## Atomic Scale Computer Simulations of L1$_o$ Nanoparticles: Thermodynamics, Kinetics and Irradiation Effects

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FePt nanoparticles are a promising candidate material for ultra high density data storage because of their large e magnetic anisotropy energy in the chemically ordered $L1_o$ phase (fct). Particles can be prepared in ordered arrays, but are mostly disordered and also occur in multiply twinned configurations. In this contribution we use atomic scale computer simulations in order to study the thermodynamic stability, ordering kinetics and ion irradiation effects in $L1_o$ nanoparticles. Particles in multiply twinned and single crystalline morphologies are investigated by means of molecular statics calculations based on a recently developed analytic bond-order potential. A continuum model is parametrized which allows to assess the contributions of elastic strain, surface and and twin boundary energies, separately. The static model calculations predict a strong energetic preference for single crystalline morphologies in the ordered and disordered phases, if the particle size exceeds 2.6 nm, while smaller particles tend to form icosahedral structures. Kinetic Monte Carlo simulations are finally employed to investigate the ordering kinetics of single-crystalline FePt nanoparticles. In non-supported particles, the A1 to $L1_0$ transition proceeds with a higher rate in layers at the surface than in the volume of the particles. Because of the statistical nucleation of the ordered phase, however, no single domain particles are obtained and an elimination of the antiphase boundaries can not be observed within the time scales accessible by the simulations. Finally, Molecular dynamics simulations are used to investigate defect production and sputtering as well as local melting processes in twinned and single-crystalline nanoparticles. Lattice-based Kinetic Monte Carlo $L1_o$ simulations are then employed in order to study the influence of ion-irradiation on the kinetics of the ordering process. We compare the case of He-irradation at low and elevated temperatures while taking into account defect production and sputtering yields as obtained from our MD-simulation.