How Peculiar Can the Temperature Variation of Magnetic Anisotropy be: Limitations by a General Theorem

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Abstract—The variation of anisotropy constants is studied within the three-constant approximation to the anisotropy free energy. The anisotropy-flow concept for tracing the evolution of the system in the anisotropy space of the system is introduced. Unexpected features of the variation of anisotropy are uncovered for realistic values of the intrinsic parameters as, e.g., two zero points for the first anisotropy constants and, correspondingly, two successive reorientation transitions between phases with different easy axes of magnetization. The question of the ultimate possible peculiarity of variation of anisotropy and magnetostriction is addressed by formulating and proving a far-reaching theorem by virtue of which the superposition of p different functions with certain widely met properties may not have more than $p-1$ zeroes or internal extrema.

I. Introduction

Magnetic anisotropy (MA) can be characterized either by the set of *anisotropy constants* K_i or by the equivalent set of *anisotropy coefficients* $\bar{\kappa}_n$ [1], [2]. These sets carry the temperature (T) and field (H) dependence of the anisotropy energy. The variation of magnetostriction (MS) with the magnetization m in a given ferromagnetic system can be addresed within the fundamental theory of [1], whereby one needs to know once again the anisotropy coefficients $\bar{\kappa}_n(m)$. One way to get the T and H dependences of the MA constants $\{K_i\}$ and of the MS constants $\{\lambda_j\}$ is by inserting the experimentally measured dependences $m(T, H)$. The theoretic alternative is to compute the functions $\bar{\kappa}_n$ within a statistic-mechanical treatment. It has recently been shown how to carry out effectively the required calculations [3] for a whole class of untrivial theories [4]. On the first stage, the MA and MS constants are expressed as linear combinations of the fundamental anisotropy coefficients $\bar{\kappa}_n$. These are defined as the normalized statistical averages of the Stevens' operator equivalents [5]:

$$\bar{\kappa}_n(T) \equiv < \hat{O}_n^o > (T) / < \hat{O}_n^o > (0) . \qquad (1)$$

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The bracket denotes statistical averaging with respect to the dominant exchange-interaction part of the Hamiltonian. It has already been explained in detail how to implement a powerful parametric approach to compute the canonic dependences $\bar{\kappa}_n(m)$ [3], [6] and this comprises the second stage of the computation. On the last stage, the temperature dependence can be obtained with the help of the same parametric approach by computing $m(T)$ within the mean-field theory or, for cubic lattices, within the random-phase approximation [7]. At this level the dependences $\bar{\kappa}_n(T)$ are already specific for each particular theory from within the class of [4].

It turns out possible to exploit the method for an exhaustive classification by general arguments of the possible types of variation of single-ion MA in the two-constant free-energy approximation [3]. One is naturally led to introduce the concept of temperature-driven flows in the anisotropy space of the corresponding system. The trajectory described by a given system under variation of temperature can be explicitly computed and monitored which, beside the rather appealing presentation of the anisotropy-related phenomena in the system, allows one to quantify in great detail the possible exchange of stability of preferential axes of orientation of magnetization.

II. Uniaxial systems with higher-order single-ion anisotropy

Below, we neglect in-plane anisotropies to avoid a redundant complication. In the case when three constants $K_i (i = 1, 2, 3)$ have to be considered in the phenomenologic free energy

$$F_A = K_1 \cdot \sin^2\theta + K_2 \cdot \sin^4\theta + K_3 \cdot \sin^6\theta \ , \qquad (2)$$

the matrix relating the set of experimentally measured *constants* $\{K_i\}$ to the theoretically computed *coefficients* $\{\bar{\kappa}_n\}$ is a three-dimensional triangular one and contains two independent parameters [8]. They can profitably be cast as the ratios K_2^0/K_1^0 and K_3^0/K_1^0, where $K_i^0 \equiv K_i(T=0)$ are the *intrinsic* anisotropy constants. The intrinsic constants play the role of initial conditions for the temperature-driven flow in the anisotropy space [3]. Any given trajectory or flow is in this sense deterministic. The relations between constants and coefficients for this case are given by [9]:

