As shown in the accompanying Letter by Koehler and Moon,[6] the predictions of this work are found to be in very good agreement with the neutron measurements. This good agreement lends greater credence to the predictions of APW energy-band determinations of wave functions and magnetization densities in metals. Hence, additional experimental and theoretical studies of rare-earth metals are called for, in order to clarify the situation with regard to Gd metal in particular and our understanding of the magnetic properties of the different rare earths, in general.

Finally, we may speculate on the observed lack of superconductivity in Sc metal whereas band theory predicts, on the basis of the calculated density of states, a large value (0.6) for the electron-phonon enhancement factor, λ, and a sizable T_c. The large expansion of the wave function may be responsible for sharply reduced electron-phonon matrix elements and hence a smaller electron-phonon interaction. (By contrast, the wave functions at E_F for Nb metal which is superconducting appears to be close to the free-atom result.) The validity of this idea awaits detailed comparison studies of the wave functions and electron-phonon matrix elements in Sc ($T_c \approx 0$ even at high pressure), Y ($T_c \approx 2.5$ K at 150 kbar pressure) and La ($T_c \approx 6$ K for double-hexagonal close packed La at zero pressure).[12]

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Field-Induced Paramagnetic Form Factor in Metallic Scandium*

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The magnetic form factor of metallic scandium has been measured at a temperature of 100 K in an applied field of 57.2 kOe by the polarized-neutron technique. Contrary to results on other 3*d* metals, the form factor is significantly different from that for the 3*d* electron in the free atom. Our results agree rather well with those of a calculation by Gupta and Freeman based on APW wave functions.

Polarized-neutron diffraction experiments have been carried out on metallic scandium in order to determine its magnetic form factor. This study of scandium was motivated by an earlier study of the form factor of gadolinium.[1] In the earlier experiment it was found that the total experimental form factor could be separated, logically and consistently, into a localized part, corresponding to a magnetic moment density arising from the 4f electrons, and a diffuse component which was attributed to a moment density associated with the conduction electrons. The localized part of the form factor was found to be in definite disagreement with predictions based on the free-ion Hartree-Fock wave functions of Freeman and Watson.[2] This disagreement was the motivation for new form factor calculations based on relativistic Hartree-Fock-Slater[3] wave functions and the more fundamental Dirac-Fock type.[4] These relativistic form factors, especially those based on the Dirac-Fock wave functions, proved to be in excellent agreement with experiment. The diffuse density derived from the experiment was neither d-like nor s-like. It had its largest positive value at the atomic sites [A and B sites of the hexagonal close-packed (hcp) structure] and it changed sign on moving away from these sites, reaching its largest negative value at the vacant C sites. Harmon and Freeman[5] subsequently made spin-polarized augmented plane-wave (APW) calculations of the conduction electron spin density and of the corresponding magnetic form factor. Their calculated density was found to have the same shape as the experimental diffuse density but differed from it quantitatively. In particular the calculated negative density at the c sites was very much smaller than that of the experiment.

Even though the separation of localized and diffuse components of the experimental form factor appeared to be a valid one, it should be emphasized that the diffuse component is obtained as a difference between two large numbers and may be subject to large errors. In order to reduce these errors and to provide an additional and possibly more meaningful confrontation with the theory we decided to study Sc which has the same hcp structure as Gd and a similar electronic structure, but which has no strong localized $4f$ moment. Scandium is also of interest because it is the first of the $3d$ transition metals. As such its properties are determined by electrons near the bottom of the $3d$ band. It is a well known and remarkable fact that neutron diffraction data on the $3d$ metals studied to date can be interpreted in terms of free-ion form factors.[6] For Sc, however, we find a much more expanded density and a form factor totally unlike those of the other $3d$ metals.

A number of crystals of Sc were investigated during the course of this study but the results reported here were obtained from a specimen cut from a crystal of exceptionally high purity which was produced at Ames Laboratory.[7] The specimen was cut in the form of a pillar $1.4\times2.0\times6.6$ mm^3 with the long edge parallel to an a direction. The crystal was lightly deformed several times, with each deformation monitored by measurement of an intense Bragg reflection, in order to minimize extinction effects. When the specimen was suitably prepared it was inserted with the long dimension vertical into the gap of a split-coil superconducting solenoid capable of producing 57.2 kOe at the specimen. Most of the measurements were made at 100 K, a temperature high enough to minimize corrections to the data due to polarization of the Sc nuclei and low enough for good helium economy.

