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Magnetic and chemical ordering properties of FePt nanoparticles¹

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The presence of anisotropic $L1_0$ type chemical order in self- assembled, monodispersed FePt nanoparticles produces an extremely high magnetic anisotropy thus making these particles potentially useful for information storage. However, it has been difficult in experiments to achieve a high degree of $L1_0$ order in 3.5-nm-diam nanoparticles. To explore the possible reasons for this observed low degree of order, we studied theoretically the equilibrium chemical ordering of $L1_0$ type for spherical FePt nanoparticles of different sizes (2.5 to 6-nm- diam) in a wide temperature range. In our study we used first-principles calculations together with the cluster expansion technique and Monte Carlo simulation. Our results indicate that the theoretical equilibrium chemical order is higher than that observed experimentally in 3.5-nm-diam nanoparticles annealed at 600 C or below. Using first-principles calculations we considered one of the possible reasons for this difference - the surface segregation in FePt and Fe-Pt-X (X=Ag, Au, Cr, and Cu) nanoparticles. It was established that surface segregation has only a small effect on ordering. We conclude that the experimental absence of (relatively) high $L1_0$ order is primarily a problem of kinetics rather than equilibrium. The recent experimental data supporting such a conclusion are discussed.

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