ing in the outer part of the atom, one can vary the initial capture distribution and its evolution during the early part of the de-excitation, and hence the l distribution at $n=(M/m)^{1/2}$; these changes are about the right size to give the observed absolute-yield variations (increased scattering producing lower yield). This same change for a given element in a compound will increase capture on that element, which accounts for the inverse correlation between the yield data [Figs. 1(a)–1(c)] and the capture-ratio data [Fig. 1(d)]. Now positron annihilation is mostly on loosely bound electrons, and the valleys in Fig. 1(e) presumably reflect an increased density of electrons in the outer part of the atom.[13] Since such an increase necessarily implies increased electron-meson scattering in the outer parts of the atom, we think that this is the basic physical property underlying the variations in yield and capture ratios.

Future theoretical and (hopefully) experimental work will attempt to test this idea quantitatively.

*Work supported in part by the U. S. Energy Research and Development Administration and the National Research Council of Canada.

†Present address: Battelle Pacific Northwest Laboratory, Richland, Wash. 99352.

[1]C. E. Wiegand and G. L. Godfrey, Phys. Rev. A 9, 2282 (1974).

[2]D. Quitmann *et al.*, Nucl. Phys. 51, 609 (1964).

[3]D. Kessler *et al.*, Phys. Rev. Lett. 18, 1179 (1967).

[4]V. G. Zinov *et al.*, Yad. Fiz. 2, 859 (1965) [Sov. J. Nucl. Phys. 2, 613 (1966)].

[5]R. Kunselman, UCRL Report No. UCLRL-18654, 1969 (unpublished).

[6]The correlations between kaonic and pionic absolute yields and muonic relative intensities have already been noted by C. E. Wiegand and G. L. Godfrey, Ref. 1, and Phys. Lett. 56B, 255 (1975); G. T. Condon, Phys. Rev. Lett. 33, 126 (1974); and A. Backenstoss, in *Atomic Physics 4,* edited by G. zu Putlitz, E. W. Weber, and A. Winnacker (Plenum, New York, 1975), p. 163.

[7]I. K. MacKenzie *et al.*, Phys. Rev. Lett. 34, 512 (1975).

[8]Condo, Ref. 6.

[9]M. Leon and J. Miller, LASL Report No. LA-UR-75-1268 (to be published).

[10]We do not make use of the *relative* kaonic intensities because (i) the ratios of the $\Delta n=-1$ transitions are very insensitive to variations in l distribution and hence give little information, and (ii) the yields of $\Delta n\leq -2$ transitions have much larger errors.

[11]M. Leon and R. Seki, LASL Report No. LA-UR-75-1267 (to be published).

[12]Second reference to Godfrey and Wiegand, Ref. 6.

[13]W. Brandt *et al.*, Phys. Rev. Lett. 35, 1180 (1975).

Comment on de Haas–van Alphen Measurements in Gadolinium*

J. E. Schirber
Sandia Laboratories, Albuquerque, New Mexico 87115

and

F. A. Schmidt and B. N. Harmon
Ames Laboratory, Ames, Iowa 50010

and

D. D. Koelling
Argonne National Laboratory, Argonne, Illinois 60439

(Received 22 December 1975)

Fermi-surface cross sections for field along principal symmetry directions for Gd are presented which are in serious disagreement with those of previous investigators. This disagreement stems from the use of an incorrect value for the saturation magnetization. The new frequency values are compared with the results of a relativistic augmented-plane-wave band calculation.

The only direct measurements of the Fermi surface of a rare-earth metal with an incomplete 4*f* shell were reported by Young, Jordan, and Jones, who observed several de Haas–van Alphen (dHvA) frequencies[1] for Gd and reported effective masses associated with some of these frequencies.[2] Assuming a rigid-band splitting of 1.14 eV for a relativistic augmented-plane-wave

(APW) band structure of paramagnetic Tb,[3] they were able to identify their larger frequencies with orbits on the spin-up and spin-down Fermi surfaces. This splitting is considerably larger than expected from the measured[4] conduction-electron polarization, using the Tb density of states.

