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RECENT MAGNETIC STRUCTURE STUDIES BY NEUTRON DIFFRACTION<sup>(1)</sup>

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**Résumé.** — L'auteur expose les résultats de plusieurs études sur les structures magnétiques réalisées récemment par les méthodes de diffraction de neutrons. Il signale une étude par Hamilton de la transition de  $\text{Fe}_3\text{O}_4$  à basse température et des expériences de Roth sur la structure magnétique mal connue des mono-oxydes des éléments de transition. L'auteur décrit les travaux récents utilisant la technique des faisceaux de neutrons polarisés et présente des données sur la diffraction du fer et du nickel.

**Abstract.** — A review is presented of several magnetic structure studies performed recently by neutron diffraction methods. These include a study of the low temperature transition in  $\text{Fe}_3\text{O}_4$  by Hamilton and experiments by Roth on the magnetic structure ambiguities of the transition element monoxides. Recent studies using polarized neutron beam techniques are described and data presented on the ferromagnetic scattering by iron and nickel.

In the eight years that have passed since the neutron diffraction technique was first utilized in determining magnetic structures, much information of value in understanding magnetic phenomena has been obtained by these methods. These studies have fallen into three categories: (1) intratomic, (2) interatomic and (3) macroscopic magnetic phenomena. Information obtained in the first classification by neutron scattering include the determination of the magnitude and quality of an atom's magnetization i.e., its magnetic moment value and the spatial and angular momentum characteristics of this moment as represented in the form factor for neutron scattering. Within the second classification are to be included the knowledge gained from studies of magnetic crystallography in which the interatomic coupling of atomic moments are demonstrated to be of a wide degree of complexity. Lastly, the correlations that exist between the magnetic and the crystalline axes and studies of the macroscopic domain structure of a magnetic material are of aid in understanding bulk phenomena.

In spite of the limitations that exist on the availability of neutron sources, a sizeable number of experimental groups are engaged in such research studies and the research literature is being increased by three or four dozen experimental reports annually along with an equal number of theoretical investigations. At the present time in the United States, three centers of magnetic investigation by neutron methods are flourishing, namely at the Oak Ridge, Brookhaven and Argonne National Laboratories. It is, of course, to be recognized that in many cases this centra-

lization is dictated by practical problems and that the basic roots of a number of research groups reside at other research institutes or laboratories. Dr. Koehler will be describing in his talk at this Conference, some of the recent activities of the Oak Ridge group and I propose to discuss a few very recent and representative investigations accomplished elsewhere. In selecting illustrations I have been guided primarily by my own familiarity with the various problems, with no implication whatsoever that these represent the most critical or important investigations. The last few years have seen very considerable advances in experimental technique and, if anything, the present illustrations, as well as those of Dr. Koehler emphasize this aspect.

**Low temperature ionic ordering in magnetite.** — Magnetite ( $\text{Fe}_3\text{O}_4$ ) has been known to be of the inverted spinel structure and the relative orientation of its  $\text{Fe}^{++}$  and  $\text{Fe}^{+++}$  ions has served as a classic example of Néel's theory of ferrimagnetism. Of the two  $\text{Fe}^{+++}$  molecular ions one is to be found at the tetrahedral sites (surrounded in tetrahedral coordination by oxygen ions) and the other is located, along with the  $\text{Fe}^{++}$  ion, at the octahedral positions. At room temperature the distribution of the  $\text{Fe}^{++}$  and  $\text{Fe}^{+++}$  ions among the octahedral sites is considered to be characterized by dynamic disorder, a fact which accounts for the rather high electrical conductivity. At low temperatures below 119 °K however, the conductivity decreases greatly and Verwey and colleagues [1] have proposed that an ionic ordering within the octahedral sites takes place.

This low temperature ionic ordering has been looked for recently by Hamilton [2] utilizing very refined neutron diffraction techniques and the

<sup>(1)</sup> The preparation of this report and some of the research studies described herein have been supported by the United States Air Force Office of Scientific Research.

