Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Generalized stacking fault energetics in FePt nanoparticles and effects of extended defects on magnetocrystalline anisotropy AHMAD ALSAAD, NABIL AL-AQTASH, RENAT SABIRIANOV, Department of Physics University of Nebraska at Omaha 6001 Dodge Street Omaha, NE 68182 — *ab inito* calculations are carried out to study the generalized stacking faults energetics of extended defects observed experimentally in FePt nanoparticles. We calculated γ-surface energy of FePt with antiphase boundary by shifting two crystallites against each other. The γ-energy is calculated using *slab approach.* Each crystallite is stacked along the [001] direction and terminated by Pt layer at the antiphase boundary. We used eight layers of $L1_0$-FePt, four of Fe layers and the other four are Pt layers. The aligned crystals position atoms of Pt directly on top of each other across the interface of two crystallites (point C). In this case, it appears that Fe layer is missing from the regular FePt lattice. A shift by (0.5, 0.5, 0.0) aligns crystallites perfectly in terms of site position of $L1_0$ lattice, but Fe and Pt interchange their site occupancy across the boundary (Point A). Another, high symmetry point of γ-surface is located at the shift of (0.25, 0.25, 0) (point B). In this case, Pt atoms are coordinated by two Pt atoms across the interface and it corresponds to a bridge position between two global minima of γ-surface. We calculated γ-surface energy along the path connecting the above high symmetry points A$\rightarrow$B$\rightarrow$C$\rightarrow$A and estimate the defect energy to be about 0.5eV/atom. Magnetocrystalline anisotropy energy (MAE) of the defect at point A is found to be 54.11 Merg/cm^3 along c-axis, while MAE decreases to 42.34 Merg/cm^3 at points C. Thus, extended defects may affect the magnetization reversal of FePt nanoparticles.

Ahmad Alsaad
Department of Physics University of Nebraska at Omaha
6001 Dodge Street Omaha, NE 68182

Date submitted: 14 Nov 2013 Electronic form version 1.4