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Extraordinary Hall Effect in Paramagnetic Gadolinium†

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The extraordinary Hall coefficient R_s of gadolinium has been measured in the temperature range 300–360 °K by analysis of the dc voltages accompanying electron spin resonance in thin oriented gadolinium films. These results extend the single-crystal data of R_s for M parallel to c, known up to 275 °K, into the paramagnetic range and give a temperature-independent value $R_s = -1.4\times10^{-9}$ V cm/AG at high temperatures. Combined with conventional Hall-effect measurements, the data also yield the strongly temperature-dependent ordinary Hall constant for the same orientation in this temperature range.

I. INTRODUCTION

Although primarily associated with ferromagnetics, the extraordinary Hall effect, which depends on electron polarization, exists also in paramagnetic conductors. Here its strength and sign can provide information about details of the effect of spin-orbit interaction on the band structure and on electron scattering. However, preliminary to such detailed application, it is still necessary to devise methods of identifying this effect unambiguously in paramagnetics and then to compare the results with the existing simplified general theories for it. We have developed a new method for isolating the extraordinary Hall effect in paramagnetic materials exhibiting electron spin resonance and have applied it to gadolinium in the strongly paramagnetic temperature range above the Curie point.

The extraordinary Hall effect is that portion of the Hall effect which, phenomenologically, is proportional to the magnetization of the material rather than to the applied magnetic field. It results from spin-dependent scattering by polarized groups of electrons interacting in a number of possible ways. Theories suitable for transition elements, where the d electrons provide both the magnetization and polarized charge transport, rely on spin-orbit interaction of the conduction electrons.[1] The role of localized magnetic electrons is emphasized by Kondo,[2] who considers their interaction with almost-free polarized conduction electrons, and by Maranzana,[3] who has proposed a model based on the interaction between the spin of the localized electrons and the orbital angular momentum of the conduction electrons. Kondo's model has become relevant ever since the recent assignment of partial d character to the conduction electrons in Gd,[4] which permits coupling to low-lying f electrons. Maranzana's approach has the advantage of not relying on the orbital angular momentum of the localized electrons, which is known to be quenched in Gd. In principle, both of these theories are applicable to the rare earths, and both predict an extraordinary Hall constant in the paramagnetic region which is independent of temperature.

Phenomenologically, the total Hall field may be written as the sum of two terms:

$$\vec{E}_H = -R_s \vec{J}\times\vec{M} - R_0 \vec{J}\times\vec{B} , \quad (1)$$

where R_s is the extraordinary Hall coefficient, R_0 is the ordinary Hall coefficient, $\vec{M}$ is the magnetization, $\vec{B}$ is the magnetic induction, and $\vec{J}$ is the current density. In the paramagnetic region, $\vec{M}$ does not saturate, and hence both terms in Eq. (1) increase with $\vec{B}$, making a separate identification of the two contributions difficult. In such a case, it becomes necessary to vary $\vec{M}$ independently of $\vec{B}$, as, for instance, by changing the temperature. This approach was applied to paramagnetic gadolinium by Volkenshtein and Fedorov,[5] and by Babushkina,[6] who analyzed conventional static Hall data over a range of temperatures by plotting the Hall voltage vs $\vec{M}$ while $\vec{B}$ was held constant. In each experiment, the constant-high-temperature slope of the plot was identified with a temperature-independent R_s. This method could not be extended to the vicinity of the Curie point because of the rapid temperature variation of all quantities there. The two experiments yielded $R_s = -5\times10^{-9}$ and -2×10^{-9} V cm/AG, respectively, at high temperatures.

This paper reports measurements of the extraordinary Hall constant in thin paramagnetic-gadolinium films[7] using a technique originally developed by Egan and Juretschke[8] for studying ferromagnetic resonance in thin films. The method is based on the detection of the nonlinear microwave interactions implied by Eq. (1), and employs the dynamic situation at spin resonance in which the alignment of the magnetic fields ($\vec{M}$, $\vec{H}$, and $\vec{B}$) is upset. By responding only to the extraordinary Hall effect, it eliminates the need for separating terms in Eq. (1), and R_s is directly obtained, once the magnetization $\vec{M}$ is known, at any given temperature.

