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Modeling of properties of a droplet on a partially wetted solid surface

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Analytical and numerical modeling of some physical properties of droplet on a partially wetted solid surface in thermodynamic equilibrium is carried out. The modeling technique is based on the use of the Lennard–Jones pair interatomic potential and the continuum approximation for interacting atoms. The density functional theory in the electron gas approximation is used to calculate the potential parameters. New formulas for the potential energy of interaction of a droplet with a substrate and the work of adhesion are derived, the condition for the stability failure of a droplet is formulated. Numerical calculations are performed for the Li (droplet)–Ni (substrate) system.

Keywords: density functional theory, droplet, work of adhesion, stability, continuum approximation, pairwise interatomic interaction.

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Introduction

Small drops of liquids and particles of solid materials with the sizes of units — dozens of nanometers on the surfaces of solid bodies are both of theoretical and of practical interest. The methods of molecular dynamics and Monte Carlo's have become the most common in theoretical studies of these nanoobjects [1–3]. It is quite hard to count even an approximate number of published articles where these methods were used. Unfortunately, analytical thermodynamic and statistical methods of study have become less popular, though these allow to obtain valuable results (see the studies [4–12] and references therein). In practice, simulation and forecasting of the properties of small drops and particles on the surfaces of solid bodies is very important for various applications in nanotechnologies, microelectronics, and microfluidics [13,14].

It is known that single 3D islands of condensed phase on the solid body surface are formed according to Volmer–Weber mechanism, when interaction of atoms of that phase between each other is comparable or stronger than their interaction with the atoms of the substrate [15]. Depending on the temperature and composition these islands could be both liquid (drop) and solid (particle). In case of a drop, when thermodynamic conditions change, the transition from partial wetting of the surface with contact angle $\theta < \pi/2$ to full wetting, when $\theta \to 0$, is possible. It is appropriate to attribute such a transition to the first-nature phase transition, since in this case the derivatives of thermodynamic potentials in terms of the temperature face the step changes [16]. Note that the phase transition of wetting within the region of small-size drops has some common features with the primary crystallization. As a result of reduction of superficial tension and action of gravity forces from the substrate side a small drop could spread very fast, turning into a structurally rigid thin film, whose thickness corresponds to the region of action of these forces. The process of fast spread of liquid over a partly or poorly wetted surface sometimes is called superspreading. Physical and chemical reasons for that phenomenon are now being actively discussed [17].

This study is devoted to simulation of equilibrium thermodynamic properties of a small drop on partly wetted and atomically smooth surface. The theoretical approach is based on the application of paired interatomic potential of Lennard–Johnes (LJ) and additive continual approximation [18]. The method of electron density functional is used for calculation of the parameters of interatomic potential; electron densities are taken in the approximation of Hartree–Fock subject to the shell structure of interacting atoms. Numerical calculations of potential energy of drop-substrate interaction and specific adhesion work were performed. The condition of mechanical stability failure of the drop was formulated by means of the Laplace equation generalization. The approach is reasonable not only for drops, but also for sparse island films, in which the distances between separate islands exceeds the radius of action of interatomic forces.

1. Calculation of LJ potential parameters

In the study for simulation of properties of a drop in-situ we offered using a paired interatomic LJ potential, whose parameters are derived from the theory of functionality of the electron density [19,20]. At that, the LJ potential ceases to be purely empirical.

In section 1 all formulas use atomic system of units ($\hbar = e = m_e = 1$). Non-valent interaction of two atoms is considered. Coulomb component of the interaction potential includes repulsion between nuclei, repulsion between electron clouds and gravity between nuclei and electron clouds of atoms:

$$\varphi_1 = \frac{Z_a Z_b}{r} + \iint \frac{\rho_a(\mathbf{r}_1)\rho_b(\mathbf{r}_2)}{r_{12}}\, d^3\mathbf{r}_1 d^3\mathbf{r}_2 - Z_b \int \frac{\rho_a(\mathbf{r}_1)}{r_{1b}}\, d^3\mathbf{r}_1 - Z_a \int \frac{\rho_b(\mathbf{r}_2)}{r_{2a}}\, d^3\mathbf{r}_2,$$

where indices „a“ and „b“ denote interacting atoms, r is the distance between atoms, $Z_{a,b}$ and $\rho_{a,b}$ are the charges and electron densities of atoms, r_{12} is the distance between electrons of atoms, r_{1b} and r_{2a} are the distances from electrons to nuclei. In spherical coordinates all parts of that functionality are grouped into one expression

