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Magnetic Anisotropy in Antiferromagnetic Corundum-Type Sesquioxides

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Evaluations of the magnetic dipolar anisotropy K_{MD} are made for the antiferromagnetic Cr, Fe, Ti, and V sesquioxides isomorphous to α-$\mathrm{Al_2O_3}$. In the first two systems the fine structure anisotropy K_{FS} is found by substracting K_{MD} from the total anisotropy K obtained from antiferromagnetic-resonance (AFMR) data. In Shull magnetic configuration type (c), of which $\mathrm{Cr_2O_3}$ is the prototype, K_{MD} was found to be very sensitive to lattice geometry. Owing to the use of inappropriate crystal data, a previous $\mathrm{Cr_2O_3}$ K_{MD} calculation is shown to be in serious error. The $\mathrm{Cr_2O_3}$ AFMR results are reinterpreted accordingly. An analysis is also made for α-$\mathrm{Fe_2O_3}$[Shull case (a)] for which some AFMR data have recently become available. The α-$\mathrm{Fe_2O_3}$ spin flip near 250 °K is predictable on a thermodynamic basis. The K_{FS} results in the Cr and Fe cases show little correlation with the corresponding quantities derived from EPR in diluted magnetic systems. The results of variation of lattice parameters are given for possible application to temperature and stress experiments and to diluted crystals. Since the antiferromagnetic properties of the Ti and V oxides currently are not clear, we present the appropriate K_{MD} calculations for each of the three possible spin configurations.

I. INTRODUCTION

A NUMBER of transition-metal ion sesquioxides are isomorphous in crystal structure with corundum, α-$\mathrm{Al_2O_3}$ [space group $D_{3d}^{6}(R\bar{3}c)$]. Under appropriate conditions, long-range antiferromagnetic ordering of the unpaired metal ion spins is possible. The specific magnetic properties of such antiferromagnetic structures have been studied most directly by neutron diffraction and magnetic susceptibility techniques. More recently the methods of antiferromagnetic resonance (AFMR) and magnetoelectric effect (ME) have also been employed.[1]

These sesquioxide antiferromagnets are composed of two coupled antiparallel magnetic systems or sublattices. The static and dynamic properties of such magnetic structures have been discussed in some detail. The magnetic anisotropy field H_A, the subject of immediate interest in this paper, is obtained most directly from AFMR.

For sublattices aligned along the c axis the resonance condition[2] is

$$\omega/\gamma=[2H_EH_A+(\tfrac{1}{2}\alpha H_0)^2]^{1/2}\pm H_0(1-\tfrac{1}{2}\alpha)\,, \qquad (1)$$

where ω is the angular frequency, γ the magnetogyric factor, H_E the exchange field, H_0 the applied field, and α is the ratio of the parallel (c axis) to perpendicular susceptibilities $\chi_{\parallel}/\chi_{\perp}$. Often it is convenient to substitute $H_E=\lambda M$, $H_A=K/M$, where M is the sublattice magnetization and to a good approximation $\lambda=1/\chi_{\perp}$. K is the "magnetic anisotropy energy." Since the χ's and γ are evaluable separately, the results of an AFMR experiment can determine H_A (or K). (The values of λ and K derived from experiments do not involve an explicit evaluation of M.)

Contributions to K are the exchange anisotropy (presumed to be negligibly small here[3] and hence not discussed further), the dipolar anisotropy K_{MD} arising from magnetic dipolar interaction, and the fine structure anisotropy K_{FS} of the individual metal ions arising from higher order spin-orbit effects. The latter corresponds to the ground-state splitting $2D$ frequently investigated in diluted magnetic systems by EPR. (Direct experimental evaluation of $2D$ in concentrated systems usually is not feasible, neither is a theoretical computation from first principles.) However, the experimentally deduced K in conjunction with a computed K_{MD} can be used to assign a value to K_{FS}.