$$\begin{aligned}\bar{K}_1 &= \left(1+\frac{8}{7}x+\frac{8}{7}y\right)\bar{\kappa}_2-\left(\frac{8}{7}x+\frac{144}{77}y\right)\bar{\kappa}_4+\frac{8}{11}y\bar{\kappa}_6,\\ \bar{K}_2 &= \left(x+\frac{18}{11}y\right)\bar{\kappa}_4-\frac{18}{11}y\,\bar{\kappa}_6\,, \qquad (3)\\ \bar{K}_3 &= y\,\bar{\kappa}_6 \qquad (x=K_2^0/K_1^0,\ y=K_3^0/K_1^0).\end{aligned}$$

If one is interested in studying the variation of the anisotropy constants, one recognizes in (3) a clearly posed mathematical problem of investigating the outcome of superposing a set of functions $\{\bar{\kappa}_n\}$ for different values of the constitutional parameters x and y. An analytic exhaustion of the possible types of variation of the K_i's as in the case with only K_1 and K_2 included does not seem possible. The only guiding lines remain the parametric approach which underlies the anisotropy-flow concept and the experience gained in analyzing the much simpler two-constant case [3].

Applying the parametric approach to probe the anisotropy space systematically, one finds several unexpected features for the variation of single-ion MA. In the first place, three generic types of variation of K_2 are possible depending on the ratio of the intrinsic constants K_2^0 and K_3^0 only: a monotonic-type variation and two non-monotonic, untrivial types of variation with an additional maximum or with a zero point of K_2 at some internal point between 0 and T_C, respectively. Second, we find a range of values of the intrinsic parameters where K_1 develops *two* internal extrema upon varying the temperature (Fig. 1). Besides, the *first* anisotropy constant K_1 exhibits *two zero points* (*two changes of sign*, respectively) for realistic values of the constitutional parameters (the lowest-lying curve in Fig. 1). Finally, we have detected regimes of variation of the anisotropy constants which bring about *two successive reorientation transitions* of the easy axis of magnetization. This feature is intimately connected with the number of zeroes of K_1 and could only be studied by implementing the parametric approach to track down the trajectories of the system in the anisotropy space. In Fig. 2(a,b) we give a typical flow diagram exhibiting the feature of a system crossing over from an easy axis along the c-axis to a canted-axis phase and then back along the c-axis upon increasing the temperature. When K_1 tends to its first zero, the trajectory goes to infinity in the chosen standard presentation and, following the change of sign of K_1, reemerges in another section of the anisotropy space where the magnetization prefers another direction. This runaway to infinity takes place twice for each of the internal zero points of K_1. Physically, we have detected two successive reorientations c-axis $\rightarrow$ canted easy axis $\rightarrow$ c-axis. Besides, this particular trajectory as well as all other possible trajectories which are computed with the help of the parametric method are valid for the whole class of theories, since they are parametrized by the generalized effective field x of [4], although physically the evolution is driven by the variation of temperature.

