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Droplet on an elastic substrate: Finite Element Method coupled with lubrication approximation

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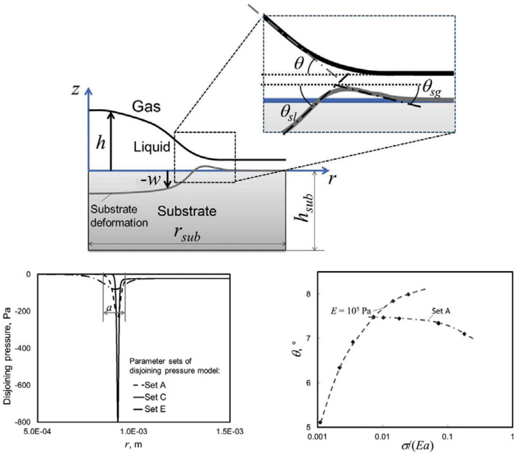
HIGHLIGHTS

- New modelling strategy for description of wetting of soft substrates combines numerical solution of elasticity problem in the substrate with the solution of a thin film equation for spreading of sessile droplet.
- Substrate deformation and the apparent contact angle depend on the parameters of the disjoining pressure model.
- The solid angle formed due to the substrate deformation is determined by the surface tension, Young modulus and the width of a region, in which the effect of disjoining pressure is significant.

GRAPHICAL ABSTRACT



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ABSTRACT

Sessile liquid droplets deposited on soft substrates may cause substrate deformation. The substrate elasticity affects the apparent contact angle and the spreading dynamics of the sessile drop. In the present work, a model for description of a droplet on an elastic substrate is developed using the disjoining pressure concept. A Finite Element Method for the elasticity problem in a substrate is coupled with lubrication approximation for the modelling of droplet spreading. The disjoining pressure model allows an independent definition of contact angle and the thickness of the adsorbed layer. Simulations are performed to quantify the influence of mechanical properties, the substrate size and the parameters of the disjoining pressure model on the substrate deformation and apparent contact angle. It is shown that the dimensionless substrate deformation peak height scales with the dimensionless parameter $\sigma \sin\theta/(Ea)$, and the solid angle appearing in the deformed substrate near the apparent cotact line scales with $\sigma/(Ea)$, where σ denotes the surface tension, E is the Young modulus, θ is the apparent contact angle and a is a width of the region in which the disjoining pressure plays an important role.

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1. Introduction

It is known that soft substrates are deformed in the vicinity of the contact line of sessile drops [1,2]. In addition, the equilibrium contact angle is modified in comparison with the value measured on a rigid substrate, and the drop spreading dynamics is governed by the mechanical properties of the solid [3,4]. As a result, the mechanical properties of substrates affect numerous phenomena governed by wetting, such as droplet spreading dynamics [4], evaporation [5], condensation [6], deposition of particles after the drying of droplet [7] and the nucleation of ice [8].

The reason of the substrate deformation is the normal component of the liquid surface tension acting at the contact line, $\sigma \sin\theta$, where θ denotes the contact angle [1,9]. At equilibrium this force leads to development of a stress field in the solid. A rigid body can be considered as an elastic material with infinitely high elastic modulus, E, in which the stresses are not accompanied by deformation. In soft substrates (elastic or viscoelastic) the substrate is deformed, and maximal deformation increases with decreasing E [10].

Numerous theoretical and numerical works have been devoted to the description of phenomena taking place in soft substrates in the vicinity of contact lines and to the prediction of substrate deformation field [1,9,11–13]. The models used in these works are based on the theory of elasticity. The deformation is computed from the prescribed surface traction distribution on the surface of the elastic body. In [1] the stress distribution produced by a sessile drop has been modelled as a constant capillary pressure distributed over an area occupied by the droplet and a constant stress directed upwards and distributed over a ring area around the contact line. The range of distribution of the upward-directed stresses, which in the work of Lester [1] is associated with the capillary layer thickness, was assumed to be of the order of 1 nm. The integral of the stress distribution over the whole area is equal to zero. In [9] the tangential stress in the vicinity of the contact line is taken into account. This additional stress results from the deviation of the local contact angle from the Young angle leading to the appearance of an unbalanced tangential force.

The deformation of the substrate and the angles formed between the phase interfaces strongly depend on the width of the area around the contact line, in which the upward stress is distributed [1,9,14]. However, this width cannot be determined from a macroscopic model and is therefore an adjustable parameter. This is changed in the models taking into account micro-scale phenomena [12,13,15,16]. In the molecular dynamic simulations [16] the width of the region around the contact line over which the stress is distributed is mostly determined by the parameters of the Lennard-Jones interaction potential. If the concept of disjoining pressure is used for description of intermolecular forces and their influence on the phenomena taking place near the contact line [12,15,17,18], the functional form of the disjoining pressure determines the area over which the stress is spread.