To compute K_{MD} the details of the crystal geometry must be specified. In hexagonal geometry these are the hexagonal axis and basal plane lattice parameters (C_0 and A_0) and the metal ion special position parameter w. The value of v, the oxygen special position parameter, is not relevant. The results of K_{MD} calculations for the Cr, Fe, Ti, and V sesquioxides are presented here. In the cases of Cr and Fe sufficient information is available to determine K_{FS}. No consistent

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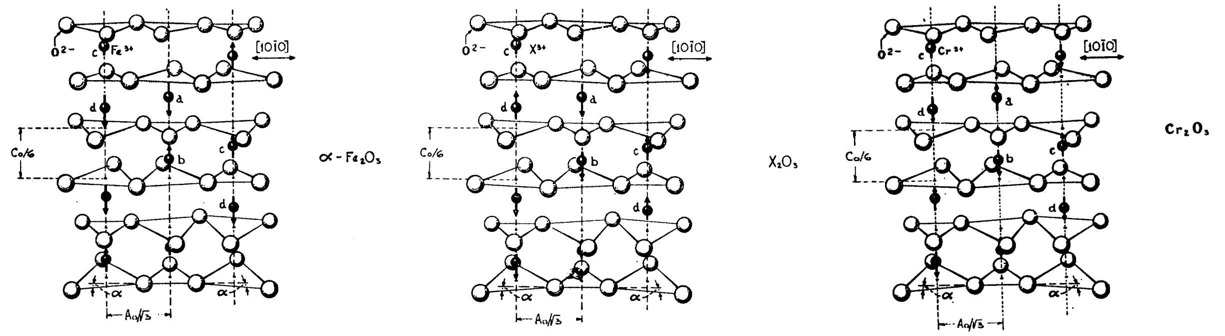
[†] Supported by Bureau of Naval Weapons, Department of the Navy, under Contract No. NOw 62-0604-c with The Johns Hopkins University.

[‡] Supported by the U. S. Air Force Office of Scientific Research.

[1] For a recent general review see *Magnetism*, edited by George T. Rado and H. Suhl (Academic Press Inc., New York, 1963). An earlier review by T. Nagamiya, K. Yosida, and R. Kubo is presented in *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1955), Vol. 4.

[2] T. Nagamiya, Progr. Theoret. Phys. (Kyoto) **6**, 350 (1951); C. Kittel, Phys. Rev. **82**, 565 (1951); F. Keffer and C. Kittel, *ibid.* **85**, 329 (1952).

[3] M. Tachiki and T. Nagamiya, J. Phys. Soc. Japan **13**, 452 (1958).



(a) (b) (c)

FIG. 1. Spin orientations in Shull structures (a), (b), and (c). The moments are directed parallel to the hexagonal axis.

correlation with the dilute system EPR value of $2D$ is found for either α-Fe_2O_3 or Cr_2O_3. The "spin flip" in α-Fe_2O_3 is shown to be consistent with a reversal in sign of H_A. Owing to the use of inappropriate crystal data a previous calculation of K_{MD} for Cr_2O_3 is shown to be in serious error. Cr_2O_3 AFMR results are reinterpreted on the basis of the present calculations.

II. MAGNETIC DIPOLAR FIELD AND ENERGY CALCULATIONS

Three distinct dispositions of relative spin orientations exist which, following Shull,[4] we designate as (a), (b), and (c). For the sequence of ions along the c axis in a magnetic unit cell these are (a) $+--+$, (b) $--++$ and (c) $-+-+$. (We take these orientations to refer to the *site* sequence *bacd* in corundum structures.[5] Two simple modes for the *geometrical* moment orientation are (1) along the c axis, (2) normal to the c axis, possibly directed parallel to one of the three twofold axes. Figure 1 displays the three Shull structures when the moments are along the c axis.

In such an array the magnetic dipolar field $\mathbf{H}$ at a metal ion site, bearing an individual moment $\boldsymbol{\mu}$, is

$$H_i = D_i \mu_i\,,\qquad i = x,\, y,\, z\,, \tag{2}$$

where $\mathbf{D}$ includes geometrical as well as orientation factors. The c-axis direction corresponds to $\hat{z}$. As in the familiar Lorentz calculation $\sum_i D_i = 0$; hence, $D_x = D_y = -\frac{1}{2}D_z$. (This is the result for an m-fold axis of rotation where $m > 3$. For $m = 2$ either $D_x = D_y = D_z = 0$ or $D_x \neq D_y \neq D_z$.)

