Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Molecular Dynamics Study of Phase Transitions of Transition Metal Alloy Nanoparticles[1] LIJUN MENG, KAIWANG ZHANG, LIZHONG SUI, CHAO TANG, HUAPING XIAO, Xiangtan University, China, G. MALCOLM STOCKS, Oak Ridge National Laboratory, USA, JIANXIN ZHONG, Xiangtan University, China — We have investigated structures of FeCo, FeNi and CoNi alloy nanoparticles using molecular dynamics simulations based on generalized embedded-atom potentials. The pair correlation function (PCF), the Honeycutt and Andersen index (HA index), and bond-order analysis techniques were employed for characterization of the atomic structures of the nanoparticles. Structural transitions in alloy nanoparticles in the size range of 300 to 800 atoms were identified through continuous variation of the compositions. We found that a FeCo nanoparticle exhibits a phase transition from a BCC structure to an icosahedral structure as the cobalt composition is larger than 60%. FeNi nanoparticles possess a BCC or an icosahedral phase if nickel is smaller than 30% or higher than 70%, respectively. In the range of 30%-70% nickel, a FeNi nanoparticle shows features of both BCC and FCC phases. However, a CoNi nanoparticle always has an icosahedral structure in the whole composition range of Ni.

[1]Supported by CNSF and DOE.

Jianxin Zhong
Xiangtan University, China

Date submitted: 25 Nov 2007 Electronic form version 1.4