On the other hand, the signal in this experiment must be subjected to detailed analysis and matched to the electromagnetic theory of the nonlinear effects before R_s can be extracted. This requires a series of systematic measurements to verify the proper dependence of the signal on various parameters of the theory. In addition, since the nonlinear effects studied here can only be detected in very thin films, it is necessary to establish how closely the thin-film properties correspond to those of bulk material.

We have determined the value of R_s in paramagnetic-gadolinium films up to 65° above the Curie point. In order to establish the applicability of the theoretical analysis for interpreting the microwave data, films of different thickness were studied, and in each case their quality relative to bulk gadolinium was determined by measurements at dc. The systematic program applied to a group of films consisted of (i) controlled preparation of Gd films; (ii) thickness, resistivity, static Hall effect, and static-susceptibility measurements over a range of temperatures; (iii) measurements of microwave resonance as a function of temperature and at various field geometries and power levels; and (iv) detailed analysis of the resonance data for determination of the microwave conduction parameters. The resonance measurements were made at microwave frequencies. However, we expect the values of R_s so obtained to be the same as those which would be measured at dc since $\omega\tau' \ll 1$ at the frequencies considered, where τ' is the collision relaxation time for the conduction electrons. In line with this, the microwave resistivities for the films are found to be comparable to their dc resistivities.

The results of our measurements of R_s are compared to those of Babushkina and those of Volkenshtein *et al*. and are also shown in relation to the results reported by Lee and Legvold[9] for ferromagnetic single-crystal gadolinium. Furthermore, the results add to and confirm various other transport and magnetic properties of gadolinium and gadolinium thin films.

II. ELECTROMAGNETIC THEORY

The principle of the experimental method is based on the fact that, if both $\vec{J}$ and $\vec{M}$ in Eq. (1) have components oscillating at the same frequency, this equation predicts a dc electric field proportional to R_s. The electromagnetic theory of such dc effects in metallic films during ferromagnetic and paramagnetic spin resonance has been presented by Juretschke,[10] Wald (née Weintraub),[11] and Moller.[12,13] It has been worked out specifically for a conductor in the form of a thin film of thickness Δ ($\Delta \ll \delta$, where δ is the skin depth of the material) located, as shown in Fig. 1, a distance D above a perfect short and subject to a microwave field propagating normal to the plane of the film. The propagation constants above, below, and within the film are k_0, k_1, and k_2, respectively. A steady magnetic field $\vec{B}_0$ in the

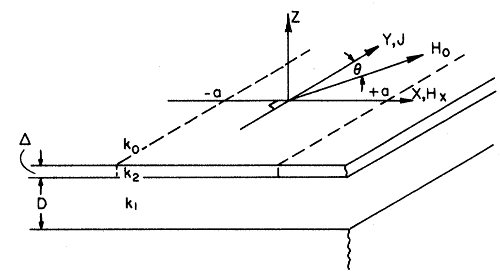

FIG. 1. Idealized experimental geometry. A film of thickness Δ is situated a distance D above a shorting plane. The film is cut at $x = \pm a$. H_0 lies in the film plane at an angle θ to the Y axis.

plane of the film defines the precession direction of the magnetization $\vec{M}$ of the film material. This precession is maintained by the $\vec{H}$ component of the microwave field, while the $\vec{E}$ component gives rise to an eddy current $\vec{J}$ in the film.

Under such conditions, Ohm's law in a magnetic conductor contains terms such as those in Eq. (1) and is given more fully by

$$\vec{E} = \rho \vec{J} - R_s \vec{J} \times \vec{M} - R_0 \vec{J} \times \vec{B} + (\Delta\rho / B^2)(\vec{J} \cdot \vec{B})\vec{B} , \quad (2)$$

where ρ is the resistivity normal to the direction of the magnetic field, $\Delta\rho$ is the magnetoresistive anisotropy, and the magnetic fields $\vec{B}$ and $\vec{M}$ are the sum of steady ($\vec{B}_0$ and $\vec{M}_0$) and microwave ($\vec{B}_1$ and $\vec{M}_1$) components. All terms except the first on the right-hand side of this equation couple two or more microwave quantities and give rise to harmonics of the microwave frequency.

