Ferrimagnetism in Classical Vector Spin Models

Thomas Falk and J. Oitmaa

School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia.

We have used Monte Carlo simulations to study classical vector spin models of the rare-earth iron garnet ferrimagnets YIG and GdIG. Critical temperatures agree well with experiment. A compensation point is observed in GdIG, again in good agreement with experiment.

1. Introduction

Ferrimagnets are materials in which different sublattices have opposing magnetic moments of unequal magnitude. Thus, unlike antiferromagnets, they have a net moment at low temperatures which vanishes at a critical temperature T_c. Furthermore, since the sublattice magnetizations will not, in general, have the same temperature dependence, there is the possibility of their cancellation at some lower temperature T_{comp}, known as a compensation point.

Real ferrimagnets, such as the garnets and spinels [1,2], have a complex structure, and theoretical treatments have been mostly at the molecular-field (MFA) level [3]. However it is well known that MFA is quantitatively, and even sometimes qualitatively, incorrect. In the present work we go beyond MFA, and use Monte Carlo simulations to study the garnet materials yttrium iron garnet (YIG) and gadolinium iron garnet (GdIG). Our only approximation is to represent the quantum spins by classical vectors which can point in any direction in space. For large quantum number S (here S = 5/2, 7/2) this should be a good approximation, except at very low temperatures.

The iron garnets are cubic, with each cubic unit cell containing 8 formula units $R_3Fe_5O_{12}$, i.e. 160 ions. The Fe3+ cations lie on 2 inequivalent sublattices (conventionally labelled ‘a’ and ‘d’) and the rare-earth cations lie on a 3rd sublattice (conventionally labelled ‘c’). Figure 1 shows the positions of cations in one unit cell.

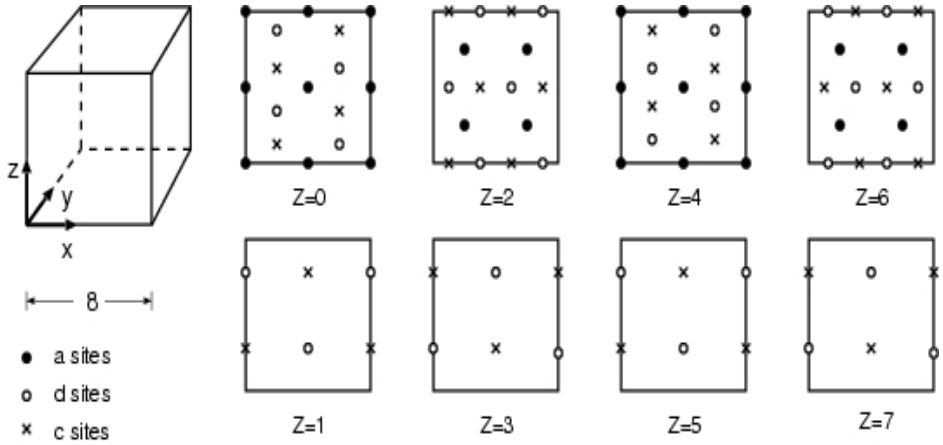


Figure 1. Positions of a,d,c sites in a single cubic unit cell of the garnet structure. The panels show slices parallel to the (x,y) plane, for z=0-7.

The spin Hamiltonian for the rare-earth iron garnets is usually assumed to have the isotropic Heisenberg form

$$H = 2 \sum_{<ij>} J_{ij} \mathbf{S}_i \mathbf{S}_j$$

with interactions restricted to nearest neighbours. Values of the various exchange constants have been estimated by fitting to a range of experimental data [2,4], but considerable uncertainty remains.

Yttrium iron garnet (YIG) is a ferrimagnet with a critical temperature of 560K. The magnetic Fe^{3+} ions have L=0, S=5/2 . and order antiferromagnetically. The ferrimagnetism is due to differing numbers of sites in the a and d sublattices. The most recent values for the exchange constants are [2,4] J_{ad} = 39.8K, J_{dd} = 13.4K, J_{aa}=3.8K. All interactions are antiferromagnetic. Thus there is a degree of frustration in each sublattice, overcome by the dominant coupling J_{ad}.

Gadolinium iron garnet (GdIG) has a critical temperature of 564K and a compensation point at 290K. The Gd^{3+} ions, occupying the c sublattice, have L=0, S=7/2 . The exchange parameters for GdIG are less well known – we take the values from Harris[5] J_{ad} = 45.7K, $J_{aa} = J_{dd}$ = 9.13K, J_{ac} = 2.52K, J_{dc} = 10.07K.

2. Method and Results

We use a standard Monte Carlo procedure with single-spin updates [6], with classical vector spins of length $\sqrt{(S(S+1))}$. As the system is rotationally invariant in spin space, the total moment can rotate freely without energy cost. To avoid difficulties associated with this we include a small magnetic anisotropy in the Hamiltonian, to yield a preferred ordering axis. Our results are not affected by this. A number of runs are taken at each temperature, to ensure reasonable statistics. The results shown are for a system of 4^3 unit cells, containing a total of 4096 cation sites. We have found this to be large enough to avoid significant finite-size effects.

