Where is magnetic anisotropy field pointing to?

Marek W. Gutowski
Institute of Physics, Polish Academy of Sciences, 02–668 Warszawa, Poland

The desired result of magnetic anisotropy investigations is the determination of value(s) of various anisotropy constant(s). This is sometimes difficult, especially when the precise knowledge of saturation magnetization is required, as it happens in ferromagnetic resonance (FMR) studies. In such cases we usually resort to ‘trick’ and fit our experimental data to the quantity called anisotropy field, which is strictly proportional to the ratio of the searched anisotropy constant and saturation magnetization. Yet, this quantity is scalar, simply a number, and is therefore of little value for modeling or simulations of the magnetostatic or micromagnetic structures. Here we show how to ‘translate’ the values of magnetic anisotropy constants into the complete vector of magnetic anisotropy field. Our derivation is rigorous and covers the most often encountered cases, from uniaxial to cubic anisotropy.

Index Terms—magnetic anisotropy, micromagnetic simulations, magnetic modeling

I. INTRODUCTION

In technically important simulations of magnetic systems at meso- or macroscopic scale one is confronted with the problem of finding the equilibrium orientation of local magnetization in each part of a system under study. Similarly to the micromagnetic calculations, the searched orientation is the one that minimizes the free energy of each small element of such a system. At mesoscopic scale this seems easy: the free energy is nothing else but the potential energy of a magnetic moment \( \mathbf{M} \) in magnetic field \( \mathbf{B}_{\text{eff}} \), namely \( F = -\mathbf{M} \cdot \mathbf{B}_{\text{eff}} \). Consequently, the lowest energy orientation of \( \mathbf{M} \) is strictly parallel to \( \mathbf{B}_{\text{eff}} \). In what follows, we will rather talk about the free energy density, and therefore write \( F = -\mathbf{M} \cdot \mathbf{B}_{\text{eff}} \), where we retain the same symbol \( F \) for free energy density, but \( \mathbf{M} \) denotes now the (local) magnetization.

It has to be stressed that we have to speak about \( \mathbf{B}_{\text{eff}} \), and not about \( \mathbf{H}_{\text{eff}} \), as of the effective field. This is in contrast with micromagnetic calculations, where the distinction between \( \mathbf{H} \) and \( \mathbf{B} \) fields is less important. Inside the ferromagnetic bodies the fields \( \mathbf{H} \) and \( \mathbf{B} \) are not proportional to each other, not even necessarily parallel, as they have to satisfy the relation \( \mathbf{B} = \mu_0 (\mathbf{H} + \mathbf{M}) \), with \( \mathbf{M} \neq 0 \) (in SI units). It is nothing unusual to observe that the vectors \( \mathbf{B} \) and \( \mathbf{H} \) are very often nearly antiparallel.

II. THE UNIAXIAL CASE

We start with probably the most often encountered situation of a single easy axis magnetic anisotropy. While it is natural to think about some crystal structures as being uniaxial, the same property is also given to the well known Stoner-Wohlfarth particle. Even nominally amorphous materials are sometimes successfully described as being magnetically uniaxial, see for example [1].

The free energy density with uniaxial anisotropy is usually written as

\[
F = K \sin^2 \theta \quad \text{with} \quad K > 0
\]

or, equivalently (since \( \sin^2 \theta = 1 - \cos^2 \theta \) and we are only interested in orientation-dependent part), as

\[
F = -K \cos^2 \theta,
\]

where \( K \) (often written as \( K_u \)) is the uniaxial anisotropy constant, and the angle \( \theta \) is made by vectors \( \mathbf{M} \) and easy axis direction \( \mathbf{e} \) (unit vector). We prefer the form (2), since it exhibits similar angular dependence as the potential magnetostatic energy usually written as

\[
F = -\frac{1}{2} \mathbf{M} \cdot \mathbf{B} = -\frac{1}{2} MB \cos \theta,
\]

where the subscript “eff” has been dropped for sake of clarity. Besides, the field \( \mathbf{B} \) above is the one generated by all surrounding magnetic moments, not by the object under study. This is why the factor \( 1/2 \) appears in formula (3). Neglect of self-interaction is justified, as it by no means depends on orientation of the object. In this spirit we may rewrite the Eq. (2)

\[
F = -K \left( \frac{\mathbf{M} \cdot \mathbf{e}}{|\mathbf{M}| \cdot |\mathbf{e}|} \right)^2 = -\frac{K}{M^2} (\mathbf{M} \cdot \mathbf{e})^2
\]

Equating (3) and (4) we obtain

\[
-\frac{1}{2} \mathbf{M} \cdot \mathbf{B} = -\frac{K}{M^2} (\mathbf{M} \cdot \mathbf{e}) (\mathbf{M} \cdot \mathbf{e})
\]

and thus immediately

\[
\mathbf{B} = \frac{2K}{M} \left( \frac{\mathbf{M} \cdot \mathbf{e}}{|\mathbf{M}|} \right) \mathbf{e} = \frac{2K}{M} \cos \theta \cdot \mathbf{e}
\]