$$\varphi_1(r) = 16\pi^2 \int_0^{\infty}\int_0^{\infty} \rho_a(x)\rho_b(y) I(r,x,y) x^2 y^2 dx dy, \tag{1}$$

$$I(r,x,y) = \frac{1}{r} + F(r,x,y) - \frac{2}{r + x + |r - x|} - \frac{2}{r + y + |r - y|}, \tag{2}$$

$$F(r,x,y) = \begin{cases} \dfrac{2}{r + x + |r - x|}, & y < |r - x|, \\ \dfrac{1}{2}\left(\dfrac{1}{x} + \dfrac{1}{y}\right) - \dfrac{r}{4xy} - \dfrac{(x-y)^2}{4rxy}, & |r - x| < y < |r + x|, \\ \dfrac{1}{y}, & y > r + x. \end{cases} \tag{3}$$

Quantum correction is derived by using the formula

$$\varphi_2 = \int \Big\{ \big[\rho_a(\mathbf{r}_a) + \rho_b(\mathbf{r}_b)\big] e_g(\rho_a + \rho_b) - \rho_a(\mathbf{r}_a) e_g(\rho_a) - \rho_b(\mathbf{r}_b) e_g(\rho_b) \Big\} d^3\mathbf{r},$$

where $e_g(\rho)$ is the volumetric density of electron gas. In ellipsoidal coordinates we have the integral

$$\varphi_2(r) = \frac{\pi r^3}{4} \int_1^{\infty}\int_{-1}^{1} \big[(\rho_a + \rho_b) e_g(\rho_a + \rho_b) - \rho_a e_g(\rho_a) - \rho_b e_g(\rho_b)\big] d\mu\, d\lambda. \tag{4}$$

Volumetric density of energy of electron gas is

$$e_g(\rho) = \frac{3}{10}(3\pi^2\rho)^{2/3} - \frac{3}{4}\left(\frac{3}{\pi}\rho\right)^{1/3} + e_c(\rho), \tag{5}$$

$$e_c(\rho) = \begin{cases} 2.711816\rho^{1/2} - 0.706052\rho^{1/3} - 3.819822\rho^{2/3} - 1.319676\rho^{5/6}, & \rho < \eta_1, \\ -0.7062 - 0.00633\ln(\rho), & \eta_1 \le \rho \le \eta_2, \\ -0.010367\ln(\rho) - (0.001861\ln(\rho) + 0.008869)\rho^{-1/3} - 0.062849, & \rho > \eta_2, \end{cases}$$

$$\rho_a(r;\lambda,\mu) = \rho_a\left(\frac{r(\lambda+\mu)}{2}\right),\ \rho_b(r;\lambda,\mu) = \rho_b\left(\frac{r(\lambda-\mu)}{2}\right),$$

where separate members of sum in (5) refer to kinetic, exchange and correlation contributions, accordingly, $\eta_1 = 2.387324 \cdot 10^{-4}$ and $\eta_2 = 0.696013$ are the cross-link parameters in correlation contribution. Resultant potential energy of interaction of two atoms is

$$\varphi = \varphi_1 + \varphi_2. \tag{6}$$

In (1)–(6) it is required to set $\rho_{a,b}$. It can be done in the most correct way, if quantum-mechanical electron densities of atoms, derived by using Hartree–Fock method, are used [21]. According to [22], we have the formula

$$\rho(\xi) = \frac{Z}{4\pi\xi}\left[\sum_i A_i \exp(-\alpha_i\xi) + \sum_j B_j(\beta_j\xi - 2)\exp(-\beta_j\xi)\right], \tag{7}$$

where Z is the atom nucleus charge, A_i, α_i, B_j, and β_j are the numerical coefficients, which are determined based on the data from [22], ξ is the coordinate counted from the atom nucleus. Calculation of paired interatomic potential as per (1)–(7) does not impose any constrains in terms of temperature during further consideration of interaction in condensed phases.

Integration in (1)–(7) was performed by trapezias method in constrained regions, within which are „effective“ parts of functions. The integration region for (1) referred to a square with the size of 60×60, and for (4) — a rectangle with the size of 2×60. Wherein the distances in 40–60 a.u. are already quite big to be a good approximation to the infinity. The distance between atoms in all calculations changed within a wide interval from 0.5 to 20 a.u. with the pitch of 0.05 a.u. The calculation mesh consisted of $\approx 5 \cdot 10^8$ dots, which eventually guaranteed 4–6 true digits after dot. The algorithm itself was paralleled to perform calculations in graphic processor and was implemented within the CUDA C++ software environment. It enabled reducing the software working time dozens of times.