We have measured dHvA frequencies on a $\frac{1}{8}$-in.-diam sphere of Gd of purity comparable to the best reported to date (residual resistivity ~260) which was purified by an electrochemical process as described by Peterson and Schmidt.[5] Our frequencies are in serious disagreement with those published by Young, Jordan, and Jones,[1] stemming primarily from the use of the wrong value for the magnetization throughout their work. The purpose of this communication is to present the correct frequencies along principal symmetry directions and to discuss briefly the implications that these values of the frequencies have on the band structure of ferromagnetic Gd.

The dHvA frequencies were obtained by standard field-modulation techniques in a 55-kOe superconducting solenoid. The use of the usual *in situ* field calibration (NMR or a known dHvA frequency)[6] is precluded by the field distortion near a ferromagnetic sample such as Gd. Therefore the H-versus-current value was checked using a known dHvA frequency in a separate experiment. The sample orientation was determined to within 2° by standard x-ray techniques and the crystal was fixed with respect to the applied-field direction by gluing with epoxy to a rigid sample holder.

In a ferromagnetic material the saturization magnetization, M_s, and demagnetizing factors must be known because the dHvA oscillations are periodic in the reciprocal of the magnetic induction, B^{-1}. For a spherical sample $B = H_a + 8\pi M_s/3$, where H_a is the applied field. We determined our frequencies by fitting our data by a straignt-line plot of integers versus $(H_i + 8\pi M_s/3)^{-1}$, where the H_i are zero crossings of the oscillations. We found values of $8\pi M_s/3$ of 18.6 ± 0.7 kG. This agrees well with the direct measurement[4] of $(7.63 \pm 0.02)\mu_B$/atom which corresponds to 18.1 kG. We also checked for consistency by measuring the effective mass of the strongest frequency at widely separated applied fields. The magnetization contribution obtained using this less accurate method was 17 ± 3 kG.

Our results using 19 kG for $8\pi M_s/3$ are shown in Table I and differ substantially from those of Young, Jordan, and Jones[1] who used 7 kG. The values are increased by roughly 50% for most of the frequencies. It should be noted that the frequencies cannot be corrected accurately without a knowledge of the applied-field values used in the measurement. Recalculations for the data of Ref. 1 using the correct magnetization are in substantial agreement with the values shown.[7]

TABLE I. de Haas–van Alphen frequencies for Gd using 19 kG for $8\pi M_s/3$ (in units of 10^6 G).

Field direction	Frequency
[0001]	0.3
	1.96
	16.9
	13.9
	40.7
$[10\bar{1}0]$	1.6
$[11\bar{2}0]$	0.5
	1.71
	2.8 [a]
	46.6

[a] From Ref. 1.

These new frequencies were compared with the results of a relativistic APW calculation for paramagnetic gadolinium. The larger frequencies could be tentatively identified with the Fermi-surface orbits suggested by Young, Jordan, and Jones, but with a rigid-band splitting of about 0.95 eV instead of 1.14 eV (using a rigid-band splitting the largest orbits could be fitted nicely, but there was only qualitative agreement for the smaller orbits). This splitting along with the calculated Gd density of states predicts a spin moment of nearly $0.78\mu_B$/atom from the uncompensated spin-up electrons. If the orbit identifications are correct (and we believe they are for the major pieces), then the simple nonrelativistic and linear picture of pure spin states split by an exchange field cannot be reconciled with the observed conduction-electron moment of $0.63\mu_B$/atom.[4] To obtain this moment, it would be necessary to reduce the splitting to $\frac{2}{3}$ the above value required for reasonable agreement with the major dHvA orbits, which would totally destroy any agreement in Fermi-surface topology. This implies that one must eliminate the nonrelativistic view of pure spin states (thus changing the g factor), the linearized-exchange-field approach, or both. A relativistic ferromagnetic calculation is being undertaken to examine these questions and provide more quantitative orbit infor-

mation.

