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Surface Energy and Production Micro-and Nanowire

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ABSTRACT

The theory of surface phenomena in the production of micro- and nanocylinder for important cases is considered. Analytical solution to Gibbs–Tolman–Koenig–Buff equation for micro- and nanowire surface is given. Analytical solutions to equations for case the cylindrical surface for the linear and nonlinear Van der Waals theory are analyzed. But for a nonlinear theory, this correspondence is absent.

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Introduction

The cast glass-coated micro- and nanowires (GCAMNW) were first introduced in 1924 by Taylor [1]. They consist of an inner metallic nucleus (core, kernel) covered by a Pyrex-like coating (shell). The GCAMNWs are manufactured by means of a modified Taylor-Ulitovsky process [1]. The preparation of microwires and studies of the magnetic properties were reported in many publications by various research groups.

In this article the surface tension in nanowires production by the Taylor–Ulitovsky method are studied. Surface tension is a fundamental thermodynamic parameter that significantly influences the creation of nanowires.

The chemical and physical properties of interphase boundaries in nanowires, as well as for nanoparticles, have been studied in a huge number of publications (fundamental monographs and literature, and also my researches. We can single out the following theoretical approaches: Gibbs-Tolman-Koenig-Buff equation method end the linear and nonlinear Van der Waals theory [1-28].

The study aims at derivation and detailed analysis of expressions for the surface tension for the microwire in thermodynamic equilibrium on the Gibbs-Tolman-Koenig-Buff equation method and on the Van der Waals theory.

The given theory can find application in microwire production technology.

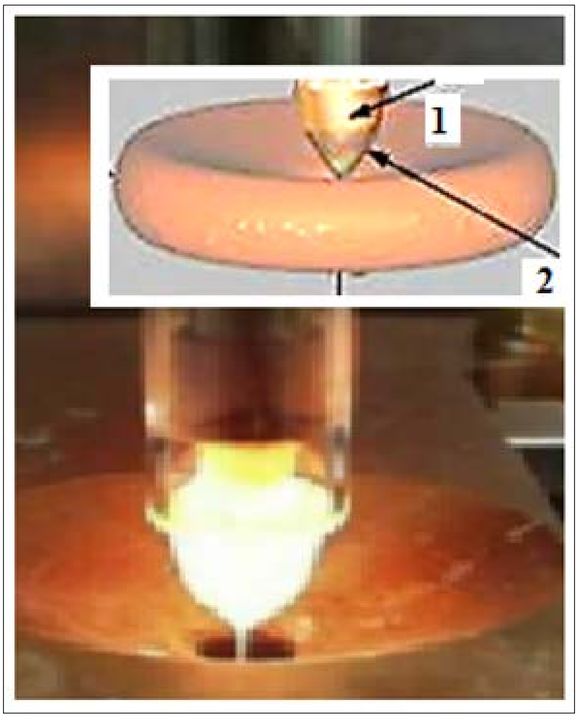

Figure 1: Process of casting glass-coated amorphous magnetic micro-and nanowires.
1. Cylindrical zone 2. Cone zone.

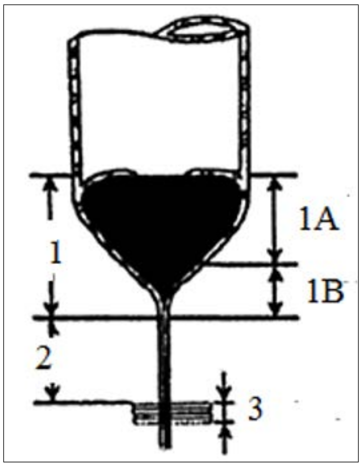

Figure 2: Drawing of micro- and nanowire fabrication process by the Taylor–Ulitovsky method.
1. Microbath: 1A). Primary cone of microbath. 1B). Secondary cone of microbath. 2. Extension zone. 3. Crystallizer

As you can see from the figures, we must study cylindrical and conical surfaces.

