beryllium,[8] and another method is necessary to predict the magnitude of the quantum oscillations in the heat capacity of this metal.

Adiabatic temperature oscillations—the change in temperature of a metal as the magnetic field is varied adiabatically—can be used to estimate the amplitude of the oscillations of the heat capacity ΔC by the relation

$$\frac{(\Delta C)_T}{C} \approx -\frac{\partial}{\partial T}(\Delta T)_S.$$

From the magnetothermal measurements of Halloran[8] the estimated peak-to-peak amplitude of the high-frequency heat-capacity oscillations ranges from 0.25 to 0.4% while the estimate for the slow oscillation is less than 1%. Considering the very large uncertainties in these estimates from the published data, the agreement with these measurements is considered satisfactory.

[8] See J. H. Condon, Phys. Rev. **145**, 526 (1966).

CONCLUSIONS

An ac temperature technique for measuring heat capacities has been developed which possesses several advantages: (1) The sample may be coupled thermally to a bath; (2) the method is a steady-state measurement; (3) changes in heat capacity with some experimentally variable parameter may be recorded directly; (4) extremely small heat capacities may be measured with accuracy; and (5) the method possesses a precision an order of magnitude better than existing techniques. Heat-capacity measurements are reported that have an absolute accuracy of 1%, and no serious problem appears to exist in improving on this figure to the limit imposed by the accuracy of the thermometer calibration. The sensitivity of the present measurements to changes in heat capacity is 0.04% with a lock-in time constant of 30 sec. This precision was limited entirely by thermal noise which can easily be reduced by an order of magnitude with improved dc temperature regulation.

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Energy Bands and Fermi Surface of Scandium*

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The energy bands for hexagonal close-packed scandium have been calculated using the augmented-plane-wave method. From these calculations, the Fermi surface, density of states at the Fermi energy, and electronic specific-heat coefficient were determined. An important feature of the Fermi surface is the existence of large relatively parallel portions perpendicular to the c axis. This feature has also been reported for Y, Lu, Er, and Dy and in the present case can be related to the wave vector of the periodic moment arrangement occurring in alloys of Sc and Tb. Comparisons with the limited number of experimental data are made. There is no indication that the electronic specific-heat coefficient enhancement (due to electron-phonon and electron-electron interactions) is significantly greater for Sc than for Y and the heavy rare earths.

I. INTRODUCTION

CALCULATIONS have been made of the electronic energy bands and Fermi surface of Sc using the augmented-plane-wave (APW) method proposed by Slater[1] and reviewed by Loucks.[2] The atomic structure of Sc is $3d4s^2$, and the hexagonal close-packed crystal structure is considered here.[3] In the next section some of the details involved in the APW calculation are described. This is followed by a section in which the results are presented and compared with available experimental data[4] and with the results of Altmann and Bradley[4] who used the cellular method. The similarities between the present results and those presented by Loucks[5] for Y and by Keeton and Loucks[6] for Lu, Er, and Dy are also pointed out.

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[1] J. C. Slater, Phys. Rev. **51**, 846 (1937).
[2] T. L. Loucks, *Augmented Plane Wave Method* (W. A. Benjamin, Inc., New York, 1967).
[3] For previous applications of the APW method to the iron transition metals and hcp structures see, for example, L. F. Mattheiss, Phys. Rev. **134**, A970 (1964); A. J. Freeman, J. O. Dimmock, and R. E. Watson, *Quantum Theory of Atoms, Molecules and the Solid State* (Academic Press Inc., New York, 1966), p. 361; J. O. Dimmock and A. J. Freeman, Phys. Rev. Letters **13**, 750 (1964); J. O. Dimmock, A. J. Freeman, and R. E. Watson, in *Proceedings of the International Colloquium on the Optical Properties and Electronic Structure of Metals and Alloys, Paris, 1965* (North-Holland Publishing Co., Amsterdam, 1966), p. 237; A. J. Freeman, J. O. Dimmock, and R. E. Watson, Phys. Rev. Letters **16**, 94 (1966); L. F. Mattheiss, Phys. Rev. **151**, 450 (1966).
[4] S. L. Altmann and C. J. Bradley, Proc. Phys. Soc. (London) **92**, 764 (1967).
[5] T. L. Loucks, Phys. Rev. **144**, 504 (1966).
[6] S. C. Keeton and T. L. Loucks, Phys. Rev. (to be published).

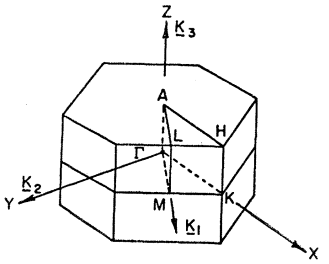

FIG. 1. Primitive Brillouin zone for the hexagonal close-packed crystal structure.

