Symposium A2 (Oral)

Size, Shape, and Compositional Effects on the Order-Disorder Phase Transitions in Au-Cu and Pt-M (M = Fe, Co, and Ni) Nanocluster Alloys

Forrest H. Kaatz[1] and Adhemar Bultheel[2]

[1] *Mesalands Community College, 911 South 10th Street, Tucumcari, NM, 88401, USA*
[2] *Department of Computer Science, KU Leuven, Celestijnenlaan 200A, 3001 Heverlee, Belgium*

Abstract

Au-Cu and Pt-M (M = Fe, Co, and Ni) nanocluster alloys are currently being investigated worldwide by many researchers for their interesting catalytic and nanophase properties. The low temperature behavior of the phase diagrams is not well understood for alloys with nanometer sizes and shapes. These systems have similar bulk phase diagrams with the L_{12} (Au_3Cu, Pt_3M, $AuCu_3$, and PtM_3) structurally ordered intermetallics and the L10 structure for the AuCu and PtM intermetallics. We consider two models for low temperature ordering in the phase diagrams of Au-Cu and Pt-M nanocluster alloys. These models are valid for sizes $\sim$ 5 nm and approach bulk values for sizes $\sim$ 20 nm. We study the phase transition in nanoclusters with cubic, octahedral, and cuboctahedral shapes, covering the compositions of interest. These models are based on studying the melting temperatures in nanoclusters using the regular solution, mixing model for alloys. Experimentally, it is extremely challenging to determine thermodynamic data on nano-sized alloys. Reasonable agreement is found between these models and recent experimental data on nanometer clusters in the Au-Cu and Pt-M nanophase systems. From our data, experiments on nanocubes about 5 nm in size, of stoichiometric AuCu and PtM composition, could help differentiate between the models. Dispersion data shows that for the three shapes considered, octahedra have the highest percentage of surface atoms for the same relative diameter. Some available evidence indicates that ordered intermetallic nanoclusters have better catalytic properties than disordered ones. We conclude with a discussion of physical mechanisms whereby ordering could improve the catalytic properties of nanocluster alloys.