In the present experiment we look for the dc effects. The contribution from the $\Delta\rho$ term is too small to be seen, since $\Delta\rho$ of Gd is very small. The R_0 term has no dc components in the film plane because by continuity the field B_{1z} vanishes identically within the film. Hence, the ideal experimental configuration, described in Fig. 1, focuses specifically on any effects due to R_s.

The x component of the dc electric field resulting from the nonlinear interaction involving R_s is given by the time and volume average

$$e_{0x} = R_s \langle J M_{1z} \rangle , \quad (3)$$

where, for convenience, we define $J \equiv |\vec{J}| = J_y$. This average is related to measurable quantities, such as applied microwave power and applied dc magnetic field, by solving to lowest order the appropriate electromagnetic boundary-value problem within the waveguide and across the region of the film sample. In the detailed calculations the Bloch equations of motion for the precessing magnetization have been used to determine M_{1z} in terms of H_{1x}.

If the extent of a paramagnetic field is limited in the x direction, as shown in Fig. 1, and no dc currents flow in this direction, the dc voltage generated

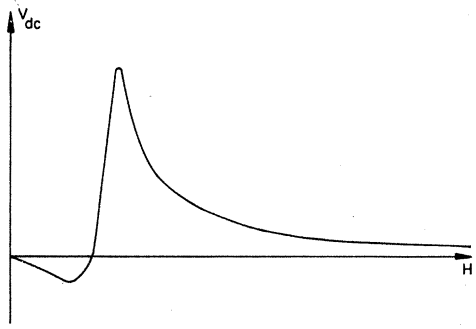

FIG. 2. Magnetic field dependence of V_{dc} as predicted by Eq. (2).

across the resulting strip is[11]

$$V_{dc}=\frac{-R_s a\sigma\omega}{2ck_1}\ \gamma\chi_0 H_1^2 \sin 2k_1 D(1+\tan^2\phi_4)^{1/2} \times\left[H_0\left(\frac{\omega^2+1/\tau^2}{(\omega_0^2-\omega^2)^2+4\omega^2/\tau^2}\right)^{1/2}\sin(\phi_2-\phi_1+\phi_4)\right], \quad (4)$$

where γ is the gyromagnetic ratio; ω is the microwave frequency, χ_0 is the static susceptibility, τ is the paramagnetic relaxation time, and the other quantities are defined by

$$\omega_0^2=\gamma^2 H_0^2(1+4\pi\chi_0)+\frac{1}{\tau^2}\ ,\quad \delta^2=\frac{c^2}{2\pi\omega\sigma}$$

$$\tan\phi_1=-\omega\tau,\ \tan\phi_2=\frac{-2(\omega/\tau)}{\omega_0^2-\omega^2}\ ,$$

$$\tan\phi_4=\frac{\Delta}{\delta k_1}\ \tan k_1 D\ .$$

The magnetic-field-dependent part of V_{dc} is contained in the square brackets. It has the general form shown in Fig. 2. The $\sin(\phi_2-\phi_1+\phi_4)$ factor, which modulates the resonance, has one zero whose position as a function of dc magnetic field depends upon the film thickness and on D, but always occurs below the resonant field. The field-independent factor is proportional to the applied microwave power through H_1^2, and is related to the film dimensions a and Δ, to D, and to the film's electrical and magnetic properties σ, χ_0, τ, γ, and R_s.

When the static magnetic field is applied at angle θ with respect to the Y axis, the dc effects based on Eq. (2) have the angular dependence

$$e_{0x}=-(\Delta\rho/B)\langle JB_{1x}\rangle\cos 2\theta\cos\theta+R_s\langle JM_{1z}'\rangle\cos\theta\ . \quad (5)$$

This angular dependence can be used to test for any contribution due to $\Delta\rho$.