Verwey picture has been completely substantiated. An early neutron diffraction study [3] of  $\text{Fe}_3\text{O}_4$  was confined to polycrystalline specimen examination and, although the Néel room temperature ferrimagnetic structure was shown to be correct, it was demonstrated that the polycrystalline scattering data was not sensitive to the presence of the Verwey low temperature ordering scheme. In figure 1 is shown the difference between the two

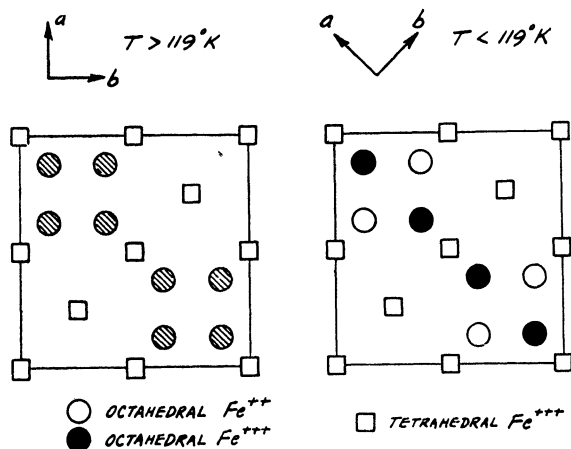


FIG. 1. — Projections on the base plane of ionic positions in  $\text{Fe}_3\text{O}_4$  at high and low temperature.

structures illustrated as ionic projections upon the base plane, that is, perpendicular to the  $c$  axis. In the high temperature phase, which is cubic, there is no distinction between the  $a$ ,  $b$ , and  $c$  axes but the Verwey structure can be envisaged as an orthorhombic structure with a unique  $c$  axis perpendicular to the plane of projection in figure 1.

Hamilton's study was performed on single crystals (both synthetic and natural) which were cooled through the ordering temperature in the presence of a large magnetic field directed along one of the cubic axes. Earlier measurements [4] on magnetization, electrical properties and unit cell distortion had demonstrated that this was necessary to insure a unique  $c$  axis in the low temperature structure although the development of a unique  $c$  axis can still result in a twinned crystal in which the  $a$  and  $b$  orthorhombic axes are undefined. A completely untwinned crystal can be obtained however if the field on cooling is applied [5] at a favorable angle to the unique  $c$  axis.

Single crystal reflectivities were measured by Hamilton for both twinned and untwinned crystals with very elegant and convincing corrections being applied to the observations for the extinction effects necessarily present. The interpretation of these neutron intensities showed without question that the Verwey structure was correct. Of critical significance in the interpretation is the appearance of an (002) reflection which should be completely

absent for the disordered high temperature structure and which should be proportional to the difference between the  $\text{Fe}^{+++}$  and  $\text{Fe}^{++}$  magnetic scattering amplitudes in the ordered structure. Numerically this difference is not great so that the intensity is not large. Figure (2) shows a typical

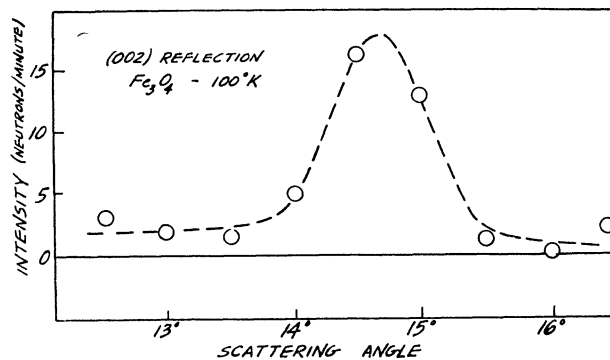


FIG. 2. — Neutron intensity in the (002) reflection of  $\text{Fe}_3\text{O}_4$  at low temperature (Hamilton).

curve obtained by Hamilton for the (002) reflection by pulling the magnetic axis away from the unique  $c$  axis with a magnetic field applied to the scattering crystal. This is necessary since even with a finite magnetic structure factor for (002) the intensity of scattering will be zero for moments aligned along the easy direction, the  $c$  axis.