The susceptibility χ_a for the field applied parallel to the a direction of a specimen of comparable purity at 100 K is 8.05×10^{-6} emu/g.[8] In the field of 57.2 kOe this corresponds to an induced moment of 3.71×10^{-3} Bohr magnetons per atom, a magnetic moment which is easily detected in a polarized-beam experiment. The quantity that is actually measured in polarized-beam diffractometry is the polarization ratio R which is the ratio of the peak intensities of a Bragg reflection for the neutron spin parallel and antiparallel to the magnetizing field. When the magnetic scattering amplitude, $p(\vec{\tau})$, is small compared to the nuclear scattering amplitude, b, as is the case in this experiment, one may express the magnetic scattering amplitude in terms of the residual polarization ratio

$$r = R - 1 = 4p(\vec{\tau})/b, \qquad (1)$$

where $\vec{\tau}$ is a reciprocal lattice vector and b is the nuclear scattering amplitude of Sc,[9] which is $b_{\mathrm{Sc}} = (1.18 \pm 0.03)\times10^{-12}$ cm.

Polarization ratios were measured for eight Bragg reflections in the $(h0l)$ zone. In every case the measurement was made at a minimum of four incident "window" wavelengths, chosen by computer calculation, to minimize multiple Bragg scattering effects. For the longer wavelengths, especially, polarization ratios were measured at several angular positions over the Bragg peak. This was done because the peak position can be displaced for neutrons of the two spin states and this displacement can lead to significant errors in the measured polarization ratios.[10] Corrections must be applied to account for the lack of perfection of the polarization in the incident beam, and for the neutron-spin–neutron-orbit scattering.[11] These corrections are readily calculable and are generally small. In addition, in order to make a comparison with theoretical predictions of the induced *paramagnetic* density an estimate of the diamagnetic[12] and nuclear susceptibilities must be made. The latter may be calculated with considerable accuracy since measurements have been made at Saclay[13] of the difference, $a_+ - a_-$, of the scattering lengths of the scandium nucleus for the two spin states $I+\frac{1}{2}$ and $I-\frac{1}{2}$. This contribution was verified in the present experiments by measuring the temperature dependence of the polarization ratio of the (004) reflection. The electronic contributions to the magnetic scattering amplitude of this reflection

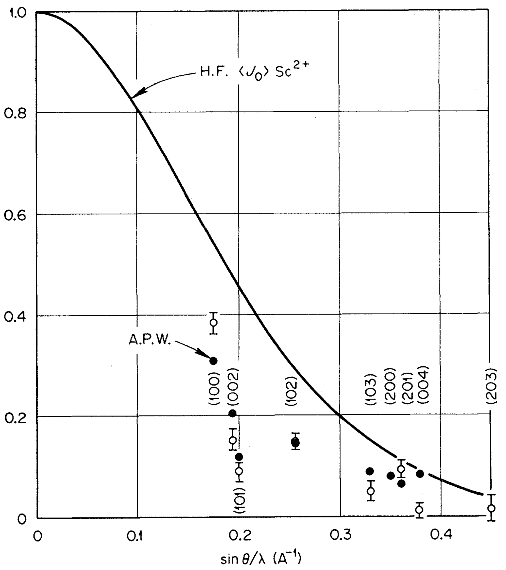

FIG. 1. The paramagnetic form factor of metallic scandium. The experimental points, shown as open circles, have been corrected for nuclear polarization, diamagnetism, and neutron-spin–neutron-orbit interaction. The closed circles are from an APW calculation by Gupta and Freeman (Ref. 15) and the solid line is a free-ion calculation by Watson and Freeman (Ref. 14).

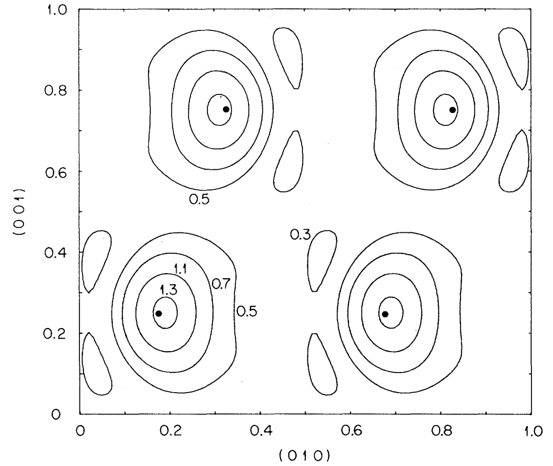

FIG. 2. Projected magnetic moment density in paramagnetic scandium at 100 K and 57.2 kOe. The contours are in units of $10^{-3}\mu_B/\text{Å}^2$ with errors in the range 0.03 to 0.08. Atomic sites are indicated by solid circles.

are very close to zero so that the temperature dependence of the amplitude is due almost exclusively to change with temperature of the nuclear polarization. The corrections to the data for the induced diamagnetic susceptibility are somewhat less certain; we have made them by calculating the free-atom susceptibility assuming a $3d^2 4s^1$ configuration outside an argon core. The resulting correction is outside our experimental errors only for the first three reflections where it amounts to approximately twice the standard deviation in each case.

