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Monte Carlo simulation of incommensurate helical ordering in a frustrated FCC lattice of Heisenberg spins SEONGWEON PARK, CH. M. SULLIVAN, G. SCHNEIDER, T.M. GIEBULTOWICZ, Oregon State University — The zincblende structure of MnSe can be stabilized in thin films and is expected to exhibit Type III FCC antiferromagnetic ordering. The expected magnetic order is indeed observed in MnSe/ZnSe superlattices where the MnSe layers experience compressive strain. However, in the MnSe/ZnTe system, in which MnSe layers experience tensile strain, the Mn spins form incommensurate helical structures¹. Mean field theory can explain the basic mechanism leading to helical ordering but cannot explain details such as the temperature dependence of the pitch of the helical ordering. We report results of Monte Carlo simulations using classical 3D Heisenberg spins and “free” boundary conditions. The simulations were performed for a range of systems with different sizes (including “bulk” thickness) and exchange constants. The change of helical pitch with temperature is correctly reproduced in our results and our data indicate that it is at least partially a finite-thickness effect. We compare our results with earlier simulations using XY spins and “self-determined” boundary conditions².

¹T.M.Giebultowicz et al, Phys Rev B, 46, 12076-12079 (1992)

²M. Collins and W.M. Saslow, Phys Rev B 53, 8533-8538 (1996)

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