

# Energy Estimation of Wettability of a Charged Dielectric Surface by a Conductive Drop

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**Abstract**—This work estimates the energy of wetting of a dielectric substrate by a conducting drop charged by an external electric charge fixed on it. It was found that the wettability of such a surface decreases if the average density of the charge induced at the base of the droplet exceeds the threshold value.

**Keywords:** wettability, conductive liquid, electric charge, contact angle

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Wettability is of scientific and practical interest as an object of research. The problem of wetting control for various technical applications remains particularly relevant. In electrowetting on a dielectric, the electric field of the electrodes is used to increase its wettability by a liquid [1]. The opposite effect—a decrease in wettability—is observed when a conductive drop is placed on a precharged dielectric substrate [2]. In this work, the behavior of wettability under experimental conditions [2] is studied based on the energy approach.

We consider the equilibrium axisymmetric state of a conducting liquid droplet in a gas placed on a horizontal solid dielectric substrate, uniformly charged by an external electric charge with a known surface density  $\sigma_0$  fixed on its bounding plane (Fig. 1). In the electric field of this charge, physically homogeneous phases become polarized. Therefore, the induced and bound charges appear only at the boundaries separating them, which are approximated as infinitely thin surfaces. The distribution of the total (external, induced, and bound) charge on these surfaces based on the Greenberg approach [3] is determined by the system of integral equations

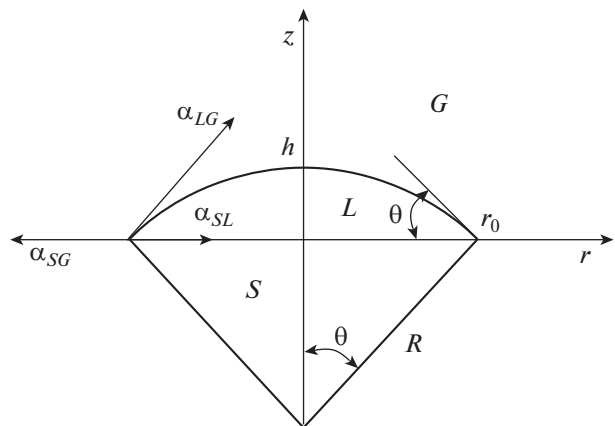
$$\begin{aligned} \sigma_{SL} &= 2\epsilon_0 E_{SL}(\sigma_{LG}), \\ \sigma_{SG} &= \frac{2}{\epsilon_G + \epsilon_S} \sigma_0 - 2\epsilon_0 \frac{\epsilon_S - \epsilon_G}{\epsilon_S + \epsilon_G} E_{SG}(\sigma_{LG}), \\ \sigma_{LG} &= 2\epsilon_0 [E_{LG}(\sigma_{LG}) + E_{LG}(\sigma_{SL}) + E_{LG}(\sigma_{SG})], \end{aligned} \quad (1)$$

where  $\sigma$  is the surface charge density,  $\epsilon$  is the dielectric constant,  $E$  is the projection onto the normal (outer to the droplet surface and opposite to the unit vector of the  $z$  axis at the  $SG$  boundary) to the element of the contact surface of the electric field vector generated by all charges located outside this element, and  $\epsilon_0$  is vac-

uum permittivity. Here and below, the single subscript denotes that the quantity belongs to the phase, while the double subscript denotes that it belongs to the interphase boundary (Fig. 1).

The stationary stable state of the considered system occurs at the minimum of its energy  $W$ . The drop is assumed to be small enough that the effect of gravity on its shape can be discarded in comparison with the effect of surface tension.  $W$  is, then, the sum of surface  $W_s$  and electrical  $W_e$  energies:

$$\begin{aligned} W_s &= \alpha_{LG} A_{LG} + \alpha_{SL} A_{SL} + \alpha_{SG} A_{SG}, \\ W_s &= \alpha_{LG} A_{LG} + \alpha_{SL} A_{SL} + \alpha_{SG} A_{SG}, \\ W_e &= 0.5 \phi_L q_L + 0.5 \int \phi_{SG} \sigma_{SG} dA. \end{aligned} \quad (2)$$



**Fig. 1.** Geometry of a three-phase system.  $S$ , solid;  $L$ , liquid;  $G$ , gas.

Here,  $\alpha$  is the surface tension coefficient at the contact interface with area  $A$  and  $\phi$  is the scalar potential at the location of the  $\sigma dA$  charge.

