

## Phase diagram prediction of Ag, Au and Ni systems

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