As expected, \( \mathbf{B} \parallel \mathbf{e} \) and \( \mathbf{B} \propto \frac{2K}{M} \). Moreover, \( \mathbf{B} \) is insensitive to easy axis reversal/reflect the \( \mathbf{e} \) as it should be. This result is in full agreement with customary definition (2) of anisotropy field as \( H_a = \frac{2K}{\mu_0 M} \). On the other hand one can see that the magnitude of anisotropy field depends on orientation of local magnetization with respect to local easy axis, ranging from \( B = 0 \) for \( \mathbf{M} \parallel \mathbf{e} \) to \( B = \frac{2K}{M} \) when \( \mathbf{M} \parallel \mathbf{e} \).

In what follows we will be using shortened notation: \( \mathbf{M}/M = \mathbf{m} \), and also \( \mathbf{m} \cdot \mathbf{e} = \cos \theta \).

III. MORE THAN ONE EASY AXIS

The FMR spectral features in presence of exactly two different (i.e. non-parallel) easy axes were extensively investigated by Cochran and Kambersky [3]. They were interested in...
surface anisotropy of ultrathin layers, which may differ for substrate-side and free side of a layer.

Our extension of the earlier described procedure for samples having even more easy axes \{e_1, e_2, \ldots\} is straightforward, if only their anisotropy may be written as a sum

\[ F = K^{(1)} \sin^2 \theta_1 + K^{(2)} \sin^2 \theta_2 + \cdots \]  \hspace{1cm} (7)

or, equivalently

\[ F = -K^{(1)} \cos^2 \theta_1 - K^{(2)} \cos^2 \theta_2 - \cdots \]  \hspace{1cm} (8)

We have to stress that all anisotropy constants, \(K^{(i)}\), have to be positive, otherwise we deal with easy plane(s) rather than with easy magnetization directions. Anisotropy field is then

\[ \mathbf{B} = \frac{2K^{(1)}}{M} (\mathbf{m} \cdot \mathbf{e}_1) \mathbf{e}_1 + \frac{2K^{(2)}}{M} (\mathbf{m} \cdot \mathbf{e}_2) \mathbf{e}_2 + \cdots \]  \hspace{1cm} (9)

The last formula applies to thin films of cubic, tetragonal or hexagonal symmetry, as well as to strained amorphous materials, whenever higher order anisotropy terms (i.e. containing terms like \(K^{(q)} \sin^q \theta\)) can be neglected. It is worth noticing that presence of more than one easy axes makes orientation of the anisotropy field a linear combination of easy directions. Thus generally \(\mathbf{B} \parallel \mathbf{e}_1, \mathbf{B} \parallel \mathbf{e}_2, \) and so on, even if \(K^{(1)} = K^{(2)}\). A very special case will occur when easy axes are perpendicular to each other, see later discussion concerning cubic anisotropy case.

IV. HIGHER ORDER SINGLE EASY AXIS

The magnetocrystalline anisotropy of bulk tetragonal and hexagonal materials is often written as \[^4\]:

\[ F = K_1 \sin^2 \theta + K_2 \sin^4 \theta. \]  \hspace{1cm} (10)

Proceeding as before we obtain

\[ F = \left[ -(K_1 + 2K_2) \cos \theta + K_2 \cos^3 \theta \right] (\mathbf{m} \cdot \mathbf{e}) / M \]  \hspace{1cm} (11)

and anisotropy field takes the form

\[ \mathbf{B} = \frac{2}{M} \left[ (K_1 + 2K_2) \cos \theta - K_2 \cos^3 \theta \right] \mathbf{e} \]

\[ = \frac{2}{M} \left[ (K_1 + 2K_2) (\mathbf{m} \cdot \mathbf{e}) - K_2 (\mathbf{m} \cdot \mathbf{e})^3 \right] \mathbf{e} \]  \hspace{1cm} (12)

Again, like in single easy axis case, \(\mathbf{B} \parallel \mathbf{e}\), with magnitude varying with orientation of magnetization \(\mathbf{M}\).

A. Non-positive anisotropy constants

Formula (12) was derived somewhat mechanically, without paying much attention to the magnitudes and signs of anisotropy constants \(K_1\) and \(K_2\). In order to find the possible equilibrium positions of the vector \(\mathbf{m}\) one has to solve the equation \(\partial F / \partial \theta = 0\) for \(\theta \in [0, \pi]\). It is easy to see that there may be up to 4 possible solutions (not necessarily corresponding to the local free energy minima!)

\[ \theta_1 = 0, \quad \theta_2 = \pi/2, \quad \theta_3 = \pi, \quad \text{or} \quad \sin^2 \theta_4 = -\frac{K_1}{2K_2} \]  \hspace{1cm} (13)

The first three solutions always exist, while the fourth is obviously only possible when

\[ 0 < -K_1 / (2K_2) < 1 \]  \hspace{1cm} (14)

(we write sharp inequalities, since the limiting cases coincide with first three solutions). The fourth solution is interesting in itself as it corresponds to the not so frequent case of easy cone magnetization.

