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Comments

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Comment on "Prediction of Fermi-surface pressure dependence in Rb and Cs"

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We present experimental evidence for formation via pressure of a multiply connected Fermi surface in Cs, resulting from contact of the Fermi surface with the Brillouin zone, for direct comparison with the predictions of the volume-dependent band calculations of Jan, MacDonald, and Skriver. Agreement is found to be excellent.

In a recent article, Jan, MacDonald, and Skriver[1] (JMS) presented predictions of the pressure dependence of Fermi-surface parameters for Rb and Cs. The results for the pressure dependence of the cross-sectional areas of the Fermi surface (FS) of Cs for various field directions were found to be in essential agreement with our published experimental results.[2] The Fs of Cs is well documented[3] to be nearly spherical with substantial protuberances in the ⟨110⟩ directions such that the Fermi surface nearly touches the bcc zone boundary at the symmetry point *N*. Increasing pressure increases the nonsphericity and, with sufficient pressure, contact is made and necks joining spheres in adjacent Brillouin zones are formed. JMS predict, on the basis of their linear muffin-tin orbitals method, the change in lattice parameter at which this multiply connected Fermi surface first occurs. In this comment we present heretofore unpublished data on the Fermi surface of Cs as a function of pressure for direct comparison with this prediction.

Most of our samples were randomly grown from 99.99% pure material from Leico Industries and oriented optically. A few crystals were cut by spark erosion along desired directions in a cooled (−20 °C) kerosene bath. All samples were right circular cylinders 0.14 in. diam by $\frac{3}{8}$ in. long. This cylinder axis is along the applied magnetic field direction in our geometry. Pressures were generated in solid He to 10 kbar as described earlier.[4] de Haas–van Alphen (dHvA) frequencies were determined with the use of the field modulation scheme[5] at 1.1 K in a 55-kOe superconducting solenoid.

The dHvA frequency is directly proportional to the extremal cross-sectional area for a given field direction. Thus in Cs the largest cross section is observed when the most ⟨110⟩ protuberances are encountered, i.e., for an applied field in the [111] direction. The smallest cross section is for a field direction 11° from [110] in a (001) plane where *no* protuberances are traversed in the extremal orbit. We find that the large "belly" orbits disappear abruptly at a pressure of about 5 kbar when the orbit cuts through ⟨110⟩ directions. This was observed for several randomly oriented crystals whose cylinder axes were such that belly orbits for fields along these axes passed through ⟨110⟩ directions. This same loss of belly orbits with pressure above 5 kbar was observed in the spark cut [100], [110], and [111] crystals. If the orbit comes within about 6° of a ⟨110⟩ direction the belly orbit persists to 6.1 kbar and to 8 kbar for an orbit passing 10° from the nearest ⟨110⟩. For the minimum area orbit which best avoids all the ⟨110⟩ directions, the belly orbits persist to our highest pressures of ~10 kbar.

We interpret this angular dependence of the occurrence of belly oscillations as a function of pressure as a direct indication of interception of the Fermi surface with the Brillouin zone at the point *N* at 5.0 (±0.2) kbar. We searched for oscillations associated with the resulting ⟨110⟩ directed necks and were unable to detect any sign of them whatsoever. We would expect the bands to be very flat in this region so the effective masses might be quite large. The belly oscillations have effective-mass ratios of 1.4–1.6 at zero pressure which increase 3–4%/kbar.

The neck frequency can be estimated to be only about 1% of the belly frequency at our highest pressure. It would be very difficult to detect this combination of high mass and low frequency because of the high modulation field amplitude required. We also attempted to observe the "rosette"-type hole orbits predicted for the [100] direction which are comprised of four necks and four segments of belly orbits from four adjacent Brillouin zones. Oscillations associated with these orbits are probably very weak because, with small necks, they exist over very small angular extent and again are expected to have large effective-mass ratios. Thus our only evidence for the formation of necks is the disappearance of the belly orbits, but the strict correspondence of this behavior with intersection of the orbit with ⟨110⟩ directions is quite convincing.

Jan, MacDonald, and Skriver predict that the intersection of the FS with the Brillouin zone should occur with a lattice constant change of −6.7%. Using the zero temperature pressure-volume-temperature (*PVT*) data of Anderson *et al.*[6] this corresponds to a pressure of 6.7 kbar. Our experimental evidence gives a value of 5 kbar which is very reasonable agreement, probably well within combined experimental and calculational uncertainties, so we conclude that the calculation of JMS faithfully represents the pressure dependence of the band structure of Cs.

ACKNOWLEDGMENT

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