III. FILM PREPARATION

Gadolinium film samples were evaporated onto carefully prepared glass substrates using three sources at an initial vacuum of 1.6×10^{-6} Torr. Simultaneous evaporation of three types of samples was carried out so that thickness, dc, and microwave measurements could be made on films with identifical properties.

The 99.9%-pure-Gd source was contained in a molybdenum or tungsten trough or was wound on tungsten filaments. Tungsten was used for most of the evaporations because the Gd tends to eat holes into the molybdenum during evaporation. Since the geometry of the container was found to have no effect on the properties of the films, the final choice of a trough was governed by the ease with which uniform substrate coverage could be obtained with minimum difficulty in preparation of the source. A separate source of Gd was used as a very effective preliminary getter to bring the pressure down to the value at which the films were evaporated. A third source in the vacuum station contained SiO in order to coat all the films, except the thickness plates, before they were exposed to air. Magnetization and resistivity measurements of films with and without the protective SiO layer show that coated films have properties much closer to bulk.

X-ray diffractometer runs and the results of the dc and microwave resistivity measurements indicate that, although the films are polycrystalline, there is significant c-axis orientation normal to the plane of the films.

IV. MICROWAVE EXPERIMENT

The experimental arrangement for measuring the dc effects is similar to that described by Moller and Juretschke.[13] The microwave film geometry was that originally used by Egan.[8] It offers little disturbance to the field patterns normally found in the waveguide, thus permitting use of the analysis of Sec. II which is valid for plane waves incident normally on a film of infinite lateral extent situated above a perfect short. Details of mounting the sample are discussed in Ref. 7.

The static magnetic field was swept in both directions up to 22 kG. The output appears directly as an x-y recorder trace of dc signal vs magnetic field. During any given run the temperature was maintained constant to within 1 °C.

Typical resonance signals obtained for a 1360-Å film of width $a=0.25$ cm are shown in Fig. 3. The signal observed at $\theta=45°$ is reduced but identical in shape to that observed at $\theta=0°$, indicating that the contribution of magnetoresistive anisotropy to the signal predicted by Eq. (5) is negligible. This is also confirmed by dc resistivity measurements where it was found that $\Delta\rho/\rho<10^{-3}$. This was true for all the films and, since V_{dc} followed a $\cos\theta$ dependence as the dc magnetic field was rotated in the film plane, the observed line shapes are expected to conform to those predicted for the extraordinary Hall contribution alone.

The rf power and D dependences of the resonance amplitude and line shape agree with the predictions of Eq. (4). Figure 4 shows recorder traces for the

1360-Å film at room temperature at six values of incident power. The magnetic field in each case was swept between − 9 and + 9 kG in the direction indicated by the arrow under each curve. The difference in noise level between curves is due to the change in recorder sensitivity. One sees from Fig. 4 that the line shape is independent of power in the range of power considered, with maxima, minima, and zeros occurring at the same magnetic fields in all curves. The resonance amplitudes vary linearly with power over most of the power range but exhibit some evidence of sample heating above 0.4-W average power (≈ 0.4-kW peak pulse power). Studies of the resonance line shape as a function of D show that it becomes more symmetric and the resonance amplitude smaller as D is increased; this is in agreement with the D dependence predicted by theory.

The temperature dependence of the resonance signal for the 1360-Å film is shown in Figs. 5 and 6. The amplitude decreases with increasing temperature as the material becomes less magnetic. The low-field crossover, which is the zero discussed in Sec. II and which is a function of the resistivity and relaxation time, is almost independent of temperature in the paramagnetic region. Below the Curie point the line broadens and the zero moves to lower fields. The second crossover at fields above resonance is connected with an additional signal not predicted by the theory.[7] Complete analysis of the curves has been somewhat complicated by this signal. However, its over-all effect on the basic numerical results is small, since the signal in the neighborhood of the resonant field is not significantly affected by this addition.

