Effect of pressure on the Fermi surface of Nb_3Sb

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The pressure dependences of three cross sections of the Fermi surface of Nb_3Sb are determined from de Haas—van Alphen measurements in solid He to several kbar. A large negative derivative is observed for the smallest cross section of the hole ellipsoid at M.

In spite of the enormous interest in the $A15$ compounds owing to their superconducting properties, very little direct Fermi-surface information is available. Arko *et al.*[1] reviewed the status of Fermi-surface (FS) measurements and comparisons to band calculations in these materials, and it appears that the best candidate for detailed study (although its T_c of 0.2 K makes it uninteresting technologically) is Nb_3Sb. High-quality crystals can be obtained by iodine-vapor-transport techniques and fairly comprehensive de Haas—van Alphen (dHvA),[1,2] Shubnikov—de Haas, and high-field magnetoresistance[3] data have been reported. The first attempts[2] to understand the FS involved rigid-band shifting of Mattheiss's band structure[4] for Nb_3Sn. Very rough qualitative agreement with the data was obtained by rigid-band shifting E_F by $\approx$ 0.5 eV (considerably more than required by the addition of two electrons, but within the stated accuracy of the calculations). Van Kessel *et al.*[5] subsequently did a non-self-consistent augmented-plane-wave calculation for Nb_3Sb but incorporated nonspherical corrections both inside and outside the muffin-tin spheres. They obtained not only qualitative but also fairly quantitative agreement with the dHvA data. Indeed they predicted additional pieces of the Fermi surface subsequently found in the measurements. With agreement between theory and experiment approaching that found in pure transition metals it becomes useful to measure parameters which can further refine the calculations and discriminate between the various approaches. In this study we present data for the pressure dependence of the Fermi surface of Nb_3Sb which should provide further insight into the details of the band structure of this material and its interesting sister compounds.

The samples used were from the same lot as in the original dHvA studies of Arko *et al.*[1] The [100] oriented parallelopiped slipped into the 0.030-in. bore of 3000-turn counterwound pickup coil which in turn slips into the Be-Cu pressure vessel whose 0.125-in. bore is orthogonal to that of the pickup coil. Fields to 100 kG are generated in a split superconducting coil. Standard field modulation dHvA techniques were employed. Pressures were generated in solid[6] He and pressure derivatives were determined by the solid-He phase-shift technique.[7] Here the shift in field ΔH of a feature of a single dHvA oscillation at a given field B with a pressure increment ΔP is related to the pressure derivative of the dHvA frequency F by $d\ln F/dP = B^{-1}\Delta H/\Delta P$. This technique was required because the pressure derivatives are far too small to observe in fluid He or by direct comparison at various pressures to our maximum pressure

TABLE I. Pressure derivatives of Fermi-surface cross sections for $\vec{H}\,||\,[100]$ for Nb_3Sb.

Orbit	Frequency (10^6 G)	Pressure derivative (10^{-4} kbar^{-1})
γ_1	9.7	7.4($\pm$0.3)
γ_1'	10.1	8.1($\pm$0.3)
α_1	0.8	-69 ($\pm$8)

of 9 — 10 kbar.

Our results are shown in Table I for data taken with $\vec{H} \parallel [100]$. To date we have been able to obtain information only on the α and γ oscillations which are due to the hole ellipsoids at M (as labeled in Ref. 2). The γ frequencies increase at $\sim 8 \times 10^{-4}$ kbar^{-1}. This can be compared to the value of $\frac{2}{3}K_T$ where K_T is the volume compressibility (estimated from data on other Nb-based $A15$ compounds to be 6×10^{-4} kbar^{-1}) which would be the free-electron scaling value if the Fermi surface were to increase in step with the Brillouin zone as the pressure increases. The α frequency on the other hand shows a large *negative* value of about -70×10^{-4} kbar^{-1}. This unexpected result should provide a rather critical check on the assignment of this frequency to a particular band and a test of the validity of the band structure in general.

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