D_z (in units of number of μ_B per dipole) follows from the summation

$$D_z = \mu_B \sum_i P_i (3\cos^2\theta_i - 1)/R_i^3\,, \tag{3}$$

where P_i specifies the orientation of the dipole i ($+$ or $-$), and R_i and θ_i its location with respect to the reference site. The magnetic dipolar anisotropy *per dipole* is

$$-\tfrac{1}{2}\boldsymbol{\mu}\cdot\mathbf{H} = -\tfrac{1}{2}\mu^2 D_z (3\cos^2\theta - 1)/2\,, \tag{4}$$

where θ is the angle between $\boldsymbol{\mu}$ and $\hat{z}$. It is customary to write the anisotropy energy as $K_{MD}\sin^2\theta$. From Eq. (4) we then set the anisotropy constant

$$K_{MD} = \tfrac{1}{2} n^2 \mu_B D_z \times \tfrac{3}{2}\,, \tag{5}$$

where n is the number of μ_B/dipole.

Machine computation programs previously used for determining electric fields in corundum-type lattices[5] were adapted readily to the magnetic summation required [Eq. (3) and Fig. 1]. In Shull cases (b) and (c) the bipyramid spherical cluster method was used. (See Ref. 5 for geometrical details.) Convergence was obtained in all cases by including clusters located within spheres of radius $6A_0$ about the centroid of the reference c-d bipyramid. The results for c and d reference positions were appropriately averaged. For Shull case (a) a *double* bipyramid cluster grouping gave slightly better convergence.

III. DISCUSSION OF D_z COMPUTATIONS

Computations of D_z for the Cr, Fe, Ti, and V sesquioxides are given in Table I in units of gauss/(number of μ_B per dipole). Although the configurations for Cr_2O_3 and Fe_2O_3 have been established as types (c) and (a), respectively, the calculations were made as a matter of form for each of the above four crystals in all three Shull cases. Unless otherwise specified the crystallographic data are those obtained by Newnham and de Haan[6] at 25°C. The D_z values for structures (a) and (b) are comparable in magnitude but differ in algebraic sign. Structure (c) evidently is one in which the magnetic geometry is almost cubic! Comments on specific sesquioxides follow:

Ti_2O_3. The antiferromagnetic structure is in dispute. Abrahams,[7] from single-crystal neutron diffraction work, identifies it as type (a)-(2). According to Al'shin

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[4] C. G. Shull, W. A. Strauser, and E. O. Wollan, Phys. Rev. **83**, 333 (1951).

[5] J. O. Artman and John C. Murphy, Phys. Rev. **135**, A1622 (1964).

[6] R. E. Newnham and Y. M. de Haan, Z. Krist. **117**, 235 (1962).

[7] S. C. Abrahams, Phys. Rev. **130**, 2230 (1963).

TABLE I. Values of D_z [units of kilogauss/(number of μ_B per dipole)] at a positively oriented dipole site for various sesquioxide structures and magnetic symmetry configurations. The crystallographic data are those of Newnham and de Haan (Ref. 6) except for the one marked SCA, obtained from Abraham's low-temperature experiments (Ref. 12), and the one marked GNH, obtained by scaling the NdH results to low temperatures by S. Greenwald's Cr_2O_3 variation factors [Nature **177**, 286 (1956)]. The oxygen special position parameter v (which does not enter into these calculations) and the Al_2O_3 data are given for reference purposes.

	Magnetic symmetry configuration (Shull notation)			Lattice parameters [space group $D_{3d}^6(R\bar{3}c)$]			
	(a)	(b)	(c)	A_0	C_0	w	v
Crystal							
Cr_2O_3	−1.839	1.453	**0.028**	4.9607 Å	13.599 Å	0.0975	0.306
	−1.856	1.464	**0.039**	4.9466	13.601		(GNH)
Fe_2O_3	**−1.339**	0.982	0.159	5.0345	13.749	0.105	0.300
Ti_2O_3	−1.772	1.531	−0.161	5.149	13.642	0.0950	0.317
V_2O_3	−1.931	1.467	0.102	4.952	14.002	0.0963	0.315
	−1.876	1.412	0.126			0.0973	0.3077 (SCA)
Al_2O_3	···	···	···	4.7589	12.991	0.1020	0.306

and Astrov[8] the ME experiments suggest type (c)–(2) symmetry. The magnetoelectric effect can only arise in magnetic structures of *IR* symmetry [types (b) and (c) but not (a)]. Blume[9] suggests that type (b)–(2) symmetry might be compatible with these data. [To date type (b) symmetry has not been found in nature.] Further investigations currently are being pursued elsewhere to clarify the situation. Although a crystallographic transformation to monoclinic symmetry occurs, crystal data for D_{3d}^6 geometry are sufficient for our purpose. n equals 0.2 (Ref. 7).