LJ potential parameters — equilibrium distance r_0 and the depth of potential well D were determined by using tabulated curve $\varphi(r)$ by direct data enumerating. At that the error of distance corresponds to the breakdown pitch and does not exceed 0.05 a.u in our case. Herein we considered the system Li–Ni. The calculation results are shown in Fig. 1. The values of equilibrium distance and potential well found by us are equal to 6.071

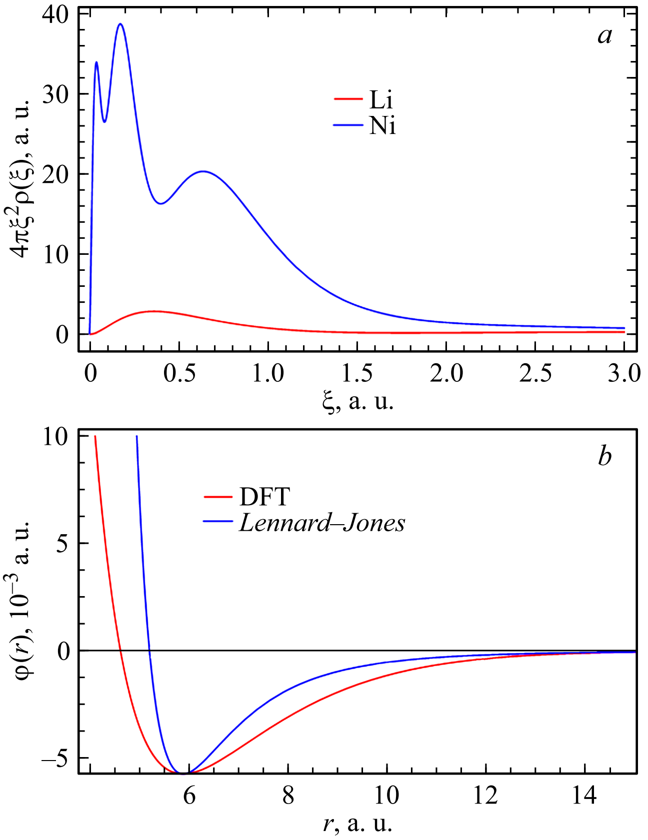

Figure 1. The results of calculation of paired interatomic interaction Li–Ni: *a* — distribution of radial electron densities; *b* — potential curves.

and 0.00572 a.u. [23] refers to empirical values of parameters of potential of the type „*n–m*“ for interaction of homoatomic pairs Li–Li and Ni–Ni. Application of Lorentz–Berthelot mixing rules to these data [2] for heteroatomic pair Li–Ni results in close values of 5.443 and 0.00557 a.u.

2. Mathematical model of drop

A small drop of non-polar and non-compressible liquid in the form of spherical segment adjacent to flat surface of solid body is considered. Contact angle $\theta < \pi/2$. Fig. 2 illustrates the geometry of the system. It is assumed that Gibbs adsorptions on all boundaries of phases separation are equal to zero or negligible, i.e. there are no long interphase layers on these boundaries. In this case, from Gibbs equation for any interphase boundary in the system we have $d\sigma = 0$ and $\sigma = \text{const}$, where σ is the superficial tension on that boundary. Medium densities of contacting phases are also considered to be constant, i.e. independent on the pressure and spatial coordinates. The systems with these properties are observed in the steady-state process at $t \to \infty$ in many numerical experiments as per the method of molecular dynamics (see, e.g., [24–27]): at intensive interatomic interaction virtually all steam atoms are captured by drop forming its equilibrium volume. The assumptions made, in our opinion, are the most acceptable for liquid metals far from the evaporation phase transition. Due to a high value of superficial tension a small drop of typical liquid metal shall have the shape closer to spherical (see, e.g., [28,29]). For the same reason, for the metal at the boundary of „liquid–steam“ separation the density distribution profile is approximately stepwise, the interphase region thickness tends to zero and dimensional dependencies of the superficial tension and contact angle can be ignored.

