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Neutron Diffraction Studies of Various Transition Elements

C. G. SHULL AND M. K. WILKINSON

Oak Ridge National Laboratory, Oak Ridge, Tennessee

Neutron diffraction measurements are reported on a series of transition elements as an investigation into their magnetic structures. Scattering data have been taken for W, Mo, Nb, V, Cr, Mn, and Fe at various temperatures as low as 4.2°K, and these data are interpreted in terms of the magnetic structure existing in the pure metals. For the first four-named elements, no magnetic scattering either coherent or incoherent is found. Cr and α-Mn are established as being antiferromagnetic with Néel temperatures of 475°K and 100°K, respectively. Paramagnetic scattering has been observed in manganese at room temperature, and the atomic moments determined for Cr and Mn follow the general trend of the Slater-Pauling curve. Magnetic superstructure effects and magnetic disorder scattering were looked for in iron and neither was found.

INTRODUCTION

IN striking contrast to the situation in crystals containing ions of the transition elements or the rare-earth elements, the magnetic structures existing in the transition elements can be considered as being very poorly understood. Aside from the relatively few cases of ferromagnetism for which an average, effective magnetic moment per atom can be ascertained from magnetic measurements, the magnetic susceptibility data are not too informative. Temperature-independent susceptibility values are the rule for the transition elements and the interpretation of this is certainly not straightforward. Recent researches by Zener and coworkers have followed the atomistic viewpoint in which the electronic structure of a given atom in the metal lattice is considered to be much the same as the configuration in a free atom. These considerations have suggested the presence of strong localized atomic moments arranged in an antiferromagnetic manner, and hence their presence is not easily evidenced in macroscopic magnetic properties. Since neutron diffraction measurements are able in principal to determine the strength and relative orientation of atomic moments in a scattering lattice, it was to be hoped that such measurements would offer illuminating information on the magnetic structures.

The transition elements which have been investigated in the present study are listed in Table I along with the characteristic configuration of the outer electron assembly in the atom as determined from spectroscopic data on the free atoms. If these configurations were representative of the metallic atoms, we should expect large atomic moments in the metals, for example $5\mu_B$ for chromium, since the five $3d$ electrons are arrayed with parallel spin according to usual spectroscopic rules. Such atomic moments should contribute (a) pronounced coherent scattering to the neutron diffraction pattern if there is any alignment correlation between neighboring moments or (b) measurable diffuse scattering in the pattern if the moments are uncorrelated in orientation. Powder diffraction data were obtained for these elements both at room temperature and when held at very low temperature in a double-jacketed vacuum cryostat. All were examined at liquid hydrogen temperature (20.4°K), some were cooled to liquid helium temperature (4.2°K), and others were studied at various intermediate temperatures including examination at elevated temperatures up to 500°C in a furnace. Temperature gradients within the sample container were studied by superconductivity observations at the very lowest temperatures and with calibrated thermocouples at higher temperatures.

TABLE I. Electronic configuration existing in isolated atoms of the various transition elements for which neutron diffraction studies are reported.

	$3d$	$4s$	$4d$	$5s$	$5d$	$6s$
V	3	2				
Cr	5	1				
Mn	5	2				
Fe	6	2				
Nb			4	1		
Mo			5	1		
W					4	2

EXPERIMENTAL RESULTS

V, Nb, Mo, and W

The data for these elements are discussed collectively since they indicate the complete absence of any measurable coherent or incoherent magnetic scattering in the powder diffraction patterns for these materials. All of these materials were of the highest purity available (spectroscopically 99.9 percent or higher) and were examined in the form of filings or fine powder. The samples were sealed in a thin-walled aluminum specimen capsule which in turn was placed in a double-jacketed Dewar cryostat. The cryostat construction was such that a minimum of neutron scattering occurred from the vacuum walls and thermal radiation shields, and corrections were made for this scattering in the neutron

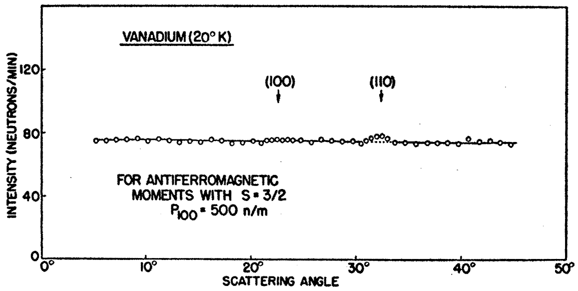

FIG. 1. Neutron diffraction pattern for V taken at 20°K. No antiferromagnetic reflection at the (100) position is to be noted.

diffraction patterns. Typical patterns taken at liquid hydrogen temperature (20.4°K) are shown for V and for Mo in Figs. 1 and 2.

