Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Phase stability, ordering, and magnetism of single-phase fcc Fe-Au alloys JOONHEE M. AN, University of Nebraska-Lincoln, SERGEY V. BARABASH, Intermolecular Inc., KIRILL D. BELASHCHENKO, University of Nebraska-Lincoln — Motivated by experimental evidence of $L1_0$ ordering in single-phase fcc Fe-Au nanoparticles, we study the structural thermodynamics of Fe-Au alloys. First, separate cluster expansions for fcc and bcc lattices are constructed for fully optimized ferromagnetic structures using density functional theory calculations. The optimized structures were assigned to fcc or bcc lattice by a structural filter. Although the lowest formation enthalpy at 50% Au is reached in the bcc lattice, the fcc lattice is preferred for the random alloy. Dynamical stability of specific orderings strongly depends on the magnetic configuration. To analyze the ordering tendencies of the fcc alloy, we restrict uniform lattice relaxations and separate the contributions of chemical interaction and local relaxations. By using the effective tetrahedron model (Ruban *et al.*, Phys. Rev. B 67, 214302 (2003)) and explicit calculations for ordered and special quasi-random structures, we find that the local relaxation energies depend weakly on the magnetization. Although the $L1_0$ ordering is the ground state at 50% Au on the ideal lattice, local relaxations make it unfavorable compared to the random alloy. Moderate compression due to the size effect tends to slightly stabilize the $L1_0$ ordering.

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Date submitted: 09 Nov 2012 Electronic form version 1.4