hyperfine field H(Sn) at the tin sites in the ferromagnetic Heusler alloy Ni<sub>2</sub>MnSn. The results at 300 and 77  $^{\circ}$ K were, respectively,  $\pm$  45  $\pm$  5 and  $\pm$  87  $\pm 2$  kOe. The Bloch  $T^{3/2}$  law was used to extrapolate the results to 0 °K, to obtain a saturation field of  $\pm 93 \pm 3$  kOe. This agrees with the result of Shinohara<sup>2</sup> who found H(Sn) = 97.0 kOe at 0°K by observing nuclear magnetic resonances in Ni<sub>2</sub>MnSn, using the spin-echo technique.

An extension of the virtual-bound-state, or resonance, model, first proposed by Caroli and Blandin,  $^{11}$  was used to calculate H(Sn). The hyperfine field at the tin sites is considered to be due to the Fermi contact interaction between the spin polarization, induced in the conduction band by the Mnion-spin splitting, and the nuclear magnetic moments at the tin sites. The electronic  $\xi$  factor, which determines the reduction in s-wave character of the electronic wave functions at the Sn sites in going from a free atom to a metallic environment,

was taken as  $\xi = 0.04$ . The magnetic moment per Mn ion, M, was taken from neutron-diffraction data<sup>5</sup> and thermomagnetic measurements<sup>2</sup> as 4.0  $\pm$  0.1  $\mu_{B}$ . H(Sn) was then calculated for a range of values of the d-level occupation,  $Z_d^{\text{tot}}(Ni)$ , at the Ni sites. The theoretical calculations were found to be sensitive to the value of  $Z_d^{tot}(Ni)$ . Agreement with the experimental result was obtained for  $Z_d^{\text{tot}}$ (Ni) = 8.6.

Finally, it should be emphasized that although the values obtained for the parameters  $\xi$  and  $Z_d^{\mathsf{tot}}$ (Ni) are reasonable in view of other experimental evidence, they are dependent upon the model which was used in the present calculation.

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PHYSICAL REVIEW B

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## Rare-Earth Spin-Disorder Resistivity and Spin-Orbit Coupling\*

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Without corrections for Fermi-surface effects, the total-spin-disorder electrical resistivity of heavy-rare-earth single crystals is accidentally proportional to S(S+1) in the basal plane and to  $(\lambda-1)^2J(J+1)$  in the c direction. When Fermi-surface effects are included, results show  $(\lambda - 1)^2 J(J+1)$  dependence in both directions.

For some time it has been understood that the total-spin-disorder resistivity ( $\rho_{m,sat}$ ) in the heavy-rare-earth metals should be proportional to  $(\lambda - 1)^2 J(J+1)$  because of spin-orbit coupling<sup>1-3</sup>; here J is the total angular-momentum quantum number and  $\lambda$  is the Landé factor. While analyzing recent electrical-resistivity measurements4-9 in rare-earth single crystals, we looked into the total-spin-disorder resistivity in different crystallographic (hcp) directions and found a surprising result which we report here.

The electrical resistivity in the basal-plane direction for each metal showed a nearly linear behavior in the paramagnetic range so it was easy to extrapolate this back to the resistivity axis, subtract the residual resistivity from the intercept

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TABLE I. High-temperature resistivity-curve slopes of single-crystal heavy rare earths in units of  $\mu\Omega$  cm/K.

	Gd	Tb	Dy	Но	$\mathbf{Er}$	Tm	Lu	
$\frac{d\rho_b}{dT}$ ( $T \gtrsim 300 \text{ K}$ )	0.095	0.13	0.15	0.185	0.20	0.22	0.25	
$\frac{d\rho_c}{dT}$ (T> 300 K)	0.08	0.085	0.09	0.11	0.11	0.12	0.12	

found, and obtain the total-spin-disorder resistivity. In the c direction it was necessary to extrapolate back from much higher temperatures because of the superzone (hump) effect 10-12 around the highest ordering temperature. By a careful analysis of the resistivity at 100 K above the characteristic minimum just above the highest ordering temperature, it was possible to get slopes in a linear range. The slopes thus found, as well as the slopes in the basal plane, are shown in Table I. By using the slopes of the table and the extrapolation process described it was possible to get quite accurate total-spin-disorder resistivities in the c direction. A graphical presentation of results found by this process is given in the upper part of Fig. 1. Here the spin-disorder resistivity in the basal plane turns out to be proportional to S(S+1), while in the c direction there is a good fit to  $(\lambda - 1)^2 J(J + 1)$ .