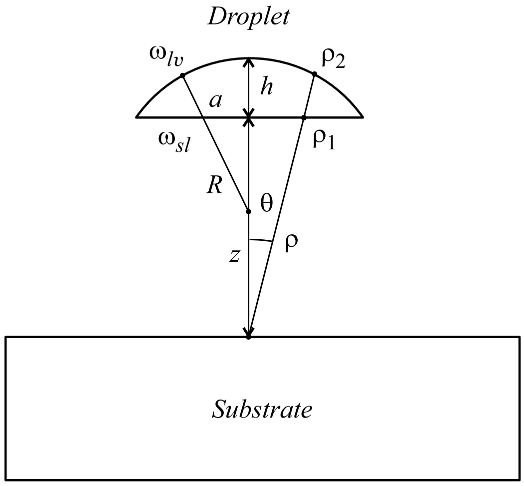

Figure 2. Drop model on partly wetted surface.

Let us write the drop free energy differential [29]:

$$dF = \Delta p dV - \sigma_{lv}\cos(\theta_c) d\omega_{sl} + \sigma_{lv} d\omega_{lv} + du, \tag{8}$$

where Δp is the excessive pressure equal to the difference between the steam pressure and the pressure in the drop, dV, $d\omega_{sl}$ and $d\omega_{lv}$ are the differentials of the drop volume and areas of the phases separation, σ_{lv} is the superficial tension at the boundary of the „liquid–steam“ separation, θ_c is the contact angle of wetting, du is the differential of drop and substrate interaction energy. From the geometry we have

$$dV = \pi\left[2 - 3\cos(\theta_c) + \cos^3(\theta_c)\right] R^2 dR,$$

$$d\omega_{sl} = 2\pi \sin^2(\theta_c) R dR,$$

$$d\omega_{lv} = 4\pi[1 - \cos(\theta_c)] R dR,$$

$$h = R[1 - \cos(\theta_c)], \quad a = R\sin(\theta_c),$$

where R is the drop radius, h is the drop height, a is the drop base radius. Subject to the formulas taken from (8) for the drop in thermodynamic equilibrium state we get generalized Laplace equation

$$\Delta p = \frac{2\sigma_{lv}}{R} + \frac{1}{4\pi R^2 f(\theta_c)}\left(\frac{\partial u}{\partial R}\right)_{eq}, \tag{9}$$

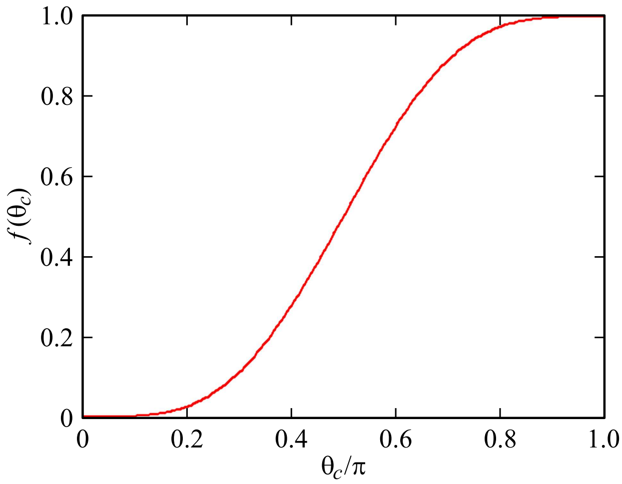

Figure 3. Dependence of wetting factor on the contact angle of wetting.

where

$$f(\theta_c) = [2 - 3\cos(\theta_c) + \cos^3(\theta_c)]/4$$

is the wetting factor that occurs in the heterogeneous nucleation theory. Graph of the function $f(\theta_c)$ is shown in Fig. 3. At a quite high R the second member of sum (9) can be ignored, so we have an ordinary Laplace equation.

Let us find now the drop and substrate interaction energy. In continual approximation

$$u = n_l n_s \iint \varphi(\mathbf{r}) dV_s dV_l, \tag{10}$$

$$\varphi(r) = D\left[\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^6\right], \tag{11}$$

where $n_{s,l}$ are the volumetric concentrations of atoms of the substrate and of the drop, which depend, generally speaking, on the temperature. The interaction energy of side atom with semi-infinite substrate is equal to

$$u_A(z) = n_s \int \varphi\, dV = 2\pi n_s \int\limits_z^\infty \varphi(r)(r^2 - rz)dr, \tag{12}$$

where z is the distance from atom to the substrate surface. By substituting (11) in (12) and making integration, we get

$$u_A(z) = \frac{u_0}{2}\left[\left(\frac{z_0}{z}\right)^9 - 3\left(\frac{z_0}{z}\right)^3\right], \tag{13}$$