V_2O_3. The presumed antiferromagnetic ordering has not been identified.[10] Evidence for a monoclinic transition at 168°K similar to that in Ti_2O_3 exists.[10,11] The ME effect has been searched for but has not yet been detected.[8] Abrahams believes that the V_2O_3 and Ti_2O_3 magnetic structures are probably the same.[12] He also has obtained a low-temperature w value[12] of 0.0973 for which the calculations are repeated.

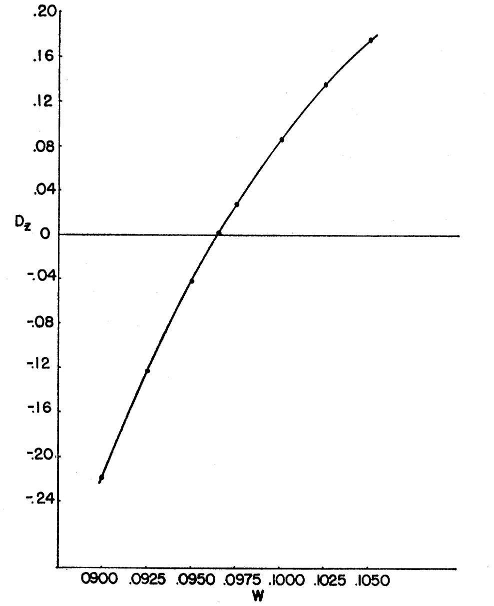

FIG. 2. D_z [units of 10^3 G/(number of μ_B per dipole)] versus w for Cr_2O_3. $A_0=4.9607$ Å, $C_0=13.599$ Å.

Cr_2O_3. Through the work of Brockhouse[13] and McGuire *et al.*,[14] the structure has been identified as (c)–(1). In the "spin-flop" configuration[15] (achieved by applying a sufficiently high magnetic field along the c axis) (c)–(2) probably would be appropriate. The sensitivity of D_z computations in structure (c) to lattice geometry is evident in Table I. It is graphically indicated in Fig. 2 for the Cr_2O_3 A_0 and C_0 values of 4.9607 and 13.599 Å, respectively and w's between 0.0900 and 0.1050. D_z is negative for w's below 0.0964. Further details of the geometrical influences on D_z are given in Figs. 3 and 4. Such nomograms may be useful in interpreting the consequences of pressure or temperature induced lattice changes.

With Newnham's crystallographic data, using $n=3$, we obtain a K_{MD} [Eq. (5)] of 0.0088 cm^{-1}/ion. The previously accepted value of Tachiki and Nagamiya[3] is 0.059 cm^{-1}/ion, six times as large. Since these authors use the Fe_2O_3 w value of 0.105 instead of the presently accepted Cr_2O_3 value of 0.0975 (the Cr_2O_3 data at the time were incomplete) the discrepancy is understandable in view of the geometrical sensitivities that we have discussed. (In particular for $w=0.105$ and Newnham's Cr_2O_3 A_0 and C_0 values we obtain D_z and K_{MD} values of 0.177 and 0.0559 cm^{-1}/ion, respectively, in good agreement with the Tachiki and Nagamiya result.) Cr_2O_3 AFMR interpretations, previously made[16] on the basis of the Tachiki and Nagamiya result, must therefore be revised. These will be discussed below.

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[8] B. I. Al'shin and D. N. Astrov, Zh. Eksperim. i Teor. Fiz. **44**, 1195 (1963) [English transl: Soviet Phys.—JETP **17**, 809 (1963)].

[9] M. Blume (private communication).

[10] A. Paoletti and S. J. Pickart, J. Chem. Phys. **32**, 308 (1960).

[11] E. P. Warekois, J. Appl. Phys. **31**, 346*S* (1960).

[12] S. C. Abrahams (private communication).

[13] B. N. Brockhouse, J. Chem. Phys. **21**, 961 (1953).

[14] T. R. McGuire, E. J. Scott, and F. H. Grannis, Phys. Rev. **102**, 1000 (1956).

[15] S. Foner and S. L. Hou, J. Appl. Phys. **33**, 1289S (1962).

[16] S. Foner, Phys. Rev. **130**, 183 (1963).

