

Mixed Ising models with two compensation temperatures

E. Machado, G.M. Buendía*

Physics Department, Universidad Simón Bolívar, Apartado 89000, Caracas 1080, Venezuela

Abstract

We calculate the free energy of a mixed Ising ferrimagnetic system from a mean field estimate of the total energy and the entropy. By minimizing the free energy we obtain the equilibrium magnetizations and the compensation temperatures. We found that compensation temperatures only appear in metastable systems, and that depending on the crystal field parameter, the system can present none, one or two compensation points.

© 2003 Elsevier B.V. All rights reserved.

PACS: 05.50.+q; 75.10.Hk

Keywords: Ferrimagnetics; Compensation temperatures

Ferrimagnetic ordering plays a crucial role in several novel materials based on molecular compounds [1]. Ferrimagnets can present compensation temperatures, T_{cp} , temperatures below the critical point at which the magnetization vanishes. At T_{cp} the coercivity of the material increases dramatically facilitating the process of writing and erasing in magneto-optical media [2]. Mixed Ising systems have proven to be very useful to understand the compensation phenomenon [3]. In this work, we study the behavior of the T_{cp} and the phase diagram of a mixed Ising model by minimizing the free energy. Compared with standard Monte Carlo (MC) algorithms, this approach requires a minimum computer effort, and allows the identification of the stable and metastable states of the system.

The model consists of a square lattice of N sites with spins $S = \pm 1, 0$ and $\sigma = \pm \frac{1}{2}$ located in alternating sites. The Hamiltonian has the form

$$\mathcal{H} = -J_1 \sum_{\langle mn \rangle} \sigma_i S_j - J_2 \sum_{\langle mn \rangle} S_j S_l - J_3 \sum_{\langle nm \rangle} \sigma_i \sigma_k - D \sum_j S_j^2 - H \left(\sum_i \sigma_i + \sum_j S_j \right), \quad (1)$$

where the J 's are the exchange interaction parameters, D is the crystal field, and H is an external magnetic field, all in energy units. The coupling between nearest neighbors is antiferromagnetic, $J_1 = -1$.

The Helmholtz free energy of the system is obtained from a mean field calculation of the internal energy and by approximating the entropy as the sum of the sublattice entropies, calculated by a direct enumeration of the number configurations. Then, the free energy per spin, f , has the form,

$$f = -\frac{1}{2} \left[J_1 z m_1 m_2 + \frac{1}{2} J_2 z (m_1)^2 + \frac{1}{2} J_3 z m_2^2 + D m_1^* + H(m_1 + m_2) \right] + \frac{T}{4} [(m_1^* + m_1) \ln(m_1^* + m_1) + (m_1^* - m_1) \ln(m_1^* - m_1) + (1 + 2m_2) \ln(1 + 2m_2) + (1 - 2m_2) \ln(1 - 2m_2) + 2(1 - m_1^*) \ln(1 - m_1^*)] - \frac{T}{2} (1 + m_1^*) \ln 2. \quad (2)$$

Besides the temperature, f is written in terms of three quantities: the magnetization per spin of the S and σ sublattices, m_1 and m_2 , respectively, and the average number of nonzero spins of the S sublattice, m_1^* . Here the temperatures are in energy units and z is the coordination number.

*Corresponding author. Tel.: +58-212-906-3910; fax: +58-212-906-3927.

E-mail address: buendia@usb.ve (G.M. Buendía).

