Letters to the Editor

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Microwave Resonance Absorption in Gadolinium Metal*

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MICROWAVE resonance absorption in gadolinium metal has been measured near 9000 and 24 000 Mc/sec in the ferromagnetic and paramagnetic regions. Gadolinium is known to exhibit a saturation magnetization¹ corresponding closely (± 2) percent) to the value expected for an ⁸S state, where the magnetic moment of each atom is due to the seven electrons in the 4f shell. It is therefore likely, as Van Vleck² has emphasized, that Gd is a good realization of the atomic model of a ferromagnet, in contrast to the ferromagnetic metals of the iron group, all of which show saturation magnetizations which cannot be explained on such a simple basis. From this point of view, we wished to determine how closely the g value corresponds to the value for free electron spin, as expected for a half-filled shell. Our results suggest that there may be spin-orbit coupling effects, perhaps between the spin of $4f^7$ shell and the orbit of the 5d electron, which partly spoil the purity of the assumed ${}^{8}S$ ionic state.

An annealed circular disk of polycrystalline Gd, 2.3 cm in diameter and 0.04 cm thick, was used in these experiments. The sample contained no more than 0.1 percent of other rare earth elements. Absorption measurements were made by clamping the sample behind a hole of area 0.049 cm² drilled into the end wall of a resonant cavity, so that the sample effectively forms a small part of this wall. Figure 1 shows a typical resonance curve.

Results in the 9000 Mc/sec range were consistent with the 24 000 Mc/sec results, but because of the greater accuracy of the measurements at the higher frequency, only the latter will be given. Measurements were made in the temperature range between -196°C and +105.5°C. The Curie temperature is 16°C, according to Trombe. Figure 2 summarizes the results at 24.30×10^3 Mc/sec for the positions of maximum absorption vs temperature. The principal cause of the shift of the peak position in going from the paramagnetic to the ferromagnetic region is the increase in





FIG. 2. Gadolinium metal peak position vs temperature, at 24.3×10^{3} Mc/sec.

magnetization of the sample. The individual absorption curves in the paramagnetic range exhibit the typical shape of resonance curves in metals, as found by Yager³ and Bloembergen⁴ in the case of supermalloy and nickel. The width of the absorption curves in the paramagnetic region is approximately 1000 oersteds at the halfpower points. Below 20°C the width increases rapidly, and below 0°C the width is so great that no estimate can be made of the width, using external fields from 0 to 10 000 oersteds. The cause of the extreme width in the ferromagnetic region is not understood, but may be associated with a high crystalline anisotropy energy and polycrystalline broadening. The value of the magnetization in the ferromagnetic range was obtained from unpublished data of Elliott, Legvold, and Spedding.

The g factor obtained in the paramagnetic region is 1.95 ± 0.03 , taking into account shifts in the peak position due to demagnetizing factors and relaxation effects, as well as the effect of varying eddy current losses. In the ferromagnetic region the extreme breadth of the absorption curve prevents accurate determination of the g value. However, we have made calculations of the ferromagnetic g value, ignoring possible shifts in peak positions arising from relaxation effects. These calculations lead to a ferromagnetic g value of 1.94. A limit of uncertainty cannot be assigned to this value because of the extreme breadth of the absorption curves, but the g value is not inconsistent with that in the paramagnetic range.

Our results are to be compared with recent unpublished results of Elliott, Legvold, and Spedding on the saturation magnetization extrapolated to 0°K and infinite applied field. The g value obtained from this value of saturation magnetization is 1.96.

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Electronic Structure of the Germanium Crystal

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HE method of orthogonalized plane waves,¹ recently applied to the diamond crystal,² has been used to study the energy band structure of the germanium crystal. The calculation is based on the usual one-electron approximation. A crystal model constructed from isolated atoms [Ge(4s)¹(4p)³] arranged as a germanium lattice was used to determine the Coulomb potential. The constituent atomic wave functions were taken from the selfconsistent field calculations for Ge.3 The effect of exchange was not considered due to the complexity of available approximate treatments.



FIG. 1. Energy band structure of the germanium crystal. The present study was restricted to the points $\mathbf{k} = 000$ and $k = 2\pi(100)/a$. The curves joining the calculated eigenvalues indicate the estimated trends, based on the slopes and curvatures at the end points. The symbols denote degeneracy and symmetry classification. The notation is fully described in references 4 and 5.

The energy band structure predicted for germanium is shown in Fig. 1. The notation used is fully described by Bouckaert et al.4 and Herring.⁵ The nondegenerate conduction bands represented by Γ_1 and Γ_2 at $\mathbf{k} = 000$ have spherical energy surfaces at this point. The energy surfaces associated with the three lower-lying conduction bands do not have spherical symmetry in E vs k. A similar band structure was found for diamond.² Although the theory of electron mobility commonly employs spherical energy surfaces for the lowest conduction band for reasons of mathematical simplicity,6 recent measurements^{7,8} have led to interpretations to the contrary.9,10 These inferences are borne out by the present calculation.

