THE FERMI SURFACE OF PLATINUM

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The Fermi Surface of Platinum†

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THE FERMI SURFACE OF PLATINUM*

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The two high mass (ε,β) orbits on the open hole surface of platinum predicted by band structure calculations but not observed in previous de Haas van Alphen studies have now been measured, providing a complete set of area data for this transition metal. A phase shift fit to this area data using a non muffin tin relativistic KKR formalism has been calculated, with an RMS error of about 0.2%. From this fit the Fermi radii have been determined for all surfaces. As a check, the total volume of the hole surfaces has been calculated and compared with that of the electron surface, yielding agreement to within 1%. Effective mass data have also been fit, with an RMS error of 3.4%, constraining the density of states calculated from the fit to agree with the specific heat value; Fermi velocities have been determined for all surfaces.

With the availability of high magnetic fields, we have observed de Haas-van Alphen frequencies corresponding to two extremal orbits on the open hole surface of platinum which were predicted by band structure calculations (Anderson and Mackintosh, 1968; Watson-Yang et al., 1977) but not observed in previous studies (Stafleu and deVroomen, 1965; Ketterson et al., 1966; Ketterson and Windmiller, 1970). These orbits are the electron orbit centered at Γ in a (100) plane (ε) and the hole orbit centered at X in a (110) plane (β). Owing to the high masses of these orbtis, they were detectable only at fields above 120 KG at a temperature of 0.35 K. Table I gives the areas for these orbits, as well as the areas and masses for seven other symmetry orbits observed in a previous study (Ketterson and Windmiller, 1970).

These nine areas have been fit with seven parameters using the RKKR formalism for two values of the Fermi energy: $E_f = 0.5556$ Ry and $E_f = 0.6335$ Ry with rms errors of 0.22% and 0.19% respectively. The areas calculated from the latter fit are given in Table I. Table II lists the phase shift parameters for this fit, which include six phase shifts and a parameter, α, which describes the relative importance of spin orbit and crystal field effects; $\alpha = 0$ for the pure spin orbit case, while $\alpha = -0.8861$ for the pure crystal field case (Ketterson et al., 1972). Also included in Table II are the carrier densities for the electron, open hole, and X-centered ellipsoidal surfaces. The total volume yields the necessary charge neutrality for this even-valent metal to within 1%. From this set of phase shift parameters, the Fermi radius in any direction may be computed. Table III lists the Fermi radii as computed from the best fit for selected directions on the various surfaces, along with the values calculated by Watson-Yang, Freeman and Koelling (Watson-Yang et al., 1977). Figs. 1a and 1b show the angular dependence of the radii in the (110) plane for the electron and open hole surfaces, respectively. The agreement between theory and experiment is quite good on both surfaces.

A fit to 17 experimental masses was carried out using the phase shift derivatives with respect to energy $\{\eta'\}$ as adjustable parameters. The experimental masses and those calculated from the fit are listed in Table I, and Table II lists the fitting parameters $\{\eta'\}$. In this fit two constraints were placed on the $\{\eta'\}$: first, that each η' be non-negative, and second, that the density of states as calculated from the $\{\eta'\}$ agree with the value determined by specific heat measurements (Dixon et al., 1965). The first constraint was found to be necessary to insure that the velocities remain well behaved at all points on the surface; the second was introduced to compensate for the lack of mass data for the two highest mass orbits (ε and β), which would contribute heavily to the density of states.

Figs. 2a and 2b show the angular dependence of the magnitude of the Fermi velocity in the (110) plane for the electron and open hole surfaces, respectively. Table III gives a comparison between theory and experiment for selected directions on the various surfaces. The enhancement, due to many body electron-phonon and paramagnon effects, appears to be fairly constant over each surface, although there is some variation from surface to surface.

TABLE I. Experimental and calculated areas and masses.