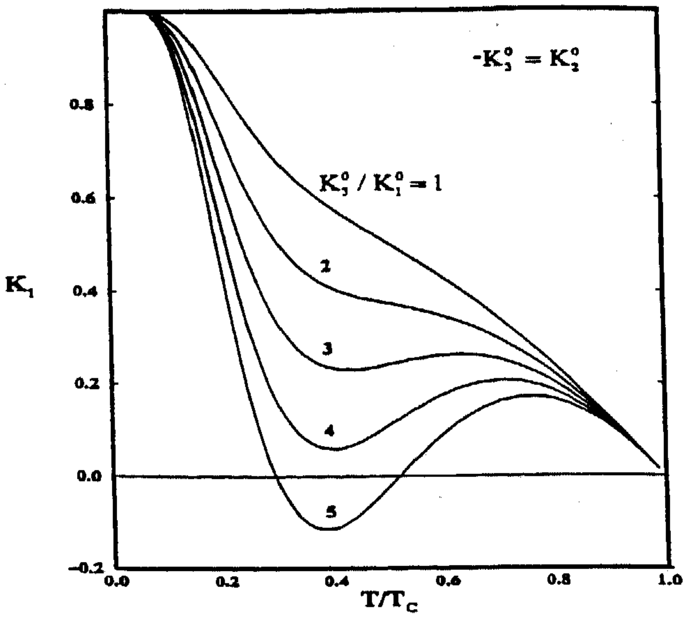

Fig. 1. Regimes with two internal extrema of K_1 and with two zero points of K_1 ($K_i^0 \equiv K_i(T=0)$).

III. Ultimate Peculiarity of Variation

The question arises about the admissible ultimate peculiarity of variation of MA and MS constants in the general cases when any one of them is represented by a superposition of p basis functions $\{g_\mu\}$ ($\mu = 1, 2, ..., p$). It makes no physical sense to consider more than three basis functions in *uniaxial* symmetry ($g_\mu(x) = \bar{\kappa}_{2\mu}(x)$, $\mu = 1, 2, 3$) or more than two basis functions ($g_\mu(x) = \bar{\kappa}_{2(\mu+1)}(x)$, $\mu = 1, 2$) in *cubic* symmetry if only single-ion contributions are considered. However, there are a number of physical effects whose account naturally leads to extending the basis of functions. Such effects are, e.g., the *two-ion* contribution to MA and MS, *higher-order perturbation effects*, *magnetoelastic contributions* to MA, etc. To address generally such realistic and, in fact, unavoidable extensions of the physical effects considered, we have been able to formulate and prove a rather general theorem whose validity is independent of whether one is examining single-ion contributions only. The theorem states that, given p sufficiently smooth, strictly monotonic, bounded functions which are defined on a finite interval and given that there they are of constant-sign convexity, one can always construct a p-term linear superposition which has at most $p-1$ internal zeroes and/or extrema. *On the existence side*, sufficiently peculiar variation of MA or MS constants is guaranteed for *some* values of the constitutional parameters; the set of such parameters will itself be extended to include all relevant ground-state propeties and not only the K_i^0's of the pure single-ion case. *On the restricting side*, no more than $p-1$ internal extrema or zeroes are allowed for *any* values of the constitutional parameters. The conditions of the theorem can be relaxed, but for the present applications may it suffice to observe that the typical functions which appear in the theory of MA and MS qualify. Apart from $\bar{\kappa}_n$, such are the powers of the magnetization m which appear in the $n(n+1)/2$-law for $\bar{\kappa}_n(m)$ at low temperatures [1] or in the mean-field treatment of two-ion contributions to anisotropy where one assumes a m^2-variation [11]. Moreover, products of the type $\bar{\kappa}_s\bar{\kappa}_q$ ($s = q$ being allowed) which may appear in a higher-order perturbative treatment or may originate in non-negligible magnetoelastic effects, also possess the required properties.

