THEORY OF NUCLEATION

S.A. Baranov

CCPF TM "TEHMED", 3/3 Academy str., MD-2028, Chisinau, Republic of Moldova
E-mail: tatiaserg@araxinfo.com

Abstract

The analogy of problem of micromagnetism and nucleation of particles is considered. The anisotropy influence for processes in the nucleation problem is investigated.

1. The goal of the present work is to find function of free energy at the description nucleation of a cylindrical particle. The analogical problems were considered in [1-3]. We will pay attention to analogy of problem in the processes of magnetization and nucleation.

The statistical sum may be determined by a local minimum of energy (see [1]). We used the variation principle of a minimum of exchange energy:

$$\delta\int E(r)dv=0, \tag{1}$$

where the integration is spread for all volume, and E(r) can be written as [1-4]:

$$E(r) = (A/2)\,[(\theta')^2 + (\sin\theta)^2/r^2], \tag{2}$$

where $0 < \theta(r) < \pi/2$ is the angle with the cylinder axis and the "magnetization" vector (classical analog spin vector), A is the "exchange" constant in the continuum Heisenberg theory, r is the radial cylindrical coordinate. Minimization of function (2) gives results as the nonlinear equation, which in more complex type is used for problems of micromagnetism (see [1 - 4]):

$$\theta''(\rho) + \theta'(\rho)/\rho - 1/\rho^2 \sin\theta\cos\theta = 0, \tag{3}$$

where $\rho = r / rc$ is the relative radial coordinate cylinder: $0< \rho< 1$, and rc is the limit of "single domain" radius, and

$$\theta(\rho) = \pi, \text{ when } \rho = 0. \tag{4}$$

$$\theta(\rho) = \pi/2, \text{ when } \rho = 1. \tag{5}$$

Exact solution of (3) can be written as [3,4]:

$$\mathrm{tg}(\theta/2) = 1/\rho. \tag{6}$$

The similar solution is presented as two-dimensional soliton and is an example of the exact analytical solution of a nonlinear problem [3]. The model corresponds to the physical problem of distribution of magnetization in thin amorphous nanowire with zero magnetostriction.

2. By analogy with the problem considered in [4], we use the equation:

$$(\theta a)'' + (\theta a)'/\rho - a^2/\rho^2 \sin(\theta a)\cos(\theta a) = 0, \tag{7}$$

where a^2 is the ratio between the anisotropy energy and the "exchange" constant A.

The exact solution can be written as [3,4]:

$$\mathrm{tg}(\theta a / 2) = 1/\rho^a. \tag{8}$$

The energy formula is:

$$E(\rho) = T + W, \tag{9}$$

where T is determined in (2), and W is determined as:

$$W = A(a^2-1)\sin^2\theta / 2\rho^2. \tag{10}$$

We use solution (8) in equation (9), and we find:

$$T + W = 2Aa^2(\rho)^{2a}/[\rho^2(1+\rho^{2a})^2]. \tag{11}$$

Let's analyze solution (11). In this specific case of absence of anisotropy (when $a^2=1$) energy of the cylinder surface (at $\rho^2=1$) goes to *A*. In the case when $a^2>1$, the energy on the cylinder surface goes to A a^2. It is possible to consider the given parameter A a^2 as the value of the surface energy.

The energy inside a particle goes to not zero value if $a^2=1$. On the other hand the energy is equal to zero if $a^2>1$. Characteristic gap of free energy can correspond to phase transition, when in system there is infinitesimal anisotropy. Such phase transition can give the result in jump of change of the magnetization distribution. The similar phase transitions are known. Here simple analytic solutions were obtained. The energy T of particles, in a case $a^2=1.$, is equal to *A*.

With decrease of particle sizes the role of a thermodynamic condition on the surface is increasing. The given elementary model showed that in this case it becomes difficult to separate thermodynamic functions on the volumetric thermodynamic functions and the surface thermodynamic functions. It is possible to do if is large parameter $a^2 >10$.

3. We will consider electrochemical nucleation. In this case anisotropy can be initiated by distribution of the electrical field in a cathodic area. If particles become comparable with the sizes of the cathodic area the electrical field will be able to become a cause of anisotropy. It will allow changing of superficial energy according to the Lippman equation:

$$- d\sigma = q d\varphi, \tag{12}$$

where *q* and *φ* is the charge and the potential on the surface .
If it is possible to enter a concept of capacity C for change of superficial energy σ will receive:

$$\sigma = C (\varphi)^2 /2 \quad , \tag{13}$$

The given change of superficial energy can initiate the anisotropy. If the particle is small we can obtain:

$$\varphi \sim 1/\rho, \tag{14}$$

That is possible to obtain the mathematical model used in (7).

Generally the results of consideration have qualitative character.

This work was supported by received Program RFFI–Moldova, grant No 06.11CRF.

References

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