The pattern for V in Fig. 1 shows the presence of a very weak (110) reflection and this is a regular body-centered cubic lattice reflection. It is very weak because the coherent nuclear scattering cross section for vanadium is very small, amounting to only 0.035 barn as determined in the reflection. Practically all of the vanadium nuclear scattering is nuclear spin disorder scattering, and this appears as a completely isotropic diffuse scattering in the pattern. Of interest here is the absence of any measurable (100) intensity. If an antiferromagnetic body-centered cubic lattice existed in vanadium, magnetic reflection should be observable at the (100) position with an intensity commensurate with the strength of the vanadium magnetic moment. Calculating the expected intensity on the basis of a magnetic moment of 3 Bohr magnetons (for the three electrons in Table I) leads to an expected (100) peak intensity of 500 neutrons/minute whereas nothing like this is observed. An upper limit on the possible (100) intensity can be estimated, and this implies that any *aligned* moments in vanadium must be smaller than about 0.1 Bohr magneton. Likewise, the diffraction data can be used to evaluate the strength of any *unaligned* moments in vanadium from the appearance of the diffuse scattering. If unaligned moments are present, then incoherent diffuse scattering should be observable and this should be recognizable by its form factor angular variation. In Fig. 3 is shown the observed diffuse scattering for vanadium after correction for the isotropic nuclear spin incoherent scattering of 5.1 barns and for comparison the calculated scattering for unaligned moments of 3 Bohr magnetons. Again the data do not support such a large moment and from the sensitivity of observation an upper limit of about 0.1 Bohr magneton for the possible *unaligned* moments is the most that would be consistent with the data.

Unlike the vanadium pattern, the pattern for Mo given in Fig. 2 contains strong nuclear reflections at the regular b.c.c. positions. In addition to the principal reflections at the (110), (200), etc., positions produced with the primary neutron wavelength of 1.212A, there exists a series of weak reflections produced by a beam of second-order neutron wavelength (0.606A) which is obtained from the monochromating crystal in the neutron diffraction spectrometer. The relative intensity of second-order neutrons to primary neutrons has been determined accurately, and the observed intensities of the secondary peaks in Fig. 2 are such as to be explained entirely by this contaminant wavelength. Thus, there is no observable (100) intensity in the pattern, and this indicates the absence of an antiferromagnetic lattice in Mo. Arguments similar to those used for vanadium would place an upper limit of about 0.3 Bohr magneton for the possible aligned moments and about 0.2 Bohr magneton for the possible

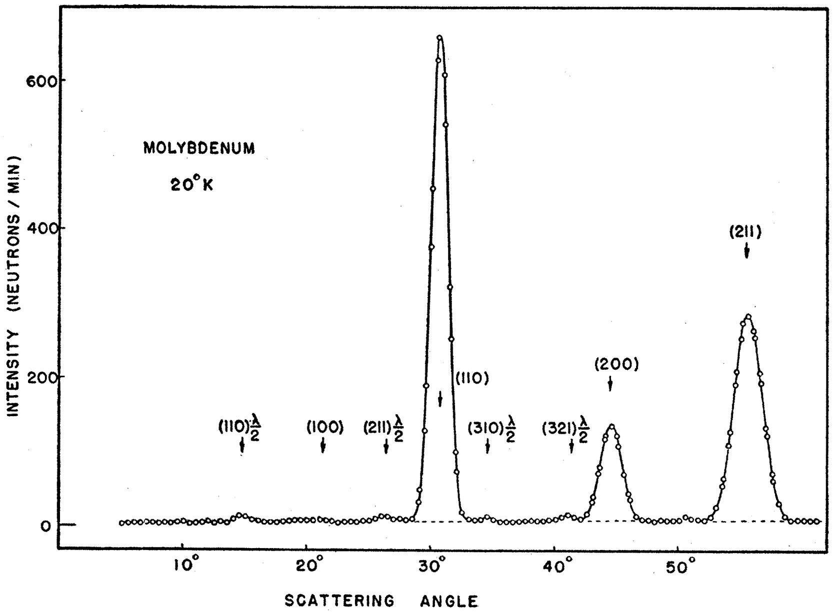

FIG. 2. Neutron diffraction pattern for Mo taken at 20°K. Large nuclear reflections are seen along with secondary weak reflections of half-wavelength origin.