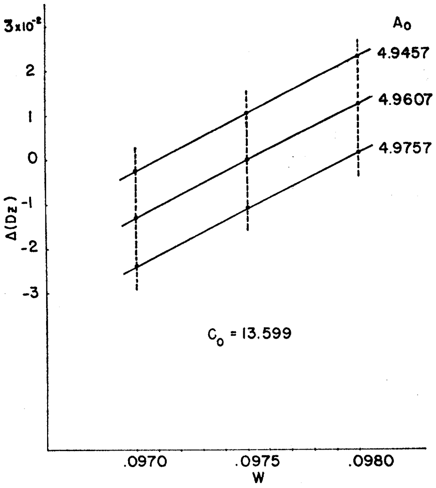

FIG. 3. Families of curves of $\Delta(D_z)$ versus w for Cr_2O_3. $C_0=13.599$ Å, $A_0=4.9457$, 4.9607, and 4.9757 Å. Fiduciary point at $A_0=4.9607$, $C_0=13.599$, $w=0.0975$.

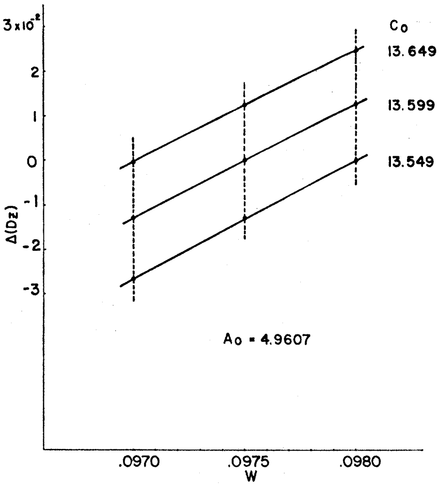

FIG. 4. Families of curves of $\Delta(D_z)$ versus w for Cr_2O_3. $A_0=4.9607$ Å, $C_0=13.649$, 13.599, 13.549 Å. Fiduciary point at $A_0=4.9607$, $C_0=13.599$, $w=0.0975$.

α-Fe_2O_3. Shull *et al.*[4] established that below the "spin-flip" transition, circa 250°K, the magnetic and geometric configurations are types (a) and (1), respectively; above the transition the configurations are (a) and (2). Tachiki and Nagamiya[3] quote a K_{MD} value, computed by Hirota *et al.*,[17] of -1.15 cm^{-1}/ion. For $n=5$ our D_z value corresponds to -1.172 cm^{-1}/ion which compares favorably. In Figs. 5, 6, and 7 we have prepared a sequence of curves, similar to the preceding Cr_2O_3 examples, which may prove useful in lattice variation considerations.

IV. APPLICATIONS TO AFMR

From the definition [Eq. (5)] we note that K_{MD} has the same algebraic sign as D_z. $K_{FS}\equiv -S(S-\frac{1}{2})D$ (Ref. 18) where S is the spin quantum number (equivalent to one-half the previously defined n); hence K_{FS} is opposite in sign to D. Low-temperature values of K (from AFMR), K_{MD} from our calculation and K_{FS} are listed in Table II for Cr_2O_3 and Fe_2O_3. In the case of Cr_2O_3 the AFMR derived K_{FS} value is about 0.05 the EPR value.[19] K_{MD} and K_{FS} are comparable in magnitude. (The previous K_{MD} value[16] led to a small *negative* K_{FS}.) Statistical effects which appear as T increases from 0°K toward T_N would be expected to decrease both K_{MD} and K_{FS}. Since they are of the same sign no unusual magnetic behavior is expected from this source.

TABLE II. Tabulation of K, K_{MD}, and K_{FS} for Cr_2O_3 and Fe_2O_3 units of 10^5 erg/cm^3. $K_{FS}=K-K_{MD}$. Cr_2O_3 entries (a) and (b) correspond to room and low-temperature crystal geometries, respectively (see Table I). (c) is the K_{FS} value derived from EPR of diluted ions. For Fe_2O_3 (d) represents a current experimental estimate by S. Foner and (e) is the EPR K_{FS} value for diluted ions.