The basal-plane result is believed to be accidental and may be understood in an empirical fashion by use of the relaxation-time approximation and the assumption that anisotropy in the Fermi surface is principally responsible for the effect. It is proposed that the "trunk" of the Fermi surface 13 changes in going from Gd to Tm. Evidence for this comes from Table I where the slopes of the resistivity-vs-temperature data above the orderdisorder temperature are given. These slopes are taken to be inversely proportional to the projected Fermi-surface areas. We see that the slopes scarcely change in the c direction, while those in the basal-plane direction change by a factor of 2. We use this information and assume an isotropic relaxation time to get the expression

$$\rho_{b\,(\mathrm{spin})} \propto (\lambda - 1)^2 J(J + 1) / \int_{E_m} dS_b \,, \tag{1}$$

which permits us to make the appropriate resis-

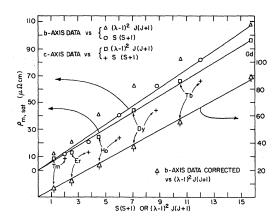


FIG. 1. Total spin-disorder resistivity of the heavy-rare-earth metals plotted against S(S+1) and  $(\lambda-1)^2J(J+1)$ .

tivity normalization. We divide the basal-plane resistivity by the ratio of the projected Fermi-surface areas

$$\int_{E_E} dS_c / \int_{E_E} dS_b$$
,

which comes from the ratio of the high-temperature slopes

$$\frac{d\rho_b/dT}{d\rho_c/dT}$$

from Table I. The corrected basal-plane points thus found are shown on the lower-right part of Fig. 1 and now fall on a straight line when plotted against  $(\lambda-1)^2J(J+1)$  as expected. The small shift in the slope of the line indicates anisotropic relaxation time or other minor effect is present. It is rather remarkable that the relaxation-time approximation could work so well for these metals. We now understand why attempts to establish spin-orbit coupling in polycrystalline samples neglecting Fermisurface effects gave obfuscate results 4 save for the work of Mackintosh and Smidt. 15 It is a relief to put this matter to rest.

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## Origin of the Magnetic "Surface Anisotropy" of Thin Ferromagnetic Films

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A very thin crystal (i. e., single-crystal film) of a cubic metal such as nickel is no longer truly cubic. This departure from cubic symmetry is reflected in the nature of the electronic states. We study the appearance of terms of lower than cubic symmetry (i. e., of axial symmetry with respect to the film normal) in the magnetic anisotropy energy associated with this change. The present paper considers the origin and nature of this additional axial anisotropy within the framework of the itinerant electron theory of magnetism. Within the localized-moment picture, as treated by Néel, this axial anisotropy is associated with effects occurring only at the surface planes, and therefore has come to be known as "surface anisotropy." We retain this nomenclature even though in our itinerant-electron picture the changes in anisotropy can be associated with electronic states extending into the interior of the film. The most striking qualitative result of our model is the marked variation of surface anisotropy with thickness possible for very thin films. This constrasts with the behavior in the Néel model, where for very thin films the surface anisotropy energy is almost independent of the film thickness. Physically this difference in behavior can be understood, since the itinerantelectron model allows the presence of coupling between the behavior at the two surfaces of the film, while such coupling cannot exist in the Néel model. We discuss the relevance of this difference to the existing experimental observations and to possible future experiments.

## I. INTRODUCTION

The free energy of a ferromagnetic metal crystal depends on the direction of its magnetization with respect to the crystal axes. This anisotropy energy<sup>1-6</sup> can be measured by obtaining magnetization vs external-field curves for several directions of the applied field, by torque experiments, or by ferromagnetic resonance, and reflects both the sample's inherent crystal symmetry and its shape. For example, the observed free energy of a bulk cubic material such as Ni<sup>1,7,8</sup> or Fe<sup>1,7</sup> may be expanded in terms of cubic harmonics:

$$F(\alpha_1, \alpha_2, \alpha_3) = K_0 + K_1(\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_1^2 \alpha_3^2) + K_2(\alpha_1^2 \alpha_2^2 \alpha_3^2) + \cdots,$$
 (1. 1)

where the  $\alpha_i$  are the direction cosines of the magnetization with respect to the crystal axes.

A very thin crystal (i.e., single-crystal film) of a cubic metal such as nickel is no longer truly cubic, and this departure from cubic symmetry is reflected in the nature of the electronic states. One therefore anticipates the appearance of terms

of lower than cubic (i.e., of axial symmetry) in the magnetic anisotropy energy. This is true in both the localized moment<sup>6,9</sup> and itinerant-electron<sup>10</sup> points of view. The present paper considers the origin and nature of this additional axial anisotropy within the framework of the itinerant-electron theory of magnetism. Within the localized-moment picture used by Néel, 6,9 this axial anisotropy is associated with effects occurring only at the surface planes, and therefore has come to be known as "surface anisotropy." We shall retain this nomenclature even though in our band treatment of the electronic structure the changes in anisotropy can be associated with electronic states extending into the interior of the film. In addition to the anisotropy effects caused by changes in the nature of the electronic states due to the intrinsically lower symmetry associated with the film geometry. experimentally there can be anisotropic contributions to the energy due to various impurity and stress effects associated with film growth. We shall concern ourselves here only with the intrinsic surface anisotropy. The other important source