Phase Diagram Prediction of Ag, Au, Ni and Pt Systems

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The phase diagram of the alloy nanoparticles (nanoalloys) were investigated by CALPHAD method. The binary nanoalloys Ag-Au, Ag-Ni, Au-Ni, Ni-Pt and AuPt were predicted with respect to nanoparticle size and temperature. The thermodynamic approach was developed by surface contribution for different shapes of particles. There is presented combination of fully miscible system Au-Ag with two fully immiscible systems Ag-Ni and Au-Ni. The calculation was completed by theoretical values of surfaces energy and cohesive energy from density functional theory (DFT).