Using the formulas  $\sigma_{LG} = \sigma^i_{LG}/\epsilon_G$ ,  $\sigma_{SL} = (\sigma_0 + \sigma^i_{SL})/\epsilon_S$  (where  $\sigma^i$  is the density of the induced charge of the conductor at the boundary with the dielectric and  $\int \sigma^i_{LG} dA + \int \sigma^i_{SL} dA = 0$ ), total charge  $q_L = \int \sigma_{LG} dA + \int \sigma_{SL} dA$  on the droplet surface can be reduced to

$$q_L = [1/\epsilon_S + (1/\epsilon_G - 1/\epsilon_S)\gamma]\sigma_0 A_{SL}. \quad (3)$$

Here,  $\gamma = -\int \sigma^i_{SL} dA / \sigma_0 A_{SL}$  is the ratio of the average density of the charge induced at the base  $SL$  to density  $\sigma_0$ , taking into account the opposite signs of these charges.

The problem of finding the shape of a drop that provides a minimum  $W$  taking into account (1)–(3) for given volume of liquid  $V$  can be solved only by detailed numerical calculation due to the peculiarities of the charge density and electric field on the three-phase interface. Therefore, to estimate the wettability, the problem is simplified. The meniscus of a small drop is assumed to be spherical.

At  $V = 2\pi R_0^3/3$  ( $R_0$  is the radius of a hemisphere with volume  $V$ ) the spherical segment is given by contact angle  $\theta$  (Fig. 1) in the known geometric formulas for radii of curvature  $R = R_0 f(\theta)$ , base  $r_0 = R \sin \theta$ , height  $h = R(1 - \cos \theta)$ , and areas  $A_{LG} = 2\pi R h$ ,  $A_{SL} = \pi r_0^2$ , where  $f(\theta) = [2/(2 - 3\cos \theta + \cos^3 \theta)]^{1/3}$ . On an uncharged substrate ( $\sigma_0 = 0$ ) minimizing  $W_s$  gives Young's formula [4]:  $\alpha_{SG} = \alpha_{SL} + \alpha_{LG} \cos \theta_Y$ . The dimensionless variable part of energy  $W_s$  with the scale  $2\pi R_0^2 \alpha_{LG}$  from the first expression (2) can be written as follows:

$$W'_s = (1 - \cos \theta - 0.5 \sin^2 \theta \cos \theta_Y) f^2(\theta). \quad (4)$$

Conductor potential  $\phi_L$  is found by the average potential method [5], the results of which agree with the experimental data with an accuracy acceptable for evaluating integral values. First, the potential from charges at all interfaces is calculated at each point of the droplet surface. For this, it is assumed that the distribution of the induced charge is uniform both on boundary  $LG$  and on boundary  $SL$ . Since the average density of the induced charge at the base of the droplet is  $-\gamma\sigma_0$ , we obtain  $\sigma_{SL} = (1 - \gamma)\sigma_0/\epsilon_S$ . For the total charge on the meniscus, we obtain  $\sigma_{LG} = (\gamma\sigma_0/\epsilon_G)\cos^2(\theta/2)$ . Density  $\sigma_{SG}$  is calculated by the corresponding formula (1). The calculated potential is then averaged over the droplet surface, and this mean surface potential is taken as  $\phi_L$ . Such a calculation does not allow an analytical result. Therefore,  $\phi_L$  is found numerically. The generatrix of the drop shape is composed of an arc of a circle of radius  $R$ , which is cut out by central angle  $\theta$ ,