SURFACE	ORBIT CENTER	ANGLE OF FIELD FROM (100)	PLANE OF FIELD ROTATION	EXPT. AREA (Atomic units)	CALC. AREA	EXPT. MASS	CALC. MASS
Electron	Γ	0° (100)	(110)	0.770	0.768	2.44	2.50
Electron	Γ	8.5°	(110)	0.769*	0.767	2.40	2.45
Electron	Γ	22.2°	(110)	0.769*	0.765	2.31	2.38
Electron	Γ	29.1°	(110)	0.756*	0.761	2.43	2.43
Electron	Γ	41.0°	(110)	0.721*	0.716	2.20	2.28
Electron	Γ	54.7°(111)	(110)	0.687	0.688	2.06	2.17
Electron	Γ	90°(110)	(110)	0.857	0.858	3.16	3.04
Electron	Γ	9.9°	(100)	0.774*	0.767	2.40	2.44
Electron	Γ	24.3°	(100)	0.790*	0.786	2.50	2.51
Electron	Γ	36.0°	(100)	0.832*	0.829	2.80	2.78
Open Hole	W	0°(100)	(110)	0.0740	0.0740	-1.53	-1.59
Open Hole	W	30.5°	(110)	0.0901*	0.0909	-2.30	-2.40
Open Hole	W	33.0°	(100)	0.0925*	0.0936	-2.30	-2.35
Open Hole	Σ'	90°(110)	(110)	0.217	0.217	-3.28	-3.53
Open Hole	Σ'	79.7°	(110)	0.228*	0.229	-3.68	-3.89
Open Hole	X	90°(110)	(110)	0.341	0.341	--	-9.12
Open Hole	Γ	0°(100)	(110)	1.890	1.898	--	6.41
Ellipsoids	X	0°(100)	(110)	0.00298	0.00298	-0.272	-0.282
Ellipsoids	X	90°(110)	(110)	0.00467	0.00467	-0.426	-0.425

*This off-symmetry area data was not included in the fit.

TABLE II. Fitting parameters, carrier densities, and densities of states from area and mass fits.

FITTING PARAMETERS

	$a = 3.9233\ \mathring{A}$	$E_f = 0.6335$ Ry
	Area parameters $\{\eta\}$	Mass parameters $\{\eta'\}$
Γ_6^+	-0.099986	0
Γ_6^-	0.133533	0
Γ_8^-	-0.095679	0
$\Gamma_8^+(3/2)$	-0.351516	0.43230
Γ_7^+	-0.487969	1.13875
$\Gamma_8^+(5/2)$	-0.495917	0.61392
α	-0.003243	0
RMS error	0.19% to 9 areas	3.4% to 17 masses
Surface	Carrier density (a_o^{-3})	Density of states (states/atom-Ry)
Electron	4.097×10^{-3}	6.35
Open Hole	-4.052×10^{-3}	-30.7
Ellipsoidal Hole (total of three)	-4.620×10^{-6}	-0.2025
Total	4.038×10^{-5}	37.3*

*Partially constrained to agree with the specific heat value of 37.9[5].

TABLE III. Comparison of Fermi surface dimensions (in atomic units) and velocities (in Rydberg-atomic units) between theory and experiment. The column labeled "enhancement" denotes the ratios of experimental and theoretical velocities.

SURFACE	DIRECTION	THEORY k_F	THEORY $\lvert\vec{v}_F\rvert$	EXPERIMENT k_F	EXPERIMENT $\lvert\vec{v}_F\rvert$	ENHANCEMENT
ELECTRON	$\Gamma - X$	0.590	0.398	0.590	0.266	1.50
	$\Gamma - L$	0.586	0.310	0.584	0.217	1.43
	$\Gamma - K$	0.436	0.744	0.436	0.485	1.53
X-CENTERED	$X - \Gamma$	0.0445	0.207	0.0482	0.150	1.38
ELLIPSOIDS	$X - K$	0.0303	0.298	0.0308	0.219	1.36
	$X - W$	0.0309	0.301	0.0308	0.218	1.38
OPEN HOLE	$X - \Gamma(\Delta)$	0.177	0.855	0.172	0.555	1.54
	$X - \Gamma(\Sigma)$	0.286	0.301	0.288	0.178	1.69

LIST OF LEGENDS

1. a) The Fermi radii in the (110) plane of the Γ centered electron surface.

   b) The Fermi radii in the (110) plane centered at X of the open hole surface.