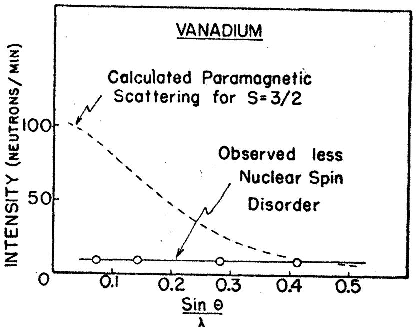

FIG. 3. Diffuse scattering observed for V after correction for nuclear spin disorder scattering. The expected paramagnetic scattering for $S=3/2$ is shown.

unaligned moment strength. The room temperature pattern for Mo, which is not shown, was completely similar to the low temperature pattern except for a slight decrease in the intensities of the lines (the normal Debye-Waller temperature effect) and a noticeable change in the amount of thermal diffuse scattering from the lattice.

A study of the patterns for Nb and W gave results completely analogous to those of V and Mo. There was no observable (100) intensity in any of the patterns, either at 20°K or 295°K, and no suggestion of an angularly dependent diffuse scattering. Thus no localized atomic moment, either aligned or unaligned, could be attributed to the metallic lattice.

In addition to the patterns taken at liquid hydrogen temperature, two of the elements, V and Nb, were also studied at liquid helium temperature (4.2°K) below their superconducting transition. This produced no change in their patterns so that the magnetic structure conclusions are unaltered. Further details of these last-mentioned measurements will be given in a separate publication.

Cr

A sample of electrolytic chromium flake was the principal source of diffraction specimens. This flake was given a quantitative spectroscopic assay and found to be 99.98+ percent pure with less than 0.01 percent Fe and less than 0.01 percent Mn as the only detectable impurities. The flakes were ground in a mortar and the examination was carried out on a fine powder. A typical pattern obtained at 20°K is shown in Fig. 4. Normal nuclear reflections are seen at the (110), (200), and (211) positions, along with secondary peaks of second-order wavelength contribution. In this case, however, the intensity at the (100) position is about five times what it should be if there were only $\lambda/2$ contribution from the (200) reflection. Thus, there appears to be a weak but perfectly measurable (100) reflection for Cr which suggests an antiferromagnetic lattice.

This reflection has been studied in detail to see if it really were of magnetic origin. It was found to be temperature sensitive, much more so than the other nuclear reflections, either the large normal reflections or the weak secondary ones. Figure 5 summarizes this temperature dependence, and it is seen that the (100) reflection disappears at temperatures above 200°C. The temperature dependence is strongly suggestive of a magnetic reflection since it follows a Brillouin function variation with a suggested Néel temperature of 200°C. It was found to be perfectly reversible. The possibility that this might be an impurity reflection and not a true Cr lattice reflection was studied in a variety of ways. An x-ray diffraction pattern of the sample showed no lines other than for the pure metal, and a very careful study* of the x-ray pattern in the region of the (100) reflection showed the complete absence of a (100) reflection. Moreover, the angular position and temperature dependence of this reflection were such as to rule out it being a magnetic reflection

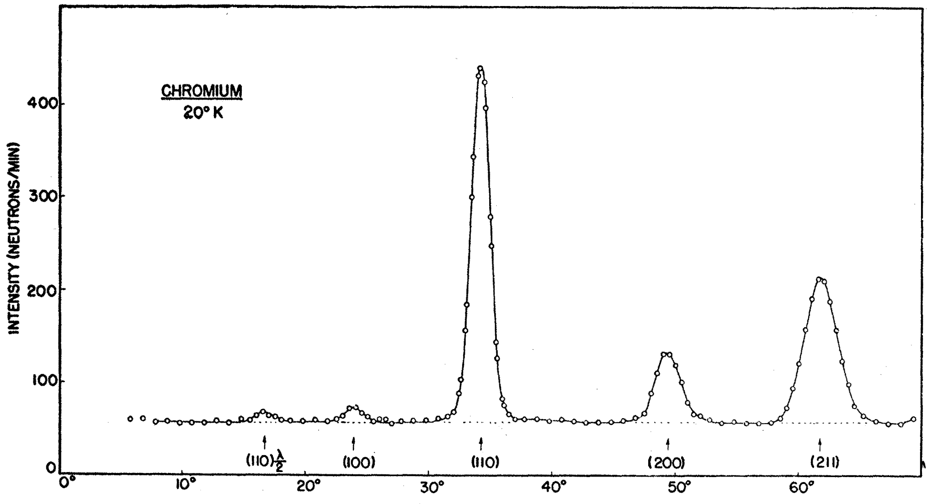

FIG. 4. Neutron diffraction pattern for Cr taken at 20°K. Extra antiferromagnetic intensity exists in the (100) reflection over and above a weak $\lambda/2$ contribution (compare with Fig. 2).

