the individual atom. (Mass and volume are of course important, but are neglected for the moment to preserve the simplicity of the picture.) Thus, an alloy containing 5% Fe and 5% Ni shows a behavior similar to that of an alloy with 10% Co. In the same way, an alloy with 5% Ru and 5% Pd duplicates the one with 10% Rh.

Carrying this concept further, it was possible to ob-tain a superconducting compound which seemed com-parable to $CoSi_2$, which becomes superconducting at 1.4°K. It is $CoZr_2$ which becomes superconducting at 6.3°K. We found also that $NiZr_2$ becomes superconduct-ing at 1.52°K.

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Magnetic Moment Arrangements and Magnetocrystalline Deformations in Antiferromagnetic Compounds*

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The neutron diffraction data of Shull *et al.* on the powder specimens of MnO, FeO, CoO, etc., are re-examined. It is found that except for FeO the observed Debye-Scherrer patterns may be produced by a number of magnetic moment arrangements with the same antiparallel coupling among the moments on the next nearest neighboring ions, but with different sublattice correlations and different orientations of mag-netic axis (or axes). The symmetry change observed at the Néel point is interpreted as a strong effect of spontaneous anisotropy magnetostriction. As a consequence the uniaxial direction of the modified symmetry must coincide with that of the magnetic axis. Assignments of antiferromagnetic arrangements for the com-pounds are reached. Our prescription does not agree with that of Shull *et al.* except in the case of FeO. The sharp readjustment of lattice parameters at the transition temperature and the orientation of spin axis in other antiferromagnetic compounds are discussed from the viewpoint of the anisotropy magnetostriction approach.

I. INTRODUCTION

IN this note we intend to give a close re-examination of the neutron diffraction data obtained by Shull *et al.*[1] on MnO, FeO, CoO, NiO, MnS, and MnSe in powder form. This study is of interest in view of the fact that whereas FeO, MnO, NiO, and MnS are dis-torted slightly from the cubic to rhombohedral sym-metry and CoO becomes tetragonal at temperatures below the Néel point, yet the arrangements of moments on magnetic ions assigned by Shull *et al.* to MnO, NiO, MnS, and CoO are all the same, both as to the con-figuration of + and − spins and the direction of spin axis.[2] It should be remarked that the symmetry changes stated above are established results of more than one author[3,4] using x-ray techniques. The explanation of this magnetocrystalline effect put forward by Smart and Greenwald[5] is not consistent with the same discrepancy.

From our analysis of the neutron diffraction data and the hypothesis of anisotropy magnetostriction we pre-scribe for these compounds (except FeO) antiferro-magnetic arrangements different from those assigned previously. We shall also discuss the crystallographic position of the magnetic axis in other antiferromagnetics such as Cr_2O_3, MnF_2, etc.

The neutron diffraction patterns of MnO, MnS, MnSe, CoO, and NiO below their respective Néel points are alike. The pattern of FeO is slightly different with the singular absence of a certain magnetic diffrac-tion line. Shull *et al.* find that the magnetic unit cell dimensions are twice as large as the dimensions of a chemical unit cell and that the *next nearest* neighboring magnetic ions must have the spins opposite. These statements are conclusive and can be verified with little effort. However, there are two types of spin arrange-ments, both consistent with the next nearest antiparallel coupling, but different in the coupling among the *nearest* neighboring magnetic ions. They are illustrated in Fig. 1. In type *A* the four face-centered cubic (f.c.c.) sublattices of antiparallel spins are correlated such that on each (111) plane the spins are parallel and the spins on two neighboring (111) planes opposite; in type *B* this particular coupling among the nearest spins is absent. The four f.c.c. sublattices divide the full f.c.c. lattice in such a way that no two *nearest* neighboring ions are in the same sublattice. Shull *et al.* have shown that a satisfactory agreement is obtained between the