2. a) The magnitude of the Fermi velocity in the (110) plane of the Γ centered electron surface.

   b) The magnitude of the Fermi velocity in the (110) plane centered at X of the open hole surface.

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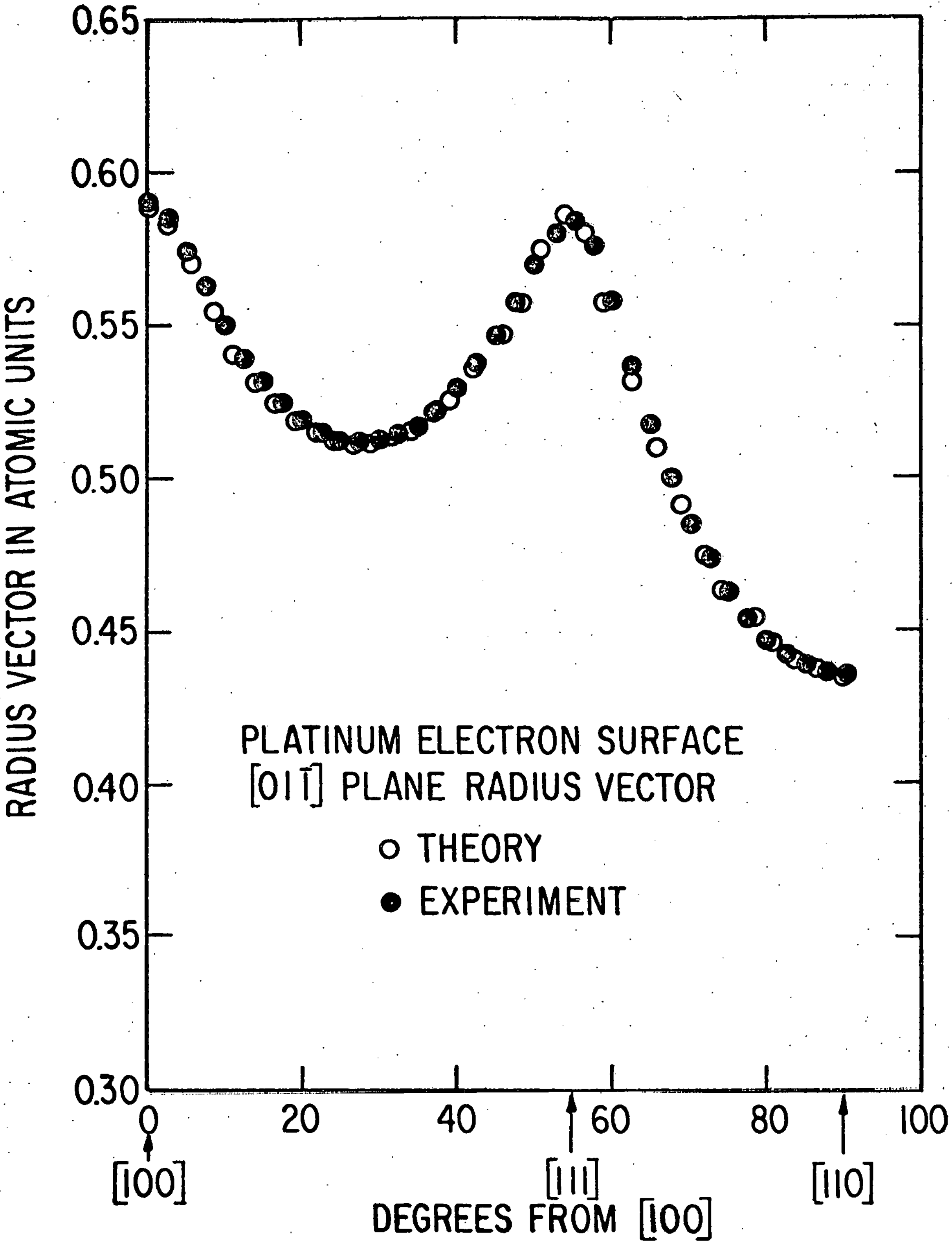