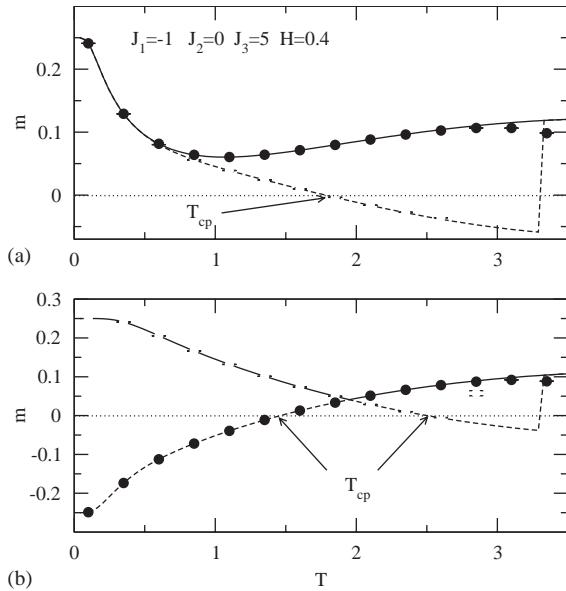


Fig. 1. Magnetizations of the metastable (dashed lines) and stable (continuous lines) states, obtained from the free-energy, and magnetizations calculated with a MC algorithm (circles) from different starting configurations. (a) $D = -2$, (b) $D = -1$.

In Fig. 1 we show the equilibrium magnetizations obtained by minimizing the free energy and also by a MC algorithm that starts from different regions of the phase diagram. The agreement between both techniques is very good, up to very close the critical temperature. An interesting result, that cannot be deduced from the MC data alone, is that only metastable states present T_{cp} , suggesting that the preparation of the system determines the existence of compensation points. Experimental results show that the T_{cp} of molecular ferrimagnets depends on whether the magnetization is measured in cooling or warming mode [4]. The behavior of the T_{cp} also depends on the crystal field, D . In Fig. 2 we observe that there is a range of values of D for which the system presents: none, one, or two T_{cp} . The limiting values of D in these regions depend on the other

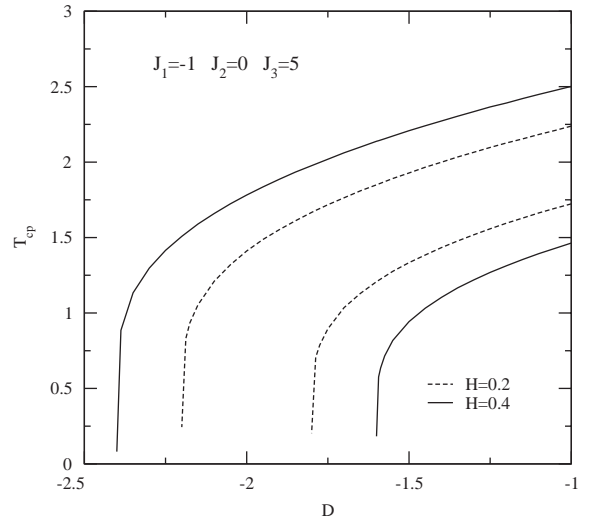


Fig. 2. Dependence of T_{cp} , calculated from the free energy, with the crystal field.

parameters in the Hamiltonian. The figure shows how these limiting values change for two values of H . Two T_{cp} have already been measured in molecular-based ferrimagnets [4].

References

- [1] J.V. Alvarez, R. Valenti, A. Zheludev, Phys. Rev. B 65 (2002) 184417; C.J. Nuttall, S.G. Carling, P. Day, Inorg. Chem. 35 (1996) 1201.
- [2] A.E. Berkowitz, K. Takano, J. Magn. Magn. Mater. 200 (1999) 552; M. Kiwi, J. Magn. Magn. Mater. 234 (2001) 584.
- [3] G.M. Buendía, E. Machado, Phys. Rev. B 61 (2000) 14686; A. Bobak, D. Horvath, Phys. Stat. Sol. (b) 203 (1999) 449.
- [4] O. Cador, M.G.F. Vaz, H.O. Stumpf, C. Mathoniere, J. Magn. Magn. Mater. 6 (2001) 234; S.I. Ohkoshi, Y. Abe, A. Fujishima, K. Hashimoto, Phys. Rev. Lett. 82 (1999) 1285.