[1] Shull, Strauser, and Wollan, Phys. Rev. **83**, 333 (1951).
[2] Since we do have in some cases orbital contributions to the magnetic moment, it is preferable to use the terms "antiferro-magnetic axis" or "magnetic axis" instead of "spin axis." We shall use them alternatively with the same meaning. Similarly, "spins" and "magnetic moments" are used interchangeably.
[3] H. P. Rooksby, Acta Cryst. **1**, 226 (1948); N. C. Tombs and H. P. Rooksby, Nature **165**, 442 (1950); H. P. Rooksby and N. C. Tombs, Nature **167**, 364 (1951).
[4] S. Greenwald and J. S. Smart, Nature **166**, 523 (1950); S. Greenwald, Acta Cryst. **6**, 396 (1953).
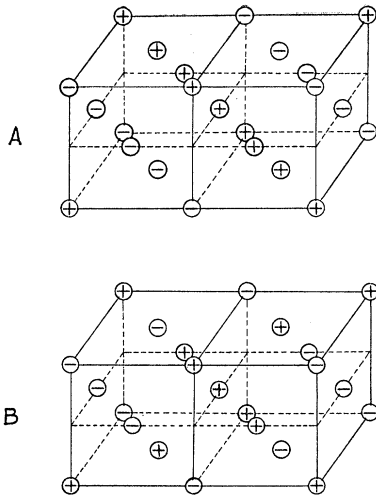[5] J. S. Smart and S. Greenwald, Phys. Rev. **82**, 113 (1951).

FIG. 1. Two different arrangements of magnetic moments with antiparallel coupling between the *next nearest* neighbors on the f.c.c. lattice.

observed diffraction pattern of MnO and the calculated peak intensities by assuming a configuration of type A with the spin axis in a cubic direction, and that the pattern in FeO can be accounted for by assuming a type A arrangement with a [111] spin axis. They also conclude that CoO, NiO, MnS, and MnSe have the same spin arrangement as MnO. They recognize the alternative arrangement of type B but reject it on the grounds that no distortion of the cubic symmetry would be expected at the antiferromagnetic transition. We shall take a different point of view on this matter in the coming discussion.

II. DEBYE-SCHERRER INTENSITY AND ALTERNATIVE ASSIGNMENTS OF MAGNETIC STRUCTURE

Before we proceed to state our viewpoint, it is necessary to consider, in detail, the Debye-Scherrer intensity of these compounds. Since unpolarized neutrons were used in the experiments, the observed intensity is the sum of nuclear and magnetic diffractions. The former is independent of the magnetic structure and so we need only to discuss the magnetic diffraction intensity factor $|\mathbf{q}F_m|^2$, where F_m is the magnetic structure amplitude of a magnetic unit cell and $\mathbf{q}$ is $\kappa(\kappa\cdot\mathbf{n})-\mathbf{n}$, where κ and $\mathbf{n}$ are respectively the unit vector in the direction of the scattering vector and the magnetic axis. We have for the type A configuration

$$F_m = 8f_m\{1-\exp i\pi(h+k)/2$$
$$-\exp i\pi(k+l)/2-\exp i\pi(l+h)/2\}, \quad (1A)$$

and for type B

$$F_m = 8f_m\{1+\exp i\pi(h+k)/2$$
$$-\exp i\pi(k+l)/2-\exp i\pi(l+h)/2\}, \quad (1B)$$

where

$$f_m = (e^2/mc^2)\nu Sf \quad (2)$$

is the magnetic scattering amplitude of the magnetic ion concerned, whose spin quantum number is S. ν is the magnetic moment of the neutron, and f is an atomic form factor which takes care of the decrease of the scattered amplitude as a result from the finite extension of the magnetically active electrons. h, k, and l are the indices referred to the magnetic unit cell and are all odd numbers in the equations. ($F_m=0$ for h, k, and l not all odd.) The factor 8 is found in the equations, because for odd indices the diffractions by the 8 chemical unit cells in a magnetic unit cell are coherent. Let α, β, and γ be the direction cosines of the magnetic axis. We write

$$q^2 = 1 - (\alpha h + \beta k + \gamma l)^2/N, \quad (3)$$

where

$$N = h^2 + k^2 + l^2.$$

For type A we derive:

$$|F_m/8f_m|^2 = \begin{cases} 16, \text{ when } \begin{matrix} h-k \\ k-l \\ l-h \end{matrix} \right\} \text{are divisible by 4,} \\ 0, \text{ otherwise;} \end{cases} \quad (4A)$$

and

$$q_{Av}^2 = \tfrac{2}{3}\{1-(\alpha\beta+\beta\gamma+\gamma\alpha)(hk+kl+lh)/N\}. \quad (5A)$$