and radius  $r_0$  of the drop base (Fig. 1). The arc is split into  $N$  equal parts. When the arc is rotated around the axis of symmetry, it forms charged coaxial circular bands, the potential of each of which is identified with the known field of the ring charge  $\Delta q_{LG} = \sigma_{LG} 2\pi r_n R \theta / N$  passing through the center of the band with coordinates  $(r_n, z_n)$ :  $r_n = R \sin \theta_n$ ,  $z_n = R(\cos \theta_n - \cos \theta)$ ,  $\theta_n = \theta(n - 0.5)/N$ ,  $1 \leq n \leq N$ . The surface charge at the base of the droplet is approximated by a system of ring charges  $\Delta q_{SL} = \sigma_{SL} 2\pi r_n R [\sin(\theta n/N) - \sin(\theta(n - 1)/N)]$ . Likewise, at the  $SG$  border,  $\Delta q_{SG} = \sigma_{SG} 2\pi r_m + 0.5(r_{m+1} - r_m)$ ,  $r_m = r_0 + (5R_0 - r_0)m/M$ ,  $0 \leq m \leq M$ . Therefore, at an arbitrary point  $(r, z)$ , the potential has the form

$$2\pi^2 \epsilon_0 \phi(r, z) = \sum_{n=1}^N \left[ \frac{\Delta q_{LG}}{R_{1n}} K \left( \frac{2\sqrt{rr_n}}{R_{1n}} \right) + \frac{\Delta q_{SL}}{R_{2n}} K \left( \frac{2\sqrt{rr_n}}{R_{2n}} \right) \right] + \sum_{m=1}^M \frac{\Delta q_{SG}}{R_{2m}} K \left( \frac{2\sqrt{rr_m}}{R_{2m}} \right), \quad (5)$$

where

$$R_{1n} = \sqrt{(r + r_n)^2 + (z - z_n)^2}, \quad R_{2n} = \sqrt{(r + r_n)^2 + z^2},$$

and  $K$  is a complete elliptic integral of the first kind.

For averaging over the droplet surface, bypassing singularity  $K(1) = \infty$ , using formula (5), we find  $\phi$  at points with coordinates  $r_l = R \sin \theta_l$ ;  $z_l = R(\cos \theta_l - \cos \theta)$  (for the points of base  $z_l = 0$ ), where  $\theta_l = \theta l/N$ ,  $0 \leq l \leq N$ , and the integrals for the mean potential  $\phi_L = (\int \phi_{LG} dA + \int \phi_{SL} dA) / (A_{LG} + A_{SL})$  of the drop and the second term of energy  $W_e$  (2) calculated by the trapezoidal rule.

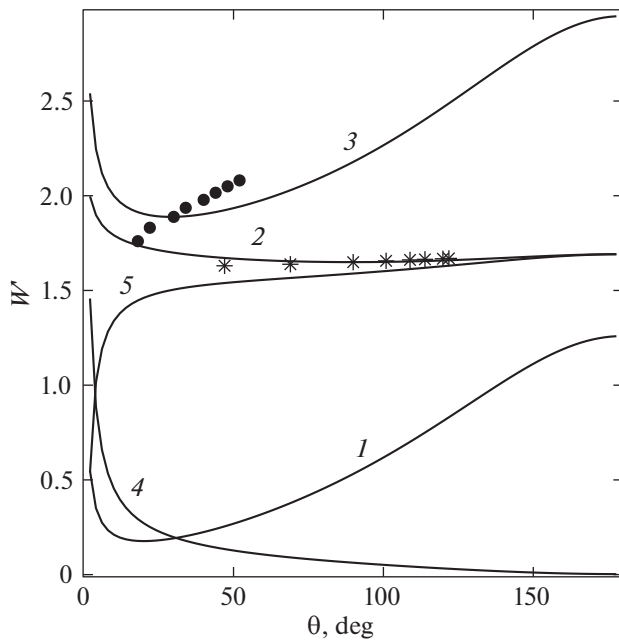
Electric energy  $W_e$ , which is dimensionless with the same scale as (4), is written in the form

$$W'_e = 0.5\beta(\phi'_L q'_L + \int \phi'_{SG} \sigma'_{SG} dA'), \quad (6)$$

where  $\beta = \sigma_0^2 R_0 / 4\epsilon_0 \alpha_{LG}$  is the ratio of characteristic values of electric energy (with scales  $\sigma_0 R_0 / 2\epsilon_0$  for the potential and  $\sigma_0 \pi R_0^2$  for the charge) and surface energy.