	K	K_{MD}	K_{FS}
Cr_2O_3	2.0	0.73 (a)	1.3
		1.00 (b)	1.0
			23.4 (c)
Fe_2O_3	2.0 (d)	-92.0	$\sim+94.0$
			-67.4 (e)

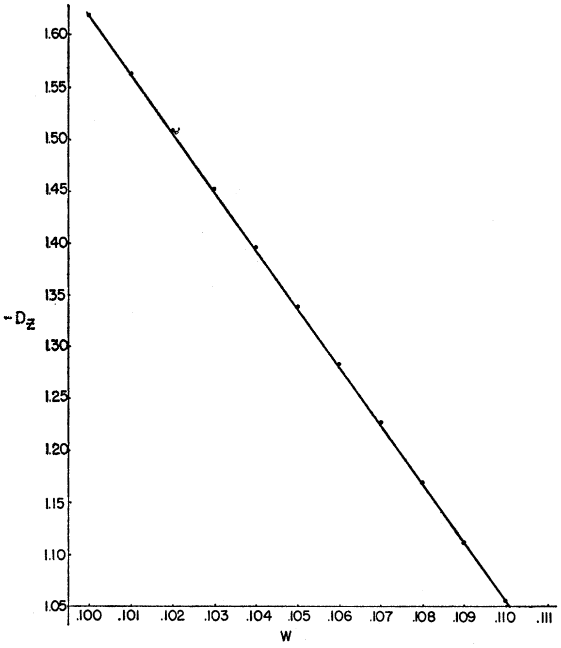

FIG. 5. $-D_z$ [units of 10^3 G/number of μ_B per dipole)] versus w for Fe_2O_3. $Å_0=5.0345$ A, $C_0=13.749$ Å.

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[17] A. Hirota, H. Suzuki, A. Tsubaki, and T. Nagamiya, presented at the Japanese Physical Society Meeting of April 1957, quoted in Ref. 3

[18] K. Yosida, Progr. Theoret. Phys. (Kyoto) **6**, 691 (1951).

[19] A. A. Manenkov and A. M. Prokhorov, Zh. Eksperim. i Teor. Fiz. **28**, 762 (1955) [English transl.: Soviet Phys.—JETP **1**, 611 (1955)].

The situation in Fe_2O_3 is quite different. Here at low temperatures $K_{\rm MD}$ and $K_{\rm FS}$, though differing in magnitude by only 2%, are opposite in sign. The positive $K_{\rm FS}$ predominates resulting in a K comparable to that of Cr_2O_3. The AFMR $K_{\rm FS}$ value is -1.4 times the EPR value.[20] Although the *angular* dependence of the magnetic dipolar and fine-structure anisotropy energies is the same, their temperature variations expected on a quantum statistical basis are different since $K_{\rm MD}\propto\langle S_z\rangle^2$, $K_{\rm FS}\propto\langle S_z^2\rangle$ (Ref. 3). As T rises toward T_N we may anticipate from this mechanism a reversal in the sign of K and a consequent "flip-over" of the spins into the basal plane. The necessary equations[3,18] are given below,

$$\begin{aligned} &K_{\rm MD}(T)=K_{\rm MD}(0)B_S^2(X),\\ &K_{\rm FS}(T)=K_{\rm FS}(0)[2(S+1)-3B_S(X)\coth X/(2S)]\\ &\qquad\qquad\times(1/2S-1), \qquad (6)\\ &\quad X=(3S/S+1)(T_N/T)B_S(X),\\ &\quad S=\tfrac{5}{2} \quad \text{for} \quad Fe_2O_3. \end{aligned}$$

The results of computations of $-K_{\rm MD}(T)$ and $K_{\rm FS}(T)$ for Fe_2O_3 are presented in Fig. 8.[21] The data of Table II are used. The quantities actually plotted are the effective anisotropy fields $-H_{\rm MD}$ and $H_{\rm FS}$ set equal to 100.4×10^2 and 102.6×10^2 G, respectively, at absolute zero. The curves cross at $T/T_N=0.281$ in surprisingly good agreement with the commonly accepted T_N and $T_{\rm flip}$ values of 948 and 253°K, respectively, $(T/T_N=0.267)$. The consensus of more recent investigations seems to be that T_N and $T_{\rm flip}$ are 961 and 263°K, respectively.[22] These correspond to a ratio of 0.274.

This agreement may be fortuitous although the general character of the result is reasonable. We assume that the spin-wave corrections are relatively small at low temperatures and that the magnetization approximates $B_{5/2}$ over the limited temperature range examined. The AFMR and spin-flop evaluations of $(2\lambda K)^{1/2}$ at this time are known to within 10%. The transition temperature usually is not defined to better than 10°. Furthermore, the small changes in lattice parameter usually occurring at the magnetic transition have not been included. As seen from the almost complete annulment of $H_{\rm MD}$ and $H_{\rm FS}$, $T_{\rm flip}$ would be affected strongly for instance, by small changes in $H_{\rm MD}$ arising from the presence of impurities. Such effects make difficult the correlation of data obtained from various sources.