Besides confirming the basic high temperature Néel structure and establishing the ionic positional parameters for this crystal with great accuracy, Hamilton's study has thus shown the correctness of the Verwey low temperature model and has demonstrated that :

- (a) the octahedral ferric ions lie in rows parallel to the orthorhombic  $a$  axis ;
- (b) the octahedral ferrous ions lie in rows parallel to the  $b$  axis ;
- (c) the magnetic moments of all ions are parallel or antiparallel to the  $c$  axis ;
- (d) the  $a$  axis is longer than the  $b$  axis.

**Magnetic structures of monoxides of the transition metals.** — Among the earliest of the antiferromagnetic structures to be investigated by neutron scattering methods were those of the simple oxides of the transition metals.  $\text{MnO}$ ,  $\text{NiO}$ ,  $\text{FeO}$  and  $\text{CoO}$ . All of these oxides exhibit Néel magnetic ordering transitions at temperatures ranging from 120 °K for  $\text{MnO}$  to 640 °K for  $\text{NiO}$ . The early investigations [9] were carried out on polycrystalline specimens and the diffraction patterns were interpreted as indicating (a) that the magnetic unit cell was twice enlarged (in a linear dimension) over the chemical unit cell and (b) that the magnetic structure consisted of ferromagnetic sheets of alternating spin orientation, with some

differences from one oxide to another of the absolute orientation of the spin axis relative to the ferromagnetic sheet. Associated with the Néel ordering is to be found a crystallographic distortion and precision x-ray investigations have shown that in MnO and NiO the structure becomes rhombohedral with  $\alpha > 60^\circ$ , FeO rhombohedral with  $\alpha < 60^\circ$  and CoO tetragonal with  $(c/a) < 1$ . These distortions were not easily correlated with the suggested magnetic structures and Li proposed [7] an alternative magnetic structure which would account not only for the polycrystalline neutron intensities but would also show consistency with the structural distortions assuming that the latter arises from anisotropy magnetostriction rather than exchange-striction effects. These structural ambiguities have been recently investigated by Roth [8] in a comprehensive series of neutron diffraction studies on both single crystal and polycrystalline specimens and the following will summarize briefly some of these results.

(A) POLYCRYSTALLINE DATA. — Comparison between the originally proposed ferromagnetic sheet model and the alternative Li model is shown in Figure (3). As Li has demonstrated, the poly-

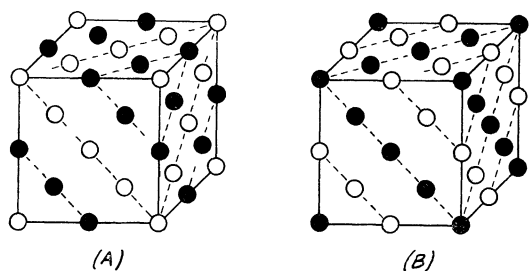


FIG. 3. — Alternative magnetic structures proposed for MnO and other transition-metal oxides. The full and open circles represent magnetic ions of opposite spin orientation.

crystalline neutron intensities to be expected for his structural model, (B) in the figure, are independent of the spin axis assignment and moreover are identical to those given by model (A) when the unique spin direction is along the [100] pseudocubic direction as originally proposed. Thus polycrystalline scattering data cannot serve to distinguish between these two alternatives. To be sure, if a single crystal, single domain specimen were to be studied then differences could be obtained and one would be favored over the other. Roth has been able to show however that his recent polycrystalline scattering data [9] are not in agreement with either model (B) or model A [100], in which the spins are along the [100] direction. Table 1 summarizes the intensities found by Roth at 4.2 °K for MnO along with the expected inten-

sities for the above two models and for a model A (111) which is found in agreement with observation. In the acceptable model A (111), the