TABLE I. Reciprocal lattice vectors used in APW expansion.

$(ijk)=i\mathbf{K}_1+j\mathbf{K}_2+k\mathbf{K}_3$							
			$(00\bar{3})$				
$(0\bar{1}\bar{2})$	$(\bar{1}1\bar{2})$	$(\bar{1}0\bar{2})$	$(00\bar{2})$				
$(0\bar{1}\bar{1})$	$(\bar{1}1\bar{1})$	$(\bar{1}0\bar{1})$	$(00\bar{1})$	$(10\bar{1})$	$(1\bar{1}\bar{1})$	$(01\bar{1})$	$(\bar{2}1\bar{1})$
$(0\bar{1}0)$	$(\bar{1}10)$	$(\bar{1}00)$	(000)	(100)	$(1\bar{1}0)$	(010)	$(\bar{2}10)$
$(0\bar{1}1)$	$(\bar{1}11)$	$(\bar{1}01)$	(001)	(101)	$(1\bar{1}1)$	(011)	$(\bar{2}11)$
	$(\bar{1}12)$	$(\bar{1}02)$	(002)				

II. PROCEDURE

The energy bands were determined by an APW calculation, using 32 reciprocal lattice vectors in the wavefunction expansion. This set was found to give convergence for energy eigenvalues to within 0.001 Ry for energies below the Fermi energy at the high-symmetry points in the primitive Brillouin zone shown in Fig. 1. The reciprocal lattice basis vectors used were

$$\mathbf{K}_1=(2\pi/a\sqrt{3})(\sqrt{3}\mathbf{i}+\mathbf{j}),$$
$$\mathbf{K}_2=(4\pi/a\sqrt{3})\mathbf{j},$$
$$\mathbf{K}_3=(2\pi/c)\mathbf{k},$$

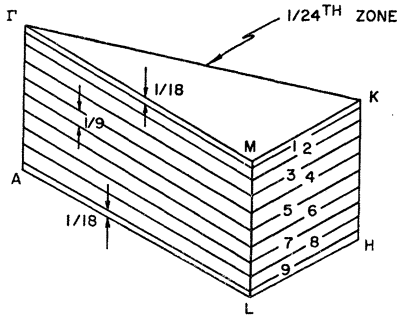

FIG. 2. 1/24 zone showing the planes on which constant-energy contours were calculated.

and the set of reciprocal lattice vectors used in the expansion is listed in Table I. The lattice constants used were $a=6.253$ a.u. and $c=9.965$ a.u.[7]

In these calculations the crystal potential was approximated by a muffin-tin potential constructed from a superposition of atomic potentials[8] including exchange in the $\rho^{1/3}$ approximation. The radius of the APW sphere was 3.004 a.u.

Constant-energy surfaces were generated by a computer program which evaluated the secular determinant at 45 grid points in each of the nine planes in the 1/24 zone shown in Fig. 2. An interpolation scheme was then used to generate the surface for a particular value of the energy. The Fermi energy was then chosen according to the requirement that the volume of the hole portion of the Fermi surface equal that of the electron portion. The results obtained from these calculations are presented in Sec. III.

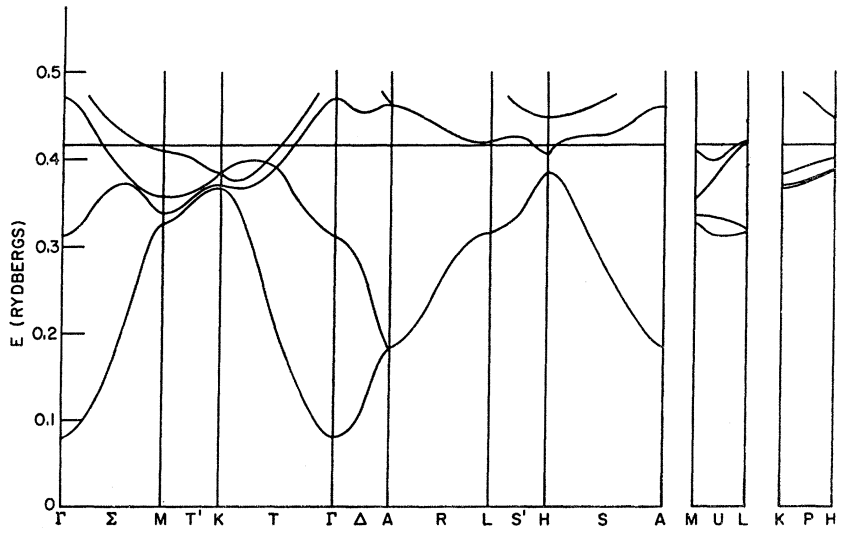

FIG. 3. Energy bands for scandium.

