Mean-Field and Beyond: Temperature Dependence of Spontaneous Magnetisation and Anisotropy

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Magnetic anisotropy energy is defined as part of the non-equilibrium thermodynamic potential of a ferromagnet that depends on the direction of the magnetization vector $\boldsymbol{M}$. The approach is valid on condition that $|\boldsymbol{M}|$ = const. The anisotropy energy is usually presented as an expansion in powers of $\boldsymbol{m} = \boldsymbol{M}/|\boldsymbol{M}|$ or, alternatively, in trigonometric functions of the spherical angles θ and φ. The form of this expansion is determined by the point symmetry group of the crystal. For example, for the hexagonal point groups C_{6v}, D_6, D_{3h} or D_{6h} one has

$$E_a = K_1 \sin^2 \theta + K_2 \sin^4 \theta + K_3 \sin^6 \theta + K_3' \sin^6 \theta \cos 6\varphi \; + ... \tag{1}$$

The coefficients in this expansion are known as anisotropy constants.

One of the most important sources of magnetic anisotropy is crystal (electric) field. It can be presented as an expansion of the effective (electrostatic) potential around the position of a particular atom over a suitably chosen basis. Alternatively, the crystal field is expanded in Stevens' operator equivalents O_n^m, which are functions of the operator of total angular momentum. Thus, e.g., $O_2^0 = 3J_z^2 - J(J+1)$ etc. The form of the crystal field expansion is dictated by the local symmetry group of the corresponding site. So for the hexagonal point groups C_{6v}, D_6, D_{3h} or D_{6h} the expansion of the crystal field Hamiltonian in the Stevens operators is as follows:

$$\mathcal{H}_{CF} = B_{20}O_2^0 + B_{40}O_4^0 + B_{60}O_6^0 + B_{66}O_6^6 \tag{2}$$

The quantities B_{nm} are called crystal field parameters.

The single-ion model of magnetic anisotropy relates the coefficients in both expansions, (1) and (2). Namely, in the above example,

$$K_1 = -3J^2 B_{20} B_J^{(2)}(x) - 40J^4 B_{40} B_J^{(4)}(x) - 168J^6 B_{60} B_J^{(6)}(x)$$
$$K_2 = 35J^4 B_{40} B_J^{(4)}(x) + 378J^6 B_{60} B_J^{(6)}(x)$$
$$K_3 = -231J^6 B_{60} B_J^{(6)}(x)$$
$$K_3' = J^6 B_{66} B_J^{(6)}(x)$$

(3)

where

$$x = \frac{\mu H_{\mathrm{mol}}}{kT}$$

(4)

and H_{mol} is the molecular field. Thus, temperature dependence of the anisotropy constants is described by three special functions, $B_J^{(n)}(x)$, $n = 2, 4, 6$, called generalised Brillouin functions.

The main postulate of the molecular field theory is the proportionality relation, $H_{\mathrm{mol}} = \lambda M$, where λ is the molecular field constant. Depending on the nature of the electronic states – carriers of magnetism – one can formulate a localised or an itinerant version of the theory. Temperature dependence of spontaneous ($H = 0$) magnetization in the localised theory is given by a pair of parametric equations,

$$kT = \mu \lambda M_0 x^{-1} B_J(x)$$

(5)

$$M = M_0 B_J(x)$$

(6)

The parameter x runs from 0 to ∞. A pair of equations similar to (5, 6) is also obtained in the itinerant version of the theory.

The molecular field approximation is inaccurate in the limiting cases $T \to 0$ ($x \to \infty$) and $T \to T_C$ ($x \to 0$). For $T \to 0$ it predicts an exponential approach to saturation, whereas in real ferromagnets the magnetization follows Bloch's $^3/_2$ power law: $M \approx M_0(1 - \mathrm{const.}\, T^{3/2})$. This behaviour finds an explanation in the spin-wave theory.

Near the Curie point the prediction of the molecular field theory is that $M \approx$ const. $\times(1 - T/T_C)^\beta$, with $\beta = \frac{1}{2}$. The real situation rather more like a cross-over from $\beta = \frac{1}{4}$ to $\beta = \frac{1}{2}$, so that no power law is strictly fulfilled. Sometimes a power law with $\beta \approx \frac{1}{3}$ is used, but this is an approximation valid in a rather limited interval of temperatures. In practice, it is more convenient to use an empirical formula,

$$M = M_0 \left[1 - s \left(\frac{T}{T_C} \right)^{3/2} - (1-s) \left(\frac{T}{T_C} \right)^{5/2} \right]^{1/3}, \tag{7}$$

where s is an adjustable parameter describing the shape of the curve ($0 < s < 2.5$). Equation (7) applies anywhere between $T = 0$ and T_C.

Recommended Literature

1. J. S. Smart, Effective Field Theories of Magnetism (Saunders, Philadelphia, 1966).

2. M.D. Kuz'min and A.M. Tishin, Theory of Crystal-Field Effects in 3d-4f Intermetallic Compounds. In: *Handbook of Magnetic Materials*, edited by K.H.J. Buschow (North-Holland, Amsterdam, 2008), Vol. 17, Ch. 3.