TABLE I

OBSERVED AND CALCULATED POLYCRYSTALLINE MnO  
MAGNETIC INTENSITIES

	OBSERVED	A[100]	(B)	A[111]
(111)	1 002	673	673	1 009
(113)	258	331	331	256
(331)	110	105	105	113
(333) (115)	88	56	56	75

alternating ferromagnetic sheet structure is retained but the spin axis is now positioned within the ferromagnetic sheet rather than along the cube axis. The polycrystalline intensities are rather insensitive to the assigned direction within the (111) sheet and it has not been possible to unambiguously assign the spin axis direction. Recent studies on the NaCl-type phase of MnS by Corliss, Elliott and Hastings [10] have shown a similar type of ordering and magnetic axis alignment.

Completely similar results were obtained for NiO and the magnetic structure is considered to be the same as for MnO, namely the ferromagnetic sheet model with spin axis within the (111) sheets. For FeO however, the absence of the (111) magnetic intensity requires a model A [111] in which the spin axis is normal to the ferromagnetic sheets, agreeing with the earlier neutron interpretation.

Similar studies on CoO by Roth showed that models (B), A [100] and A (111) were all in disagreement with the neutron scattering data. The best agreement was obtained by using model A but tipping the spin axis about  $11^\circ$  from the [100] direction, along an odd direction [117]. This conclusion agrees with that of Nagamiya and Motizuki [11] who have extended the Kanamori treatment and who suggest that the spin axis may be tipped as much as  $10^\circ$  from the [100] direction.

In all of the above polycrystalline specimen analysis, Roth has assumed the existence of a single magnetic axis for all four of the interpenetrating sublattices that make up the unit cell. Roth considers the possibility of multispin-axis models and shows that it is necessary to have single crystal, single domain specimens in order to determine the magnetic structure without ambiguity.

(B) SINGLE CRYSTAL OBSERVATIONS ON NiO. —

Roth has complemented his polycrystalline specimen studies with observations taken on single crystals of NiO. Optical examination on thin sheets of crystal with faces parallel to (110) performed after annealing at 1 500 °C showed the

presence of untwinned regions and Roth examined the neutron scattering from such regions. Magnetic intensity was observed from four of the eight (111) reflections whereas intensity should have been observable from only two (111) reflections if the spin axis were unique within the (111) plane of a single antiferromagnetic domain. This suggested either (a) the presence of a multidomain structure in spite of the absence of optically detectable domains or (b) the presence of a multi spin-axis structure within a single domain. Unfortunately three dimensional single crystal data are not available to remove this ambiguity. The present data do, however, eliminate certain of the multi-spin-axis models and demonstrate that the antiferromagnetic spin arrangement in NiO does not have three-fold symmetry.

**Magnetic scattering by iron and nickel.** — The metallic elements forming the 3*d*-transition group have served as the classic examples of ferromagnetism and a great volume of literature is available describing and interpreting their magnetic properties. They have served as attractive subjects for neutron scattering studies during the last five years and a number of reports have appeared on the neutron scattering, elastic and inelastic as well as coherent and incoherent, at various temperatures with varying conditions of magnetization. These studies have concentrated mostly on metallic iron in both polycrystalline and single crystal form with only slight attention being paid to metallic nickel scattering. For both of these cases, the magnetic scattering effects are unfortunately rather small, particularly so for the case of nickel, and this has placed limitations upon the quantitative significance of the scattering results. For example in iron, the magnetic scattering contribution to the dominant Bragg reflection is only 8 per cent of the nuclear scattering, only 0.7 per cent for nickel, and severe problems arise in interpreting this to the accuracy desired.