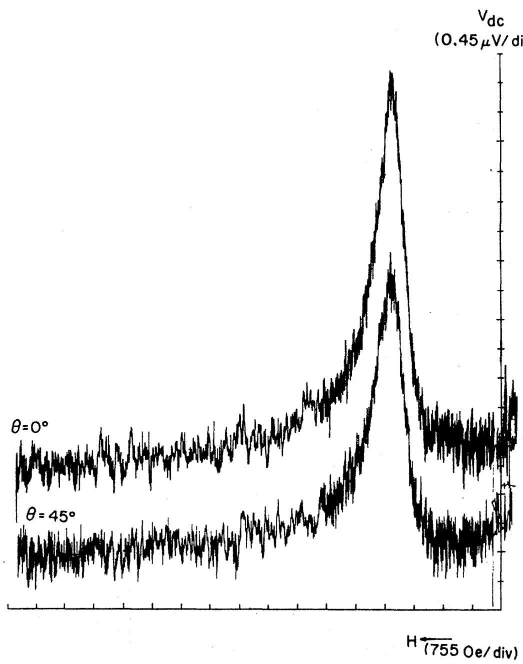

FIG. 3. Recorder traces of V_{dc} as a function of applied magnetic field at $\theta=0°$ and $\theta=45°$ for the 1360-Å film at room temperature: $D=0.05$ cm; $P_{av}=0.5$ W.

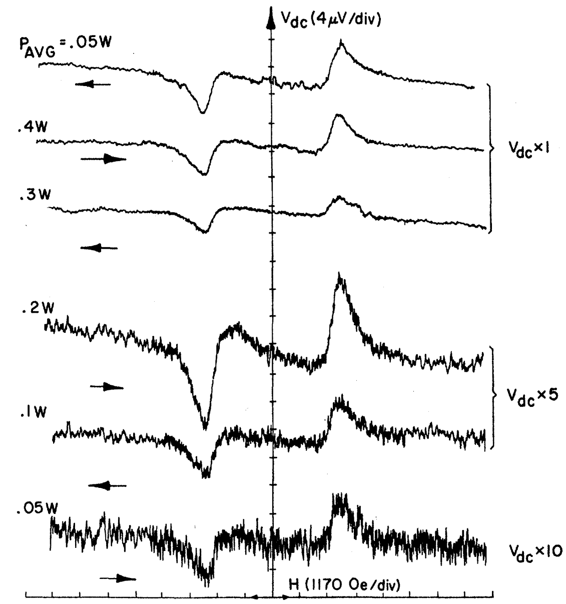

FIG. 4. Recorder traces of V_{dc} as a function of applied magnetic field for the 1360-Å film at room temperature at six values of incident power.

The magnetic field at resonance, determined by the analysis of these curves, increases with increasing temperature and follows fully the curve reported by Kip[14] for bulk gadolinium. The resonance linewidth in the paramagnetic region is constant at 420 ± 50 Oe, in agreement with results reported by Kip and by Rodbell and Moore.[15] As the temperature is reduced through the Curie point the linewidth increases in the manner observed in bulk gadolinium. The g value of all gadolinium films, obtained from detailed analysis of the resonance curves, is close to 1.96, as in bulk. The good agreement between the various bulk and film parameters confirms that we are observing the true gadolinium resonance.

V. RESULTS AND DISCUSSION

The room-temperature properties of five gadolinium films are summarized in Table I, together with pertinent bulk data. The first three columns refer to magnetic properties. The resonance parameters are identical in films and in bulk, but the susceptibilities decrease with film thickness, largely as a result of a slight drop in Curie temperature, but perhaps also because of oxidation of part of the film depth. In all subsequent analyses the experimentally found value of χ_0 was used. The dc resistivities show no thickness dependence. R_{dc} is the initial slope of the static-Hall-effect curve of E_H

