

Physico-Chemical nanomaterials science

Effects of size, surface and depletion on melting loop of individual Cu-Ni nanoparticle

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Modified thermodynamic approach to describe the thermodynamic properties including the size effect is suggested taking into account the nucleation and chemical depletion so that the Gibbs free energy of a nanosystem was reassessed as function of composition, temperature and particle size [1]. Such methodology has been applied for the size- and composition-dependent melting of the isolated solid Cu-Ni spherical nanoparticle at 25nm radius. Equilibrium states in two-phase region are investigated from 1000K up to 1700K, and the melting characteristics are determined. It is shown that nanomelting loops in temperature-composition phase diagram (at fixed initial composition and the number of atoms) do not coincide with solidus and liquidus [2]. It is found that Cu-Ni nanoparticle can melt in different stages whereas the dominant transition morphology is surface-induced melting that proceeds from the surface bob like liquid part towards the core region and then whole nanoparticle.

1. Shirinyan, A. S.; Wautelet, M. Phase separation in nanoparticles // *Nanotechnology*.-2004.-**15**.-P. 1720–1731.

2. Shirinyan, A.; Gusak A.; Wautelet M. Phase diagram versus diagram of solubility: What is the difference for nanosystems? // *Acta Materialia*-2005.-**53**.-P. 5025-5032.