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* We are much indebted to Mr. B. S. Borie and Mr. R. S. Steele for these x-ray measurements.

(and hence not measurable with x-rays) of the two stable chromium oxides, Cr_2O_3 and CrO_2. Additionally, several samples which were obtained from different sources or had been subjected to different treatment were examined. These included (1) a sample of very fine electrolytic chromium powder from a different source than the chips, (2) a sample of the electrolytic flakes which had been crushed only to 30<40 mesh rather than a fine powder, (3) a sample of relatively impure chromium (containing 0.96 percent Fe and 0.2 percent Mn) manufactured by an aluminum reduction method, (4) a sample of electrolytic flake which had been degassed by high vacuum heat treatment at 500°C, and (5) a sample of electrolytic flake which had been heat treated in air at 500°C until noticeable oxide had been formed. Examination of all of these samples showed the same anomalous neutron intensity at the (100) position relative to the large (110) intensity or the (110) ($\lambda/2$) intensity.

The intensity in the (100) reflection has been placed on an absolute scale in terms of differential scattering cross section, and this has been plotted in Fig. 5. It is seen to saturate at a value of 0.0038 barn/steradian per Cr atom, and this can be used to evaluate the magnetic moment of the Cr atoms arranged in a simple antiferromagnetic array. This results in an effective magnetic moment of 0.40 Bohr magnetons per atom, a value which is still very much smaller than that predicted on the atomistic viewpoint expressed in Table I.

Again it is instructive to look at the diffuse scattering in the Cr pattern to see if there might be any unaligned moment contribution. Figure 6 shows the observed diffuse scattering obtained for Cr at a temperature of 20°K and for comparison purposes the calculated magnetic diffuse scattering for unaligned moments of strength 5 Bohr magnetons. From the apparent isotropy in the observed intensity an upper limit on the possible magnetic diffuse scattering places the maximum strength of the unaligned moments at about 0.1 magneton. Thus the large difference between the predicted atomistic moment and the $0.40\mu_B$ which is observed in antiferromagnetic alignment can by no means be accounted for by an unaligned component.

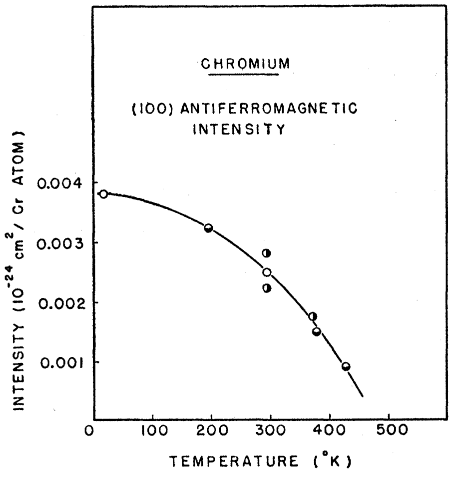

Fig. 5. Temperature dependence of the Cr (100) antiferromagnetic intensity in absolute units of differential scattering cross section.

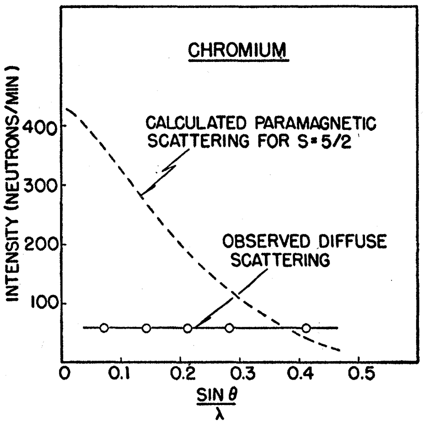

Fig. 6. Diffuse scattering observed in the neutron diffraction pattern for Cr showing the absence of any appreciable component of paramagnetic scattering.

