Monte Carlo simulation of equilibrium L1₀ ordering in FePt nanoparticles

R.V. Chepulskyy and W. H. Butler

MINT Center - The University of Alabama

Abstract

First, second and third nearest neighbor mixing potentials for FePt alloys, were calculated from first principles using a Connolly-Williams approach. Using the mixing potentials obtained in this manner, the dependencies of equilibrium long range order (LRO) on temperature and concentration were studied for bulk and for spherical nanoparticles by use of Monte Carlo simulation and the analytical ring approximation. These nanoparticles exhibit very large anisotropy and are therefore promising for high density recording applications. We find that the LRO parameter is a continuous function of temperature for nanoparticles, but 3.5nm diameter particles should have an equilibrium LRO parameter > 0.8 at 600°C. We conclude that the absence of LRO in such nanoparticles after annealing is more an issue of kinetics than of equilibrium LRO.

Conclusions

- For nanoparticles of finite size, the order parameter changes continuously from unity to zero with increasing temperature. Rather than having a discontinuity indicative of a phase transition (as in bulk), we obtained an inflection point in the order parameter as a function of temperature.
- Our calculations predict that 3.5nm diameter particles in configurational equilibrium at 600°C (a typical annealing temperature for promoting L1₀ ordering) have an L1₀ order parameter of 0.83 (compared to a maximum possible value equal to unity).
- The experimental absence of (relatively) high L1₀ order in 3.5nm diameter nanoparticles annealed at 600°C or below is primarily a problem of kinetics rather than equilibrium.

For more information and reprints contact:
R. Chepulskii, MINT Center. E-mail: roman.chepulskyy@ua.edu