But which solution corresponds to our particular case? Of course, the one making the global minimum of the free energy density \(F\). The values of \(F\) corresponding to each solution are:

\[ F(\theta = 0) = F(\theta = \pi) = 0 \]  \hspace{1cm} (15)

\[ F(\theta = \pi/2) = K_1 + K_2 \]  \hspace{1cm} (16)

\[ F(\theta_4) = - \frac{K_1^2}{4K_2} \]  \hspace{1cm} (17)

The necessary condition for (local!) minimum of \(F\) is: \(\partial^2 F / \partial \theta^2 > 0\). Thus for easy axis case (\(\theta = 0\) or \(\theta = \pi\)) we should have

\[ K_1 > 0, \]  \hspace{1cm} (18)

for easy plane (\(\theta = \pi/2\)):

\[ -K_1 - 2K_2 > 0, \]  \hspace{1cm} (19)

while for easy cone

\[ -4K_1 \left( \frac{K_1}{2K_2} + 1 \right) > 0. \]  \hspace{1cm} (20)

Looking at inequality (19) we immediately conclude that expression contained in parentheses in (20) must be positive, thus the easy cone may only be realized when

\[ K_1 < 0 \]  \hspace{1cm} (21)

We stop the discussion concerning the correspondence between values and signs of anisotropy constants \(K_1\) and \(K_2\) and the kind of magnetization of a sample. Here we are interested only in the direction and magnitude of an anisotropy field.

B. Conclusion

The formula (12) produces the correct result in every case, regardless of the relations between the anisotropy constants \(K_1\) and \(K_2\). A surprising part of our result is the fact that rotational symmetry axis \(\mathbf{e}\) (of \(C_\infty\) type) of a system dictates the alignment of the anisotropy field, equally well for easy-axis, easy-plane or easy-cone magnetization.

To decide which type of equilibrium position (easy axis, easy plane or easy cone) is currently at play, one has to carefully analyze the conditions from (13) to (20). Of course, we are always looking for the global minimum of a free energy density, \(F\).

V. CURVED SURFACE CASE

The case of otherwise amorphous ferromagnetic microwire is specific. In addition to the energy given in Eq. (10) we should consider one more, rather unusual term\[^5\], namely

\[ F_s = K_s |\cos \theta| \]  \hspace{1cm} (22)

It is specific as the constant \(K_s\) is always positive and inversely proportional to the wire’s diameter squared. For this reason it promotes an easy plane, perpendicular to the wire, rather than
easy axis. Therefore, using its hard axis, i.e. the one parallel to wire length, \( e \), the anisotropy field in Eq. (12) should be appended with

\[
B = -\frac{2K_s}{M} \text{sign}(\mathbf{m} \cdot e) \mathbf{e}
\]  

Here we have exploited the identity \( |x| = x \cdot \text{sign}(x) \). Note the minus sign and that again \( B \parallel e \).

It is interesting that the surface-generated anisotropy described by formula (12) applies equally well to rippled MBE grown surfaces [6], not just to microwires only.

VI. CUBIC ANISOTROPY

In cubic materials the density of anisotropic part of the free energy takes the shape:

\[
F = K_1 (\alpha^2 \beta^2 + \beta^2 \gamma^2 + \gamma^2 \alpha^2)
+ K_2 \alpha^2 \beta^2 \gamma^2
+ K_3 (\alpha^4 \beta^4 + \beta^4 \gamma^4 + \gamma^4 \alpha^4) + \cdots
\]  

(24)

Here \( \alpha, \beta, \gamma \) are direction cosines in Cartesian coordinate frame. Depending on relation between \( K_1 \) and \( K_2 \), the easy axes are \([100]\) or \([111]\) when \( K_1 > 0 \), while for \( K_1 < 0 \) the easy axes are aligned with \([111]\) or \([110]\) directions [4]. Under no circumstances easy cone or easy plane appears. This discussion, strictly speaking, is only valid when \( K_3 \), and higher terms of magnetic anisotropy are negligible.

From now on we will not pay attention to the relations between \( K_1 \), \( K_2 \), and \( K_3 \). Our goal is to find the orientation and strength of local magnetocrystalline anisotropy field. The natural choice for three orthogonal directions is to take as ‘easy’ axes the ones coinciding with the coordinate frame, namely: \( e_1 = (100) \), \( e_2 = (010) \), and \( e_3 = (001) \). Needless to say that other three orthogonal, highly symmetrical, directions may be used as well. For this reason, in the following, we will use only their general symbols, i.e. \( e_1 \), \( e_2 \), and \( e_3 \).

