EFFECT OF HYDROSTATIC PRESSURE ON THE ELECTRON FERMI SURFACES IN Pd AND Pt[†]

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We present measurements of the pressure derivative $d(\ln S)/dp$ of the Fermi surface cross section S at [100] and [111] for the electrons in Pd and Pt in the range 0-25 atm. The results suggest that the electron pressure derivatives in these metals are nearly isotropic. Along [100] $d(\ln S)/dp = (4.0 \pm 0.4)\times 10^{-4}$ and $(3.2 \pm 0.3)\times 10^{-4}$ kbar^{-1} for Pd and Pt, respectively.

There has recently been a considerable amount of interest in the electronic structures of Pd and Pt, metals whose magnetic spin susceptibilities are unusually large.[1] The dimensions and effective masses of their Fermi surfaces have been derived from the de Haas–van Alphen (dH-vA) data for Pd[2] and Pt,[3-6] and these results have contributed a great deal of information about their band structures. We present here dH-vA measurements of the change in cross sectional area of the electron sheets of these two similar Fermi surfaces as a function of hydrostatic pressure, and this yields additional information about the energy bands in these metals.

The band structure in Pd and Pt, like that in other transition metals, is represented to a good approximation by a nearly-free-electron s-p band crossing and hybridizing with a relatively narrow tight-binding d band.[7] The Fermi level in Pd and in Pt lies just below the top of this d band.[8] The corresponding Fermi surface then consists of an electron sheet of primarily s-p character and a hole sheet, part of which is open,[9] of primarily d character. According to our measurements, this electron surface expands under pressure by an amount that is greater than the compressibility prediction by a factor of about 1.2 in Pd and 1.3 in Pt, and these results are used to discuss the effect of pressure on their d bands.

The change in cross-sectional area of the Fermi surface with pressure was measured by the fluid-helium phase-shift method[10] at temperatures as low as 0.95°K. A 55-kG Westinghouse superconducting solenoid with a 1-in. bore supplied the magnetic field, which was homogeneous to one part in 10^5 over 1 cm. The dH-vA phase measurements were made with a crystal symmetry axis aligned parallel to the field with sufficient accuracy to eliminate spurious phase changes dependent on orientation. Single-crystal specimens of Pd and Pt were grown by the rf floating-zone technique. The residual resistivity ratio of typical specimens varied from 2000 to 4000.

Some phase measurements for the electrons in a [100] Pd sample are shown in Fig. 1. The corresponding oscillations were nearly sinusoidal, indicating that they were not strongly interacting. The dH-vA phase φ, apart from a constant of order unity, is related to the extreme Fermi surface cross section S by the expression[11]

$$\varphi = \hbar c S/eH = 2.351\times 10^9 S/H \tag{1}$$

if the magnetic interaction with other oscillations is neglected. The phase is expressed in radians when S is in a.u. and the field H is in gauss. Pressure derivatives obtained with Eq. (1) for the electron surface in Pd and Pt are given in Table I. The effect of the d-band hole oscillations on the electron phase was neglected. The hole phase shift with pressure was below the present level of detection and estimates of the upper limit of the hole contribution to the electron phase were small compared with the specified limits of error in the phase measurements. When the field is directed along [111], two extremal sections exist (central and noncentral) producing beats in the dH-vA oscillations.[2,4] Measurements of the phase at beat maxima were made for this direc-

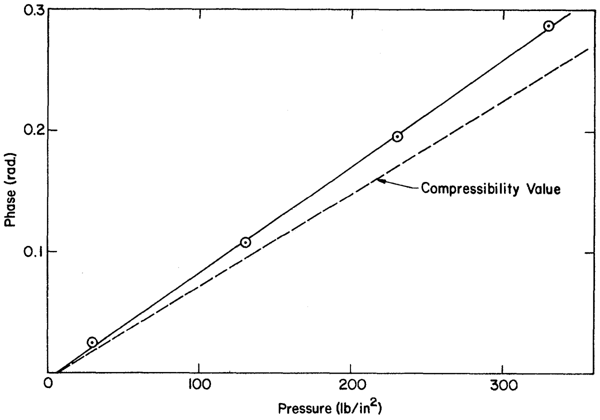

FIG. 1. The relative dH-vA phase dependence on pressure for the electrons in Pd with the field H parallel to [100] and $H = 52.2$ kG.

Table I. Pressure derivatives for the extremal cross section S of the electron Fermi surfaces in Pd and Pt. For comparison, the free-electron value $\frac{2}{3}K$ is given where K is the compressibility. All values are positive numbers. The values of S were taken from Refs. 2 and 4.

	$d(\ln S)/dp$ (in units of 10^{-4} kbar^{-1})	
Orientation	Pd	Pt
100	4.0 ± 0.4	3.2 ± 0.3
111	3.9 ± 0.4	2.8 ± 0.3
$\frac{2}{3}K$	3.412^{a}	2.311^{b}

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[b] R. E. Macfarlane, J. A. Rayne, and C. K. Jones, Phys. Letters 18, 91 (1965).

tion and, therefore, the value quoted in Table I represents the dominant or central section.

The electron pressure derivatives in Table I show little variation with orientation. The electron surface is not highly anisotropic; it is located at the center of the Brillouin zone, and it occupies only about $\frac{1}{5}$ of the zone volume.[2,4] Pressure, therefore, is not expected to change the anisotropy of this surface very much.

Average values of the pressure derivatives in Table I are greater than the corresponding compressibility values by about 16% in Pd and about 30% in Pt. Since these are compensated metals, the d-band hole surface and the electron surface are constrained to remain equal in volume. The calculated d-band density of states[12] at the Fermi level, however, is larger than that for the electrons by at least a factor of 4. Because the pressure derivatives are not much greater than the compressibility values, then, the shift with pressure in the center of gravity of the d bands relative to the core levels is probably much smaller than the shift in the electron band relative to the Fermi level.

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ELECTROREFLECTANCE STUDY OF NiO

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By using a thin NiO single-crystal sample, it has been possible to observe electroreflectance spectra between 3.0 and 5.0 eV. The results of this study and a recent photoconductivity investigation suggest that an energy-band description which includes the 3d electrons is necessary for a full description of NiO interband optical properties.

The sensitivity to detail in the joint density of states made possible by modulation techniques[1] has not previously been utilized in studies of interband optical transitions in transition-metal compounds. This note reports electroreflectance spectra obtained for NiO and discusses their implications for three current models of electronic structure for this material.

NiO is a NaCl-type antiferromagnet with a Néel temperature of 523°K. The specimens used in this study were prepared from a single crystal of 10^7 Ω cm resistivity grown by the flame fusion technique.[2] Reduction in a hydrogen atmosphere at 700°C for about 10 min produced a thin nickel