It has been suggested that the low value for the observed Cr moment might be associated with a rapidly changing polarity of the moment in the lattice. The observed small value of $0.4\mu_B$ would then represent a residual moment which the neutron would see during its passage time ($\sim 10^{-13}$ sec) in the vicinity of an atomic moment. If such were the case, the residual moment should be quite sensitive to the neutron's velocity or wavelength. As a test on this, a pattern was taken with a neutron wavelength of 0.900A rather than the usual 1.212A, and this showed no significant change in the intensity of the (100) reflection relative to that of the (110) nuclear reflection. Changing the passage time by 25 percent should have changed the residual magnetic moment by several hundred percent if there had been a coincidental phase relationship between the neutron's speed and the polarity flipping of the magnetic moments, and nothing like this was observed.

Mn

This material was examined in the form of α-manganese, which possesses a cubic unit cell of size 8.894A containing 58 atoms. The sample first examined was of electrolytic origin in the form of a very fine powder. This was found to show oxide impurity in the diffraction pattern and was discarded in favor of treated electrolytic chips. As obtained from the commercial vendor the electrolytic manganese flakes possessed a characteristic surface layer of brownish oxide. This oxide layer was removed by dipping the electrolytic flakes into dilute hydrochloric acid followed by rinsing and drying. The flakes, of bright metallic appearance, were then fragmented in a mortar and placed in a high vacuum furnace for degassing at about 300°C. Following this, the

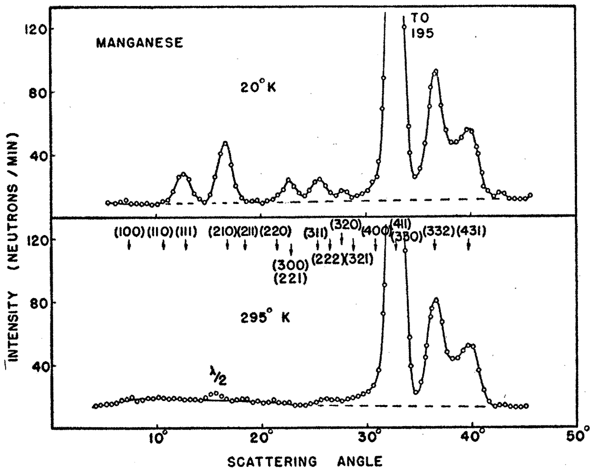

FIG. 7. Neutron diffraction patterns for α-Mn taken at 20° and 295°K. Extra antiferromagnetic reflections are to be seen in the low temperature pattern which transform into paramagnetic scattering with short-range order characteristics at room temperature.

small chips were sealed into an aluminum capsule for examination in the neutron diffraction spectrometer. This procedure of specimen preparation was found to show no measurable oxide impurity in the diffraction pattern. Spectroscopic analysis indicated a purity of 99.98+ percent with Ca and Cu as the primary impurities.

Figure 7 shows diffraction patterns for α-Mn taken at room temperature and at 20.4°K. In the room temperature pattern are observed the normal lattice reflections caused by nuclear scattering, as well as an angularly dependent diffuse scattering which is attributed to paramagnetic scattering. At the low temperature there is noticed a decrease in the paramagnetic diffuse scattering and a pronounced build-up of extra coherent scattering. The new reflections are at the (111), (210), (300)–(221), and (311) positions. Since these reflections have zero structure factors for a lattice in which every Mn atom is the same, their appearance in the low temperature neutron pattern immediately suggests an antiferromagnetic lattice. The nuclear reflections are unaltered in intensity or location, aside from a normal temperature dependence, and this can be taken as evidence that there has not occurred any gross crystallographic transformation on cooling.

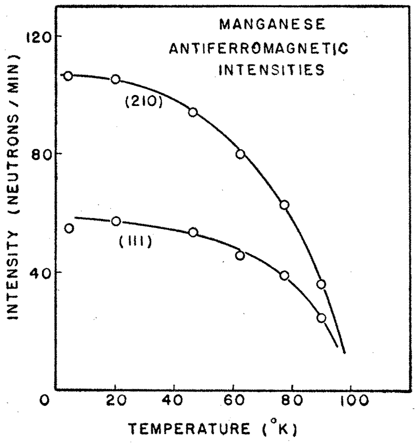

FIG. 8. Temperature dependence of the (111) and (210) antiferromagnetic reflections in α-Mn. The Néel temperature is at 100°K.

A careful study of the temperature dependence of the extra low temperature reflections at temperatures as low as 4.2°K has been made, and Fig. 8 summarizes this for the two reflections, (111) and (210). Again as with the extra reflection in Cr, a Brillouin-type temperature dependence is indicated with a Néel temperature of 100°K. The intensities are reversible and within the significance of the measurements show no hysteresis effects.

