

Dipolar Energy Anisotropy in Hexagonal Ferrites

G. Litsardakis

► **To cite this version:**

G. Litsardakis. Dipolar Energy Anisotropy in Hexagonal Ferrites. Journal de Physique IV Colloque, 1997, 07 (C1), pp.C1-341-C1-342. 10.1051/jp4:19971137. jpa-00254780

HAL Id: jpa-00254780

<https://hal.archives-ouvertes.fr/jpa-00254780>

Submitted on 1 Jan 1997

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Dipolar Energy Anisotropy in Hexagonal Ferrites

G. Litsardakis

Department of Electrical & Computer Engineering, Aristotelian University, 54006 Thessaloniki, Greece

Abstract. The dipolar energy contribution to the anisotropy of M-, W- and Y-type hexagonal ferrites is examined. The geometrical coefficients k_{ij} are given, so that a calculation for any hexaferrite with the same structure can be effected. Differences in the results of previous works are explained as due to a simplifying assumption, the validity of which is restricted. The ambiguity regarding dipolar energy anisotropy has been raised: dipolar energy anisotropy is dominant in BaZn-Y, while it is negligible in M- and W-type hexagonal ferrites. The results suggest that single ion anisotropy of the bipyramidal site is significant but the contribution of all the other sites is equally important.

1. INTRODUCTION

The origins of anisotropy in hexagonal ferrites were discussed for the first time by Smit and Duyvesteyn in Ref. [1]. They calculated the dipolar energy anisotropy and found that it is important only in Y compounds, while in M the calculated value was low and with opposite sign, compared to the experimental value. The anisotropy of M (and W compounds subsequently) was then attributed to single ion anisotropy of Fe^{3+} in the bipyramidal site of the structural block R, which does not exist in the Y-type structure. The dipolar energy was calculated again by Lotgering et al [2] for some M, W and Y-type compounds. Comparing to the earlier results of [1], the values of k_{ij} (see eq.1a) that they found were the same, except for those with $i=j$. In spite of this difference, the anisotropy constant K_1 resulted similar and their conclusions were the same: dipolar energy anisotropy is important only in the Y structure. However, calculations made by Isalgué et al [3] in M and R structures, and in W later [4], gave K_1 values very close to the experimental ones, with all but few k_{ij} equal to those of [2]. It was then proposed that anisotropy in both uniaxial and planar hexagonal ferrites is due to dipolar energy.

In this work a calculation of the dipolar energy anisotropy in M, W and Y structures of hexagonal ferrites is performed, and previous calculations are discussed, showing that the importance of dipolar energy has to be reconsidered.

2. CALCULATION OF DIPOLAR ENERGY ANISOTROPY

In previous calculations dipolar anisotropy K_1 is analysed in coefficients k_{ij} , which represent the geometric part of the interaction between two sublattices i and j with magnetic moments n_i and n_j respectively (in Bohr magnetons):

$$K_1 = 10^3 \sum_{i \neq j} k_{ij} \cdot n_i n_j \text{ (erg / cm}^3\text{)}, \quad \text{where } k_{ij} = 10^{-3} \mu_B^2 \cdot N_i \sum_{n(j)}^N 3 \frac{\cos^2 \theta_{\ell n}(//) - \cos^2 \theta_{\ell n}(\perp)}{r_{\ell n}^3} \quad (1)$$

The use of N_i , the number of ions of sublattice i per volume unit, presumes that, for symmetry reasons, the dipolar energy is the same for each and every cation of a sublattice. So the interaction for only one ion of each sublattice was computed and then multiplied by the crystallographic multiplicity of the sublattice. This assumption is not generally true, and the correct way is to calculate the interaction for every ion in each sublattice separately:

$$k_{ij} = 10^{-3} \mu_B^2 \cdot \frac{1}{2} \frac{1}{V_{cell}} \sum_{\ell(i)}^L \sum_{\substack{n(j) \\ n \neq \ell}}^N 3 \frac{\cos^2 \theta_{\ell n}(//) - \cos^2 \theta_{\ell n}(\perp)}{r_{\ell n}^3} \quad (\times 2)_{i \neq j} \quad (2)$$

The results for M, W and Y type structures are given in tabl. 3-5.

Expression (1b) saves programming and computation time, but for certain sublattices, such as the 12k in M, the 6g and 12k in W and the 18h in Y, it yields $k_{ij} \neq k_{ji}$ (see tabl. 1-2). The values of k_{ij} in this case vary with the direction perpendicular to c axis, which is arbitrarily set in the calculations. Since only one half of the table of coefficients k_{ij} is required (because in eq. 1a it is $i \leq j$), and also it is not necessary to calculate for more than one direction in the basal plane

{001} (because the coefficients k_{ij} should be the same for any direction), the error resulting from (1b) has not been revealed up to now.

