Pressure dependence of the Fermi surface of cadmium*†

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We report measurements for the effects of hydrostatic pressure on several cross-sectional areas for the electron and for the hole sheets of the Fermi surface of Cd. Pressure derivatives were obtained at a temperature of 0.4 K using a fluid-He phase-shift technique in which the data are digitally recorded and analyzed. Calculations based on a semiempirical nonlocal pseudopotential band structure due to Stark are compared with the experimental results. The anisotropy observed in the pressure dependence of the electron sheet confirms the negative sign of the [0002] pseudopotential in this model. The pressure derivative of largest magnitude is for the $[11\bar{2}0]$ cross section of the cap and is given by $d(\ln S)/dp = -(13.0 \pm 0.2) \times 10^{-3}\,\mathrm{kbar}^{-1}$.

I. INTRODUCTION

Some of the physical properties of Cd, especially the galvanomagnetic properties, as a function of pressure show abrupt and unusual changes. Therefore, new information about how the electronic energy spectrum in this metal changes as a function of the lattice constants is particularly interesting. Tsui and Stark[1] have determined the Fermi surface (FS) of Cd at zero pressure with high precision using the de Haas–van Alphen (dHvA) effect, and Stark *et al.* have used this information to develop a nonlocal pseudopotential model which accurately describes the observed FS.[2] We have used this model to calculate changes in the FS brought about by straining the lattice, and we have studied these changes experimentally using the dHvA effect under generally more favorable conditions than those used in the previous measurements of the same type. The purpose of this paper is to report our measurements and calculations for the pressure-induced changes in some of the cross sections for the electron and for the hole sheets of the FS.

All of the previous detailed studies of the FS of Cd under pressure have been made at temperatures above 1 K. Schirber *et al.* have measured the effects of pressure on several of the cross sections of the hole sheets in the fluid-helium range (0–25 bar) and in the range 0.025–9 kbar using a solid-helium pressure medium.[3] The magnetoacoustic effect has been used to study some of the cross sections of the hole sheets and the spin-orbit interaction at pressures as high as 12 kbar.[4] Itskevich *et al.* have measured the magnetoresistance at pressures to 15 kbar using a frozen-oil medium, and have used their results to propose pressure-induced changes in the topology of the FS.[5]

In this paper, we report cross-sectional-area pressure derivatives obtained at a temperature of 0.4 K using a fluid-helium phase shift method.[6] The accuracy of this method is normally improved when the temperature is reduced from 1 to 0.4 K. This can be demonstrated using the relation

$$\varphi = \hbar c S/eB = 2.35 \times 10^{9}(S/B), \tag{1}$$

where φ is the phase of a fundamental dHvA oscillation in radians, S is the FS cross section in a.u., and B is the magnetic induction in G.[7] The smaller the magnitude of B, the larger the phase shift for a given change in S. There is a mininum field, however, below which the dHvA effect can not be adequately observed. This field is usually a great deal smaller at 0.4 than at 1 K, and consequently appreciably larger phase shifts are observed at the former temperature.

II. EXPERIMENTAL METHODS AND RESULTS

In the measurements reported here, the dHvA oscillations were digitally recorded and analyzed for pressure-induced phase shifts using a large computer. The phases and amplitudes of the individual oscillations were determined by a least-squares fitting to the magnetization of as many as eight sinusoidal oscillations belonging to the dHvA frequency spectrum of Cd.

The oscillatory magnetization was measured by the field-modulation technique. Single-crystal specimens were cut by acid erosion and aligned to within 1.5° of the crystallographic directions using Laue-back-reflection techniques. The fluid-^{4}He pressure medium was cooled to 0.4 K by a pumped-^{3}He bath.[8]

Our measurements for the pressure derivatives of the FS cross sections are listed in Table I. The orbit designation and diagrams are given by Tsui and Stark (see Ref. 1). In the present study, changes in the cross sections λ_1^1, γ_1^1, α_1^1, and β_1^1 were obtained when B in Eq. (1) was 26, 13, 7, and 7 kG, respectively. Individual oscillations were not always isolated in these measurements but the

computer analysis yields individual phase shifts for as many as eight oscillations at once.

