

DE HAAS—VAN ALPHEN EFFECT IN IRIIDIUM

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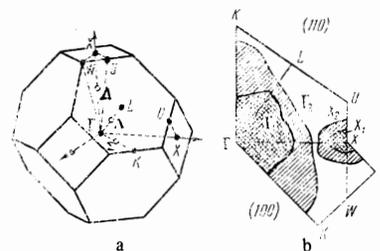
The magnetic-susceptibility oscillation periods of iridium single crystals are measured at temperatures of 2–4.2° K in magnetic fields up to 45 kOe directed along the $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$ crystallographic axes. The areas of the extremal cross sections of the hole sheet X_1 of the Fermi surface appearing for given magnetic field directions are determined. The temperature dependence of the oscillation amplitudes is studied experimentally and the effective masses of the hole carriers of the respective extremal cross sections are determined. The results are compared with available theoretical calculations of the iridium electron energy spectrum.

EXPERIMENTAL studies of the magnetoresistance and the Hall effect of iridium^[1] give a qualitative picture of its electronic structure and show that iridium is an “uncompensated” metal with a closed Fermi surface consisting of electron and hole sheets such that the volume difference of these sheets corresponds to one electron per atom ($n_e - n_h = 1$). These data substantiate a model of the Fermi surface (see the figure) based on a theoretical calculation of the electron energy spectrum using the RAPW method^[2].

In order to obtain quantitative information about the electronic structure of this transition metal, measurements of the de Haas—van Alphen effect^[1] were made. Measurements of the oscillation periods of the magnetic susceptibility and of the temperature dependence of the oscillation amplitudes were made in the 2–4.2° K range in magnetic fields up to 45 kOe. The magnetic susceptibility was measured using the Faraday method (the construction of the magnetic balance is described by Svechkarov^[3]), and a superconducting solenoid was used to produce the magnetic field.

The temperature was varied by pumping the gas over the liquid helium bath and monitored with a carbon thermometer. The signal was recorded automatically by a PDS-021M two-coordinate potentiometer.

The samples were cut by the electric-spark method from a single crystal with an electrical resistivity ratio of $\rho(298^\circ \text{K})/\rho(4.2^\circ \text{K}) = 150$ which was grown by electron-beam zone refining from the melt. The samples were in the shape of $5 \times 5 \times 0.5$ mm plates with three different orientations: the normal to the plane of the plate was along one of the principal crystallographic directions— $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$ —to within 2° . The samples were suspended in the solenoid field by a quartz filament such that the normal to plane of the plate was along the magnetic field direction. The thickness of the samples (0.5 mm) was chosen so that the gradient of the field of the superconducting solenoid was small enough over the sample thickness so as not to affect the form of the oscillatory dependence of the susceptibility $\chi(H)$. The geometry of the experiments allowed the areas of the extremal cross sections to be determined for the $\{100\}$,



Brillouin zone for FCC metals (a) and cross sections of the Fermi surface of iridium for the (100) and (111) planes according to calculations^[2] (b).

$\{110\}$, and $\{111\}$ planes, as well as the effective (cyclotron) masses of the conduction electrons corresponding to these extremal cross sections.

1. **Extremal cross sections.** As a consequence of the rather low sample purity, we observed oscillations due only to the “lighter” carriers—the holes of sheet X_1 . For the magnetic field along the $\langle 100 \rangle$ and $\langle 110 \rangle$ axes the $\chi(1/H)$ dependence showed two distinct frequencies corresponding to two extremal cross sections of sheets X_1 . When the magnetic field was along the $\langle 111 \rangle$ axis a single oscillation frequency appeared. This agrees with the distribution symmetry of the hole sheets X_1 in the Brillouin zone (see the figure).

The areas of the extremal cross sections corresponding to the observed oscillation frequencies are given in the table.

There is good agreement of our results with the results of measurements^[4] made by the torsion method. It should be noted that the areas of the extremal cross sections in the table, which are taken from Grodski and Dixon^[4], have a large error in the third significant figure. It turns out that for the torsion method the error greatly increases for magnetic fields close to the symmetry directions and is as large as 3%^[4] as can be seen from the graph given by Grodski and Dixon.

Analysis of the data obtained shows that a slightly deformed ellipsoid elongated along the ΓX direction and slightly compressed along the XW direction can be taken as an approximate model of the X_1 hole sheets. The volume enclosed by one X_1 surface is $V_{X_1} \approx 3.1 \times 10^{-3}$ atomic units. The total volume of the X_1 sheets within

¹We note that the de Haas—van Alphen effect was measured in samples prepared from the same single crystal, for which the galvanomagnetic properties were measured earlier^[1].

Direction of H	S_{extrem} (atomic units)			Cyclotron masses		
	Theory [2]	Experiment		Theory [2]	Experiment	
		Our data	Data of [4]		Our data	Data of [4]
$\langle 100 \rangle$	0.0261	0.018 ± 0.001	0.0183	0.21	0.22 ± 0.02	—
	0.0388	0.029 ± 0.001	0.0289	0.24	0.27 ± 0.02	—
$\langle 110 \rangle$	0.0293	0.021 ± 0.001	0.0213	0.22	0.25 ± 0.02	0.24
	0.0406	0.031 ± 0.001	0.0297	0.26	0.28 ± 0.02	—
$\langle 111 \rangle$	0.0318	0.024 ± 0.001	0.0228	0.22	0.25 ± 0.02	—

the Brillouin zone is $3V_{X_1}$ which corresponds to a concentration of X_1 hole carriers of 7.2×10^{-3} holes/atom.

2. Effective Masses. In addition to the periods (frequencies) of oscillation, the temperature dependences of the amplitudes of the oscillations were studied in the $2.0\text{--}4.2^\circ\text{K}$ temperature range. These measurements allowed the values of the effective (cyclotron) masses to be determined for the hole carriers of the X_1 sheet, which corresponded to the extremal cross sections studied. The data obtained for m^*/m_0 are given in the table.

It is apparent from the table that a significant deviation of the extremal cross sections of the X_1 surface was observed between the experimental measurements and the values theoretically calculated by Anderson and Mackintosh^[2]. It is very likely that this deviation is due to the fact that the model of the potential chosen for the calculation of the energy spectrum of iridium did not adequately describe the real potential. Evidently, agreement between calculated and experimental parameters of small groups of carriers at the boundaries of

the Brillouin zone such as for the X_1 hole sheets serves as a good criterion for the validity of the potential chosen.

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²C. K. Anderson and A. R. Mackintosh, Solid State Commun. 6, 285 (1968).

³I. V. Svechkarev, Pribory i Tekhnika Éksperimenta 4, 142 (1963).

⁴J. J. Grodski and A. E. Dixon, Solid State Commun. 7, 735 (1969).

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