0.65
0.60
0.55
0.50
0.45
0.40
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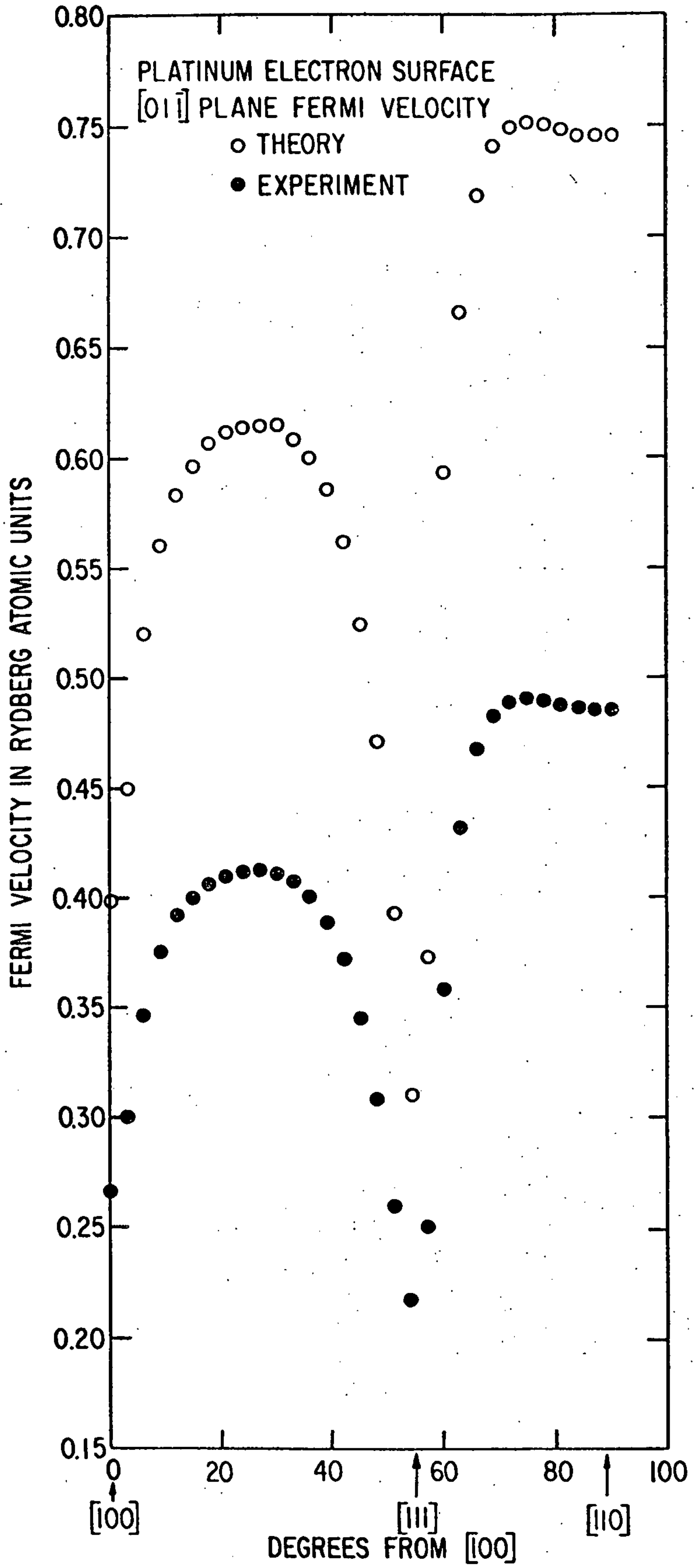
0.30
RADIUS VECTOR IN ATOMIC UNITS
PLATINUM ELECTRON SURFACE
[01$\bar{1}$] PLANE RADIUS VECTOR
○ THEORY
● EXPERIMENT
0
20
40
60
80
100
[100]
[111]
[110]
DEGREES FROM [100]