[7] W. B. Pearson, *Handbook of Lattice Spacings and Structures for Metals* (Pergamon Press, Inc., New York, 1958). Atomic units (a.u.) are used; $e^2=2$, $m=\frac{1}{2}$, $\hbar=1$.

[8] D. Liberman, J. T. Waber, and Don T. Cromer, Phys. Rev. 137, A27 (1965).

TABLE II. Electronic specific-heat coefficients (10^{-4} cal/mole °K²).

	Calculated		
	APW	Altmann and Bradley[a]	Experimental
Sc	13.0	7.4	25.8
Y	11.2[b]	6.0	24.1

[a] Reference 4.
[b] Reference 5.

III. RESULTS

The energy bands for hexagonal close-packed Sc are plotted along symmetry directions of the Brillouin zone in Fig. 3. In this plot the zero of energy corresponds to

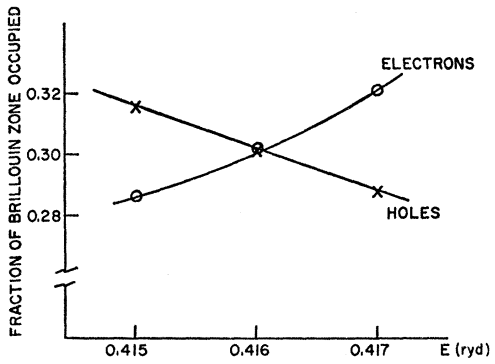

FIG. 4. Volume of hole and electron portions of constant-energy surfaces.

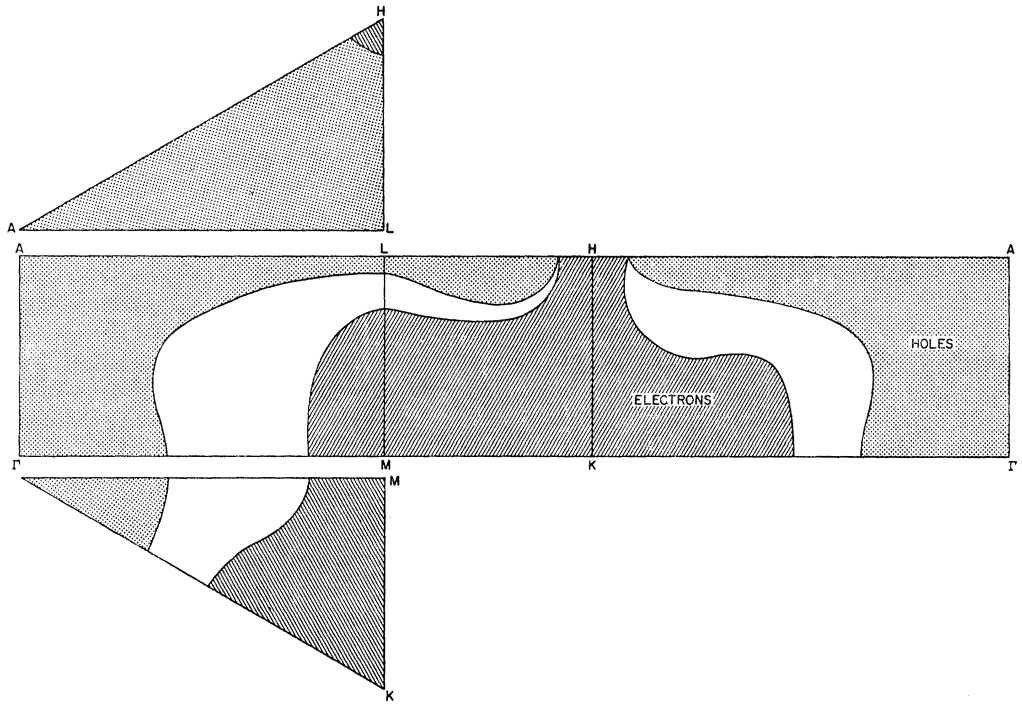

FIG. 5. Intersection of the Fermi surface with the faces of the 1/24 zone.