Deryagin et al. [15] have been, to the best of our knowledge, the first to suggest computing the normal stresses acting on the substrate from the disjoining pressure distribution. They have considered a disjoining pressure isotherm which is positive for small values of film thickness, decreases with increasing thickness, crosses the zero axis, then reaches a negative minimum, after that increases with thickness and approaches zero. In this case the liquid-gas interface doesn't cross the solid substrate, but rather smoothly transforms into a very thin adsorbed layer covering an apparently dry area of the substrate. The condition $\Pi(h_{ads}) = -\Delta P$ determines the thickness of the absorbed film at equilibrium with a liquid drop characterized by a Laplace pressure difference ΔP. The authors have shown that the integral of the disjoining pressure distribution around an apparent contact line is equal to $\sigma \sin\theta$. Moreover, the application point of the resultant force coinsides with the position of apparent contact line. However, Deryagin et al. [15] didn't compute the deformation of the elastic substrate under the action of distributed force.

White [12] distinguishes between two classes of disjoining pressure functions. The monotonously increasing function, which is negative in the whole range of film thicknesses, does not lead to the appearance of an adsorbed film beyond the apparent contact line. The second class includes the disjoining isotherms of the type considered in [15]. In the paper of White [12] an analytical expression for the elastic deformation in an infinite elastic medium beneath the sessile droplet is derived using the surface Green function. White [12] considers the asymptotic behavior of the deformation, which is independent from the form of disjoining pressure.

In [17,18] the stability and dewetting of a liquid film on a thin elastomeric layer is considered in the framework of lubrication theory, whereas a linear viscoelastic model has been chosen for description of the elastomeric layers. Both the liquid film thickness and the thickness of the substrate are assumed to be much smaller than the characteristic length of the film deformation [19]. The disjoining pressure of the form $\Pi(H) = -A/H^3 + B/H^4$ has been considered. The theory has described the instability due to the action of van der Waals forces [17] and has predicted the thinning of the liquid film and the thickening of the elastomeric solid (formation of dimples) in the case $A > 0$, $B = 0$ [18]. In the case $A > 0$, $B > 0$ the solution of the model equations describes regions of thin liquid film connecting fluid ridges.

The evolution of sessile droplets on rigid substrates has been also studied in the past in the framework of the lubrication theory, whereas the solid-fluid intermolecular interactions have been described using the disjoining pressure concept. In particular, some of these works have been focussed on droplet evaporation [20–22]. These works differ from each other not only in the choice of the evaporation model and the further physical phenomena taken into account, but also in the choice of disjoining pressure model. Murisic and Kondic [20] use the form $\Pi(H) = A/H^3 - B/H^2$, and in the work [21] the form $\Pi(H) = \frac{\varepsilon}{H^3} - d_1 \operatorname{sech}^2\left(\frac{H}{d_2} - 2\right)$ is adopted. These models predict a stable adsorbed film covering the apparently dry area and a finite contact angle. In [22] a fully wetting case is considered with the disjoining pressure isotherm in the form $\Pi(H) \sim H^{-3}$, taking into account only the repulsive van der Waals forces.

In the present work we consider a sessile droplet wetting an elastic substrate of arbitrary thickness and diameter, thus relieving the restrictions present in the works [12,17,18]. The deformation of the substrate is simulated numerically using the Finite Element Method. The shape of a thin droplet is modelled using the lubrication approximation. The models are coupled with each other through the surface traction on the elastic substrate exerted by the droplet and through the substrate topography affecting the droplet shape evolution. In this paper the steady state solutions depending on the mechanical properties and the size of the substrate, as well as on the parameters of disjoining pressure model are considered.

2. Physico-mathematical model

Consider a cylindrical substrate with a thickness h_{sub} and a radius r_{sub} (see Fig. 1). A sessile droplet of a Newtonian liquid is placed at the center of the substrate. The position of the liquid-gas interface is denoted by h, and the deformation of the substrate resulting from the traction exerted by the droplet is denoted by w, so that the film thickness is $H = h - w$. The axis r lies in the plane of undeformed substrate surface ($h = 0$). We assume that the apparently dry portion of the substrate is covered by an adsorbed liquid film. We define the apparent contact angle θ at a location of the maximal slope of the liquid-gas interface. The angles θ_{sl} and θ_{sg}

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