as well as the phase transition and lattice constant variation must be considered when treating the crystalline field in these temperature ranges.

A. BOSE : A phase change can occur in our case but as yet we have no direct evidence for such changes. The changes in most cases appear to be perfectly reversible, and hence may be only a lattice expansion effect or may be the effect you mention.

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The Energy Band Structure of Body Centred Iron

J. F. CORNWELL AND E. P. WOHLFARTH
Department of Mathematics, Imperial College
London, England

The density of states curve of iron has been calculated using the Slater-Koster interpolation scheme and data due to J. H. Wood. The relevance of the results in the theory of ferromagnetism is discussed.

Wood[1)] obtained a density of states, $N(E)$, curve for iron directly from energy levels at 55 non-equivalent points of the Brillouin zone, calculated by the augmented plane wave method. As this number of points is insufficient for an accurate calculation of $N(E)$, levels at altogether 396 evenly spaced non-equivalent points were obtained from Wood's data, using the Slater-Koster interpolation scheme[2)]. Here 9 Bloch sums

$$\psi_{nk}(\boldsymbol{r})=C\sum_{l}\exp(i\boldsymbol{k}\cdot\boldsymbol{R}_l)\phi_n(\boldsymbol{r}-\boldsymbol{R}_l),$$

based on atomic s, p and d functions ϕ_n, were used; values of 30 energy integrals were obtained which reproduced nearly all Wood's energy levels very well.

Fig. 1 shows $N(E)$ for the lowest 6 bands; this agrees well with a more accurate calculation[3)] of $N(E)$ where the critical points, which give rise to discontinuities of $N'(E)$, are taken into account. The figure shows a peak at -0.01 Ry., agreeing well with that obtained by Wood at -0.03 Ry.; elsewhere, however, the figure differs markedly from Wood's. For 'non-ferromagnetic' iron the Fermi energy is here -0.01 Ry. where $N(E)=36.9$ Ry.$^{-1}$, corresponding to an electronic heat coefficient $\gamma=15.3\times10^{-4}$ cal mol^{-1} deg^{-2}. If the exchange forces are assumed to shift completely the sub-bands containing electrons with opposite spin so as to give an unbalance of 2.2 electrons per atom, the two corresponding energies lie at -0.13 and 0.07 Ry., as shown in Fig. 1. The calculated value of γ is then 6.3×10^{-4} cal mol^{-1} deg^{-2}, compared with the experimental value 12.0×10^{-4}. Both these energies for ferromagnetic iron correspond to relatively high values of $N(E)$, agreeing with a suggested interpretation[4)] of the magnetic properties of iron alloys.

The one-electron wave functions are given by

$$\psi_k(\boldsymbol{r})=\sum_n a_n(\boldsymbol{k})\psi_{nk}(\boldsymbol{r}),$$

$$\sum_n |a_n(\boldsymbol{k})|^2=1,$$

and selected values of $A_d=\sum|a_n(\boldsymbol{k})|^2$, corresponding to the 5 atomic d functions only, are shown as functions of $E(\boldsymbol{k})$ in Fig. 2. It appears that A_d is large only in the range $-0.4<E<0.3$ Ry. approximately, over most of which range $N(E)$ is also high. Between -0.7 and -0.4 Ry., only A_s is large and both A_s and A_p are appreciable above about 0.3 Ry. Hence the original basis of the collective electron treatment of ferromagnetism[4)] of overlapping d and $s-p$ bands is not unreasonable.

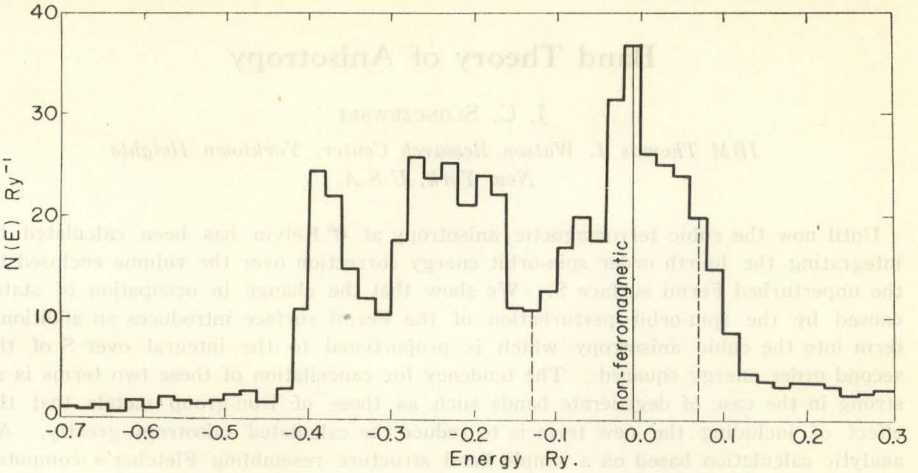

Fig. 1.

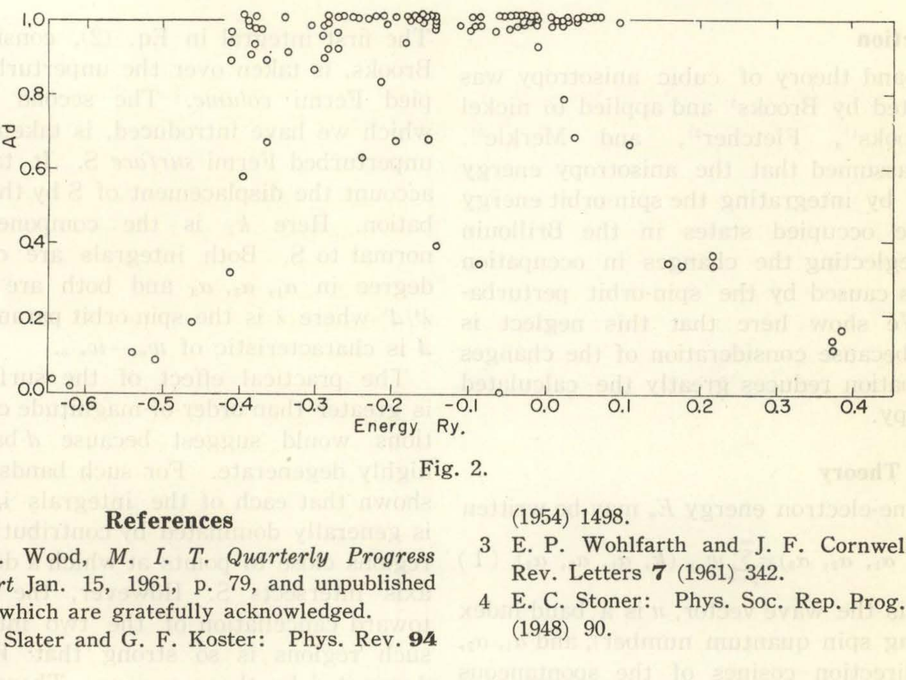

Fig. 2.

References

1 J. H. Wood, *M. I. T. Quarterly Progress Report* Jan. 15, 1961, p. 79, and unpublished data which are gratefully acknowledged.

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DISCUSSION

W. KOHN: What is the precise mathematical meaning which you attribute to what you call "amount of *d*-state"?

E. P. WOHLFARTH: The quantity A_d is as defined.

W. KOHN: In band calculation of the alkali metals a similar analysis also gives surprisingly high *p* and *d* admixtures. Nevertheless it seems inappropriate in this case to speak of the band as partly *d*-like.

E. P. WOHLFARTH: I agree about your comments on sodium.