Simultaneously measured phase shifts were used to determine the pressure derivative of one cross section relative to another. The relative measurements are thought to be more accurate in general than the individual ones because the phase shifts in the former were made simultaneously. With the field directed along [0001], the following relative pressure derivatives were obtained:

$$\frac{d(\ln\lambda_1^1)}{dp} - \frac{d(\ln\gamma_1^1)}{dp} = (0.66 \pm 0.06)\times 10^{-3}\ \text{kbar}^{-1}, \quad (2)$$

$$\frac{d(\ln\alpha_1^1)}{dp} - \frac{d(\ln\beta_1^1)}{dp} = (0.5 \pm 0.2)\times 10^{-3}\ \text{kbar}^{-1}. \quad (3)$$

The latter result yields a change of $(-2\pm3)\times10^{-3}$ kbar^{-1} for the annular area between the cap and the monster in the *AHL* plane. This agrees with the results of Schirber and O'Sullivan who report a change of $(-3\pm3)\times10^{-3}$ kbar^{-1} in the fluid-helium range (see Ref. 3).

III. CALCULATIONS AND DISCUSSION

The effects of pressure on the electron sheet (lens) can be understood using a two-orthogonalized-plane-wave (2-OPW) model.[9] In this model, the rim of the lens is rounded by V_{0002}, the [0002] Fourier coefficient of the pseudopotential, while the rest of the surface is nearly free-electron-like. The amount of rounding is a measure of the magnitude of this parameter. In Fig. 1, we schematically show the effects of pressure on the extremal orbits when the field is normal to the c axis. For a model of the Heine-Aberenkov type, the magnitude of V_{0002} decreases with pressure (assuming $V_{0002} < 0$) at such a rate that the radius ρ of the circular cross section increases, as shown in the diagram. This causes a positive sign in the calculated [0001] pressure derivative, in agreement with experiment.

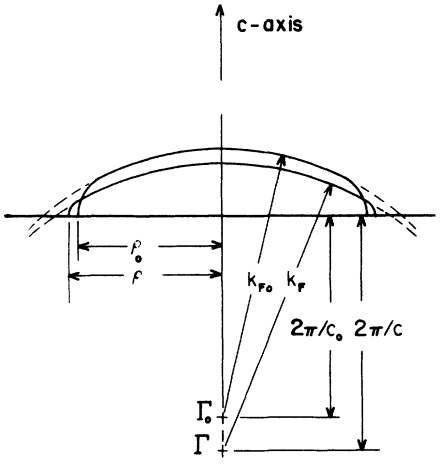

FIG. 1. Effects of pressure on the extremal lens orbits when the field is in the basal plane. The subscript 0 refers to zero pressure.

The cross-sectional area of the lens normal to $[11\bar{2}0]$ is not affected as much by V_{0002} as the [0001] area. The former area is determined primarily by the free-electron radius k_F and the lattice spacing c, as shown in Fig. 1. Because of the decrease with pressure of c/a in Cd, the increase in k_F is small enough compared to the increase in $2\pi/c$ to cause a net decrease in the $[11\bar{2}0]$ cross-sectional area. Since the lens is almost invariant to a rotation about the c axis, the pressure derivative of the electron sheet should be negative for any other field direction in the basal plane.

The hole sheets of the FS in Cd are more complicated than the electron sheet. They cannot be described by a simple local pseudopotential model. The band structure we use to calculate the pressure derivatives for both the electrons and the holes is described in detail elsewhere so our description is limited primarily to the pressure dependence of the parameters in this model (see Ref. 2). The slope of V_{0002} (= −0.0193 a.u.) is assumed to be given by

$$\left(\frac{\partial V_{0002}}{\partial q}\right)_{k_F} = 0.15\ \text{a.u.}, \quad (4)$$

which is consistent with the Heine-Aberenkov-Animalu model,[10] where q is a reciprocal-lattice vector. This slope and the Hartree dielectric-screening function yields the pressure dependence of V_{0002} (see Ref. 9). The slopes of the other local coefficients ($V_{10\bar{1}0}$, $V_{10\bar{1}1}$, and $V_{10\bar{1}2}$) are appreciably less than the [0002] slope. These coefficients are assumed to be independent of pressure because their estimated changes do not appreciably change the FS. The nonlocal coefficients and the spin-orbit parameter are also held constant.

To calculate the pressure derivatives, the calculation is repeated with lattice constants corresponding to 3.64 kbar.[11] Pressure changes much larger in magnitude than this either cause changes in the topology of the FS or introduce nonlinear changes in the cross sections. The energy levels are convergent at zero pressure so the truncation energy should not cause serious errors in the compressed metal.[12] The Fermi level E_F is found as at zero pressure by equating the number of hole and electron states.

