# Phase Diagrams of Nanoalloys

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CALPHAD method is well-known semiempirical method for thermodynamic and phase diagram calculations in materials science enabling to take into account various contributions for the total Gibbs energy of systems. In the case of nanomaterials, additional Gibbs energy term involves surface energy contribution of nano-objects. The CALPHAD technique is most effective and useful tool because thermodynamic data for various multi-component systems stored in so called thermodynamic databases can easily be used for practical applications. First-principles approach, which may also be used in this field, is restricted to the several hundred atoms only while molecular dynamic simulations have their limitations when applied to multi-component systems.
The CALPHAD method as well as a procedure of including surface dependent parameters of pure components and alloys into the CALPHAD modelling will be explained on the Ag-Au model system [1]. Cu-Ni system with practical importance in electronic industry and calculated phase diagrams of nanoalloys of variable composition as well as an example of synthesized nanoalloy characterized by electron microscopy will also be discussed in this presentation.

Reference:
[1] J. Park, J. Lee: Calphad, 32 (2008), 135.