Juniper Online Journal Material Science
ISSN: 2575-856X

Juniper Publishers
key to the Researchers

Mini Review
Volume 2 Issue 3- July 2017
DOI: 10.19080/JOJMS.2017.02.555587

JOJ Material Sci

Isolation the Influence of the Size Factor on the Eutectic Temperature and the Concentration of Binary Composites

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Submission: July 01, 2017; **Published:** July 20, 2017

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Abstract

From the first principles, universal relationships have been obtained that relate the eutectic temperature and concentration to the thickness of the composite in the form of a nanoplate. Reducing the size of the nanocomposite leads to an increase in the proportion of the strengthening phase and a decrease in the eutectic melting temperature.

Introduction

When passing from bulk crystals to nanocrystals, first of all, it is necessary to estimate the fraction of the energy of the external surface of the nanocrystal in comparison with the bulk one. The presence of an external surface leads to an increase in the total energy of the electron-ion system of the crystals. In the case of nanoparticles in the form of nanoplates (in the presence of close-packed atomic planes in the crystal structure), we assume that the outer surfaces of nanoparticles have half of the energy of interaction with the missing atomic plane [1,2]. The influence of the size factor on the interaction energy of atomic planes is taken into account using the method [2].

In the case of LaB_6 and MeB_2 nanocrystals, the energy of the outer surface can be determined from the value of the total energy of the electron-ion system of the unit cell. We distribute the total energy of the electron-ion system per one unit cell uniformly along the faces. Then for the energy density over the outer surface of the cell:

$$\rho_A = U^0_{AA}/(6\cdot a_0^2)\ ;\ \rho_B = U^0_{BB}/(4\cdot a\cdot c.+2a^2\cdot\sqrt{3}).$$

Here U^0_{AA} ; U^0_{BB} are the energies of the electron-ion system of one cell LaB_6 and MeB_2, a_0, a and c are the lattice parameters. The external surface energy pertaining to the basal planes for LaB_6 and MeB_2 will be

$$\Phi_A = -.5a_0^2\ \cdot\rho_A\ ;\ \Phi_B = -.5a^2\sqrt{3}\cdot\rho_B$$

To estimate the energy of the nanocrystal (LaB_6, MeB_2), the averaging procedure [2] is used for crystals having close-packed atomic planes, only with the difference that the energy is averaged over two neighboring cells, rather than by atomic planes. As a result, the energy of a unit cell is obtained depending on the distance to the external surface (implicit in the cell number). To calculate the concentration and temperature at the eutectic point of LaB_6-MeB_2 composites with limited dimensions, it is necessary to estimate the energy of the interfacial interaction taking into account the presence of the external surface. For this purpose, we construct a virtual cell along the interface of two components [3], which has a volume -- $\Omega_{AB} = C_E\,\Omega_A + (1-C_E)\Omega_B$ where C_E is the eutectic concentration for bulk materials, and Ω_A, Ω_B the volumes of elementary cells of the components, respectively.

The final formulas for the interaction energy of representative elements with allowance for the size factor are presented in the form:

$$\overline{U}_{AA} = U^0_{AA}(1-K_{AA}\cdot d^{-1});\ \overline{U}_{BB} = U^0_{BB}(1-K_{BB}\cdot d^{-1});\ \overline{U}_{AB} = U^0_{AB}(1-K_{AB}\cdot d^{-1}),\quad (1)$$

With coefficients K_{AA} =a0/12; K_{BB} =0,162c; K_{AB} =0,072A, Where (CE is the eutectic concentration of the A component)

$$A = \left|0{,}5\,(a^3C_E + (1-C_E)a^2c\sqrt{3})\right|^{1/3}.$$

The method for calculating the eutectic concentration and temperature for nanocomposites is the same as for bulk materials [4], but only with new values of the interaction energy between representative elements (1). In relation (1), the increase in the mean square displacement of atoms at small dimensions and the decrease in the Debye temperature are taken into account implicitly. In Fig. are presented the dependences of the eutectic concentration and temperature on the thickness (0.5≤d≤35nm) of the composite for the LaB_6-TiB_2, SiC-B_4C, Au-Ge systems Figure 1.

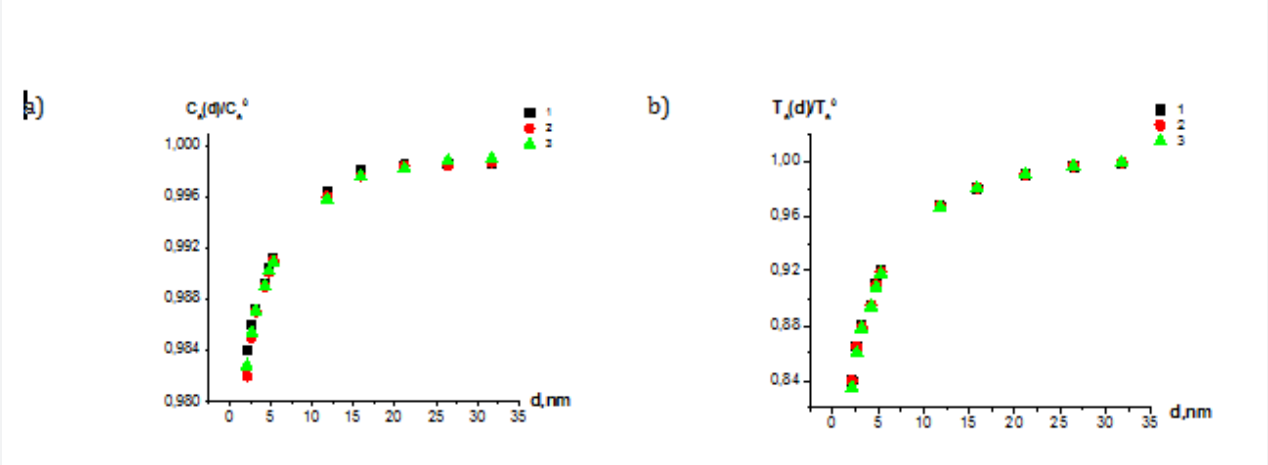

Figure 1: Dependence of eutectic 1(a) concentration and 1(b) temperature on plate thickness for 1) LaB_6-TiB_2; 2) SiC-B_4C; 3) Au-Ge. SSSSS

Based on the results of calculations with the help of an approximating function, the relations describing the relationship between the concentration and temperature of the eutectic with the plate size of two-component composites are derived:

$$C_E(d)/C_E^0 = 1 - 0{,}05\exp(-0{,}01d/r_B)\ ; \quad (2)$$

$$T_E(d)/T_E^0) = 1 - 0{,}26\exp(-0{,}01d/r_B). \quad (3)$$

Here, r_B = 0.0529nm (Bohr radius),$C_E(d)$, $T_E(d)$ is the eutectic concentration and temperature for a composite with thickness d, and a C_E^0 ,T_E^0 is the corresponding values for bulk composites. Relations (2, 3) allow us to estimate the eutectic temperature and concentration with allowance for the size factor. At d=4nm, the melting temperature of the Au-Ge system of the eutectic composition isTE(d)≈306 C0, which agrees well with experiment [5].

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DOI: 10.19080/JOJMS.2017.02.555587

How to cite this article: Dora Z.Isolation the Influence of the Size Factor on the Eutectic Temperature and the Concentration of Binary Composites. from the Gut of Estuarine Fish *Etroplus suratensis*. JOJ Material Sci. 2017; 2(3): 555587. DOI: 10.19080/JOJMS.2017.02.555587