$$u_0 = \frac{10}{9}\pi n_s D z_0^3, \quad z_0 = \frac{r_0}{\sqrt[6]{5}},$$

where z_0 and u_0 are the equilibrium state and depth of potential well during „atom–substrate" interaction. The spherical segment and substrate interaction potential is

$$u(z) = n_l \int u_A dV = 2\pi n_l \int\limits_0^{\operatorname{arctg}(a/z)} \sin(\theta)d\theta \times \int\limits_{\rho_1(z,\theta)}^{\rho_2(z,\theta)} u_A\big(r^* \cos(\theta)\big) r^2 dr, \tag{14}$$

$$\rho_1(z,\theta) = \frac{z}{\cos(\theta)},$$

$$\rho_2(z,\theta) = (h + z - R)\cos(\theta) + \sqrt{R^2 - (h + z - R)^2 \sin^2(\theta)},$$

where z is the distance between the drop and the substrate, R is the drop radius, a and h is the base radius and the drop height interrelated with each other by the ratio $a = \sqrt{h(2R - h)}$. By deriving the internal integral (14), we get

$$u(z) = \frac{10}{3}\pi^2 n_s n_l D z_0^6 \int\limits_0^{\operatorname{arctg}(a/z)} \mu(z,\theta)\sin(\theta)d\theta, \tag{15}$$

$$\mu(z,\theta) = \frac{1}{18\cos^9(\theta)}\left[\left(\frac{z_0}{\rho_1(z,\theta)}\right)^6 - \left(\frac{z_0}{\rho_2(z,\theta)}\right)^6\right] + \frac{1}{\cos^3(\theta)}\ln\left(\frac{\rho_1(z,\theta)}{\rho_2(z,\theta)}\right).$$

A multiplier before the integral in (15) can be expressed through the Hamaker constant [18]. The integral itself (15) is efficiently calculted by Romberg method.

Equilibrium state z_d, in which the drop is above the substrate, and specific work of adhesion W of the drop to the substrate are determined from the equations

$$\left(\frac{\partial u(z)}{\partial z}\right)_{z=z_d} = 0, \tag{16}$$

$$W_d = -\frac{u(z_d)}{\pi h(2R - h)} = -\frac{u(z_d)}{\pi R^2 \sin^2(\theta_c)}. \tag{17}$$

The equation (16) is solved numerically by tangent method. On the other hand, for the drop there is well known Young–Dupre equation

$$W_d = \sigma_{sl}\big[1 + \cos(\theta_c)\big] = \sigma_{sl}\big[1 + \sqrt{1 - (a/R)^2}\big], \tag{18}$$

where σ_{sl} is the superficial tension at the boundary of „solid body–liquid" separation. Equations (17), (18) can be used for theoretical determination of σ_{sl}. Equilibrium energy $u(z_d)$ depends only on R and θ_c (if a and h are excluded from it), and must be included into the equation (9).

By using the obtained formulas we can define the condition for wetting phase transition. In the absence of mutual dissolution of substances, full wetting will occur, apparently, when the pressure in the drop created by interatomic forces from the substrate side will be equal to or exceed the Laplace pressure. Relevant condition in our case is

$$\Delta p = 0. \tag{19}$$

Resolving (19) subject to (9) at the specified angle θ_c, we define the limit value of the drop radius R, there cannot be a lower one for the drop. The drop spreading rate υ is assessed from the equation of hydrodynamic and Laplace pressures: $\rho_l \upsilon^2/2 = 2\sigma_{l\upsilon}/R$, where ρ_l is the liquid density. Hence, we get the formula

$$\upsilon = 2\sqrt{\frac{N_A \sigma_{l\upsilon}}{M n_l R}}, \tag{20}$$

where M is the molar mass, N_A is the Avogadro number. In (20) R refers namely to the limit radius of the drop at the specified temperature.

The results of numerical calculations for a small lithium drop on the nickel substrate are given below. Without oxygen lithium and nickel do not form a chemical compound [30]. Initial parameters [30–34]:

$$\theta_c(T) = 488.14 - 0.72\,T, \ \text{[deg]},$$

$$\sigma_{l\upsilon}(T) = 0.447 - 1.07 \cdot 10^{-4} T - 1.351 \cdot 10^{-8} T^2, \ \text{[N/m]},$$

$$n_s(T) = 92.252 - 3.345 \cdot 10^{-3} T - 7.413 \cdot 10^{-7} T^2, \ [\text{nm}^{-3}],$$