For type B:

$$|F_m/8f_m|^2 = 4, \quad (4B)$$

and

$$q_{Av}^2 = \tfrac{2}{3}, \quad (5B)$$

independent of α, β, and γ. q_{Av}^2 is the average of q^2 calculated over all the possible permutations and combinations of signs of $(\pm h, \pm k, \pm l)$ with given h, k, and l for which F_m is not zero. For type A three out of four of all these permutations and combinations of signs do not satisfy the condition that $h-k$, $k-l$, and $l-h$ be divisible by 4. They make no contribution to the intensity. Those with $h-k$, $k-l$, and $l-h$ divisible by 4 have an intensity four times that of each diffraction maximum of $B[\alpha\beta\gamma]$. Therefore, the spin arrangements $A[100]$ and $B[\alpha\beta\gamma]$ must yield the same Debye-Scherrer pattern, although their diffraction patterns produced by a single crystal under neutron irradiation should be markedly different.

The occurrence of more than one magnetic axis among the sublattices cannot be ruled out by physical considerations. Its influence on the susceptibilities has been discussed by Van Vleck.[6] We have evidence to believe that this is the case in MnO$_2$.[7] Therefore we must, in general, allow that the magnetic axes of the four sublattices in the MnO type compounds may be all in different orientations. Let $\mathbf{n}_i(\alpha_i,\beta_i,\gamma_i)$ with $i=0, 1, 2, 3$ be the unit vectors along the four magnetic axes and

[6] J. H. Van Vleck, J. phys. radium **12**, 262 (1951).
[7] R. A. Erickson, Phys. Rev. **85**, 745 (1952); H. Bizette and B. Tsai, *Colloque sur les Phenomenes Cryomagnetiques* (Perrin-Langevin, Paris, 1948).

$\mathbf{q}_i = \kappa(\kappa \cdot \mathbf{n}_i) - \mathbf{n}_i$. Now we have

$$\left| \sum_i \mathbf{q}_i(F_m)_i \right|^2 = (8f_m)^2 \left| \mathbf{q}_0 + \mathbf{q}_1 \exp i\pi(k+l)/2 \right.$$

$$\left. + \mathbf{q}_2 \exp i\pi(l+h)/2 + \mathbf{q}_3 \exp i\pi(h+k)/2 \right|^2. \quad (6)$$

We derive the intensity of a Debye-Scherrer line

$$I(hkl) \propto \sum_{(\pm h, \pm k, \pm l)} \left| \sum_i \mathbf{q}_i(F_m)_i \right|^2 = 4(8f_m)^2 p Q_{\text{Av}}{}^2, \quad (7)$$

where $\sum_{(\pm h, \pm k, \pm l)}$ is summed over all the possible permutations and combinations of signs of $(\pm h, \pm k, \pm l)$, and p is the multiplicity factor.

$$Q_{\text{Av}}{}^2 = \tfrac{2}{3}[1 - \phi(\mathbf{n}_0, \mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)(h^*k^* + k^*l^* + l^*h^*)/N], \quad (8)$$

with

$$\phi(\mathbf{n}_0, \mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3) = \tfrac{1}{4}(\alpha_1\beta_2 + \beta_1\alpha_2 + \beta_2\gamma_3 + \gamma_2\beta_3 + \gamma_3\alpha_1 + \gamma_1\alpha_3$$
$$- \alpha_0\beta_3 - \beta_0\alpha_3 - \beta_1\gamma_0 - \gamma_1\beta_0 - \gamma_2\alpha_0 - \alpha_2\gamma_0), \quad (9)$$