The results of the calculations are shown in Table I. The pressure derivatives for the electron sheet are not appreciably different from experiment, but those for the holes are well outside the estimated error in the available measurements. It is of some interest to note that all of the calcu-

lated changes for the hole cross sections need to be shifted systematically to smaller values. Such a shift can be accomplished by increasing the change in E_F with pressure.

In Fig. 2, we show the calculated pressure derivatives of S as a function of the pressure derivative of E_F. The change in E_F for volume compensation ($n_e = n_h$) is 1.3×10^{-3} kbar^{-1}. This is nearly the same as the free-electron value $\frac{2}{3}K_T = 1.25\times10^{-3}$ kbar^{-1}, where K_T is the isothermal compressibility (see Ref. 11). According to Fig. 2, however, a change in E_F of about 1.5×10^{-3} kbar^{-1} brings most of the calculated pressure derivatives for the holes into agreement with experiment. This does not affect the electron values very much because they are not as sensitive as the holes to changes in the pressure dependence of E_F. But the pressure dependence of E_F needed to fit the data violates compensation.

This discrepancy should be removed before the calculations are used to predict changes in the FS at high pressure. Perhaps this could be achieved with the addition of the pressure dependence for the nonlocal coefficients. But the pressure dependence of these parameters is not properly understood at the present time. This problem has been avoided in Mg by Beardsley *et al.* who use a local model employing enough plane waves for convergence.[13]

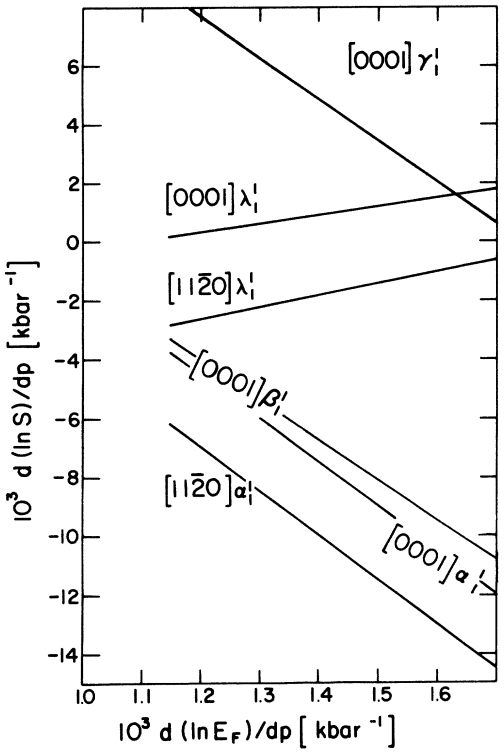

FIG. 2. Calculated pressure derivatives of the Fermi-surface cross sections S vs the pressure derivative of the Fermi energy E_F. See Table I and Ref. 1 for orbit nomenclature.

TABLE I. Comparison of experimental and calculated values for the hydrostatic pressure dependence of the cross-sectional areas S of the Fermi surface of cadmium. The units of $d(\ln S)/dp$ are 10^{-3} kbar^{-1}.

Cross section[a]	Field direction	$\frac{d(\ln S)}{dp}$ Expt.	Present calc.
Lens			
λ_1^1	[0001]	1.6 ± 0.6	0.7
λ_1^1	[11$\bar{2}$0]	-2.3 ± 0.3	-2.2
Cap			
α_1^1	[0001]	-9.7 ± 0.2	-6.0
		-10 ± 1[b]	
α_1^1	[11$\bar{2}$0]	-13.2 ± 0.2	-8.5
α_1^1	28.5° from [0001] in a [11$\bar{2}$0] plane	-9.4 ± 0.8[b]	-5.0
Monster			
β_1^1	[0001]	-9.1 ± 0.5	-5.4
		-9 ± 1[b]	
γ_1^1	[0001]		6.2
		1.0 ± 0.5[b]	

[a]Orbit nomenclature is given in Ref. 1.
[b]Reference 3.

A model of this type that accurately describes the FS of Cd has not yet been developed, however.

Summarizing, one can say that some of the largest effects of pressure on the FS in Cd are due to changes in the c/a ratio. An analogous situation in Zn is described in the pressure studies of O'Sullivan and Schirber[14] and in the alloy work of Higgins and Marcus.[15] The pressure dependence of the electron sheet in Cd is adequately described by the nonlocal pseudopotential model due to Stark *et al.*, when just the local coefficients are allowed to change with the lattice spacings (see Ref. 2). The anisotropy observed in the pressure dependence of this sheet confirms that $V_{0002} < 0$ as determined by this model.

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