SUBMISSION ROLE: 2017 Southwest Regional Meeting

CONTROL ID: 2811772

ABSTRACT SYMPOSIUM NAME: Southwest Theoretical & Computational Chemistry: Dieter Cremer Memorial Session (Invited) (Oral)

AUTHORS (FIRST NAME, LAST NAME): Forrest Kaatz[1], Adhemar Bultheel[2]

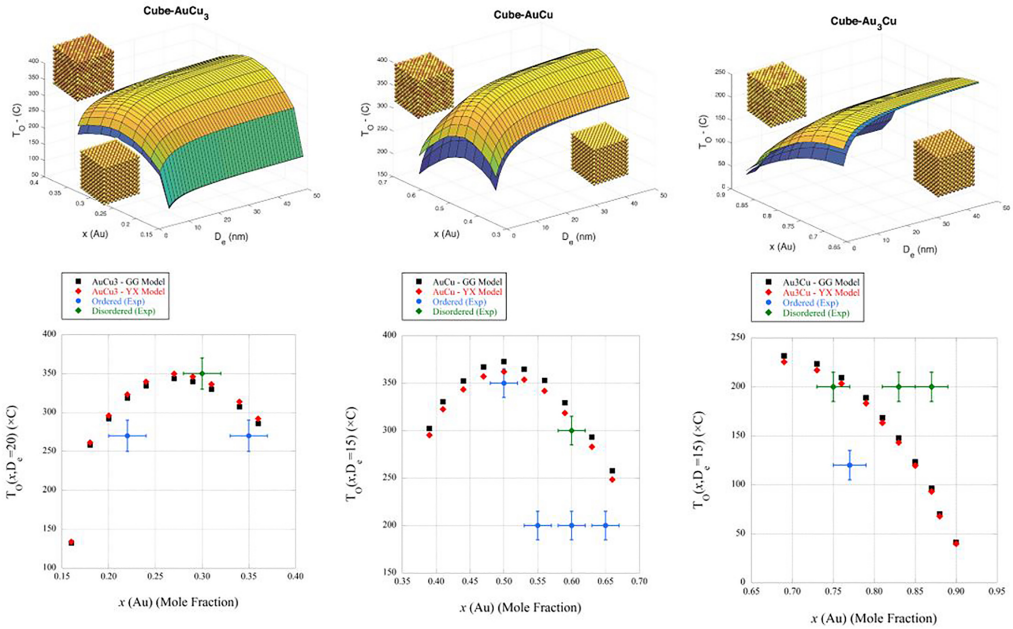
INSTITUTIONS (ALL):

1. Mesalands Community College, Tucumcari, NM, United States.
2. KU Leuven, Heverlee, Belgium.

TITLE: Size, shape, and compositional effects on the order – disorder phase transitions in gold – copper and platinum – nickel nanocluster intermetallics

ABSTRACT BODY:

Abstract: Gold–copper and platinum–nickel nanocluster alloys are currently being investigated world–wide 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 two systems have similar bulk phase diagrams with the $L1_2$ (Au_3Cu, Pt_3Ni, $AuCu_3$, and $PtNi_3$) structurally ordered intermetallics and the $L1_0$ structure for the AuCu and PtNi intermetallics. We consider three models for low temperature ordering in the phase diagrams of Au–Cu and Pt–Ni nanocluster alloys. These models are valid for sizes > 5 nm and approach bulk values for sizes ~ 50 nm. We consider 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–Ni nanophase systems. Some available evidence indicates that ordered intermetallic nanoclusters have better catalytic properties than disordered ones. We discuss physical mechanisms whereby ordering could improve the catalytic properties of nanocluster alloys. We conclude with some suggestions for future research that could help differentiate between the models.


Cube-AuCu3
Cube-AuCu
Cube-Au3Cu
T_O - (C)
x (Au)
D_e (nm)

AuCu3 - GG Model
AuCu3 - YX Model
AuCu - GG Model
AuCu - YX Model
Au3Cu - GG Model
Au3Cu - YX Model
Ordered (Exp)
Disordered (Exp)
T_O(x,D_e=20) (×C)
T_O(x,D_e=15) (×C)
x (Au) (Mole Fraction)

(no table selected)