We conclude this section by revising the Cr_2O_3 interpretation previously presented in Ref. 16. We indicate in Fig. 9 the curve of K versus T/T_N shown in this reference. We have also plotted in this figure $K_{\rm MD}$ and have subtracted to find the difference $K_{\rm FS}$ which is also noted. In the $K_{\rm MD}$ computation, allowance was made for the effects of temperature on the lattice parameters. Instead of the function $B_{3/2}$ [see

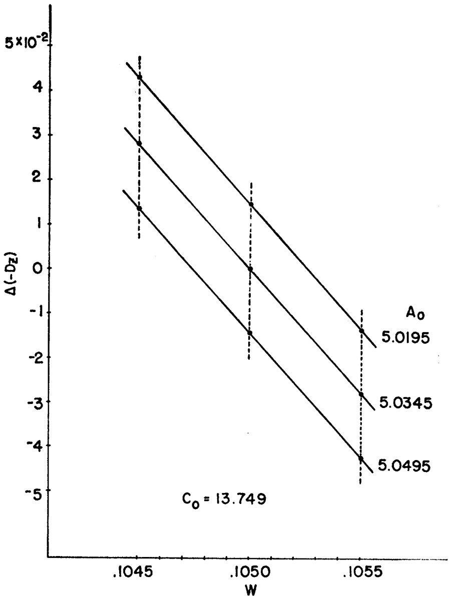

FIG. 6. Families of curves of $\Delta(-D_z)$ versus w for Fe_2O_3. $C_0=13.749$ Å, $A_0=5.0195$, 5.0345, 5.0495 Å. Fiduciary point at $A_0=5.0345$, $C_0=13.749$, $w=0.1050$.

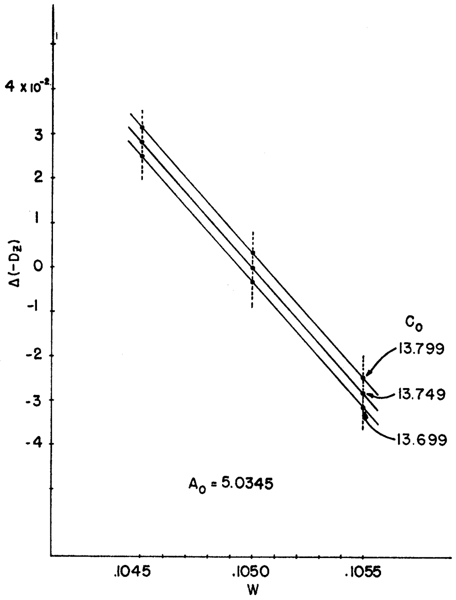

FIG. 7. Families of curves of $\Delta(-D_z)$ versus w for Fe_2O_3. $A_0=5.0345$ Å, $C_0=13.799$, 13.749, 13.699 Å. Fiduciary point at $A_0=5.0345$, $C_0=13.749$, $w=0.1050$.

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[20] H. F. Symmons and G. S. Bogle, Proc. Phys. Soc. (London) **79**, 468 (1962).

[21] The necessary thermodynamic data were obtained from the tabulations of L. P. Schmid and J. S. Smart, NAVORD Report 3640, 1954 (unpublished) and Eric D. Thompson, Lincoln Laboratory, M.I.T. (unpublished).

[22] M. Blackman and G. Kaye, J. Phys. Soc. Japan **17**, Suppl. B-II, 289 (1962) S. Freier *et al.*, Phys. Letters **2**, 191 (1962); A. H. Morrish, G. B. Johnston and N. A. Curry, Phys. Letters **7**, 177 (1963); P. Gilad *et al.*, *ibid.* **7**, 239 (1963); C. M. Isererant, G. G. Robbrecht, and R. J. Doclo, *ibid.* **11**, 14 (1964).