and (h^*, k^*, l^*) is one of those combinations of $(\pm h, \pm k, \pm l)$ such that $h^* - k^*$, $k^* - l^*$, and $l^* - h^*$ are all divisible by 4. When we put $\mathbf{n}_0 = \mathbf{n}_1 = -\mathbf{n}_2 = -\mathbf{n}_3$ the general case is reduced to the type B arrangement discussed above, and the right-hand side of Eq. (9) is zero. Similarly, when $\mathbf{n}_0 = -\mathbf{n}_1 = -\mathbf{n}_2 = -\mathbf{n}_3 = \mathbf{n}(\alpha, \beta, \gamma)$ we have the type A arrangement and $\phi = (\alpha\beta + \beta\gamma + \gamma\alpha)$. In both cases $Q_{\text{Av}}{}^2$ reduces to $q_{\text{Av}}{}^2$ given by Eq. (4A) and (4B) respectively. In general any arrangement making $\phi = 0$ must produce the same Debye pattern as that of $A[100]$ and $B[\alpha\beta\gamma]$ and those satisfying $\phi = 1$ must produce a powder diffraction pattern, the same as that of $A[111]$. Among the former we are specially interested in the case of $\mathbf{n}_0 = \mathbf{n}_1 = (100)$ and $\mathbf{n}_2 = \mathbf{n}_3 = (010)$. For this arrangement the notation $C[100][010]$ will be used.

It is inevitable to conclude that with the powder diffraction data alone a large number of spin arrangements may be assigned to each of the MnO type compounds. When we assume a single magnetic axis for the four sublattices, there is no ambiguity in the antiferromagnetic structure of FeO which must be $A[111]$, but even then the spin arrangement of MnO, NiO, CoO, MnS, and MnSe still cannot be decided. The analysis given in the preceding paragraph thoroughly illustrates the limitation of the Debye-Scherrer method in neutron diffraction work, a situation similar to that of the same method in the x-ray analysis. A precise assignment of a magnetic structure cannot be reached with the results of the powder diffraction technique alone, when there are more than two sublattices of parallel spins involved and the direction of spin axis (or axes) is not revealed by the singular absence of a certain diffraction line. In our case there are eight sublattices of parallel spins. In FeO we notice the singular absence of the (111) line.

We shall now look into the symmetry changes accompanying the magnetic transition. The rhombohedral distortion of the cubic structure of MnO and NiO produces a contraction in the [111] direction and that of the FeO an expansion in the same direction. In the

TABLE I. Crystalline deformation and assignment of magnetic moment arrangement in the MnO type compounds.

Compounds	MnO	FeO	CoO	NiO	MnS	MnSe
Symmetry[a]	Rh.	Rh.	Tet.	Rh.	Rh.	Rh.?
Rhombohedral angle, or tetragonality	$\alpha > 60°$	$\alpha < 60°$	$c/a < 1$	$\alpha > 60°$	?	?
Shull et al.[b]	$A[001]$	$A[111]$	$A[001]$	$A[001]$	$A[001]$	$A[001]$
This note	$B[111]$	$A[111]$	$B[001]$ or $A[001]$ or $C[100][010]$	$B[111]$	$B[111]$	$B[111]$

[a] Rh. = rhombohedral; Tet. = tetragonal.
[b] See reference 1.

type A arrangement a contraction or an expansion in the trigonal direction changes the distance between the antiferromagnetically coupled spins on the neighboring (111) planes. Smart and Greenwald have proposed to explain the symmetry distortion by assuming that the dependence of the exchange integral J on the distance between magnetic ions is in favor of such a contraction or an expansion. However, the tetragonal deformation of CoO directly contradicts this exchange magneto-striction hypothesis. We shall adopt the viewpoint that this magnetocrystalline effect is simply a strong manifestation of (spontaneous) anisotropy magnetostriction. The deformation amounts to a strain of 10^{-3} to 10^{-2} which is larger than the usual magnetostriction by several orders of magnitude. The term anisotropy magnetostriction is used to describe the fact that the anisotropy energy depends on the strain, and, as a consequence of this and the minimization of the internal energy, the lattice of the antiferromagnetic crystal must be a deformed one with respect to the cubic lattice of the paramagnetic state.[8] In this mechanism it is the direction of magnetic axis rather than the configuration in which the moments on magnetic ions are coupled that determines the characteristics of the magnetocrystalline deformation. By symmetry considerations we expect that the compounds with rhombohedral symmetry, when antiferromagnetic, are the ones having the spin axis in the [111] direction. MnO, MnS, and NiO must have the type B arrangement but FeO the type A correlation of sublattices. Similarly, we may assign to CoO either the A or $B[001]$ arrangement or $C[100]$ [010], in each case [001] being the tetragonal axis. For the purpose of clarity we list in Table I the compounds, their symmetry below the Néel point, and the two antiferromagnetic structures prescribed respectively by Shull et al. and by the present writer. Because of the large number of possibilities that lead to a given value of ϕ of Eq. (9), our assignments given in Table I may not be the only ones consistent with the neutron diffraction data and the anisotropy magnetostriction hypothesis. It is interesting to note that according to our assignment the $B[111]$ structure is distorted by a contraction in the trigonal direction $(\alpha > 60°)$ and the $A[111]$ structure by an expansion in the same direction