PLATINUM ELECTRON SURFACE
[01$\bar{1}$] PLANE FERMI VELOCITY
○ THEORY
● EXPERIMENT
FERMI VELOCITY IN RYDBERG ATOMIC UNITS
0.80
0.75
0.70
0.65
0.60
0.55
0.50
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0.30
0.25
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0.15
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20
40
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80
100
[100]
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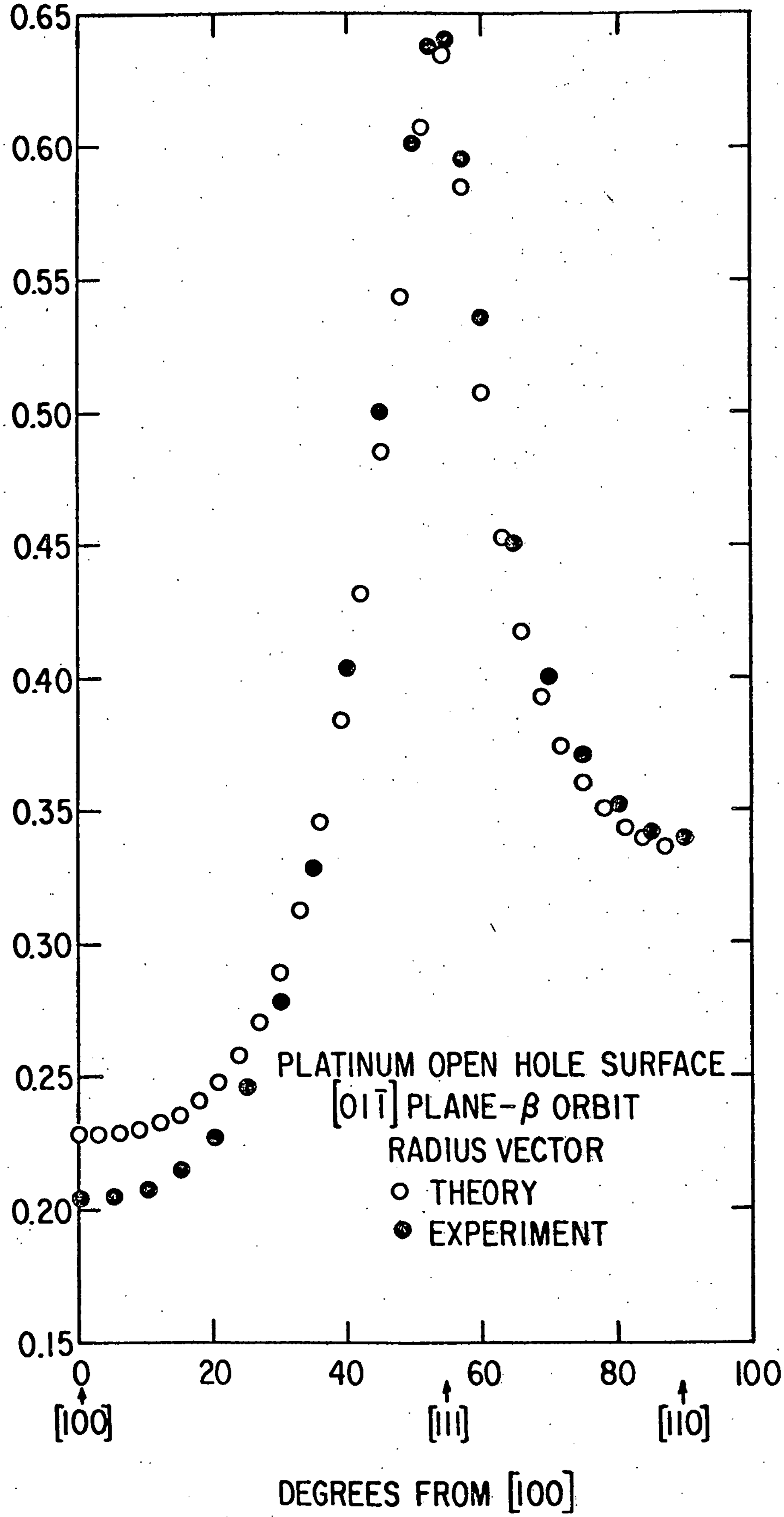
DEGREES FROM [100]



