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# Effect of Pressure on the Fermi Surface of $ReO_3$ †

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We have determined the pressure derivatives of several cross-sectional areas of the Fermi surface of $ReO_3$ as well as the isothermal compressibility at room temperature. The cross-sectional areas increase at rates of $(1.5–4.0) \times 10^{-4}$ $kbar^{-1}$ compared to the free-electron scaling prediction of $3.6 \times 10^{-4}$ $kbar^{-1}$.

The Fermi surface of the bright-red transition-metal oxide $ReO_3$ has been determined experimentally in considerable detail from the magnetothermal studies of Graebner and Greiner[1] and the de Haas-van Alphen (dHvA) work of Marcus[2] and of Phillips and Shanks.[3] These experimental results are all in substantial agreement with the augmented-plane-wave (APW) band calculation of Mattheiss[4] who found the Fermi surface to consist of two roughly spherical electron pockets centered at the center of the Brillouin zone and a multiply-connected hole sheet in the form of an array of intersecting tubes directed along [100] axes.

The purpose of this communication is to present measurements of the effect of hydrostatic pressure upon several cross sections of the Fermi surface of $ReO_3$. Such measurements have proven useful in evaluating the physical significance of model descriptions for various metals.[5,6] The simplest model prediction for a cubic system for the change with pressure of the Fermi surface is that of free-electron scaling which simply assures that the same fraction of the Brillouin zone remains filled. Scaling then requires that all cross sections of the Fermi surface increase at the rate of two-thirds of the volume compressibility. In order to be able to compare our results with even this simplest model, we need the compressibility, which to our knowledge is unavailable. We have therefore determined the room temperature compressibility for $ReO_3$ by direct measurement of the lattice constant with pressure to 3 kbar.

Single-crystal specimens were grown by a chemical-vapor reaction.[7,8] The crystals were then annealed at 350 °C for several weeks which resulted in substantial ($\sim 10^2$) increase in the amplitude of the dHvA oscillations. The largest crystals were 3–4 mm on a side. The sample used in the compressibility measurements was an irregularly shaped prism approximately $0.2 \times 0.3 \times 0.4$ $mm^3$ in size mounted on [110].

dHvA frequencies were obtained using the field-modulation technique.[9] Hydrostatic pressure derivatives of the dHvA frequencies, and therefore of the corresponding cross-sectional areas, were obtained by means of the fluid-He phase-shift technique.[6,10] Here advantage is taken of the large phase of the dHvA signal so that the change in frequency can be observed with pressures below the freezing pressure of He (25 bar at 1 °K). For a single frequency, the relation between the shift in field position of a single oscillation $\Delta H$ is related to the logarithmic pressure derivative of the dHvA frequency $F$ by

$$B^{-1}\Delta H/\Delta P = d\ln F/dP ,$$

where $B$ is the field at which the data are taken and $\Delta P$ is the increment of pressure applied. A similar but somewhat more complicated expression is obtained for the superposition of two frequencies[6]

TABLE I. Experimental values for pressure derivatives of cross-sectional areas of the Fermi surface of $ReO_3$. Values of $d\ln F/dP$ are given in units of $10^{-4}$ $kbar^{-1}$; frequencies are in $10^7$ G. Nomenclature for cross sections is from Mattheiss (Ref. 4).

| Cross section | Field direction | Frequency | $d\ln F/dP$ |
|---|---|---|---|
| $\alpha$ | [100] | 4.15 | $4.0 \pm 0.3$ |
| | [111] | 4.61 | $4.0 \pm 0.4$ |
| $\gamma_1$ | [100] | 4.88 | $1.5 \pm 0.5$ |

Scaling prediction $\sim 3.6 \times 10^{-4}$ $kbar^{-1}$

and it is usually possible by proper choice of the modulation amplitude, field direction and magnitude, and temperature to limit the signal to one or two components.

The compressibility was determined by following nine high (110–150 deg) $2\theta$ x-ray reflections as a function of pressure to 3 kbar. Pressure was generated in kerosene in a pure Be pressure vessel described earlier.[11] The value we obtained for the isothermal compressibility near 23 °C is $(5.3 \pm 0.9) \times 10^{-4}$ kbar$^{-1}$. The uncertainty is large because of the small change in the lattice parameter with 3 kbar.

Our results for the pressure derivatives of the Fermi-surface cross sections are given in Table I. We have employed the notation of Mattheiss[4] throughout. The frequency of the $\alpha$ oscillations, which correspond to the smaller of the two $\Gamma$-centered electron sheets, changes at a rate which is, within combined experimental uncertainty, equal to the scaling prediction of $3.6 \times 10^{-4}$ kbar$^{-1}$. The $\gamma_1$ frequency, corresponding to the minimum area of the multiply-connected hole sheet, on the other hand, increases at a much slower rate of $(1.5 \pm 0.5) \times 10^{-4}$ kbar$^{-1}$. We have been unsuccessful in isolating the $\beta$ oscillations associated with the larger electron pocket with sufficient amplitude to obtain pressure data.

It is not particularly surprising that the free-electron scaling fails in a transition-metal oxide as we have observed large deviations from scaling in transition metals such as Zr[12] and W.[13] It would be of considerably more interest to compare our results with predictions of a model calculation such as Mattheiss's APW description. In previous comparisons either a "first-principles" calculation is made at various volumes[5] or a parametrized fit is made at normal volume and then the volume-dependent parameters of the model are changed[14] to give the model predictions for the effect of pressure on the Fermi surface. Therefore, if the compressibilities are known, a given model can be tested to see how well it predicts the observed pressure dependence of the Fermi surface. However, in order to achieve agreement with optical data in the case of $ReO_3$, Mattheiss was forced to shift his bands relative to each other by several volts. It is not obvious then exactly how this would be most reasonably handled in a calculation at a new volume.

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# Velocity of Second Sound in $Li^7F$ and NaI

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Calculated values are given for the velocity of drifting second sound and the heat capacity per unit volume for $Li^7F$ from 15 to 48 °K and for NaI from 3 to 15 °K. Limiting values for 0 °K are also given.

In a previous paper[1] we presented the results of a detailed calculation for NaF of the velocity of drifting second sound $v_{II}$. The values obtained were used to interpret the results of the experimental investigations of second sound in NaF by Jackson, Walker, and McNelly.[2] Similar experimental investigations have also been done on $Li^7F$ and NaI, but distinct second-sound pulses like those seen