[8] R. Becker and W. Döring, Ferromagnetismus (Verlag Julius Springer, Berlin, 1939), Chap. III, Sec. 11.

($\alpha < 60°$). A possible explanation of the different sign of $\Delta\alpha$ for FeO is that in the $A[111]$ structure exchange magnetostriction must also be expected to occur but not in the $B[111]$ structure.

The issue between the different assignments can be decided either by neutron diffraction on a single crystal or by measuring the susceptibilities of a single crystal to determine the direction of spin axis. Indirect evidence concerning the spin arrangement can be obtained by conducting the following suggested experiments which may be performed either on a sintered specimen or single crystal. The sharp decrease of Young's modulus of CoO and NiO at the Néel point as shown by Street and Lewis[9] and of CoO by Fine[10] indicates the readiness of the trigonal axis in NiO and the tetragonal axis in CoO to switch to a more favorable orientation, presumably a crystallographically equivalent one, under an applied stress. Single crystals of NiO are always badly twinned even under extremely careful handling and the distribution of twinned domains can be disturbed by a light touch.[11] In Rh. $A[100]$ structure the spin axis is not at all related to the rhombohedral direction, while in Rh. $A[111]$, Rh. $B[111]$, and Tet. A or $B[001]$ the spin axis coincides with the rhombohedral or tetragonal axis. Therefore, in the former the spin axis would not have to turn when the rhombohedral axis flops under external stress, but in the latter the spin axis must turn with the uniaxis of symmetry. The change of the direction of spin axis can be detected by the difference in susceptibility before and after the application of external stress. On the other hand, with a sufficiently strong magnetic field we could switch the spin axis from one of its normal direction to an equivalent one. In Rh. $A[111]$, Rh. $B[111]$, and Tet. $B[001]$ the uniaxis of the crystal must turn with the spin axis and produce an elastic strain. In Rh. $A[100]$ the three cubic directions are equivalent with respect to the rhombohedral axis. The switch of spin axis would not demand a flop of the rhombohedral axis, say, from $[111]$ to $[11\bar{1}]$ and so no strain would be induced. According to the following discussion an extremely strong field is required in this experiment.

III. DISCUSSION

Our anisotropy magnetostriction hypothesis must face the question of why the deformation is such a large effect in the MnO type compounds as well as other antiferromagnetics to be mentioned later, being larger than the magnetostriction in the ordinary ferromagnetics by orders of magnitude. We may answer this by affirming that the large magnetostriction is tied to a high anisotropy in the antiferromagnetics, since both are under the same influence of a strong spin-orbit coupling. The argument goes as follows:

The dipole-dipole term of the anisotropy energy has been calculated by Kaplan[12] for type A arrangement on an undeformed cubic lattice. He obtains