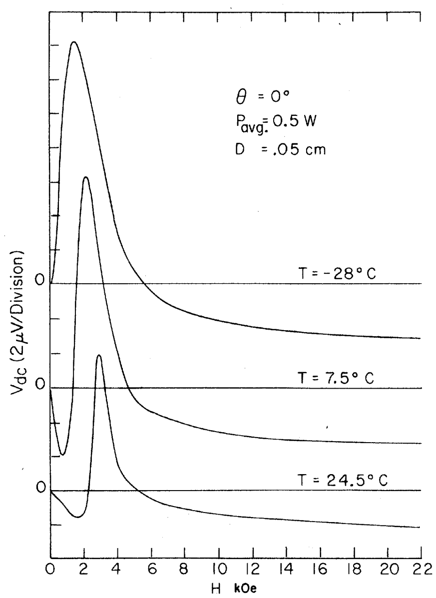

FIG. 5. Temperature dependence of microwave signal. $\Delta = 1360$ Å; $T <$ room temperature. Tracings represent an average of original recorder trace.

vs B.

The last two columns of Table I refer to values obtained from an analysis of the resonance data, using Eq. (4). ρ follows from the dependence of $\tan\phi_4$ on $\tan k_1 D$, and since it was possible to obtain a good fit to the experimental curves within a wide latitude of $\tan\phi_4$, no real difference can be ascribed to the resistivities at zero and at microwave frequencies. The last column in Table I gives R_s, the central quantity of the experiment. Although the value of

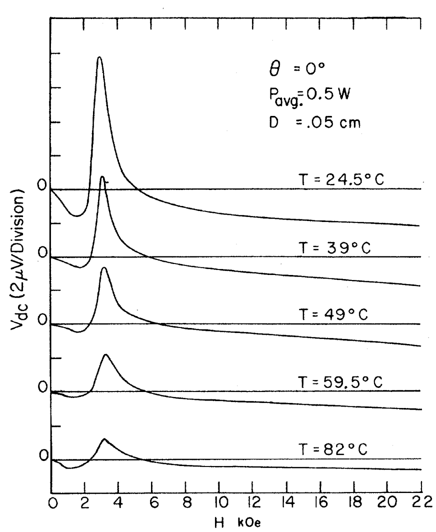

FIG. 6. Temperature dependence of microwave signal. $\Delta = 1360$ Å; $T >$ room temperature. Tracings represent an average of original recorder trace.

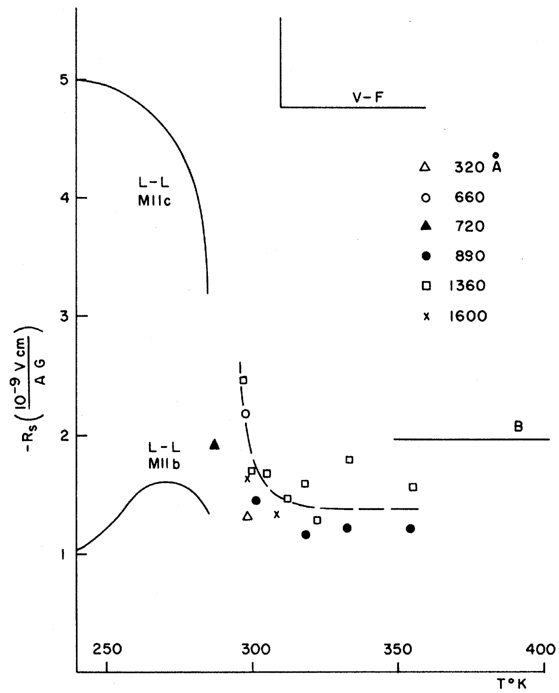

FIG. 7. Extraordinary Hall constant R_s of Gd above 300 °K obtained from six films by the resonance method. The full curves (L-L) below 280 °K are the bulk-single-crystal data of Lee and Legvold, and the high-temperature curves summarize the results of Volkenshtein and Fedorov (V-F) and of Babushkina (B). The dashed curve indicates the general trend of the film data.

