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ELECTRONIC STRUCTURE AND MANY-BODY EFFECTS IN Pd

MASTER

by

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Using extremal orbital areas and cyclotron masses measured with the de Haas-van Alphen effect we have constructed a phase shift parametrization based on the KKR method of band calculation for the Fermi surface properties of Pd. The use of magnetic fields to 13.2 T and temperatures as low as 0.3 K allowed orbital measurements on all four sheets of the Fermi surface. On the open hole sheet we observe the high mass β orbit for the first time. We have extensive data on the small L-centered hole pockets which show significant distortion from ellipsoidal shape due to a nearby van Hove singularity.

The measured data were fit with KKR phase shifts appropriate for a relativistic potential with a non-spherical charge distribution inside the muffin tin spheres for ℓ = 0, 1, and 2 (Ketterson et al 1975) augmented by a very small spherical, non-relativistic ℓ = 3 component. Similar schemes have worked successfully in other transition metals (Crabtree et al 1979). The KKR parameters used to fit the cross-sectional areas (η_ℓ) and masses (η'_ℓ) are shown in Table I.

Table I. Phase shifts η and their energy derivatives η' used in KKR parametrization of Pd.

	Γ_6^+	Γ_6^-	Γ_8^-	$\Gamma_8^+(3/2)$	Γ_7^+, $\Gamma_8^+(5/2)$	f	α
η	-0.3133	-0.1680	-0.0116	-0.2916	-0.3534	-0.0011	-0.0119
η'	3.382	6.652	-3.964	0.1521	0.8036	0.1093	7.051

E_F = 0.7437 (2π/a units)   a = 7.3398 (bohr radii)

The Fermi surface geometry is illustrated in Figure 1, where the intersection of the Fermi surface with the (100) and $(1\bar{1}0)$ planes of the Brillouin zone is shown. Charge neutrality requires the total volume of the electron sheet to equal that of the hole sheets. This is satisfied in the KKR parametrization to within .004 electron/atom.

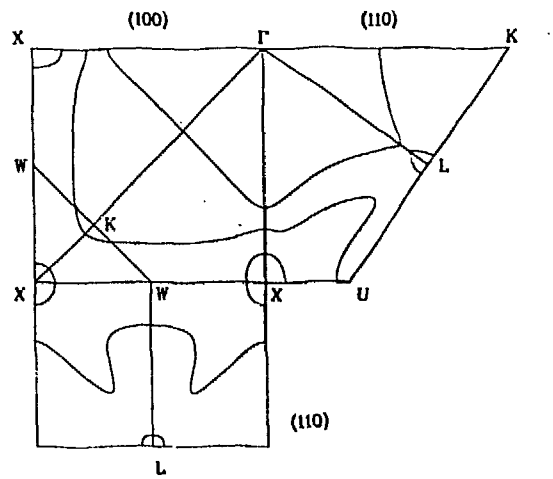

Figure 1. Intersection of Fermi surface of Pd with the (100) and (110) planes of the Brillouin zone.

The Fermi velocities predicted by the fit are shown for the two most important sheets of the surface in Figures 2 and 3 along with the band structure predictions of MacDonald et al (to be published).

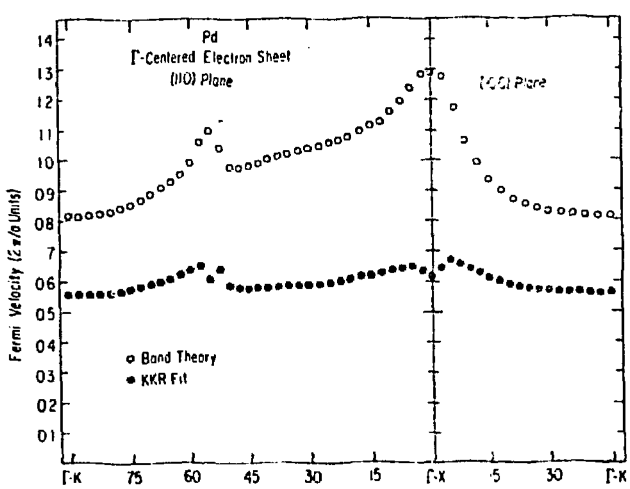

Figure 2. Magnitude of the Fermi velocity in (100) and (110) planes on the Γ centered electron sheet.

The many body renormalization due to electron-phonon and electron-electron or electron-paramagnon interactions is clearly seen as a reduction in the parametrized velocities from the band structure values. The inverse KKR velocity integrated over the Fermi surface gives the enhanced density of states consistent with the measured dHvA masses. In Pt and Nb this prediction agrees with the results of specific heat measurements to within 2% (Crabtree et al 1979 and this volume). For Pd the enhanced density of states from the KKR fit (see Table II) lies 13% below the value 2.00 states/eV-atom-spin inferred from specific heat measurements (Boerstal et al 1971). We

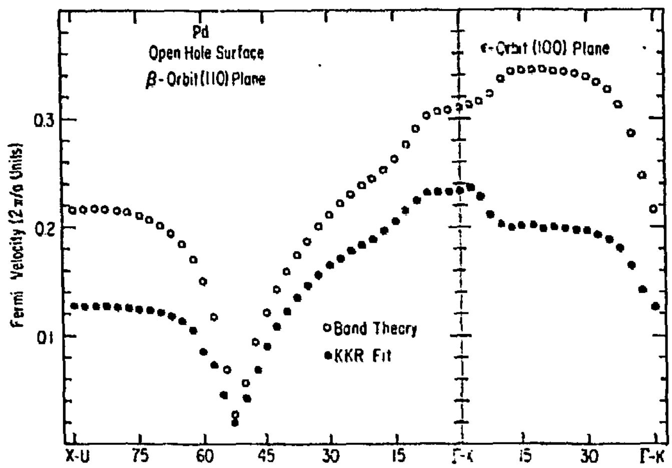

Figure 3. Magnitude of the Fermi velocity in the (100) and (110) planes on the open hole sheet.

have tried to eliminate this discrepancy by changing KKR parameter sets and fitting procedures, and by requiring the parametrization to fit the measured masses and specific heat density of states simultaneously. In all cases the discrepancy remains. We conclude that the discrepancy is not an artifact of the fitting procedure.

Table II. Fermi surface volume and enhanced density of states predicted by KKR fit

	L Holes	X Holes	Γ Electrons	Open Holes	Total
Fermi surface volume (Brillouin units)	-0.00142	-0.00537	0.3749	-0.3643	0.00381
Density of states $(\text{eV-atom-spin})^{-1}$	0.0348	0.0423	0.189	1.47	1.74

The discrepancy may reflect a difference in the way electron-electron and paramagnon effects renormalize the dHvA cyclotron mass and the specific heat, though this explanation is not consistent with the conventional picture of many body theory. Alternatively, the discrepancy may be caused by the inhibition of paramagnon enhancement by a magnetic field, since our mass measurements were made in fields up to 12.0 T while the specific heat work was done in zero field. This possibility suggests several further experiments, such as looking for a field dependence in the specific heat or in particular cyclotron masses.

Complete details of our measurements and parametrization will appear shortly (Dye et al to be published).

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