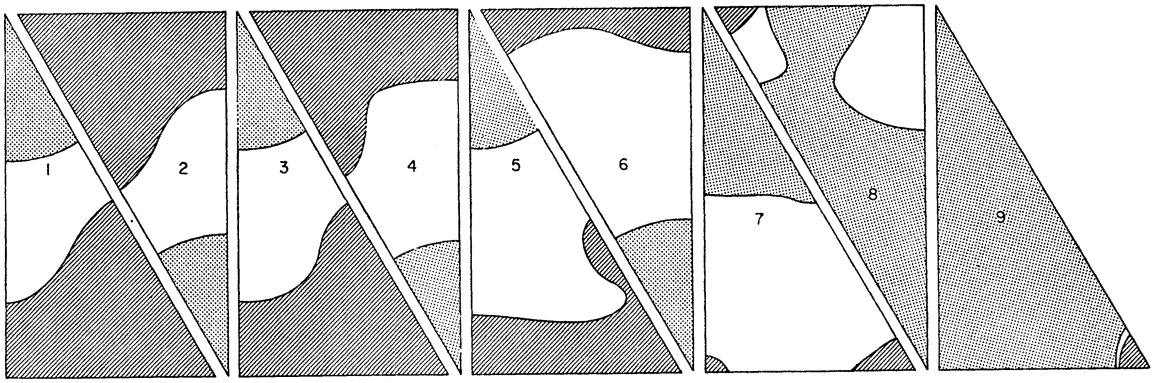

FIG. 6. Intersections of the Fermi surface with the planes shown in Fig. 2.

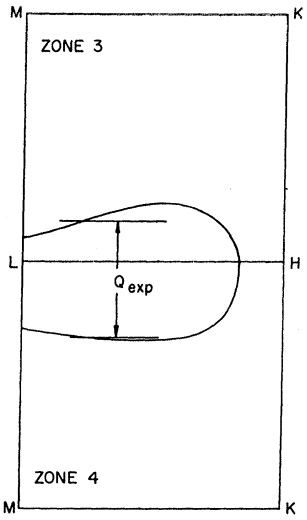

FIG. 7. Double zone representation of a portion of the Fermi surface showing the "webbing" feature.

the constant potential in the region between the APW spheres.

The volumes of the hole and electron portions of the constant-energy surfaces are plotted as a function of energy in Fig. 4. The intersection of these two curves gives the Fermi energy (0.416 Ry), and the density of states at the Fermi energy, $n(E_F)$, can be found from the slopes of the curves. This was determined to be 31.0 (electron states)/Ry/ atom.

The next two illustrations show the details of the Fermi surface; Fig. 5 shows its intersections with the boundaries of the 1/24 zone while Fig. 6 shows its intersections with the nine planes shown in Fig. 2. The principal features of the surface are the same as those described by Loucks[5] for the Fermi surface of Y($4d5s^2$) which also has a hexagonal close-packed crystal structure. However, the surface is quite different from that calculated for Sc by Altmann and Bradley using the cellular method.[4] It is interesting to note that they also obtained quite similar Fermi surfaces for Y and Sc although both differ from the present results and from those of Loucks. The differences are probably due to the methods used in constructing the potentials in each case. The impressive list of successful APW calculations[2] and the already accepted form of the rare-earth Fermi surfaces (Refs. 5, 6, and articles cited therein) speak very strongly for the present results.

The electronic specific-heat coefficient γ was calculated from $n(E_F)$ and is listed in Table II along with that of Altmann and Bradley and the experimental value obtained by Gschneidner.[9] For comparison the corresponding values for Y are also given. In all cases γ is slightly larger for Sc than for Y. Our result differs from the experimental one by a factor of approximately the same magnitude as found for Y and the heavy rare earths.[5]

Examination of the Fermi surface shows that, in the MLMKHK face of the double zone representation, there exists the "webbing" feature, the relatively flat and parallel portion shown in Fig. 7. This feature is similar to that exhibted by Y and by the rare-earth elements Lu, Er, and Dy. For these rare earths Keeton and Loucks[6] have proposed that the wave vector of the various periodic moment arrangements is determined by the average width of this "webbing." Their argument is similar to that used by Lomer[10] to account for the ordered magnetic moment in Cr.

Although Sc has no localized magnetic moment, the periodic moment arrangement in antiferromagnetic Sc-Tb alloys[11] has been determined. Extrapolation of these data to very low Tb concentration yields a turn angle of 42° per layer. The corresponding wave vector is shown in Fig. 7 and is nearly equal to the average width of the webbing. Similar agreement with experiment has been obtained for Y, Lu, Er, and Dy.[6]

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[9] K. A. Gschneidner, Jr., Solid State Phys. **16**, 275 (1964).
[10] W. M. Lomer, Proc. Phys. Soc. (London) **80**, 489 (1962).
[11] H. R. Child and W. C. Koehler, J. Appl. Phys. **37**, 1353 (1966).