R_s shows fluctuations from film to film, there is no observable thickness dependence in these data.

The temperature dependence of R_s is shown in Fig. 7, together with the Hall constants reported by Lee and Legvold for single-crystal bulk gadolinium up to the Curie temperature and with the curves reported by Volkenshtein *et al.* and by Babushkina for polycrystalline bulk gadolinium above the Curie point.

Knowing R_s and χ_0 at each temperature, it is possible to use the appropriate value of R_{dc} and Eq. (1) to determine the temperature variation of the ordinary Hall constant R_0. The results of this calculation are shown in Fig. 8, together with the curves reported by Lee and Legvold.

These results indicate that the extraordinary Hall constant of Gd is independent of temperature between 305 and 360 °K, consistent with the theoretical predictions based on the models of conduction electrons interacting with localized magnetic electrons. Below 305 °K the magnitude of R_s increases rapidly but smoothly and R_s approaches the curve obtained by Lee and Legvold for single-crystal gadolinium with the magnetic field parallel to the c axis. Some significant c-axis orientation has been found normal to the plane of the gadolinium films, and

TABLE I. Magnetic and transport properties of godolinium films at room temperature. Symbols are defined in Sec. II. The last two columns refer to values obtained from analysis of the resonance data.

Thickness (Å)	χ_0	g	τ (10^{-10} sec)	ρ_{dc} (10^{-6} Ω cm)	R_{dc} $\left(10^{-9}\ \frac{\text{V cm}}{\text{A G}}\right)$	ρ (10^{-6} Ω cm)	R_s $\left(10^{-9}\ \frac{\text{V cm}}{\text{A G}}\right)$
320	0.70	1.96	1.4				−1.3
720	1.19	1.96	1.4	142	−4.0		−1.7
890	1.29	1.96	1.3	143	−3.9	104	−1.4
1360	2.64	1.96	1.4	129	−5.6	128	−1.7
1600	3.33	1.96	1.4	142	−8.0	139	−1.7
∞	5.0	1.96	1.39	130–146			

since the resonance experiment looks at the component of the Hall coefficient for the magnetization along the film normal, the agreement between our results and those of Lee and Legvold indicates that our results directly extend the value of this particular component of R_s to higher temperatures. In a similar manner, the pattern of Fig. 8 suggests that the corresponding component of R_0 has been identified by our experimental method.

The results of this work are primarily experimental. The main agreement with the theoretical models is in the constancy of R_s at high temperatures. Since there is some question as to whether

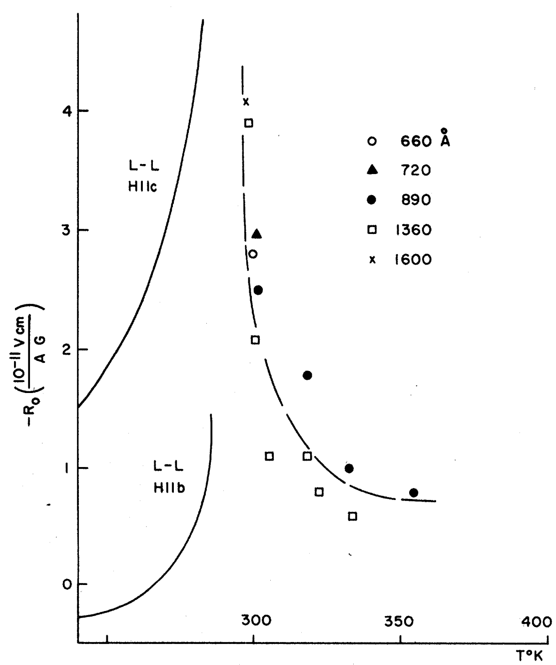

FIG. 8. Ordinary Hall constant R_0 of Gd above 300 °K, obtained by combining the initial slope data R_{dc}, the susceptibility χ_0, and the extraordinary Hall constants R_s such as given in Table I, according to Eq. (1). The uncertainty in each point is about 20%. The full curves (L-L) below 280 °K are the bulk-single-crystal data of Lee and Legvold.

the proposed models can account for the observed magnitude of R_s in terms of the values of the known parameters of Gd, more detailed identification with these theories has not been attempted.