Figure 2 shows results for YIG, in the form of normalized sublattice magnetizations and specific heat versus temperature.

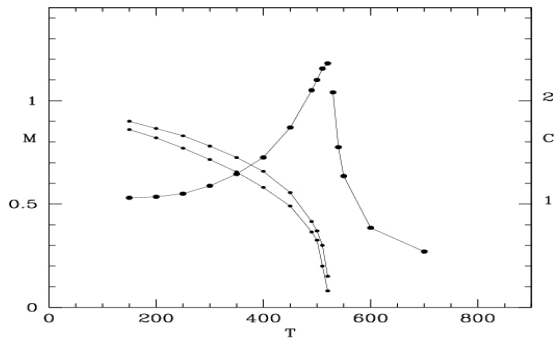
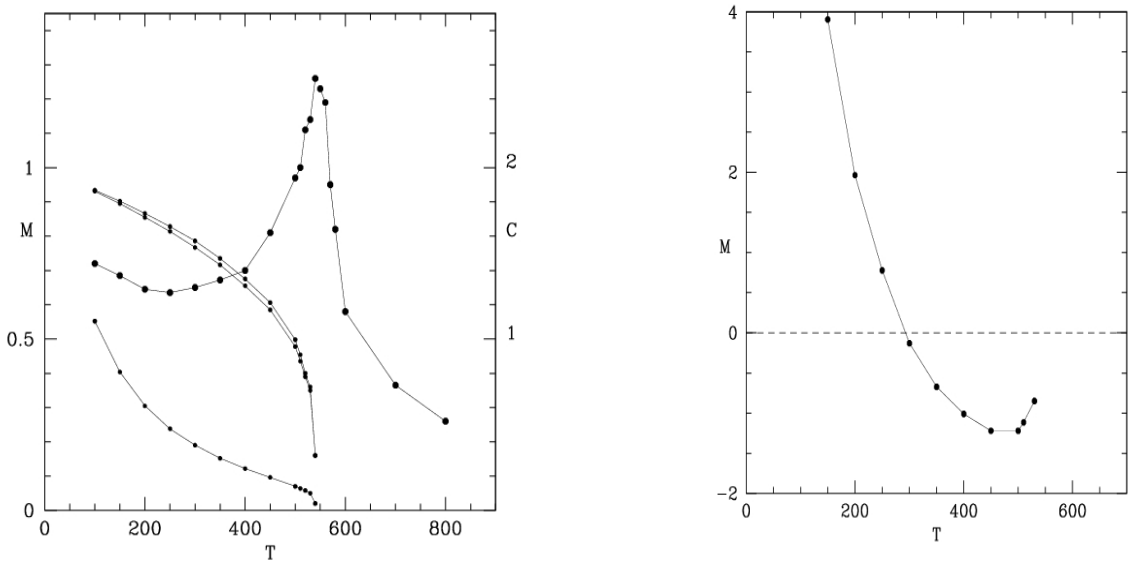


Figure 2. Monte Carlo results for YIG. The filled circles are MC results with error bars. For convenience both magnetizations are shown as positive.

We note the specific heat peak at ~500K., which is a signature of the critical point, and the similar temperature dependences of the sublattice magnetizations. There is no compensation point.

Similar results for GdIG are shown in Figure 3. The specific heat peak occurs at ~550K



(a) (b)

Figure 3. Monte Carlo results for GdIG. (a)The specific heat and the three sublattice magnetizations (all shown as positive); (b) The normalized total moment.

We note the rapid drop in the Gd^{3+} magnetization at low T. This reflects the relatively weak coupling between the Gd spins and the Fe spins.

The total magnetization of GdIG is, to within a constant factor,

$$M_{ferri} = -15\sigma_d + 10\,\sigma_a + 21\sigma_c$$

This is also shown, as a function of temperature, in Figure 3b. We note that M_{ferri} changes sign at a compensation point at 290K. This is in excellent agreement with the experimental value of 290K.

3. Conclusions

This work shows that the Monte Carlo method provides an effective technique to investigate complex magnetic structures. Our results for both YIG and GdIG are in good agreement with experiment, given the uncertainties in the experimental values of the exchange parameters. We show that the compensation point in GdIG is predicted by a simple exchange Hamiltonian.

References

[1] D.H. Martin, 'Magnetism in Solids', (MIT Press, 1967).
[2] V. Cherepanov et al., Phys. Reports 229, 81 (1993).
[3] J.S. Smart, 'Effective Field Theories of Magnetism' (Saunders, 1966).

[4] J.S. Plant, J. Phys. C. 10, 4805 (1977).
[5] A.B. Harris, Phys. Rev. 132, 2398 (1963).
[6] D.P. Landau and K. Binder, 'A Guide to Monte Carlo Simulations in Statistical Physics' (Cambridge, 2000).