It has been recognized for sometime that the employment of polarized neutron radiation, rather than the generally-used unpolarized radiation, would enhance materially the magnetic scattering and permit quantitative measurements to a much higher degree of accuracy. Accordingly a program of exploiting the use of polarized radiation in the study of magnetic scattering effects [12] was undertaken at the Brookhaven National Laboratory and the following will describe the results obtained on nickel and iron. It has been possible by these new methods to determine the absolute magnetic scattering to much higher accuracy than has been previously available and the results when combined with the recent X-ray findings of Weiss and DeMarco [13] permit interesting conclusions.

In the recent studies, a conventional neutron

diffraction spectrometer was modified to incorporate the production and use of polarized monochromatic radiation. This was done by the substitution of a polarizing ferromagnetic crystal for the usual monochromating crystal with suitable provision for controlling the beam polarization in the experiment under study. In this technique the polarizing crystal must be magnetized to as near saturation as is practicable and the resulting neutron polarization is directed along the axis of this magnetizing field. Single crystals of both Fe<sub>3</sub>O<sub>4</sub> and Co-Fe alloy (92 atomic per cent Co) were utilized as polarizing crystals and it was ascertained that their polarizing efficiencies approached 99 per cent for either case. It was found very desirable to be able to reverse the neutron polarization without altering the magnetic field distribution within the spectrometer and this was performed by the nuclear resonance technique with a radio-frequency field matched in frequency to the Larmor precession of the neutron spin.

In the iron and nickel studies, the polarized neutron beam was scattered by single crystal pillars of the metal placed in a magnetic field of about 8 000 oersteds. This magnetizing field on the crystal specimen was oriented parallel to the polarizing field with the result that the neutron, throughout its trajectory, always experienced a magnetic field along a common direction. This was necessary to avoid neutron depolarization effects. Various crystal reflections were then studied as a function of the relative orientations of the neutron polarization and the crystal magnetization. For the two cases where these are parallel and antiparallel, the intensity in the Bragg reflection becomes

$$I_{++} = c(b + p)^2$$

$$I_{+-} = c(b - p)^2$$

with *b* and *p* being the nuclear and magnetic scattering amplitudes and *c* a proportionality constant. Large intensity changes are found in this fashion (up to ratios of 3.6 to 1 in the iron case) and these can be interpreted to furnish the magnetic scattering amplitude. It is necessary to allow for extinction effects in the crystal scattering or to examine the crystals under extinction-free conditions. Both procedures were used in practice with control over the degree of extinction being exercised through its dependence upon the mosaic structure, crystal thickness and neutron wavelength.

Figure 4 shows the magnetic scattering amplitudes observed for various iron reflections plotted as a function of the Bragg angle  $\theta$ . In the forward direction (zero scattering angle) the magnetic scattering amplitude should be directly related to the magnetization and this value is shown along the ordinate axis. Also shown on the graph are theoretic-

tical form factor values for iron as calculated by Wood and Pratt [14] which are here normalized to the expected scattering at zero angle. The two

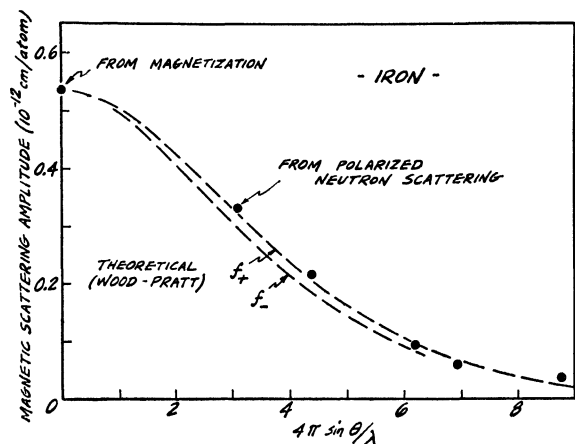


FIG. 4. — Magnetic scattering amplitudes observed in iron by polarized neutron methods as compared with theoretical form factor values.

theoretical curves correspond to the two groups of electrons of opposite spin orientation in the 3d shell and illustrate the effect of intra-atomic exchange effects. The agreement between experiment and theory is satisfactory, particularly when compared with the calculations for the positive spin group of electrons. This is interesting in light of the recent x-ray findings of Weiss and DeMarco [13] which indicate that the 3d shell in iron contains electrons of only one spin orientation.