We have shown that measurements of dc effects during spin resonance provide a useful method for separating the ordinary- and extraordinary-Hall-effect contributions to the total Hall voltage. When the magnetization is linear in applied field and not strongly temperature dependent, as it is in gadolinium at high temperatures, in principle a resonance method provides the only reliable means for such separation. In the region near the Curie point the magnetization is not linear in field and is strongly temperature dependent. Here the resonance approach has advantages over the use of conventional Hall-effect measurements in that the resonance method requires only measurements at the temperature of interest. This same method can be applied at the Curie temperature and at temperatures in the ferromagnetic region.

A possible limitation of the resonance method, especially when studying anisotropic effects in single crystals, is that the detection of dc voltages requires thin films (although this is not true for the corresponding second-harmonic signal when observed in reflection). In addition, before the resonance data for a particular sample at a specific temperature can be interpreted in detail, it is necessary to know the magnetic field dependence of the magnetization of that film at that temperature. Finally, the temperature range in which this method can be used is determined by the size of the resonance signal which can be detected. In Gd the limiting factor at low temperatures is the large linewidth of the resonance. At high temperatures, the smallness of the magnetization leads to resonance-signal levels proportionately small. Given signal levels in our temperature range of the order of 1.0–10 μV, and a noise level of 0.50–1.0 μV, the signal should still be observable in gadolinium up to 95 °C.

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Self-Consistent Warped-Muffin-Tin-Potential Energy Bands of γ-Fe with Various Exchange Approximations*

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Using a modified augmented-plane-wave expansion recently developed by us, we have calculated the energy bands and the binding energy of fcc γ-Fe. From a self-consistently calculated muffin-tin charge density, we obtained a warped-muffin-tin potential. We used the full, $\frac{7}{9}$, and $\frac{2}{3}$ Slater exchange potentials. All gave reasonable energy bands but when the "Koopmans corrections" recently suggested by Herman *et al.* were added, the *d* levels were driven below the *s* levels at all points in the Brillouin zone and an unphysical type of *s-d* hybridization was obtained.

I. INTRODUCTION

The purposes of this calculation are threefold: (i) to obtain self-consistent energy bands of γ-Fe, the fcc structure stable between 910 and 1400 °C, the only previous calculation being non-self-consistent[1]; (ii) to test the effect of various exchange potentials of the form

$$V_{ex}(\vec{r}) = -\alpha 3[3\rho(\vec{r})/\pi]^{1/3} \quad (1)$$

on both the energy bands and the binding energy of the crystal; also to test the so-called "Koopmans correction" of Herman *et al.*[2] to the one-electron energy levels; and (iii) to obtain crystal wave functions from which we can obtain the first iteration of a self-consistent true crystal potential as contrasted with the warped-muffin-tin potential used here. This will be the topic of a later paper.

The calculation is performed using the modified augmented-plane-wave expansion we have recently described.[3] In Sec. II, we explain how the warped self-consistent muffin-tin potential is obtained from a self-consistent muffin-tin charge density and calculate the energy bands for a $\alpha=1$, $\frac{7}{9}$, and $\frac{2}{3}$. In Sec. III we discuss the physics behind the various choices for α and the so-called Koopmans correction. We calculate the Koopmans correction and find that it lowers everywhere the *d* band below the *s* band leaving a peculiar unphysical sort of *s-d* hybridization. In Sec. IV, we discuss the calculation of the binding energy of the crystal and compare it with the ionization energy of the atom calculated with the same exchange approximation. We find in no case is the crystal actually bound, i.e., its binding energy greater than the ionization energy of the atom, but that it is much more nearly bound for $\alpha=\frac{2}{3}$ than for $\alpha=1$. In Sec. V, we speculate that although the Kohn-Sham (KS) ($\alpha=\frac{2}{3}$) poten-