$$E_d = K_d(\alpha\beta + \beta\gamma + \gamma\alpha), \qquad (10A)$$

where

$$K_d = 1.64 \ 10^7 \ \text{ergs/cm}^3 \ \text{for MnO.} \qquad (11)$$

For type B arrangement our calculation shows

$$E_d = 0 \qquad (10B)$$

independent of the direction of spin axis. Evidently E_d of Eq. (10) in either case cannot be taken as the anisotropy energy we wish to discuss, since we have not considered the deformed symmetry, nor included the second order effect of the dipole interaction, nor the multipole interactions.[13] Moreover, we must also take into consideration the spin-orbit coupling. A calculation of the anisotropy energy including these effects would be enormously troublesome, even to obtain a quite approximate result. Fortunately, the following observation can be made from Eq. (10A). For the spin arrangement of FeO $A[111]$, E_d is a maximum of Eq. (10A) instead of a minimum. Therefore, this dipole-dipole energy is not the dominant term of the total anisotropy, although this term already amounts to 10^7 erg/cm^3. Accordingly, we must conclude that for the MnO type compounds the anisotropy energy is of the order of 10^8–10^9 erg/cm^3. (Incidentally, we may mention that in order to overcome such a high anisotropy a field of 10^5 gauss or higher would be required to turn the spin axis.) The origin of this high anisotropy should be sought in the Mn-O-Mn super-exchange. The importance of spin-orbit coupling in the calculation of anisotropy energy has been shown by Van Vleck.[13] When this coupling is not taken into consideration the second-order perturbation calculation of the dipole energy of a cubic ferromagnetic gives a result only 1/1000 of the observed anisotropy. The anomalous magnitude of the anisotropy can be reasonably attributed to the effect of the spin-orbit coupling with the anisotropy in the energy of orbital valence. This applies as well whether or not the inclusion of the multipole interactions besides the dipole term is necessary. Vonsovsky[14] has shown that with the orbital wave function acting as the bridge between the spin and the crystal lattice, the dependence of the dipole energy and the spin-orbit energy can account for the observed magnetostriction in the metals of the iron group. Presumably, a strong spin-orbit coupling should lead to a large magnetostriction. On the grounds of these connections we may hold that a large (spontaneous) magnetostriction should be found in magnetics of high anisotropy such as the MnO-type antiferromagnetics.

We shall present the following empirical findings to

[9] R. Street and B. Lewis, Nature 168, 1036 (1951).
[10] M. E. Fine, Revs. Modern Phys. 25, 158 (1953).
[11] W. Roth (unpublished).

[12] J. I. Kaplan, J. Chem. Phys. 22, 1709 (1954).
[13] J. H. Van Vleck, Ann. inst. Henri Poncaré 10, 57 (1947).
[14] S. V. Vonsovsky, J. Phys. (U.S.S.R.) 3, 181 (1940).

demonstrate some remarkable correlations between the magnetostriction and the anisotropy energy. The magnetostrictive energy (the sum of the elastic strain energy and the magnetoelastic energy) may be expressed by an increment ΔK in the anisotropy constant. ΔK is a function of the elastic moduli and the magnetostrictive constants of the crystal. This has been explicitly shown by Kittel[15] for ferromagnets of cubic symmetry. For ferromagnetic metals and alloys the ratio $\Delta K/K$ is generally of the order of 10^{-1} to 10^{-3} and K is of the order of 10^5 erg/cm^3. For the MnO type compounds $K \approx 10^8 - 10^9$ erg/cm^3. ΔK is of the order of $Y\lambda^2$, where Y is the Young's modulus and λ the magnetostrictive strain. For CoO Greenwald[4] found $\lambda \approx 10^{-2}$ to 10^{-3} increasing with the decrease of temperature, and according to Street and Lewis[9] $Y \approx 10^{12}$ dyne/cm^2. Therefore, here again we have $\Delta K/K \approx 10^{-1}$ to 10^{-3}. It seems that the anisotropy energy and the energy of magnetostriction varies roughly in proportion from metallic ferromagnetics to the antiferromagnetic compounds.

In order to test our confidence in the anisotropy magnetostriction approach we shall examine the relation between the magnetic axis (or axes) and the crystal summetry of the antiferromagnetics for which such information is available.[16] With the exception of CuCl$_2 \cdot$2H$_2$O, which is in a different category, they are listed in Table II. No change of symmetry has been reported at the Néel point of these compounds. For several cases sharp changes of the lattice parameters[17] are found accompanying the magnetic transition. Probably all the compounds have, more or less, a readjustment of lattice spaces at the Néel point. Except the state of α-Fe$_2$O$_3$ in the temperature range of $-20°$C and $675°$C, their spin axis is in the uniaxial direction, or in the case of MnO$_2$ the spin axes are orientated symmetrically in the plane perpendicular to the uniaxial direction. This situation agrees perfectly with the concept of anisotropy magnetostriction. In the case of NiF$_2$, the deviation in the direction of spin axis from the tetragonal axis by 10 degrees should induce a slight distortion of the true tetragonal symmetry. An accurate x-ray analysis should be carried out on this compound.

