Pis'ma v ZhETF, vol. 88, iss. 4, pp. 297 – 298 © 2008 August 25

High-temperature solid/melt nanocomposites

*V. V. Belousov*1)

A.A. Baikov Institute of Metallurgy and Materials RAS, 119991 Moscow, Russia,

Submitted 27 June 2008

The interfacial energy of nanomaterials can be decreased by grain boundary wetting. Most effective is grain boundary wetting by chemically compatible melt in the two-phase area of the phase diagram where the solid and melt are in equilibrium. The possibility of the thermodynamically stable solid/melt nanocomposite existence in the two-phase area of the phase diagrams where the solid and melt are in equilibrium, is shown.

PACS: 78.67.–n, 81.07.Bc

Nanomaterials [1] have a high interfacial energy and, therefore, they are thermodynamically unstable and experience recrystallization problem at 0.2–0.3$\,T_m$ (T_m is the melting temperature). The interfacial energy can be decreased sufficiently by grain boundary (GB) wetting. Most effective is GB wetting by chemically compatible melt in the two-phase area of the phase diagram where the solid and melt are in equilibrium [2]. In this case, the solid/melt interfacial energy can be decreased largely ($\sim 1{-}80\,\mathrm{mJ/m^2}$) [3 – 4].

Here we show the possibility of the thermodynamically stable solid/melt nanocomposite existence in the two-phase area of the phase diagrams where the solid and melt are in equilibrium. The calculated, within framework of a low-angle GB wetting model [5], values of the solid/melt interfacial energies are typical for liophilic colloids [3]. This opens the way to the design of the thermodynamically stable high-temperature nanomaterials.

GB wetting by chemically compatible melt in the two-phase area of the phase diagrams has been established for both ceramic and metallic materials [6, 7]. Thermodynamic condition of the GB wetting can be written as [8]:

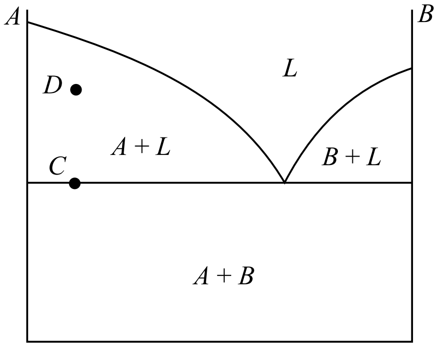
$$\gamma_{gb} \geq 2\gamma_{sl}, \tag{1}$$

where γ_{gb} and γ_{sl} are the specific free energies at the grain boundary and solid/melt interface, respectively. The γ_{gb} depends on the misorientation angle, θ. Low- and high-angle GBs are distinguished by the θ. Low-angle GBs refer to low-energy; high-angle to high-energy (with the exception of the so-called special GBs). As GBs have a wide spectrum of energies, the temperature of GB wetting will differ: the lower γ_{gb}, the higher temperature. Because size of the blocks (subgrains) in solids is 10-100 nm, let us consider the thermodynamic opportunity of low-angle GB wetting. Read and Shockley [9] have proposed a formula for γ_{gb} calculation as a function of the θ:

$$\gamma_{gb} = \frac{Ga}{4\pi(1-\sigma)}\theta(\beta - \ln\theta), \tag{2}$$

where G is the rigidity modulus, a is the lattice constant, σ is the Poisson‘s ratio, and β is approximately 0.25. According to the equation (2), the γ_{gb} increases with increasing θ and reaches a maximum, $\gamma_{gb\,(\max)}$. If the θ corresponding to the $\gamma_{gb\,(\max)}$ marks as $\theta_{\max}$, than the eq. (2) can be transformed to [10]:

$$\frac{\gamma_{gb}}{\gamma_{gb\,(\max)}} = \frac{\theta}{\theta_{\max}}\left(1 - \ln\frac{\theta}{\theta_{\max}}\right) \tag{3}$$



Phase diagram

Estimation shows that the γ_{gb} values for low-angle GBs, $10'' \leq \theta \leq 1^\circ$, is varied from $1\,\mathrm{mJ/m^2}$ to $150\,\mathrm{mJ/m^2}$ at $\theta_{\max} = 30^\circ$ and $\gamma_{gb\,(\max)} = 10^3\,\mathrm{mJ/m^2}$. Consequently, the thermodynamic condition of low-angle GB wetting (1) is fullfield at $0.5\,\mathrm{mJ/m^2} \leq \gamma_{sl} \leq 75\,\mathrm{mJ/m^2}$. These γ_{sl} values on order of magnitude are typical for liophilic colloids [3]. In particular, the liophilic colloid may form in the two-phase area of the phase diagram (Figure) where the solid A or B and melt are in equilibrium. The formation of the high-temperature liophilic colloid could be explained as follows. It is known that the GB wetting by eutectic melt occurs in the two-phase area of

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1)e-mail: vbelousov@imet.ac.ru

the phase diagrams (point C in Figure) [2]. With further rise in the temperature, γ_{sl} is decreased. If the γ_{sl} reaches a value of $0.5\,\mathrm{mJ/m^2} - 75\,\mathrm{mJ/m^2}$, the low-angle GB wetting by chemically compatible melt occurs (for example, point D in Figure). At that, the partial dissolution of the solid grains A takes place. As the result, the thermodynamically stable high-temperature solid/melt nanocomposite may exist.

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