

where \mathbf{n} and \mathbf{r} are running vectors in Fourier and crystal space respectively, magnitudes η and r , and v_a is the volume of the primitive cell.

We consider a crystal in which the total charge density at a typical lattice site, taken as origin, is $R(\mathbf{r}) = Z[\delta(\mathbf{r}) - R_S(r)]$, where Z is the atomic number, and $R_S(r)$ is a spherically symmetric electron density of content $+1$; there is no net charge at any site. Let $P(\mathbf{n}) = \mathfrak{F}(R(\mathbf{r}))$, $P_S(\eta) = \mathfrak{F}(R_S(r))$, $\Phi(\mathbf{n}) = \mathfrak{F}(V(\mathbf{r}))$, where $V(\mathbf{r})$ is the potential due to $R(\mathbf{r})$. Then from Poisson's equation,

$$\Phi(\mathbf{n}) = P(\mathbf{n})/4\pi^2\eta^2 = Z[v_a^{-1} - P_S(\eta)]/4\pi^2\eta^2, \quad (2)$$

where²

$$P_S(\eta) = \frac{2\pi}{v_a} \int_0^\infty \frac{J_{\frac{3}{2}}(2\pi\eta r)}{(\eta r)^{\frac{3}{2}}} R_S(r) r^2 dr. \quad (3)$$

The average crystal potential is $\lim_{\eta \rightarrow 0} \Phi(\eta)$. Using the Taylor expansion³ of $J_{\frac{3}{2}}(2\pi\eta r)$ in (1)-(3), we have

$$\begin{aligned} \Phi(\eta) = Z(4\pi^2 v_a \eta^2)^{-1} & \left[1 - 4\pi \int_0^\infty R_S(r) r^2 dr \right. \\ & \left. + \frac{8\pi^3}{3} \eta^2 \int_0^\infty R_S(r) r^4 dr - O(\eta^4) \right]. \quad (4) \end{aligned}$$

The first integral in (4) is $(4\pi)^{-1}$ by the normalization, so

$$\Phi(000) = \frac{2\pi Z}{3v_a} \int_0^\infty R_S(r) r^4 dr = \frac{2\pi}{3v_a} Z \langle r^2 \rangle_{av}, \quad (5)$$

which is the Frenkel-Bethe result. If the crystal has a basis, (5) must be summed over each species present.

Thus the contribution of one type of particle to the average crystal potential can be directly determined from the appropriate atomic scattering factor, $f(\sin\vartheta/\lambda) = ZP_S(\eta)$. Near $\eta=0$,

$$ZP_S(\eta) = [Z/v_a - 4\pi^2\Phi(000)\eta^2 + O(\eta^4)]. \quad (6)$$

Since the largest contribution to $P_S(\eta)$ at small η comes from the outer or valence electrons,⁴ the average crystal potential is primarily determined by the valence electron density. Crystal binding will of course greatly distort the valence electrons from their configuration in the free atom. Hence in general one cannot use the *free* atom scattering factors to determine the average crystal potential, unless accurate x-ray Fourier synthesis of the crystal electron density shows that the same scattering factors apply to the atom bound in the crystal.

For an ionic crystal the net charge at each site, $P(000)$, is not zero so it is not clear that this analysis should apply. If, however, the excess or deficiency of charge is treated separately from the neutral complex of core plus compensating charge,⁵ then (5) can apply to the neutral complex, while the excess density makes no contribution. We hope to discuss the average crystal potential again at a later date.

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¹ J. Frenkel, *Z. Physik* **59**, 649 (1930); H. Bethe, *Ann. Physik* **87**, 55 (1928), see footnotes 1 and 2 on p. 106 and Eq. (85) on p. 109.

² S. Bochner and K. Chandrasekharan, *Fourier Transforms* (Princeton University Press, Princeton, 1949), p. 67 ff.

³ G. N. Watson, *Bessel Functions* (The Macmillan Company, New York, 1945), second edition, p. 15.

⁴ R. W. James, *The Optical Principles of the Diffraction of X-rays* (G. Bell and Sons, Ltd., London, 1950), pp. 125-129.

⁵ J. L. Birman, *Phys. Rev.* **97**, 897 (1955); see also erratum, *Phys. Rev.* **98**, 1871 (1955). Note that in *both* (4.2) and (4.3) the average potential is made equal to zero, which is a consequence of the use of the sums $\psi^{(1)}(\mathbf{r}; \alpha)$ and $\psi^{(2)}(\mathbf{r}; \alpha)$.

Magnetic Susceptibility of α Manganese at Low Temperatures*

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RECENT measurements of the specific heat in α manganese¹ at liquid helium temperatures yield a value for the electronic term that is very large compared to other elements of the first transition series. This implies a very high density of states at the Fermi surface of the $3d-4s$ band which could on the band picture lead to strong magnetic effects. To investigate this, measurements of the magnetic susceptibility were undertaken in the range of temperature between 1.8°K and room temperature. Previous measurements of the susceptibility of α Mn by Serres² and Kriessman and McGuire³ show a maximum in the susceptibility in the neighborhood of 150°K but these measurements were only taken down to liquid nitrogen temperatures. Shull⁴ has studied this material by means of neutron diffraction and finds evidence for a feeble antiferromagnetism at low temperature which disappears at approximately 100°K. Since the completion of this work, more recent measurements by Kriessman and McGuire to lower temperatures⁵ have come to our attention and in these a marked increase in susceptibility is reported.