In Ref.[3] the projection direction [1,0] has been applied [5], while in Ref.[4] the use of [1,1] is reported, which explain the differences in the reported k_{ij} values of 12k and 6g. In Ref.[2] the results for M and W are practically the same with ours, although they were also obtained with the use of eq.(1b), while for Y there are significant differences in the interactions with sublattice 18h. The projection directions used in [2] are not reported, but we may comment that using eq.(1b), one can reproduce these k_{ij} values in two ways: Either calculating at certain projection directions, 45° from the a axis in M and W, 15° in Y, which however are not any particular directions in the hexagonal system, $[(1+\sqrt{3})/2, 1]$ and $[(1/2)+(\sqrt{3}/2)(\sqrt{6}+\sqrt{2})/(\sqrt{6}-\sqrt{2}), 1]$ respectively. Or taking the average of the extreme k_{ij} values that occur at different directions $[(1,2,0)]$ - $[-1,0,0]$ in M and W, $[1,-1,0]$ - $[-1,1,0]$ in Y).

Table 1. k_{ij} of Y, using (1b)

project.	18h-3a	18h-3b	18h-6c2	18h-6c3	18h-6c1	18h-18h
[1,1]	30.2	59.3	-45.0	-38.5	85.5	-114.0
[1,0]	32.7	29.8	16.6	16.1	69.4	-201.8
[1,-1]	33.5	20.0	37.1	34.3	64.0	-231.1

Table 2. k_{ij} of M, using (1b)

project.	12k-2a	12k-4e	12k-4f1	12k-4f2	12k-12k
[1,0]	85.1	70.7	-24.0	-45.4	-107.6
[1,1]	49.9	55.6	42.3	37.1	-216.1
[1,2]	38.2	50.6	65.4	64.6	-252.3

Table 3. k_{ij} of M

M	2a	4e(v)	4f(IV)	4f(VI)	12k
2a	-5.5	9.8	-57.3	15.4	61.7
4e(v)	9.8	-5.5	16.6	-33.2	59.8
4f(IV)	-57.3	16.6	-29.7	46.6	19.7
4f(VI)	15.4	-33.2	46.6	19.7	9.6
12k	61.7	59.8	19.7	9.6	-180.0

Table 4. k_{ij} of Y

Y	3a	3b	6c2	6c3	6c1	18h
3a	-5.2	5.7	45.1	11.7	-16.9	22.7
3b	5.7	-5.2	9.6	-49.6	12.7	38.9
6c2	45.1	9.6	-4.3	31.3	-31.0	-24.3
6c3	11.7	-49.6	31.3	-27.1	21.4	9.2
6c1	-16.9	12.7	-31.0	21.4	-6.8	6.1
18h	22.7	38.9	-24.3	9.2	6.1	172.3

Table 5. k_{ij} of W

W	2d	4f(VI)S	6g	4e	4f(IV)	4f(VI)R	12k
2d	-4.8	9.4	13.1	8.6	8.1	-27.0	30.3
4f(VI)S	9.4	-5.6	33.2	-37.0	-34.2	15.8	57.3
6g	13.1	33.2	-98.5	-43.7	32.2	26.4	77.7
4e	8.6	-37.0	-43.7	-0.4	-22.6	16.7	59.6
4f(IV)	8.1	-34.2	32.2	-22.6	-5.2	26.0	-16.5
4f(VI)R	-27.0	15.8	26.4	16.7	26.0	11.6	-13.7
12k	30.3	57.3	77.7	59.6	-16.5	-13.7	-157.7

3. CONCLUSION

As we can see in table 6, in M and W the contribution of dipolar anisotropy is very small compared to the experimental value. In BaZn-Y this kind of anisotropy is dominant, being about two times larger than the experimental value. In any case, besides dipolar anisotropy, a positive contribution of $1.6-4.6 \cdot 10^6$ erg/cm³ from other sources has to be taken into account in order to obtain the experimental values. The planar anisotropy of Y compounds is determined both by the large negative dipolar anisotropy and by the lack of the bipyramidal site. A comparison of K_{1exp} - K_{1dip} in all three structure types indicates that the role of the bipyramidal site may be significant but the total contribution of the other sites is also important.

A reliable calculation of dipolar energy contribution to the anisotropy of M- and Y-type hexagonal ferrites has been effected. The results reverse the conclusions of the more recent calculations and confirm the earlier ones, although in all previous cases k_{ij} were not calculated correctly.

Acknowledgments

The author wishes to thank A. Collomb for suggesting the subject, A. Isalgué and J.P. Mignot for providing their calculation programs, D. Samaras and G. Kanellis for helpful discussions.

References

- [1] Casimir H.B.G., Smit J., Enz U., Fast J.F., Wijn H.P.J., Gorter E.W., Duyvestein A.J.W., J.D. Fast J.D. and J.J. Jong J.J. *Le Journal de Physique et le Radium*, t20 (1959) 360-373
- [2] Lotgering F.K., Locher P.R. and vanStapele R.P., *J. Phys. Chem. Solids*, 41 (1980) 481-487
- [3] Isalgue A., Obradors X. and Tejada J., *J. de Physique*, C6, t46 (1985) 345-348
- [4] Collomb A., Abdelkader O., Isalgué A. and Mignot J.P., *phys.stat. sol. (a)*, 97 (1986) 896-904
- [5] Isalgué A., private communication

Table 6. Experimental and calculated K_1

	K_{1exp}	K_1 dipolar				non-dipolar $K_1(exp-dip)$
		[1]	[2]	[3,4]	this work	
M	4.4	-1.5	0.2	4.2	-0.2	4.6
W	2.8-3.8	-	0.3	1.9-2.1	0.06	2.8-3.8
Y	-1.6	-4	-4	-	-3.2	1.6