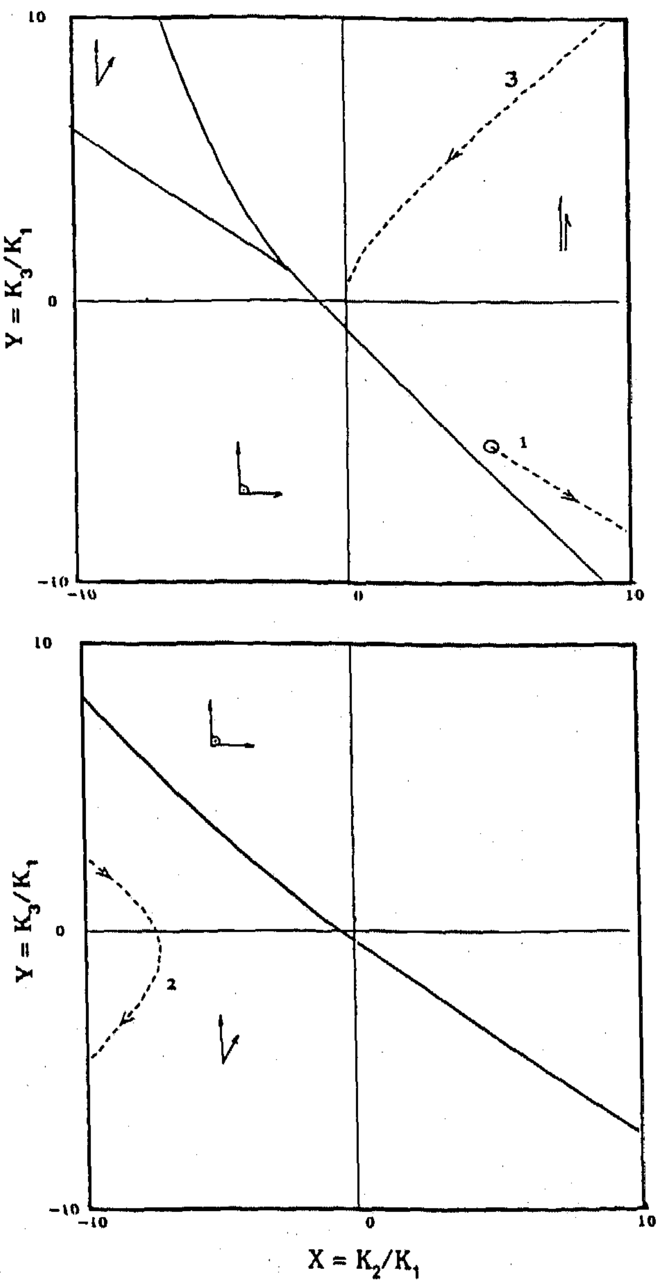

Fig. 2. Two-dimensional mapping of an anisotropy flow with two successive reorientations: (a) $K_1 > 0$; (b) $K_1 < 0$. Physically, the flow is driven by variation of temperature. Thick: borders between phases of different easy axes [10]; dashed: a trajectory consisting of 3 pieces, numbered accordingly and computed with the intrinsic parameters for the lowest curve in Fig. 1 (see text).

Since, on the other hand, the theorem given above is a purely mathematical statement, one might expect that there are other interesting situations where it should render physical insights. We point out in a way of example that by virtue of the same theorem the overall magnetization in a ferrite of p magnetic sublattices may have up to $p-1$ compensation points upon variation of temperature, provided the individual sublattice magnetizations vary with temperature as required by the theorem. The result for $p = 2$ is well-known and amounts to the existence of a single compensation point as predicted by L. Néel long ago.

IV. Discussion

We have shown that recent advances with the statistical computation of the fundamental anisotropy coefficients make possible an extensive analysis of the variation of the experimentally measured single-ion anisotropy constants. This variation is studied in the three-constant approximation to the free energy of uniaxial systems. Unexpected features are detected such as: three types of variation of K_2, up to two zero points of K_1, and up to two successive reorientations. Guided by the anisotropy-flow concept and the insights offered by the underlying parametric approach, we have addressed the problem of the ultimate possible peculiarity of variation of MA and MS by formulating and proving a far-reaching theorem by virtue of which the superposition of p functions which satisfy certain conditions may not have more than $p-1$ zeroes or internal extrema on a bounded interval. The physical applicability of the theorem to the study of MA and MS is guaranteed by the fact that the typical functions arising in statistical treatments which can be seen to form the basis set meet its requirements. A consequence of direct practical significance is that experimental observation of k zeroes or extrema mandates the use of at least $k+1$ parameters to fit data.

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