While the numerical results are highly dependent upon the assumed crystal potential and core wave functions, the Γ_2' and Γ_{15} eigenvalues are found to lie far enough apart to suggest that the present study reliably predicts their relative position.

The \mathbf{k} value at which the minimum vertical separation between valence and conduction bands occurs cannot now be predicted with certainty. One of the three conduction bands, degenerate at $\mathbf{k} = 000$ (at Γ_{15}), has a downward curvature at this point in certain crystallographic directions; the largest downward curvature occurs along the screw axis (100). The other two bands have upward curvature at $\mathbf{k} = 000$ in all directions. The lowest conduction band has a smaller downward curvature at $\mathbf{k} = 000$ than any of the three valence bands degenerate at this point (at Γ_{25}). An exploratory calculation at $\mathbf{k} = 2\pi (100)/a$ on the reduced zone face indicates that the separation between valence and conduction bands is considerably greater at this point than at the reduced zone center (k=000). In view of these results, it appears likely that the minimum vertical (optical) separation occurs at $\mathbf{k} = 000$.

That the lowest energy value reached by the lowest conduction band does not lie much below its value at k=000 is suggested by the approximate equality of the energy gaps determined by optical and thermal measurements. The calculated energy gap at k=000, 1.45 ev, is in reasonable agreement with the experimental value, 0.75 ev.⁶ The valence bands are found to span an energy range of 13.3 ev; experimental data bearing on this prediction are lacking

In the limit of an empty diamond-type lattice (V=0), the states Γ_{15} and Γ_{25}' coalesce. The crystal potential removes this degeneracy. In the case of diamond,² Γ_{15} and Γ_{25} ' are automatically orthogonal to the core bands formed from the (1s) atomic states.

The crystal potential, representing Coulomb and exchange interactions, separates these states by about 5.7 ev. In germanium, these states must be orthogonalized to the core bands arising from the (2p), (3p), and (3d) atomic states. The existence of a smaller energy gap in germanium may be attributed to the partial cancellation of the attractive crystal potential by a repulsive potential introduced by the orthogonalization. The convergence properties of the germanium eigensolutions are improved, relative to the diamond eigensolutions, by the additional orthogonality terms.

A more detailed account of the present investigation will be submitted for publication shortly.

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Proton-Proton Scattering at Intermediate Energies

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 $R_{
m pseudoscalar\ meson\ theory\ (with\ pseudoscalar\ coupling)\ has}$ been analyzed by Lévy.¹ At low energies, this interaction reduces to a potential which has the following form:

$$V(r) = \infty \quad \text{for} \quad r < r_c,$$

$$V(r) = V_c(r) + S_{12}V_t(r) \quad \text{for}$$

where

$$V_{c}(r) = \frac{G^{2}}{4\pi} \left(\frac{\mu}{2M}\right)^{2} \frac{(\mathbf{\tau}_{1} \cdot \mathbf{\tau}_{2})(\mathbf{\sigma}_{1} \cdot \mathbf{\sigma}_{2})}{3} \frac{e^{-\mu r}}{r} - 3\left(\frac{G^{2}}{4\pi}\right)^{2} \left(\frac{\mu}{2M}\right)^{2} \frac{1}{\mu r^{2}} \\ \times \left\{\frac{2}{\pi}K_{1}(2\mu r) + \frac{\mu}{2M} \left[\frac{2}{\pi}K_{1}(\mu r)\right]^{2}\right\}, \quad (1)$$
$$V_{t}(r) = \frac{G^{2}}{4\pi} \left(\frac{\mu}{2M}\right)^{2} \frac{(\mathbf{\tau}_{1} \cdot \mathbf{\tau}_{2})}{3} \left[1 + \frac{3}{\mu r} + \frac{3}{\mu r^{2}}\right] \frac{e^{-\mu r}}{r},$$

its validity being limited to energies not greater than about 50 Mev. With this potential, Lévy has studied the low and intermediate energy experimental data for the neutron-proton system. The two constants $G^2/4\pi$ and r_c were determined to fit the binding energy of the deuteron and the neutron-proton zero energy singlet scattering length, with the following results:

$$G^2/4\pi = 9.7 \pm 1.3,$$

 $r_c = (0.38 \pm 0.03)(\hbar/\mu c).$ (2)

 $r > r_c$

It seemed interesting to investigate proton-proton scattering at intermediate energies (18.3 and 32 Mev), where the accuracy of the measurements and the sensitivity of the differential cross sections to the characteristics of the potential presumably provide a more severe test for the theory.

The calculations were carried out as follows: direct numerical integration of the Schrödinger equation for L=0, to obtain the S phase shift K_0 ; Born approximation with Coulomb wave function