Monte Carlo Simulations of ABC Stacked Kagome Lattice Thin Films

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ABSTRACT: In this work, properties of thin films of the frustrated antiferromagnet IrMn3 (ordered phase) is examined by using Metropolis Monte Carlo simulations, which is a step towards better understanding of the exchange bias phenomenon in heterostructures with this fcc compound. This compound has an unusual magnetic structure composed of ABC stacked (along cubic $\langle 111 \rangle$ axes) kagome layers of magnetic Mn ions. The kagome lattice is known to exhibit a high degree of frustration for antiferromanetically coupled spins. A classical spin Heisenberg Hamiltonian is utilized, where symmetry breaking at the surfaces is modelled by introducing a local easy axis anisotropy perpendicular to the film. The impact of having an easy-axis anisotropy on the surface layers and cubic anisotropy in the middle layers is explored. The spin structure at the surface is shown to be different from that of the bulk 3D system, where spins tend to align along the surface [111] normal axis. This alignment tendency then propagates to the middle layers through exchange coupling. Results are shown for the specific heat, magnetization and sub-lattice order parameters for both surface and middle spins in three and six layer films as a function of increasing axial anisotropy. Preliminary results of simulations of the thin films with surface magnetic vacancies, which usually is present in real films, are also shown.

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