Modeling of Surface Energy for Microwires in Gibbs-Tolman-Konig-Buff`s Theory

We will use the Gibbs-Tolman-Koenig-Buff differential equation [2-6] (for a cylinder) to describe the surface tensions, σ_i, of nanowires [1]:

$$\frac{d\ln\sigma_i}{d\ln R_i} = \frac{\frac{2\delta_i}{R_i} + \left(\frac{\delta_i}{R_i}\right)^2}{2 + \frac{2\delta_i}{R_i} + \left(\frac{\delta_i}{R_i}\right)^2}, \qquad (1)$$

Where R_i are the radii of micro- and nanowires (the radius of its metallic kernel, R_m, or the total radius of glass, R_g).

Non-negative parameters Tolman length, δ_i, is characterizing the thickness of the interfacial layer (for example, between glass and glass-metal).

In surface thermodynamics the Tolman length is used as a parameter which is equal to the distance between the surface of tension and equimolar surface. The numerical values of parameter the analog
"Tolman length" for micro and nanowire are in the range from 0.1 to 1 µm.

The integral in (1) (if δ_i =const.) can be exactly taken. The final result has the form [7, 10]:

$$\sigma/\sigma^{(\infty)} = \frac{R}{\delta}\sqrt{\frac{2}{2(R/\delta)^2 + 2R/\delta + 1}}\exp\left(-\mathrm{arctg}\left(\frac{1}{1+2R/\delta}\right)\right). \qquad (2)$$

The well-known Tolman formula (for cylinder) is in special case *R>>δ* for this formula (2)

$$\sigma/\sigma^{(\infty)} \sim \frac{1}{1+\frac{\delta}{R}} \cdot \sigma \qquad (3a)$$

In case *R>>δ*: $\sigma/\sigma^{(\infty)} \sim 0.645(R/\delta)$. (3b)

We represent the Rusanov linear formula [5, 11] for the cylindrical surface.

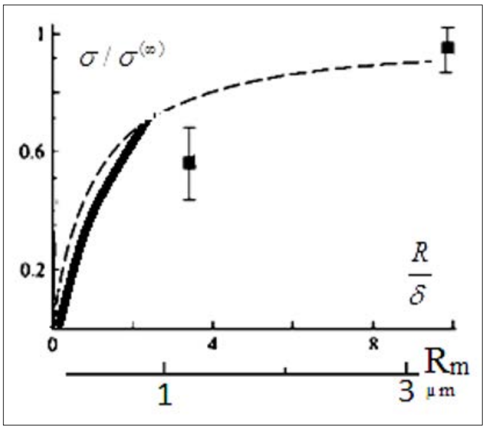

Figure 3: Functions graphs of solutions (3) (dashed line), and of solutions (10 -14) (bold line) are presented. Experimental data for the surface tension of metal-glass are presented depending on the radius of the metallic kernel, Rm.

Modeling of Surface Energy for Micro-and Nanowires in Linear Van Der Waals Theory

The basic equation of the linear Van der Waals theory of an inhomogeneous medium (see [1-3] for details) can be written in the form:

$$n'' + \frac{n'}{r} - \frac{1}{\delta^2}(n - n_{1,2}) = 0, \qquad (4)$$

Where n (x) is the function when proportional to the volume density N(x) ($x = r/\delta$, n_o=const.), or is the radial variable measured from the center of a nanoparticle, is the Tolman length [1-3].

