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Spin dynamics simulations for a nanoscale Heisenberg antiferromagnet¹ ZHUOFEI HOU, D.P. LANDAU, Center for Simulational Physics, University of Georgia, Athens, GA 30602, G. BROWN, Computer Science and Mathematics Division, ORNL, Oak Ridge, TN 37831, G.M. STOCKS, Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831 — Thermoinduced magnetization(TiM) is a novel response which was predicted to occur in nanoscale antiferromagnetic materials. Extensive Monte Carlo simulations² have shown that TiM is an intrinsic property of the antiferromagnetic classical Heisenberg model below the Neel temperature. To obtain a fundamental understanding of TiM, spin dynamics(SD) simulations are performed to study the spin wave behavior, which seems to be the cause of TiM. A classical Heisenberg model with an antiferromagnetic nearest-neighbor exchange interaction and uniaxial single-site anisotropy is studied. Simple-cubic lattices with free boundary conditions are used. We employed the fast spin dynamics algorithms with fourth-order Suzuki-Trotter decompositions of the exponential operator. Additional small excitation peaks due to surface effects are found in transverse $S(q,w)$.

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²G. Brown, A. Janotti, M. Eisenbach, and G. M. Stocks, Phys.Rev.B **72**, 140405(2005)

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