Because of the lattice complexity and the limited number of magnetic reflections which were measurable, it has not been possible to describe the antiferromagnetic structure which sets in below 100°K. A number of possible models were studied† which led to finite and reasonable intensities for the magnetic reflections, but these had to be discarded for one reason or another. In the absence of a detailed magnetic structure model it has not been possible to use the coherent intensities in assigning an effective magnetic moment for the manganese atoms in the lattice. It is by no means certain that all of the atoms possess the same magnetic moment and this complicates the picture even more. Whatever the moment distribution may be, it is certain that they must exist in balanced pairs since it has been established that manganese metal does not become ferromagnetic even at these low temperatures.

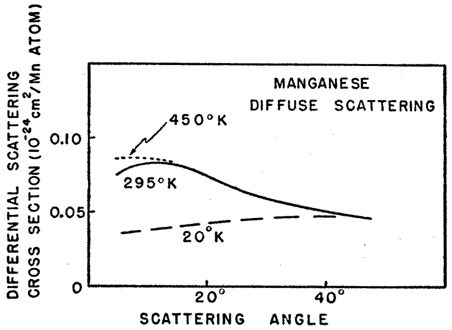

FIG. 9. Diffuse scattering observed in the neutron diffraction pattern for α-Mn at various temperatures. The paramagnetic scattering in the forward direction amounts to $0.060 \cdot 10^{-24}$ cm²/steradian per Mn atom.

Of interest in the higher temperature patterns is the observable paramagnetic scattering. At room temperature there is a suggestion of residual short range coherence in the magnetic diffuse scattering and this short-range order has been found to disappear at higher temperatures. Figure 9 illustrates the absolute intensity

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† We wish to thank Dr. B. W. Roberts for investigating some of these models.

of the diffuse scattering expressed in units of differential scattering cross section for temperatures of 20°, 295°, and 450°K. These curves have been corrected for a small amount of thermal diffuse scattering, and the differences from one temperature to another represent changes in magnetic diffuse scattering. The characteristic form factor variation of the scattered intensity with scattering angle is to be noticed in the higher temperature curves. From the absolute intensity of the magnetic scattering (that portion associated with the form factor), which is seen to amount to about 0.060 barn/steradian per Mn atom in the forward direction, it is possible to determine an average or effective magnetic moment for manganese in the paramagnetic state. Halpern and Johnson[1] have given a theoretical evaluation of the paramagnetic cross section as

$$d\sigma\text{ (para)}=0.194\cdot 10^{-24}S(S+1)\text{ cm}^2$$

in the forward direction. Here S represents the spin quantum number of the magnetic atom. A straightforward application of the above experimental cross section leads to $S=0.25$ and hence a magnetic moment of 0.5 Bohr magneton per Mn atom. However, it is rather doubtful that the above formulation can be significantly used with such a small cross section corresponding to less than one electronic magnetic moment. Perhaps a more significant interpretation of the cross section is in terms of the fraction of the atoms which possess say one Bohr magneton with the rest exhibiting no magnetic moment. In this way a distribution of 40 percent of the atoms having $1\mu_B$ and 60 percent having no moment would be in agreement with the observation.

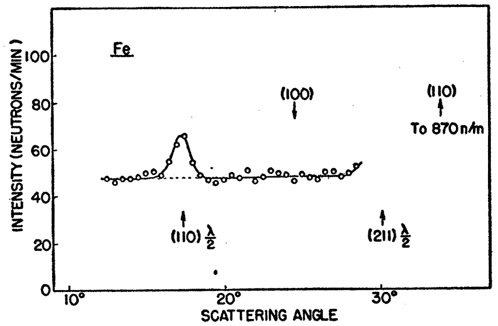

Fig. 10. Portion of the neutron diffraction pattern for Fe showing the region around the (100) reflection.

Fe

Neutron diffraction measurements on unmagnetized and magnetized Fe have been reported earlier,[2] and these have shown the presence of ferromagnetic scattering superimposed on strong nuclear reflections. The strength of the magnetic scattering was found to be in agreement with the Fe moment of $2.22\mu_B$ and the angular variation of the magnetic scattering was in satisfactory agreement with theoretical estimates of the magnetic form factor. Since that time, additional measurements have been made on the intensity at the possible superstructure line position (100) and on the diffuse scattering in order to establish limits on the possible difference between local atomic moments.