[15] C. Kittel, Revs. Modern Phys. 21, 541 (1949).
[16] The sources of information for the antiferromagnetics listed are: (a) α-Fe$_2$O$_3$: see reference 1. (b) Cr$_2$O$_3$: B. N. Brockhouse, J. Chem. Phys. 21, 961 (1953); McGuire, Scott, and Grannis, Phys. Rev. 98, 1562(A) (1955). (c) MnF$_2$: R. A. Erickson, Phys. Rev. 90, 779 (1953). (d) MnO$_2$: See reference 7. (e) CrSb: A. I. Snow, Phys. Rev. 85, 365 (1953); Revs. Modern Phys. 25, 127 (1953).
[17] The sources of information on the change of lattice parameters are: (a) α-Fe$_2$O$_3$: B. T. M. Willis and H. P. Rooksby, Proc. Phys. Soc. (London) B65, 950 (1952). (b) Cr$_2$O$_3$: S. Greenwald, Nature 168, 379 (1951). In this article Greenwald reported a contraction in the [111] direction when Cr$_2$O$_3$ is cooled below the Néel point. It has been found by R. J. Davis and W. E. Armstrong, and by Greenwald herself (reindexing her original data) that the readjustment of lattice parameters involves an expansion in the [111] direction instead of a contraction. See S. Greenwald, Nature (to be published). (c) CrSb: See reference 16(e), or B. T. M. Willis, Acta Cryst. 6, 425 (1953).

TABLE II. Crystalline structure and the orientation of magnetic axis (or axes) in antiferromagnetic compounds.

Compounds	Crystal structure	Directions of spin axis (or axes)
MnF$_2$, FeF$_2$, CoF$_2$, and NiF$_2$[a]	Tetragonal, rutile structure	Tetragonal axis
MnO$_2$	Tetragonal, rutile structure	Two spin axes within the xy-plane and mutually perpendicular
CrSb	Hexagonal, AsNi structure	Hexagonal axis
α-Fe$_2$O$_3$ (below $-20°$C) and Cr$_2$O$_3$	Rhombohedral α-Al$_2$O$_3$ structure	Rhombohedral axis
α-Fe$_2$O$_3$ (between $-20°$C and 675°C)	Rhombohedral α-Al$_2$O$_3$ structure	Within the (111) plane and direction to a nearest neighboring Fe^{+3} in the plane

[a] In NiF$_2$ the spin alignment is not exactly along the tetragonal axis but makes an angle of 10 degrees with the latter.

The degree of distortion depends, of course, on the strength of anisotropy-elastic coupling, which is not known for this compound. The spin axis in the high-temperature antiferromagnetic state of α-Fe$_2$O$_3$ is perpendicular to the trigonal axis. From our viewpoint the crystal structure should become monoclinic in the temperature range of this state. Yet, according to the x-ray analysis of Willis and Rooksby,[17] α-Fe$_2$O$_3$ remains rhombohedral with a sharp change of lattice parameters at 675°C. This should not be taken as a negative evidence of the general validity of our hypothesis, as can be explained in the following. Anderson et al.[18] find by a resonance technique that the anisotropy force in α-Fe$_2$O$_3$ is only about 60 gauss in the (111) plane, while that in a plane containing the [111] axis is 30 000 gauss. Combining this experimental fact and the concept mentioned in the preceding paragraph that a strong magnetostriction goes together with high anisotropy, we must anticipate in α-Fe$_2$O$_3$ a small magnetostriction within the (111) plane. Therefore, an x-ray experiment cannot detect the distortion of the (111) cross section of a unit cell, although the readjustment of lattice parameters is so much larger and more readily measured by x-ray technique. Another effect of concurrent interest is the $-20°$C transition of α-Fe$_2$O$_3$ at which the magnetic axis turns to the [111] direction in the lower temperature range. Willis and Rooksby report that the change, if any, of lattice parameters at this transition is considerably less than that which occurs at the high Néel temperature associated with the magnetic lattice formation. This simply means that the two antiferromagnetic states of α-Fe$_2$O$_3$, which are different only in the orientation of magnetic axis, have approximately the same spontaneous magnetostriction. No criterion on our anisotropy magnetostriction hypothesis can be derived from this effect.

[18] P. W. Anderson et al., Phys. Rev. 93, 717 (1954).