The general solution to Eq. (4) has the form

$$n(r) = n_{1,2} + A\,I_0(r/\delta) + B\,K_0(r/\delta), \qquad (5)$$

Where $I_0(r/\delta), K_0(r/\delta)$ are modification Bessel and

Hankel functions.

$$n(0) = n(R) = n_1, \quad n(+\infty) = n_2. \qquad (6)$$

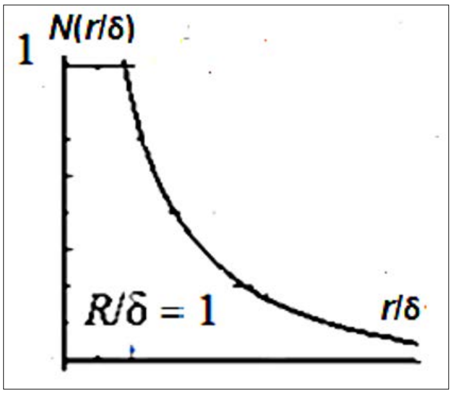

Figure 4: Function graph of volume density function, N(r/δ) is presented

We will accept for the volume density function, N(r/δ). We get:

$$N(r/\delta) \to n(0) \equiv n(R) = 1,\ N(+\infty) \to n(+\infty) = 0. \quad (7)$$

Substituting solution (5) into expression (7) and integrating, we obtain:

$$N(r/\delta) = \begin{cases} 1, & r \le R, \\ \dfrac{K_0(r/\delta)}{K_0(R/\delta)}, & r > R, \end{cases} \quad (8)$$

Solution (8) can be used for calculating adsorption, which is defined as the excess number of atoms or molecules in the surface layer of the nanoparticle per unit area:

$$\Gamma \to \delta \frac{K_1(x)}{K_0(x_0)}, \quad (9)$$

$(x = r/\delta,\ x_0 = R/\delta)$.

Taking into account adsorption (9), we obtain the differential equation

$$\frac{d\ln\sigma}{d\ln x} = \frac{1}{x\{K_0(x)/K_1(x_0)\}+1}. \quad (10)$$

If $x >> 1$

$$\frac{K_0(x)}{K_1(x_0)} \to 1 \quad (11)$$

We obtain

$$\frac{d\ln\sigma}{d\ln x} = \frac{1}{x+1} \quad (12)$$

(See formula (2) and (3a));

And if $x << 1$

$$\frac{K_0(x)}{K_1(x)} \approx x\ln\frac{2}{\gamma x}. \quad (13)$$

Where $\gamma = 1{,}781$ is Euler constant, we obtain

$$\frac{d\ln\sigma}{d\ln x} = \frac{1}{x\ln\dfrac{2}{\gamma x}+1}. \quad (14)$$

This equation is integrated numerically.

Modeling of Surface Energy for Micro-and Nanowires in Nonlinear Theory

The nonlinear equation can be written in the form

$$n_1'' + \frac{1}{r}n_1' + \frac{1}{\delta_1^2}\exp\{-n_1\} = 0, \quad (15)$$

The simple volume density function, N, may be determined:

$$N_1 = 1 + 2\ln[1 - X_1^2] \quad (16)$$

$$X_1 = r/(2\sqrt{2}\delta_1) \quad (17)$$

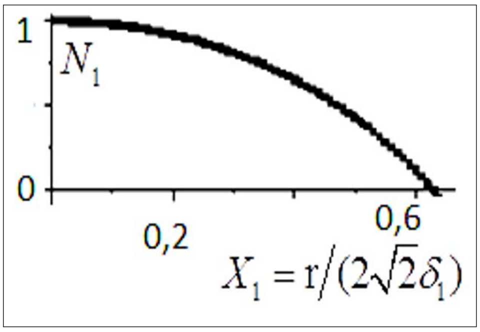

Figure 5: Function graph of solution (16) is presented

The results obtained have a physical meaning only as long as the function N_1 is positive.

The resulting density profile (see Figure 5 and (16), (17)) is very different from the results of the linear theory (see Figure 4 and (8)), and therefore the GTKB theory (see (2), (3a), (3b)).

The density profiles in [13] (see Figure 6) are very different too from the results of the Fig. 5.

Micro and nanowire will only be produced for a limited its metallic kernel, R_m.