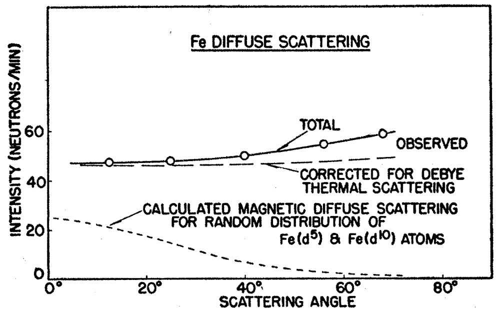

Fig. 11. Diffuse scattering observed in the neutron diffraction pattern for Fe. Magnetized sample studies permit a quantitative determination of the amount of magnetic disorder scattering which might be present in the diffuse scattering.

A concentrated study of the intensity at the (100) position for iron was carried out for two neutron wavelengths, 1.212A and 0.900A. The sample was in the form of filings from pure Armco iron which were given a vacuum heat treatment at 500°C. Figure 10 illustrates the intensity in the region of the (100) reflection, and it has been established that all of the observed reflection here can be accounted for satisfactorily by the second-order contaminant of known amount. From the sensitivity of observation it has been established that the differential scattering cross section $F^2{}_{100}$ for magnetic scattering in the (100) superstructure line must be less than $0.0010\cdot 10^{-24}$ cm^2 per Fe atom. This can then be used to set an upper limit on the difference between the magnetic moments μ_1 and μ_2 which might exist for the two unique atoms of the body-centered cubic unit cell. Such considerations show that $\mu_1-\mu_2$ must be less than $0.4\mu_B$. In other words, if an ordered array of iron atoms existed with a unit cell containing an iron atom of moment μ_1 at the corner position and an iron atom of moment μ_2 at the body-centered position, then these two atomic moments could not differ *algebraically* by more than $0.4\mu_B$. This upper limit for the difference is very much smaller than the $6.0\mu_B$ suggested by Zener's model[3] or the $5.0\mu_B$ suggested by Hume-Rothery, Irving, and Williams.[4]

In addition to the investigation of the coherent scattering effects produced by a possible ordered distribution of magnetic moments in metallic iron, a study of the diffuse scattering should yield information on the

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[1] O. Halpern and M. H. Johnson, Phys. Rev. **55**, 898 (1939). See also Shull, Strauser and Wollan, Phys. Rev. **83**, 333 (1951) for experimental results.

[2] Shull, Wollan, and Koehler, Phys. Rev. **84**, 912 (1951).

[3] C. Zener, Phys. Rev. **85**, 324 (1952).

[4] Hume-Rothery, Irving, and Williams, Proc. Roy. Soc. (London) **208**, 431 (1951).

presence of a random distribution of moments. If two magnetic ions of moments μ_1 and μ_2 were randomly distributed throughout the body-centered cubic lattice, magnetic incoherent scattering would be expected whose intensity would depend upon $(\mu_1-\mu_2)$ and which would exhibit a magnetic form factor variation of intensity with scattering angle. Figure 11 shows the diffuse scattering which is observed for Fe and after correction for normal Debye thermal scattering, this is seen to be closely isotropic. For comparison purposes there is also shown on the graph the expected magnetic disorder scattering for a randomly distributed arrangement of Fe(d^5) and Fe(d^{10}) ions. Since all of the known components in the diffuse scattering are isotropic or very nearly so, it is not considered possible that the observed scattering could contain very much of the form factor magnetic scattering.

A more quantitative estimate of the magnetic portion can be obtained if the diffuse scattering is studied with a magnetized scattering sample. By magnetizing the sample in a direction parallel to the scattering vector, thereby directing all of the atomic moments in this sense, all of the magnetic scattering should disappear according to the theory of magnetic scattering for neutrons. This has been tested experimentally by placing the sample between the pole pieces of an electromagnet capable of applying a field of about 8000 oersteds. The diffuse scattering was studied at a scattering angle of 8°, and it was found not to change by more than 1 percent upon magnetization. This upper limit on the change of intensity has been converted to absolute units and places the magnetic disorder scattering at less than $0.0035\cdot10^{-24}$ cm^2/Fe atom. In turn this implies that the difference $(\mu_1-\mu_2)$ must be less than $0.6\mu_B$, or there would have been a noticeably larger magnetic diffuse scattering in the neutron pattern. This difference is again very much smaller than those mentioned in the above references.