Equivalent magnetic scattering amplitudes for nickel were obtained and these are graphed in Figure 5 along with the amplitude at zero scat-

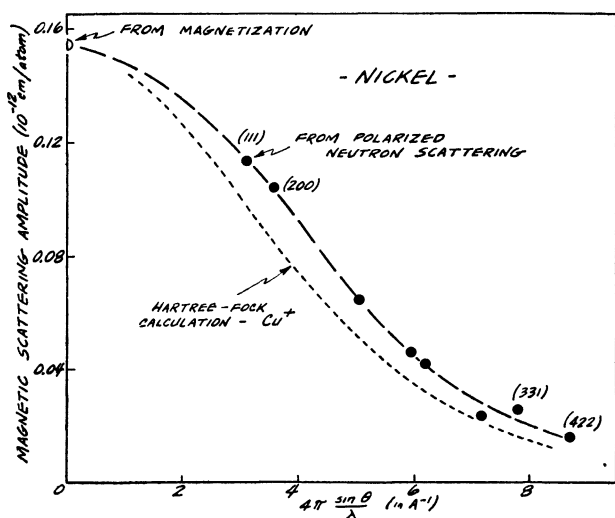


FIG. 5. — Magnetic scattering amplitudes observed in nickel by polarized neutron methods as compared with theoretical form factor values.

tering angle expected from the magnetization. Also shown is a theoretical curve for a Hartree-Fock calculation of Cu<sup>+</sup> since this ion possesses the same number of outer electrons as does nickel. For this case the experimental observations are definitely at variance with the calculated values and this is considered to result from the intra-atomic exchange effect introduced by Wood and Pratt. In the Weiss and DeMarco X-ray experiments on nickel, the absolute X-ray intensities showed the full compliment of electrons present in the 3d shell namely  $9.7 \pm 0.3$  and hence the magnetic spin density must arise from electrons of both spin states. Since there are present presumably five electrons of positive spin and 4.4 of negative spin to give the observed magnetization and since the neutron scattering depends upon the difference in spin density, the present neutron observations could be accounted for by having only a slight difference in the wave functions for the two electron groups of opposite spin orientation. A calculation of the form factor difference for the two spin states which would account for the experimental observations shows that this needs to be only about one third of that calculated by Wood and Pratt for the iron case and illustrated in Figure 4. This implies that the mean radius of the negative spin wave function  $\Psi_-$  is about 4 per cent larger than that of  $\Psi_+$  in the 3d shell of nickel.

Thus the availability of more accurate neutron scattering data for these elements obtainable by newly developed polarized neutron methods has confirmed the existence of a very subtle intra-atomic exchange effect acting upon the 3d electrons in nickel. It is of interest that the magnetic scattering amplitudes shown for the outer reflections in Figure 5 are by far the smallest that have been measured to date and illustrate the great sensitivity of the polarized beam technique.

ACKNOWLEDGEMENTS. — I am indebted to Drs. W. C. Hamilton and W. L. Roth and others among my colleagues for permission to utilize these results before their formal publication.

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in that higher resolution was employed and the observations were carried to much lower temperatures (4.2 °K) than was originally obtained (ca 70 °K).

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## DISCUSSION

*Mr. Bozorth.* — Do neutron diffraction experiments show independently that the structure proposed by Verwey is truly orthorhombic, as proposed by Bickford.

*Mr. Shull.* — Hamilton's neutron diffraction data on  $\text{Fe}_3\text{O}_4$  at low temperature do not show directly that the low temperature phase is strictly orthorhombic. The X-ray data show this convincingly, however.

