Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

**Calculation of the free energy of NiFe2O4 nanopoarticles by Monte Carlo simulation**[1] CHENGGANG ZHOU, T. C. SCHULTHESS, Computer Science and Mathematics Div., Oak Ridge National Laboratory, D. P. LANDAU, Center for Simulational Physics, Univ. of Georgia — Magnetic properties of nanoparticles are of great current interest in light of possible applications to high density magnetic storage media. Finite size and surface effect are important for magnetic nanoparticles and differentiate them from their bulk counterparts. We use Monte Carlo simulation to study a model of $NiFe_2O_4$ nanopoarticles proposed by Kodama and Berkowitz [1]. The Hamiltonian of the nanoparticle contains superexchanges between magnetic ions modeled by Heisenberg spins, and surface/bulk anisotropy terms. A continuous version of the Wang- Landau algorithm [2] is used to calculate the joint density of states $\rho(M, E)$ efficiently. From $\rho(M, E)$, we can directly evaluate the free energy of the particle, and many other physical quantities. A hysteresis loop for particles with surface disorder and surface anisotropy is observed, in agreement with previous studies [1]. We found that such a hysteresis loop is the result of interplay between surface disorder and surface anisotropy. Compared with micromagnetic modeling, our Monte Carlo simulation treats the thermodynamic effects properly and is capable of calculating physical quantities at all temperatures and magnetic fields with very limited CPU time. [1] R. H. Kodama, et. al. Phys. Rev. Lett. **77**, 394 (1996); Phys. Rev. B 59, 6321 (1999). [2] C. Zhou, et al., in preparation.

[1]This research is supported by the Department of Energy through the Laboratory Technology Research Program of OASCR and the Computational Materials Science Network of BES under Contract No. DE-AC05-00OR22725 with UT-Battelle LLC, and by NSF DMR-0341874.

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Date submitted: 06 Dec 2004 Electronic form version 1.4