We acknowledge the technical support of R. L. White.

*Work supported by the U. S. Energy Research and Development Administration.

[1]R. C. Young, R. G. Jordan, and D. W. Jones, Phys. Rev. Lett. 31, 1473 (1973).

[2]R. C. Young and J. K. Hulbert, Phys. Lett. 47A, 367 (1974).

[3]C. Jackson, Phys. Rev. 178, 949 (1969).

[4]H. E. Nigh, S. Legvold, and F. H. Spedding [Phys. Rev. 132, 1092 (1963)] measured the saturated moment of gadolinium as $7.55\mu_B$/atom, indicating a conduction-electron contribution of $0.55\mu_B$/atom; however, more recent measurements on high-purity samples by L. W. Roeland, G. J. Cock, F. A. Muller, A. C. Moleman, R. G. Jordan, and K. A. McEwen (private communication) yield $7.63\mu_B$/atom—a value confirmed by measurements performed at the Ames Laboratory (S. Legvold, private communication).

[5]D. T. Peterson and F. A. Schmidt, J. Less-Common Met. 29, 321 (1972).

[6]W. J. O'Sullivan and J. E. Schirber, Cryogenics 7, 118 (1967).

[7]R. C. Young, private communication.

Secondary Reconstruction on the Si(100) Surface via a Charge-Density Wave

Joel A. Appelbaum, G. A. Baraff, and D. R. Hamann
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 20 November 1975)

A pair of partially occupied surface-state bands found in recent calculations by the authors for the 2×1 reconstructed Si(100) surface is shown to provide a mechanism for additional reconstruction via charge-density-wave formation. This is proposed as an explanation of weak fourth-order reflections seen in low-energy electron diffraction.

The dominant reconstruction pattern of the Si(100) surface is 2×1.[1] In a recent Letter[2] the authors have shown that the self-consistently calculated spectrum for the Schlier-Farnsworth-Levine dimerization model[1,3] of this reconstruction agreed with ultraviolet photoemission and energy-loss measurements.[4,5]

In this Comment we demonstrate that residual Fermi surface or charge-density-wave (CDW) instabilities[6,7] can account for the weak higher-order spots that are observed in low-energy electron diffraction (LEED) on carefully prepared Si samples.[8,9] The position of these higher-order spots relative to the primary and half-order spots is shown in Fig. 1. These spots are almost two orders of magnitude weaker than the primary spots, and more than an order of magnitude weaker than the half-order spots.[9]

The origin of the CDW we believe to be responsible for these spots can be found in the pair of partially occupied bonding and antibonding π-like surface states calculated for the dimer model, whose dispersion relations are plotted in Fig. 2 of Ref. 2. Notice that the lower band contains a pocket of holes around the line Γ to J, and that the upper contains a pocket of electrons around the line J' to K. The electron and hole Fermi surfaces, displaced relative to each other by the vector $\vec{q}_0$ connecting Γ to K, are shown in the upper left in our Fig. 2.

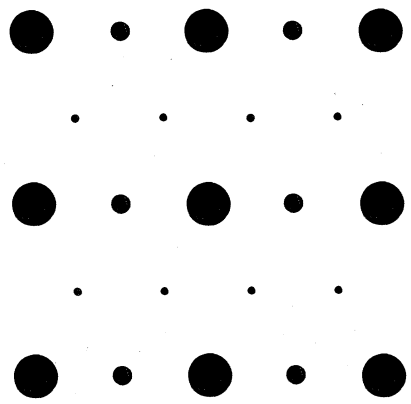

FIG. 1. Schematic representation of the LEED pattern for Si(100). The size of the first-, second-, and fourth-order spots indicates their relative intensity. While a single domain is shown here for clarity, the experimental pattern will be a superposition of this pattern and one obtained by a 90^0 rotation.