*Mr. Bacon* (Comment). — Although the single-crystal intensity measurements of NiO do not give non-ambiguous information about the orientation of the magnetic moments (since the single crystals are not single domains). They do offer a means of giving the form factor of  $\text{Ni}^{2+}$  much more accurately than with powders. This can be done by measuring the series of magnetic reflexions 111, 333, 555, ... as has been done by T. Sabine at Harwell. The f-curve is obtained without making any assumption about moment directions. We have therefore a possibility of comparing the form factor of  $\text{Ni}^{2+}$  in antiferromagnetic NiO with the very accurate measurements in metallic nickel which have been obtained from Prof. Shull's polarized beam measurements.

*Mr. Shull.* — It would be very interesting if accurate form factor data were obtained for both  $\text{Ni}^{++}$  ions and for metallic nickel.

*Mr. Dabbs.* — I think it should be emphasized to the congress that the *same* technique which permits the study with polarized neutrons of magnetic scattering amplitudes, using sums and differences between these and nuclear scattering *amplitudes* (e.g. in  $\text{Fe}_3\text{O}_4$ ) is perhaps the most important of the methods of procuring polarized neutrons.

*Mr. Shull.* —  $\text{Fe}_3\text{O}_4$  is a very good material for this purpose, but more recently an alloy 8Fe and 92Co was found to give very high polarization with higher intensity and other advantages. Polarization values up to 99 percent are rather easily obtained.

*Mr. Pratt.* — The neutron diffraction results discussed by Prof. Shull seem to support the theoretical description in which electrons of different spin are discussed on an entirely separate basis from the Hartree-Fock standpoint. One has an independent experimental source of support by measuring hyperfine splittings. In the  $\text{Mn}^{++}$  ion one has a net spin of 5/2. Thus the 1s, 2s, etc. inner electrons with opposite spins will have different exchange interactions with the d-electrons. This results in separate charge densities for inner electrons with the same *n* and *l* quantum numbers. Consequently the magnetic field at the nucleus is not self-cancelling as it would be in the ordinary picture of closed shells. This generalized method has been able to fit the observed hyperfine splitting of  $\text{Mn}^{++}$  rather satisfactorily. Therefore, both the neutron diffraction results and the hyperfine results tend to confirm the picture in which electrons of different spin are treated independently.

*M. Guiot-Guillain.* — La diffraction des neutrons a-t-elle été essayée sur l'oxyde  $\text{Fe}_2\text{O}_3$  rhomboédrique ( $\text{Fe}_2\text{O}_3\text{-}\alpha$ ) ou sur les ferrites de terres rares  $\text{FeMO}_3$  (structure pérovskite déformée orthorhombique, par exemple  $\text{FeGdO}_3$ ) dont les propriétés magnétiques sont assez analogues à celles de  $\text{Fe}_2\text{O}_3\text{-}\alpha$  ? Cet oxyde présente on le sait un faible ferromagnétisme qui n'a pas encore été expliqué de façon satisfaisante.

*Mr. Shull.* — There have been some recent polarized neutron scattering studies on  $\alpha\text{-Fe}_2\text{O}_3$  but these have not given particular information on the origin of the weak parasitic ferromagnetism found in this substance.

*M. Bertaut.* — Les différences entre les densités de charge et de spin, sont-elles réellement significatives ? Les deux densités sont obtenues par une transformation de Fourier. Pour les comparer, l'information que l'on possède devrait être équivalente, c'est-à-dire les sphères dans l'espace réciproque devraient avoir le même rayon.

Il me semble que l'on dispose dans le cas de réflexions magnétiques de moins d'informations (rayon de la sphère réciproque plus petit). A-t-on corrigé les résultats de « l'effet de sommation finie » ? Cet effet peut déplacer les maxima des courbes.

*Mr. Shull.* — The magnetic or spin density form factor is very definitely higher than the charge density form factor over the observable angular range and this can imply only that the spin density is compressed relative to the charge density. Certainly the termination effects in the Fourier inversion of the form factors are important and these will affect the precision of the calculated density curves.