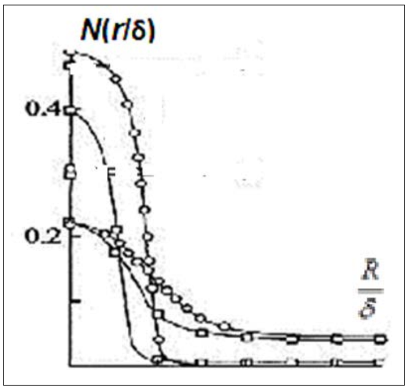

Figure 6a: Qualitative density profiles of volume density function, N(r/δ) are presented in [13]

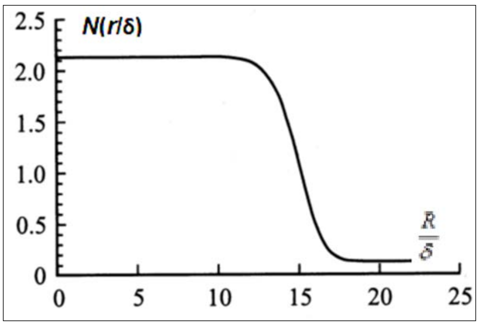

Figure 6b: Typical density profile of volume density function, N(r/δ) is presented in [13-20].

Modeling of Surface Energy for Micro-and Nanowires in the Pure Case Theory

The equation can be written (in the pure case theory) in the form:

$$n_2'' + \frac{1}{r} n_2' = 0 \quad (18)$$

A particular solution for equation (18) can have the form:

$$n_2 = c \ln(R/\delta) \quad (19)$$

We will accept the initial values

$$N_{2,0} = 1 \quad (20)$$

And get

$$N_2 = 1 + \ln(R/\delta) \quad (20a)$$

Function graph N2 is shown in Figure 7.

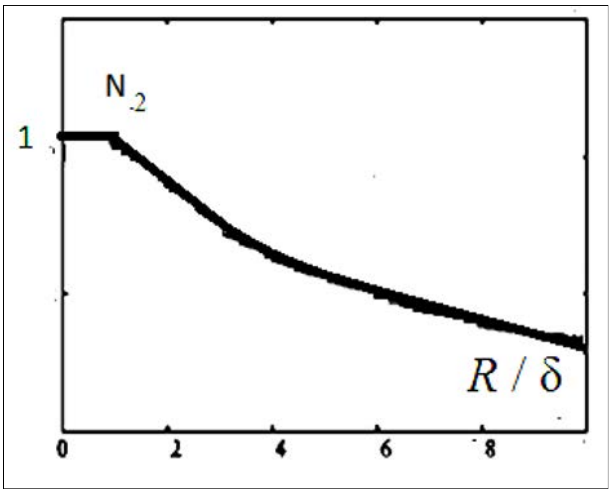

Figure 7: Function graph of solution (20-20a) is presented

Conclusion

A feature of micro- and nanowires is that these objects consist of an amorphous alloy core (metal conductor) with a diameter of (0.1...50) µm, covered with a Pyrex-like coating with a thickness of (0.5...20) µm. Therefore, the main technological parameters for the production of glass micro- and nanowires is the surface tension of the surfaces of micro- and nanowires.

According to the previous analysis, the most significant effect on the geometry of such microwire comes from the glass properties. The microwire radius Rg (the outer radius of the glass shell) is estimated as follows [1]:

$$R_g \sim \frac{\eta^{2-k}}{V_d^k \sigma_s^{1-k}} \quad (21)$$

Where k is the parameter, which is dependent on a casting rate (0 < k < 1); V_d is the casting rate; σ_s is the surface tension.

The metallic Radius, Rm , is possible to estimate approximately:

$$R_m \sim \frac{\sigma_{sm}}{V_d^{2-k_m}} \quad (22)$$

σ_{sm} is the surface tension of metal – glass ($0 < k_m < 1$).

We thus confirm that surface tension, defined as excess free energy per unit surface area, determines the radius of micro- and nanowires.

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