$$n_l(T) = 48.37 - 8.607 \cdot 10^{-3}\,T, \ [\text{nm}^{-3}],$$

where all formulas use the temperature expressed in Kelvin. The LJ potential parameters calculated in the electron gas approximation, in customary measurement units are equal to (for Fig. 1): $r_0 = 0.3213$ nm; $D = 0.1556$ eV. The presented mathematical model makes it possible to calculate the limit radius and the spreading rate of a droplet at a given temperature. For example, for a lithium sessile droplet on a nickel substrate at $R = 1$ nm, the values $T = 264.7$ K and $\upsilon = 1.8$ m/s are obtained. Numerical simulations show that the radius increases as far as the temperature rises. It is caused by simultaneous decrease of the contact angle of wetting and of the superficial tension. At the same time the spreading rate decreases, which is explained by increase of the drop volume. The obtained rate values are lower than the speed of sound (6000 m/s), this is why the assumption as to noncompressibility of liquid during spreading can be considered as reasonable.

It is reasonable to compare the small drop adhesion parameters with similar parameters for two massive samples with flat boundary of separation between them. By integration (11) for a semi-space we get specific work of adhesion and equilibrium state for two massive samples:

$$W_p = \frac{15}{8}\pi n_l n_s D z_p^4, \quad z_p = \frac{r_0}{\sqrt[6]{15}}. \tag{21}$$

At certain temperature, e.g. at $T = 264.7$ K, for lithium droplet at $R = 1$ nm and thick liquid film of lithium in contact with solid nickel substrate from (17) and (21) we get $W_d = 0.98\,\text{J/m}^2$ and $W_p = 1.02\,\text{J/m}^2$. Rough assessment by using the formula of Girifalco and Good [35] subject to reference data from [36] gives the value of specific work of adhesion of $W_p \sim 1.6\,\text{J/m}^2$. Therefore, we define that in the same conditions the specific work of adhesion of thick liquid film exceeds specific work of adhesion of droplet in-situ. Moreover, the dependences of thermodynamic characteristics on the temperature in case of a small drop are manifested heavier than in the case of thick liquid film. The reason of all of that is the system geometry playing a decisive role in the low-size region.

Conclusion

The studies of interphase phenomena occurring due to physical forces of interaction remain relevant. The study deals with analytical (without computer simulation by molecular dynamics and Monte Carlo methods) model of a small drop on partly wetted surface of a solid body, which enabled to study physical properties of the system. The model includes calculation ab initio of the parameters of paired LJ potential and calculation of potential energy based on it and the specific work of the drop adhesion. Numerical calculations were performed for the Li (drop)–Ni (substrate) system, which is interesting in terms of studying physical and chemical properties of electrodes of lithium-ion batteries. Wettability of electrodes by lithium in these batteries has paramount importance [37]. The results obtained in the study are consistent with [33].

According to the given calculations, it is natural that with a fixed value of the contact angle the equilibrium state between the drop and the substrate decreases as far as the drop volume rises. It is explained physically that in the transition from interaction between separate atoms to the interaction between 3D bodies the equilibrium state must decrease. E.g., with the Lennard-Jones potential the equilibrium state is r_0, $0.765r_0$ and $0.637r_0$ for the „atom–atom", „atom–plate" and „plate–plate" systems.

In case of incomplete surface wetting with decrease of size of the drop in-situ it specific adhesion work rises. It is caused by increase of contribution of dispersion gravity forces acting between the drop and the substrate. On the same basis the existence of a minimum drop size is predicted. If the drop in-situ is too small, then the excessive pressure caused by interatomic forces from the substrate side exceeds capillary pressure associated with the superficial tension (i.e. in fact, with the interaction of liquid atoms between each other), and the drop ceases to be stable. Such a phenomenon is observed in the machine experiments [24,27], but is not quantitatively described, nor the phenomenon physics is discussed at all in multiple publications. In our opinion, the drop spreading due to the loss of stability by it, in particular, due to decrease of superficial tension and action of superficial forces, could be associated with the first nature phase transition and to so called superspreading.

Clear advantage of the presented simulation procedure refers to its applicability not only to a small drop, but, without equations (9), (19) to a solid particle on the solid body surface too. For a drop in-situ with a low value of superficial tension it is required to consider the deviation from the spherical shape, as well as the dimensional dependence of the superficial tension, which leads to non-linear differential equations of Bashforth–Adams type [28,35,38–40]. Such problem is the subject of a separate study.

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Conflict of interest

The authors declare that they have no conflict of interest.

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