We will analyze the formula (23) term after term, \( F = F_1 + F_2 + F_3 \), remembering that \( \alpha = \mathbf{m} \cdot e_1 \), \( \beta = \mathbf{m} \cdot e_2 \), and \( \gamma = \mathbf{m} \cdot e_3 \).

Writing the first term (of fourth order) twice and rearranging the new expression we obtain:

\[
F_1 = \frac{K_1}{2} \left( \alpha^2 \beta^2 + \beta^2 \gamma^2 + \gamma^2 \alpha^2 + \alpha^2 \beta^2 + \beta^2 \gamma^2 + \gamma^2 \alpha^2 \right)
\]

\[
= \frac{K_1}{2} \left[ \alpha^2 (\beta^2 + \gamma^2) + \beta^2 (\alpha^2 + \gamma^2) + \gamma^2 (\alpha^2 + \beta^2) \right],
\]  

(25)

and consequently

\[
B^{(1)} = -\frac{K_1}{M} \left\{ \left[ (\mathbf{m} \cdot e_2)^2 + (\mathbf{m} \cdot e_3)^2 \right] (\mathbf{m} \cdot e_1) e_1
+ \left[ (\mathbf{m} \cdot e_1)^2 + (\mathbf{m} \cdot e_3)^2 \right] (\mathbf{m} \cdot e_2) e_2
+ \left[ (\mathbf{m} \cdot e_1)^2 + (\mathbf{m} \cdot e_2)^2 \right] (\mathbf{m} \cdot e_3) e_3 \right\}
\]  

(26)

The second term of (24) needs triplication in order to extract a part linear in \( \mathbf{m} \) from free energy density:

\[
F_2 = \frac{K_2}{3} \left( \alpha^2 \beta^2 \gamma^2 + \alpha^2 \beta^2 \gamma^2 + \alpha^2 \beta^2 \gamma^2 \right)
\]  

(27)

The corresponding anisotropy field is then:

\[
B^{(2)} = -\frac{2K_2}{3M} \left\{ \left[ (\mathbf{m} \cdot e_2)^2 + (\mathbf{m} \cdot e_3)^2 \right] (\mathbf{m} \cdot e_1) e_1
+ \left[ (\mathbf{m} \cdot e_1)^2 + (\mathbf{m} \cdot e_3)^2 \right] (\mathbf{m} \cdot e_2) e_2
+ \left[ (\mathbf{m} \cdot e_1)^2 + (\mathbf{m} \cdot e_2)^2 \right] (\mathbf{m} \cdot e_3) e_3 \right\}
\]  

(28)

The eight order term again should be virtually doubled and rearranged, leading finally to:

\[
B^{(3)} = -\frac{K_3}{M} \left\{ \left[ (\mathbf{m} \cdot e_2)^4 + (\mathbf{m} \cdot e_3)^4 \right] (\mathbf{m} \cdot e_1) e_1
+ \left[ (\mathbf{m} \cdot e_1)^4 + (\mathbf{m} \cdot e_3)^4 \right] (\mathbf{m} \cdot e_2) e_2
+ \left[ (\mathbf{m} \cdot e_1)^4 + (\mathbf{m} \cdot e_2)^4 \right] (\mathbf{m} \cdot e_3) e_3 \right\}
\]  

(29)

The full anisotropy field is, of course, equal to the sum \( B = B^{(1)} + B^{(2)} + B^{(3)} \). The dependence of \( B \) on \( \mathbf{m} \) appears highly non-linear and pretty complex. Nevertheless \( B(-\mathbf{m}) = -B(\mathbf{m}) \), as expected.

It is interesting to see what happens when the local magnetization vector, \( \mathbf{m} \), is oriented along one of the directions \( e_i \), \( i = 1, 2, 3 \). Then \( \mathbf{m} \cdot e_i = 1 \) but for any \( j \neq i \) we necessarily have \( \mathbf{m} \cdot e_j = 0 \), hence \( B = B^{(1)} + B^{(2)} + B^{(3)} = 0 \) – regardless of the values of \( K_1, K_2, \) and \( K_3 \). High symmetry cubic directions are always special: they point either to extrema or to saddles of free energy density.

VII. ENDING REMARKS

We have shown how to convert the various phenomenological expressions for magnetocrystalline free energy density into a vector of the so called anisotropy field. This fictitious field has nothing to do with external field, nor with dipole-type field generated by the other parts of a sample. It is nevertheless very useful during simulations based on Landau-Lifshitz-Gilbert (LLG) equation of motion [7], [8], [9], or some variants of Monte Carlo approaches as well.

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