The calculation is carried out at fixed values of  $\epsilon_G = 1$ ,  $\epsilon_S = 4$ ,  $\theta_Y = 20^\circ$ , close to the experimental data [2] for a water drop on an amorphous silicon dioxide film, and parameters  $\gamma$  and  $\beta$  are varied. Note that the expression for parameter  $\gamma$  of the model can be found for a hemispherical drop. Since the electric field at the base of a uniformly charged hemisphere is uniform and equal to  $\sigma_{LG} / 4\epsilon_0$ , it follows from (1) that  $\sigma_{SL} = \sigma_{LG} / 2$ , which gives  $\gamma = 1 / (1 + 0.25\epsilon_S / \epsilon_G)$ .

For a fixed value of  $\beta = 0.1$ , there is threshold value  $\gamma \approx 0.35$ , below which the energy minimum point practically coincides with the given Young angle (Fig. 2). When the threshold value is exceeded, contact angle  $\theta$  increases (circles in Fig. 2) and, for  $\gamma \rightarrow 1$ , reaches  $52^\circ$ .



**Fig. 2.** Dependences of (1) energy  $W_s'$ , (2) total energy  $W_e'$ , and (4, 5) its terms in formula (6), as well as (3)  $W_s' + W_e'$ , on the contact angle at  $\beta = 0.1$ ,  $\gamma = 0.5$ . Asterisks indicate the minima of  $W_e'$  at  $\gamma = 0.36, 0.4$ , and further to 1 with a step of 0.1; circles indicate the minima of  $W_s' + W_e'$  at  $\gamma$  from 0.3 to 1 with a step of 0.1.

The threshold value of  $\gamma$  separates monotonic and nonmonotonic dependences  $W_e'(\theta)$ , the minima of which (asterisks in Fig. 2) depend only on  $\gamma$ . The minima themselves are due to the opposite nature of the change in terms  $W_e'$  in (6) (lines 4 and 5 in Fig. 2). At fixed  $\gamma$ , with increasing  $\beta$ , as the contribution of  $W_s'$  to the system energy profile decreases, contact angle  $\theta$  increases monotonously and, at  $W_e' \gg W_s'$ , reaches saturation at points of minimum  $W_e'$ , that do not depend on  $\theta_\gamma$ . In Fig. 2 this corresponds to moving any of the circles to the corresponding asterisk at  $\beta \rightarrow \infty$ .

The physical explanation of the calculated increase in the contact angle follows from the equivalence of the effect of the electric charge at the interface and a decrease in the surface tension. In electrowetting, the charge is predominantly located at the  $SL$  boundary, which leads to a decrease in  $\alpha_{SL}$  and an increase in wettability. In the considered case, there is a charge at all interphase boundaries. Near the three-phase interface, where  $E_{SG}(\sigma_{LG}) \approx E_{SL}(\sigma_{LG})$ , it follows from (1) that

$$\sigma_{SG}/\sigma_{SL} = [(1 + \gamma)/(1 - \gamma) + \epsilon_G/\epsilon_S]/(1 + \epsilon_G/\epsilon_S) > 1.$$

Therefore,  $\alpha_{SG}$  decreases more than  $\alpha_{SL}$ . As a result, the tension balance is fulfilled on a smaller wetting perimeter with a larger contact angle, regardless of the changing  $\alpha_{LG}$  at  $\theta \leq 90^\circ$ . This behavior of wettability of a charged dielectric substrate by a conducting drop is in qualitative agreement with what was experimentally observed in [2].

#### CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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