The results are summarized in Fig. 1 where the experimental residual flipping ratios, after correction for the effects mentioned above, have been converted to a form factor by normalization with the appropriately corrected (for diamagnetic and nuclear susceptibilities) experimental susceptibility. This form factor resembles that of the diffuse component obtained for Gd in its abrupt drop over the first three reflections; it differs from it in that the form factor at the (102) reflection rises again to a value greater than that at the (101) peak and in that the point at the origin is much larger, relative to the first Bragg peak, in Sc than in Gd. The solid line in the figure is a Hartree-Fock free-ion calculation for the spin part of the form factor.[14] Comparison of this curve with the observations shows that, unlike the case of the other $3d$ transition metals, the form factor for Sc cannot be interpreted in terms of free-ion form factors. Inclusions of any orbital contribution would make the departure from experiment even greater. A rather good account of the observations has been given, however, by Gupta and Freeman[15] in the preceding note, on the basis of APW wave functions determined for metallic scandium. Their results are shown as the solid circles in the figure.

The nature of the moment density is shown in Fig. 2. For convenience we have represented the hcp structure in terms of an orthorhombic structure with $a = a_H$, $b = \sqrt{3}a_H$, and $c = c_H$. The atomic positions in this cell are then $(0,\frac{1}{3},\frac{3}{4})$, $(0,\frac{2}{3},\frac{1}{4})$, $(\frac{1}{2},\frac{1}{6},\frac{1}{4})$, and $(\frac{1}{2},\frac{5}{6},\frac{3}{4})$. We do not have full three-dimensional data but we do effectively have a complete set of data in a $(0kl)$ zone from which we can calculate the projection of the point density on the orthohexagonal b-c plane and which we show in Fig. 2 as a contour map. The numbers are multiples of $10^{-3}\mu_B/A^2$ and the dark circles represent the projections of the atomic sites. In the projection the moment density is a maximum near the atomic sites but it is rather large, $\sim 0.3 \times 10^{-3}\mu_B/\text{Å}^2$, and positive at the interatomic positions in contrast to the diffuse density in Gd. A map constructed with the values calculated by Gupta and Freeman exhibits the same features.

The principal conclusions are that the induced magnetization density in metallic Sc is not like that of a single $3d$ electron in atomic Sc, and that the APW calculation of Gupta and Freeman gives quite good agreement with our results. From the temperature dependence of the susceptibility, Spedding and Croat[8] have inferred that Sc behaves as though there were a single localized $3d$ electron. Our results seem inconsistent with this interpretation.

The first exploratory measurements on this problem were carried out while one of us (W.C.K.) was a guest scientist at the Brookhaven National Laboratory. This author wishes to acknowledge with thanks the hospitality extended to him by the entire staff of BNL generally and by Dr. Gen Shirane and Dr. David Cox in particular. We wish to thank Mr. J. L. Sellers of Oak Ridge National Laboratory for valuable technical assistance.

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Indirect Exciton Dispersion and Line Shape in Ge

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The effective-mass equation for indirect excitons in Ge is solved taking the degeneracy and anisotropy of the bands into account. The calculated binding energies of the anisotropy split ground state (4.18 and 3.17 meV) are in excellent agreement with experiment (4.15 and 3.14 meV). The method is then extended to calculate the energy-momentum dispersion of excitons, which are strongly nonparabolic, and account well, with no adjustable parameters, for the recently measured modulated absorption line shape.

The interest in the indirect exciton spectrum of Ge has recently been stimulated by the accurate wavelength-derivative transmission spectra of Frova *et al.*[1] This experiment has determined that the exciton ground state is split by the conduction-band-valley anisotropy into two levels separated by 1.01 ± 0.03 meV, and that the energy–translational-momentum dispersion relations of the two exciton branches are strongly nonparabolic, and display the "mass-reversal" effect predicted by Kane.[1,2]

From the theoretical point of view, the solution of the effective-mass equation for indirect excitons in cubic semiconductors is difficult be-