The measurements were made by an induction technique⁶ in which a disk-shaped sample is translated between two detecting coils connected in series opposition. The magnetic moment is obtained by measuring the dc current that must be supplied to a third coil, that is wound on the sample and which rides with the sample, in order to balance out the detected signal. The entire coil and sample assembly is suspended in a Dewar designed to eliminate the need for liquid nitrogen in the field-sensitive region⁷ and sits between the pole pieces of an A. D. Little electromagnet. With this

method, susceptibilities of the magnitude measured in this experiment may be measured to an accuracy of 1 percent.

Two samples of α Mn were employed in this investigation. One was from a cast ingot⁸ and was pickled prior to measurement; the other was a packed capsule of electrolytic flakes and was from the same sample used by Shull in his neutron diffraction investigation. The results are tabulated in Table I. The room temperature

TABLE I. Mass susceptibility of α Mn, $\chi \times 10^6$.

T°K	Electrolytic	Cast ingot	Cast ingot degassed
300	10.6	8.8	8.9
120-170	10.9	9.6	...
90	10.7	9.4	...
77	10.5	9.9	...
4.2	11.5 ^a	15.0 ^a	9.0 ^a

^a Magnetization in a field of 10 kilogauss on a virgin magnetization curve ($\times 10^6$).

susceptibility for both samples was of the order of 10^{-5} emu/g and in good agreement with previously measured values. Both samples also show the maximum below 200°K that is found by the earlier investigators.

The cast sample shows an increasing susceptibility below 100°K. At helium temperatures the sample is definitely ferromagnetic with a remanence of some 0.07 emu/g. The magnetization at each field is increased over the room temperature values by approximately the remanence. The magnetization at 10 kg is approximately 70 percent greater at 4.2°K than at 77°K. The remanence decreases rapidly between helium and hydrogen temperatures but persists to approximately 60°K. This behavior appears to be consistent with the susceptibility curve of Kriessman and McGuire. However, for the electrolytic sample, which is similar to that of Kriessman and McGuire, the increase in susceptibility at helium temperatures is nowhere near so marked, being less than 10 percent. A remanence is still observed but amounts to but 0.005 emu/g. It is well known⁹ that many alloys and compounds of manganese, including the hydride and nitride, are ferromagnetic. Chemical analysis of the case sample did indeed show the sample to contain 0.4 percent (atomic) hydrogen, 0.11 percent oxygen, and 0.09 percent nitrogen. Analysis of the electrolytic sample from the diffuse background in the neutron diffraction pattern shows the hydrogen content to be no greater than 0.02 percent. On the supposition that the observed ferromagnetism may have been caused by the presence of interstitial impurities, the "ferromagnetic" sample was given a vacuum anneal treatment of 500°C which presumably removes most of the common interstitial impurities. Following the anneal this sample showed a 2 percent increase in susceptibility at room temperature. At helium temperatures, however, its susceptibility was within 2 percent of its room temperature value and the

remanence was down to 0.003 emu/g. One may thus conclude that the onset of ferromagnetism in manganese is associated with the presence of interstitial impurities and the increase observed by Kriessman and McGuire at low temperatures is probably due to the presence of impurities in their sample and is not an intrinsic property of the manganese. Further investigation of the quantitative aspects of this effect and its interpretation is being undertaken in this Laboratory. The authors are indebted to Dr. C. J. Kriessman and Dr. T. R. McGuire for making the results of their research available in advance of publication and to Dr. G. Derge for the vacuum fusion analyses.

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² A. Serres, *J. phys. radium* **9**, 377 (1938).

³ C. J. Kriessman and T. R. McGuire, *Phys. Rev.* **90**, 374 (1953). Their curve is reproduced in a paper by C. J. Kriessman and H. B. Callen [*Phys. Rev.* **94**, 837 (1954)] who also give an interpretation based on the band theory.

⁴ C. G. Shull and M. K. Wilkinson, *Revs. Modern Phys.* **25**, 100 (1953).

⁵ C. J. Kriessman and T. R. McGuire, *Phys. Rev.* **98**, 936 (1955).

⁶ A. Arrott, thesis, Carnegie Institute of Technology, 1953 (to be published).

⁷ W. E. Henry and R. L. Dolecek, *Rev. Sci. Instr.* **21**, 496 (1950).

⁸ Supplied by National Research Corporation and obtained through the kind cooperation of Professor J. G. Daunt.

⁹ R. Becker-Döring, *Ferromagnetismus* (Verlag Julius Springer, Berlin, 1939), p. 100.

Infrared Absorption of Silicon Near the Lattice Edge

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WE have measured the absorption of a polycrystalline specimen of 100 ohm-cm silicon in the neighborhood of the lattice edge at temperatures from 20°K to 3330°K. High resolution was obtained by the use of glass prisms, the method being to measure the transmitted radiation intensity with and without the specimen present, to deduce the reflection coefficient from the constant value of the transmission coefficient at wavelengths well beyond the absorption edge, and to calculate the absorption from these data.

The results, shown in Fig. 1, indicate that, as with germanium,¹ the absorption constant, K , is well represented at low levels by a law of the form

$$K = A \left[\frac{(h\nu - E_G - k\theta)^2}{1 - e^{-\theta/T}} + \frac{(h\nu - E_G + k\theta)^2}{e^{\theta/T} - 1} \right].$$

The best fit is obtained with $\theta = 600^\circ\text{K}$, for which value the full lines in Fig. 1 are drawn. E_G , which in the theory