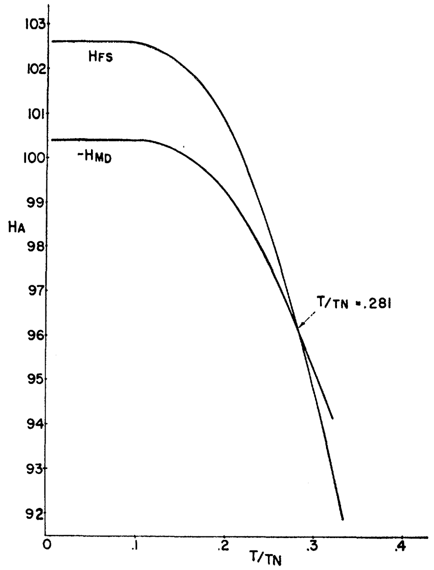

FIG. 8. Plot of the temperature variation of the effective magnetic fields due to magnetic dipolar anisotropy (H_{MD}) and fine structure anisotropy (H_{FS}) in Fe_2O_3. See Eq. (6). Units of 10^2 G are used. At $T=0°$K, H_{MD} and H_{FS} are assigned the values of -100.4 and 102.6, respectively.

Eq. (6)] we used the Cr_2O_3 reduced magnetization curve recently found by neutron diffraction techniques.[23] On this basis K_{FS} exhibits a large hump centered at $T/T_N=0.7$, a reflection of a corresponding hump in the plot of K peaked near $T/T_N=0.6$.

V. OTHER APPLICATIONS

It is apparent from the present analysis that a determination of K_{FS} in a dilute magnetic system has little correlation with the value actually existing in the concentrated system. (Some other aspects of dilute and concentrated system behavior are discussed in Ref. 5.) In systems with small atomic dilutions f, such as $Cr_{2(1-f)}Al_{2f}O_3$, we would expect $H_{\mathrm{MD}}(f)=H_{\mathrm{MD}}(0)(1-f)$, $H_{\mathrm{FS}}(f)=H_{\mathrm{FS}}(0)$. However, superimposed upon this would be changes due to specific modifications in the lattice constants upon dilution. A similar complication would ensue when the temperature is varied where the statistical effects described in Eqs. (6), (or by more appropriate analyses) would have to be combined with specific geometrical modifications. In the case of Cr_2O_3, the extreme geometrical sensitivity of D_z suggests that a sequence of low-temperature crystallographic investigations of A_0, C_0, and w would prove useful. We have prepared Figs. 2–7 in the hope that they will assist in the correlation of such research (and related stress experiments for example) with AFMR and other data.

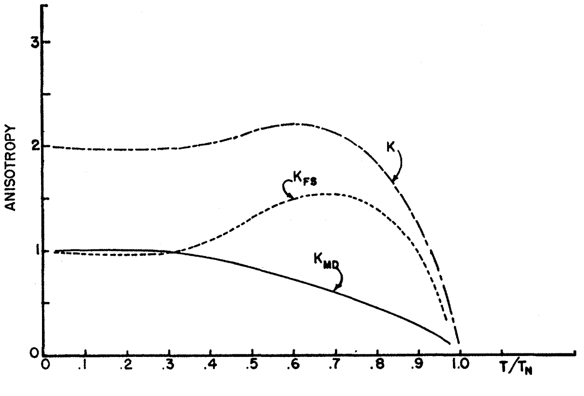

FIG. 9. Anisotropy (units of 10^5 erg/cm^3) versus reduced temperature T/T_N for Cr_2O_3. The curve of total anisotropy K is adapted from the AFMR interpretations of Foner, Fig. 17 of Ref. 16. The dipolar anisotropy K_{MD}, computed by the methods of this paper, is subtracted from K to yield the fine-structure anisotropy K_{FS}.

In the α-Fe_2O_3 case the prediction of the spin flip-over from the interplay of the opposing anisotropies is a most interesting result. The study of magnetic dilution effects from, for example, work in mixed Fe-Al sesquioxide systems is of especial interest here. In these Cr and Fe cases it may be of interest to inquire within what sphere radius are the *individual* site contributions to D_z of the same order (or more) than the total net value. The result for Fe_2O_3 is $0.38\,A_0$, for Cr_2O_3 $1.39\,A_0$. This illustrates the totally different nature of the D_z convergence in Shull cases (a) and (c).

We note an error in the Cr_2O_3 tabulation of Ref. 16, Table I. M_0 and H_E should be doubled and H_A halved. However, the values of λ and K, the quantities generally used in analysis, are stated correctly.

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