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Monte Carlo simulation of equilibrium $L1_0$ ordering in FePt nanoparticles ROMAN CHEPULSKYY, WILLIAM BUTLER, Center for Materials for Information Technology, The University of Alabama, Bevill 205, Box 870209, Tuscaloosa, AL 35487 — Mixing potentials for FePt alloys were calculated from first principles. Using the mixing potentials obtained in this manner, the dependency of equilibrium $L1_0$ ordering on temperature and concentration was studied for bulk and for spherical nanoparticles of different sizes by use of Monte Carlo simulation and the analytical ring approximation. For nanoparticles of finite size, the (long range) order parameter changed continuously from unity to zero with increasing temperature. Rather than a discontinuity indicative of a phase transition we obtained an inflection point in the order as a function of temperature. This inflection point occurred at a temperature below the bulk phase transition temperature and which decreased as the particle size decreased. Our calculations predict, for example, that 3.5nm diameter particles in configurational equilibrium at 600 $^\circ$C (a typical annealing temperature for promoting $L1_0$ ordering) have an $L1_0$ order parameter of 0.83 (compared to a maximum possible value equal to unity). According to our investigations, the experimental absence of (relatively) high $L1_0$ order in small nanoparticles (2-6 nm in diameter) annealed around 600 $^\circ$C or below is primarily a problem of kinetics rather than equilibrium. As FePt nanoparticle size is reduced, the maximum of equilibrium order parameter shifts from equiatomic concentration toward higher iron concentration.

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