0.65
0.60
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0.30
0.25
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0
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40
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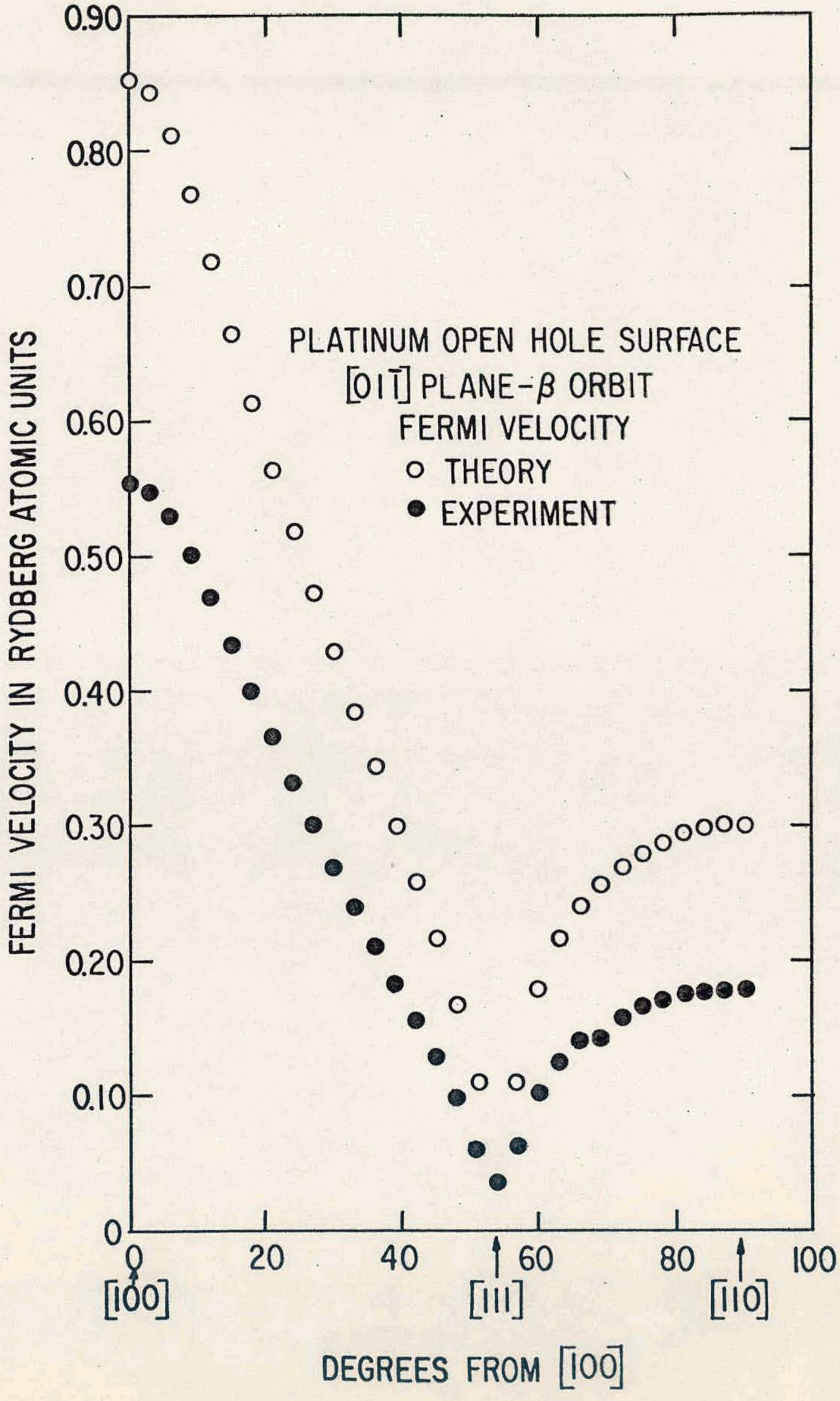
80
100
[100]
[111]
[110]
PLATINUM OPEN HOLE SURFACE
[01$\bar{1}$] PLANE–β ORBIT
RADIUS VECTOR
○ THEORY
● EXPERIMENT
DEGREES FROM [100]



0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0
FERMI VELOCITY IN RYDBERG ATOMICS UNITS
PLATINUM OPEN HOLE SURFACE
[01$\bar{1}$] PLANE-β ORBIT
FERMI VELOCITY
THEORY
EXPERIMENT
0
20
40
60
80
100
[100]
[111]
[110]
DEGREES FROM [100]