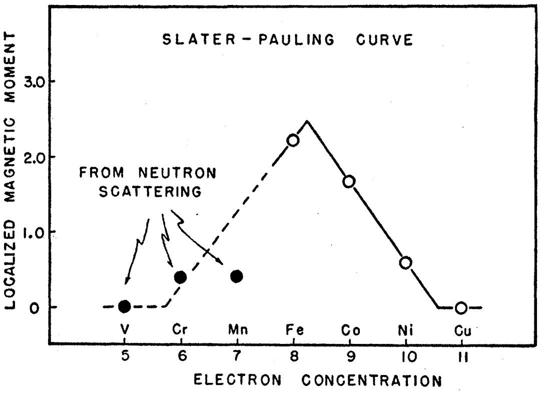

FIG. 12. Comparison between the observed atomic moments as determined by neutron scattering and the Slater-Pauling curve.

DISCUSSION

Most of the present observations on the magnetic structures existing in the transition elements can be summarized by reference to the Slater-Pauling curve shown in Fig. 12. In attempting to explain the variation of saturation magnetization among the ferromagnetic elements and some of their alloys, Slater has offered band theory arguments to account for the almost linear variation of moment with outer electron concentration. A simplified picture was independently developed by Pauling in terms of a distribution of the outer electron system among stable atomic orbitals (which contribute to the macroscopic magnetic properties) and molecular bonding orbitals (which serve valence purposes), and Pauling extended the treatment to include other nonferromagnetic elements. It is seen that the experimental data for vanadium, chromium, and manganese do indeed follow the general trend of their predictions. The manganese crystal structure is so complicated and so different from all of the other simple structures that the apparent numerical disagreement for this case may not be troublesome.

The Néel temperatures for Cr and Mn which have been reported here have not received strong confirmation from measurements of physical properties such as susceptibility, specific heat, resistivity, etc. For chromium, the recent paramagnetic susceptibility measurements of Fine, Greiner, and Ellis[5] and of McGuire and Kriessman[6] have not been suggestive of a Néel transition at 200°C. This may be a consequence of the relatively small moment which is found by neutron scattering and the relatively high Néel temperature. The anomalies in resistivity and other physical properties found by Fine *et al.* at 40°C for chromium do not correlate with the Néel temperature of 200°C. The early work of Serres[7] on the susceptibility of manganese did indeed suggest a low temperature antiferromagnetic transition, but this was open to suspicion because of possible oxide presence (both MnO and MnO_2 possess Néel temperatures in this region) as Serres has pointed out. A noticeable specific heat anomaly in manganese at 95°K has been reported by Shomate,[8] and recent unpublished measurements by Patrick have also indicated an abrupt change in resistivity at about 83°K. Both of these latter measurements may very well be associated with an antiferromagnetic transition.

The observations on iron have indicated the lack of either an ordered or disordered distribution of sizeably different magnetic ions at least as seen by neutrons in a scattering experiment. Of course, if such a distribution of ionic strength did occur and there were very rapid transitions for any one ion from one state to

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[5] Fine, Greiner, and Ellis, J. Metals **189**, 56 (1951).

[6] T. R. McGuire and C. J. Kriessman, Phys. Rev. **85**, 452 (1952).

[7] A. Serres, J. phys. et radium **9**, 377 (1938).

[8] C. H. Shomate, J. Chem. Phys. **13**, 326 (1945).

another in a time which is much shorter than the neutron passage time of 10^{-3} seconds, then the neutron would see just the average of the different states and all iron atoms would appear identical, in agreement with experiment. Since it appears necessary to admit of a mixture of states to account for the odd moment, this may very well be a reasonable picture.

ACKNOWLEDGMENT

We wish to thank Mr. L. A. Rayburn for considerable assistance in the preparation of suitable samples and in some of the later data accumulation. Very helpful conversations and correspondence with Dr. J. E. Goldman, Dr. J. C. Slater, and Dr. C. Zener have been appreciated.

DISCUSSION

W. J. Carr, Jr., *Westinghouse Research Laboratory, East Pittsburgh, Pennsylvania:* In connection with the data on Ni_3Mn and Ni_3Fe it seems worth pointing out that, since the alloys did not have perfect order, one would expect a number of Mn or Fe nearest neighbors to exist. If such Mn or Fe nearest neighbors exhibit an antiferromagnetic behavior, it would require a reinterpretation of Dr. Shull's data and lead to different calculated moments for the Fe, Mn, and Ni atoms.

H. Eckstein, *Armour Research Foundation, Chicago, Illinois:* Have you assumed purely elastic scattering? Is it possible that the spin coupling is only of the order of a fraction of an ev? Then the elastic scattering should be considered.