of $(I_1 - 3)$, $(I_2 - 3)$ and $(I_3 - 1)$. For an incompressible material $I_3 = 1$ and $W$ depends on only two independent deformation invariants [21].
- MR model: The strain energy function of this model is the first-order polynomial form; more exactly, it is only linear functions of the invariants $I_1$ and $I_2$. It is the most widely used hyperelastic constitutive relation due to its simplicity and convenience for practical use.
- Ogden model: Ogden in 1972 deduced a hyperelastic constitutive model for large deformations of incompressible rubber-like solids. The strain energy is expressed as a function of the principal stretches. For particular values of material constants, the Ogden model will reduce to either the Neo-Hookean solid or the MR material.
- Yeoh model: The Yeoh (1993) model depends only on the first strain invariant $I_1$, it applies to the characterization

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of elastic properties of carbon-black filled rubber vulcanizates. The Yeoh model is also called the reduced polynomial model.

(2) Mechanistic models deriving from arguments about underlying structure of the material
- Arruda–Boyce model: The constitutive model for the large stretch behavior of rubber elastic materials is presented by Arruda and Boyce (1993). Also sometimes called the eight-chain model because it was derived by idealizing a polymer as eight elastic chains inside a volume element. The strain stress function is based on an eight chain representation of the macromolecular structure of the rubber.
- Neo-Hookean model: The model was derived from the statistical mechanics of a molecular chain network characteristic of the amorphous structure of rubber-like material by Treloar in 1943. It is the simplest model of rubber-like elastic response, in which only the term of $I_1$ is considered. Thus, Neo-Hookean material is a particular kind of MR material.

(3) Hybrids of phenomenological and mechanistic models
- Gent model: The strain energy density in the Gent model (1996) is a simple logarithmic function of the first strain invariant $I_1$, and involves two material constants.

For the relevant applications, Feng and Huang [22] and Pamplona et al. [23] used the MR model to investigate the large deformations of cylindrical membrane under internal pressure with the software ABAQUS and made comparison between the experimental and numerical results for the membrane under traction to identify the material parameters of the model. Three-dimensional (3D) solid element analysis and the membrane approximated analysis employing the hyperelastic model were developed for the simulation of the thermoforming process by Nam et al. [24]. Bellamy et al. [25] have recently simulated the mechanical behavior of the polymer up to 50% strain using MR model and found that the solutions were in excellent agreement with analytical and experimental results. Dong et al. [26] used the MR model to obtain the critical material parameters of polymethylmethacrylate (PMMA) with experimental verification, and then derived the major material parametric functions at temperatures between 150 °C and 190 °C.

When there is a water droplet on the surface of PDMS membrane with a rigid substrate, the PDMS material was simply regarded as a linear elastic material because the deformation is very small, and then numerical simulation was carried out for the elastic deformation of the membrane due to the vertical components of liquid–vapor surface tension [27]. However, linear elastic material model is only a first-order approximation for a hyperelastic material like PDMS. The main objective of the present paper is to make a guideline for the accuracy range for the linear elastic model to simulate the elastic deformation of PDMS under the action of a water droplet.

Determination of the materials constants in the MR model is a prerequisite to use this model for the numerical simulation. Fortunately, there are some literatures on for relevant experiments [28–30]. In addition, Gent [31] has proposed some other methods to get the material constants.

Besides, we continued to study the effect of a liquid droplet on the deformation of a MCL. For macro structures, the deformation induced by liquid droplets may be neglected simply since the surface tension and the Laplace pressure are negligible compared to the rigidity of the solid body; while in MEMS/NEMS, vertical displacement induced by them may be several to hundreds nanometers and even hundreds micrometers when the materials are very soft. In such cases, the deformation cannot be neglected anymore. For example, if there are several microdrops on the MCL of an atomic force microscopy (AFM), they may decrease the precision of AFM. Therefore, it appears significant to study the effect of liquid droplets on MCL.

During the recent years, some researchers have made some relevant investigations on the deflection of MCL due to microdrops, as shown in Fig. 9. Jensenius et al. integrated resistors on flexible cantilevers to monitor the cantilever deflection [32]. Bonaccurso et al. studied microdrops on AFM cantilevers theoretically and experimentally [33,34]. Some researchers studied the influence of nanobubbles on the bending of MCLs [35,36]. Recently, Bonaccurso et al. developed a FEM model for the bending of a cantilever and measured the bending versus time [37]. Zheng et al. used the energy method to study the directional movement of liquid droplets on a microbeam with a varying or gradient stiffness and found that the droplet will move to the softer end of the beam [38].

In the first part of this paper, we first introduced the procedure to determine the material constants in the MR model. Then we used the least square method (LSM) to obtain the material constants from experimental data in Ref. [16]. At last, both the linear elastic and the MR constitutive models were used to numerically simulate the deformation of PDMS membrane induced by a water droplet. And we found the solutions with a linear elastic model are in excellent agreement with that by using the MR model for such problem. In the latter part, we theoretically analyzed the effect of a liquid droplet on the deflection of a MCL and gave some numerical simulations to demonstrate the deflection might not be neglected.

## 2. MR model and determination of material constants

A hyperelastic material is an ideally elastic material for which the stress–strain relationship derives from a strain energy density function. The strain energy density function, $W$, for PDMS is the function of the three strain invariants $I_1$, $I_2$ and $I_3$, i.e. [20],

$$W = W(I_1, I_2, I_3), \tag{1}$$

where $I_1 = \operatorname{tr}\mathbf{C}$, $I_2 = [(\operatorname{tr}\mathbf{C})^2 - \operatorname{tr}\mathbf{C}^2]/2$.

Then, corresponding stress can be expressed as

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{E}} = 2\frac{\partial W}{\partial \mathbf{C}}, \tag{2}$$

where $\mathbf{S}$ is the second Piola–Kirchhoff stress tensor, $\mathbf{E}$ is the Green strain tensor and $\mathbf{C}$ is the right Cauchy–Green deformation tensor. $\mathbf{E}$ and $\mathbf{C}$ satisfy the following relationship:

$$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I}), \tag{3}$$

where $\mathbf{I}$ is the second-order unit tensor.

To ensure incompressibility of a hyperelastic material, the constraint $I_3 = 1$ must be fulfilled. The strain-energy function, $W$, can be written as a polynomial function of $(I_1 - 3)$ and $(I_2 - 3)$ [18,21]

$$W = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} c_{ij}(I_1 - 3)^i (I_2 - 3)^j, \tag{4}$$

where $c_{ij}$ are empirically determined material parameters.

Because the deformation of PDMS material in the present paper is very small under the action of a water droplet, two-parameter MR model is used as follows [18]:

$$W = c_1(I_1 - 3) + c_2(I_2 - 3), \tag{5}$$

where $c_1$ and $c_2$ are material constants. The model has an applicable strain of about 100% in tension and 30% in compression. Then, the constitutive equation for hyperelastic incompressible materials can be expressed as: