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THE FERMI MOMENTUM OF ALUMINUM FROM 0 TO 100 KBARS

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In this letter we report the results of a study of the Fermi momentum of aluminum from 0 to 100 kbars carried out at room temperature through the utilization of positron annihilation. We have found that, over this pressure range, the Fermi momentum of aluminum is very well described by the free electron model which predicts that the Fermi momentum, p_F, of a metal is given by

$$p_F = \hbar \left(\frac{3\pi^2 Z}{V} \right)^{1/3}$$

where Z is the number of valence electrons per unit cell in the lattice and V is the volume of the unit cell. Melz[1] has studied the details of a small region of the Fermi surface of aluminum to 7 kbars with the de Hass- van Alphen effect and has shown that his results cannot be explained by the free electron model. We will show that our results for the average momentum at the Fermi surface are not inconsistent with those of Melz.

It is well known that the angular distribution of two quantum annihilation of positrons in alkali metals, alkaline earths, and aluminum is characterized by a central parabola with a tail at large angles.[2] The interpretation of the tail is not yet certain; it has been explained by assuming that the positrons have a large effective

mass or temperature.[3] It could also be due to the population of states above the Fermi level at absolute zero which was found by Luttinger for a system of interacting electrons.[4] However, it is well established that the angle at which the central parabola extrapolates to zero, θ_F, is related to the Fermi momentum by

$$\sin \theta_F = p_F/mc$$

where m is the mass of an electron and c the velocity of light.[5] A study of the variation of θ_F with pressure yields the pressure dependence of the Fermi momentum.

We used 500 μc of Na^{22} in the form of NaCl as the source of positrons. The NaCl was placed between two 1/8" diameter discs of 1/2 mil Nylar. This source was put between two discs of 99.9999% Al which were 5/16" in diameter and 7 mils thick to form a sandwich. The entire sandwich was contained by a 1/2" × 3/32" × 20 mil pyrophyllite ring and placed between 1/2" Bridgman anvils (Fig. 1). 2" NaI detectors located 1 meter from the source with lead slits 1-1/2" high and 20 mils wide were used. The slits were perpendicular to the plane of the sample.

The zero pressure annihilation spectrum of the positron source was obtained initially. It was assumed that pressure changes in the annihilation spectrum of the source were small in comparison to the total pressure change in the spectrum and possible changes in the source spectrum were neglected in analyzing the data. The source contributed roughly one-third of the total annihilation spectrum.

Annihilation spectra were taken at 0, 27, 54, 81, and 108 kbars. The pressure calibration was based on the phase transitions of bismuth in the same geometry using silver chloride as the pressure transmitter.

In going from 0 to 100 kbars, the γ emission rate of the source was found to decrease by 20%; this was not surprising as in Mössbauer studies to 100 kbars the intensities of the Fe^{57} lines have been found to decrease as much as 80% because of deformation of the anvils. The raw data at each pressure were corrected for the pressure and time decrease in count rate. The aluminum spectrum at each pressure was obtained by subtracting the source spectrum from the corrected data assuming that the ratio of total source to total aluminum counts was constant over the pressure range of interest and that the shape of the source spectrum did not vary with pressure. The results for the Fermi momentum at each pressure did not depend greatly on these two assumptions.

At each pressure studied, the central portion of the observed annihilation spectrum of the aluminum was fit with a parabola. In fitting the data with a parabola we neglect the effects due to the finite resolution of the experimental apparatus and the finite width of the source; errors introduced by this assumption are small compared to the statistical uncertainty in the results.

The Fermi momenta at the five pressures examined are plotted in Fig. 2 as a function of pressure. The line in this figure is the Fermi momentum curve predicted by the free electron model assuming three free electrons per atom and using the volume data for aluminum of Bridgman[6] and Jamieson.[7] Figure 2 shows that the Fermi momentum of aluminum is very accurately described by the free electron model within the errors of this experiment.

We have found that the Fermi momentum of aluminum to 100 kbars is very accurately described by the free electron model. This is intui-

tively reasonable as the Fermi surface of aluminum at zero pressure is fairly close to that predicted by the free electron model assuming three electrons per atom. We would not expect the number of free electrons to increase with pressure as this would involve stripping core electrons off the aluminum ions which is energetically unfavorable.

Melz[1] has found in experiments to 7 kbars that the Fermi surface of aluminum does not grow as predicted by the free electron model. Ashcroft[8] showed that the zero pressure Fermi surface of aluminum can be fitted with two Fourier coefficients of a weak pseudo-potential

$$V_{111} = .0179 \text{ Ry}$$

$$V_{200} = .0562 \text{ Ry}$$

in an OPW calculation. Melz obtained the pressure derivatives of the pseudo-potential coefficients based on form factors proposed by Harrison[9]

$$\frac{dV_{111}}{dP} = 1.6 \times 10^{-4} \text{ Ry/kbar}$$

$$\frac{dV_{200}}{dP} = 2.1 \times 10^{-4} \text{ Ry/kbar}$$

He found that these pressure derivatives adequately explained his data.

Using Melz's[1] values of the derivatives of the pseudo-potential coefficients we have calculated the average value of the momentum at the Fermi surface for a number of pressures between 0 and 100 kbars assuming that the coefficients are linear in pressure. The calculated average momenta at the Fermi surface agreed with the values obtained

from the free electron model to within .1% over the entire range. Though the band gaps of aluminum are pressure dependent, very little of the Fermi surface lies close to the zone boundaries. Thus the average momentum at the Fermi surface does not depend strongly on the band gaps so long as the band gaps are small.

This work suggests that positron annihilation studies of Fermi momenta may be an excellent tool for investigating either the pressure dependence of the volume of free electron metals or the high pressure electronic properties of metals for which the pressure dependence of the volume is well established. Positron annihilation would be most useful for studying metals with a large compressibility because of the difficulties involved in getting sufficient accuracy in the data and the weak expected volume dependence of the results.

ACKNOWLEDGMENTS

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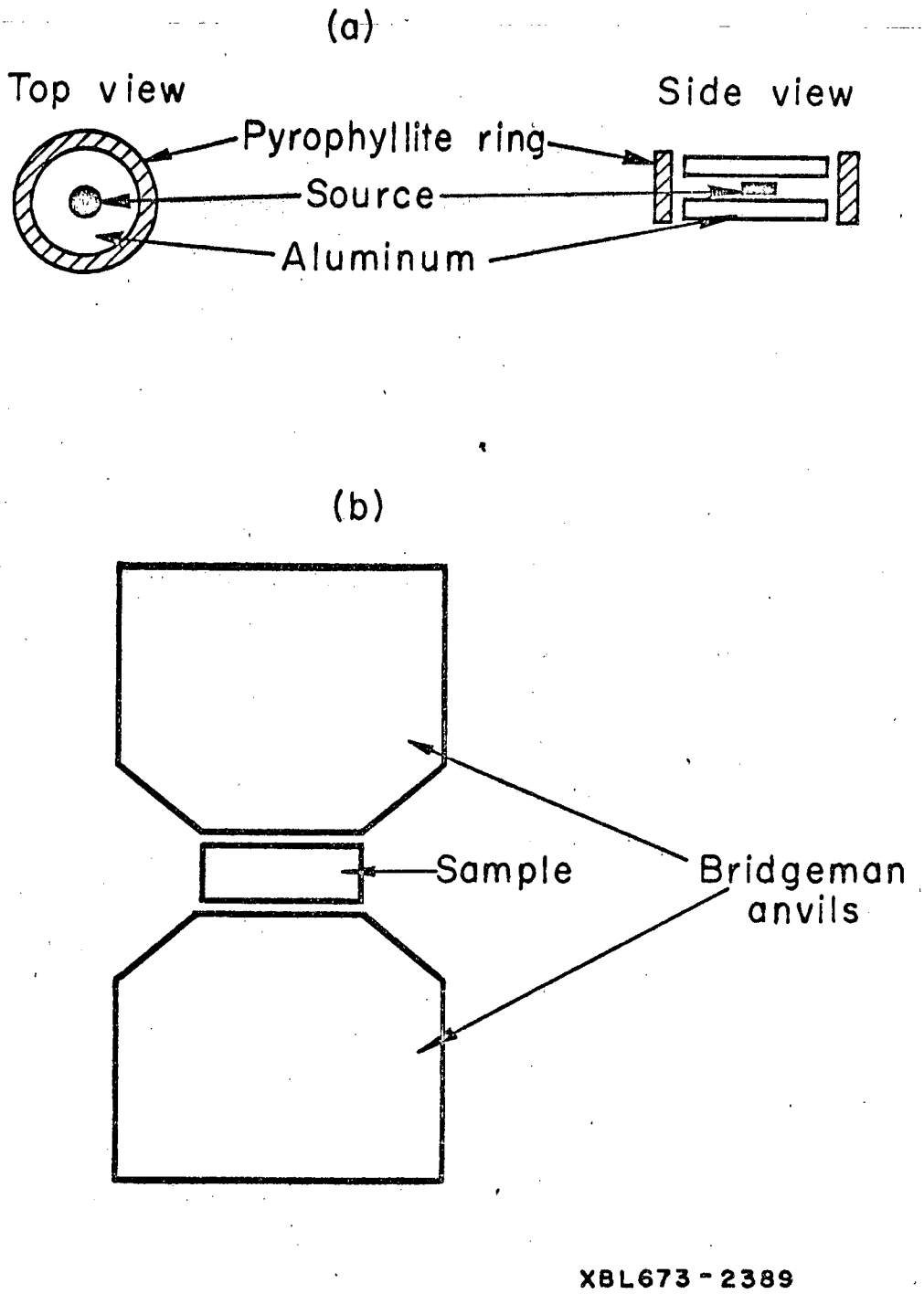
FIGURE CAPTIONS

Fig. 1 (a) The positron source, aluminum, and pyrophyllite containing ring.

(b) The assembled sample sandwich between Bridgman anvils.

Fig. 2 The Fermi momentum of aluminum as a function of pressure. The line is that predicted by the free electron model.



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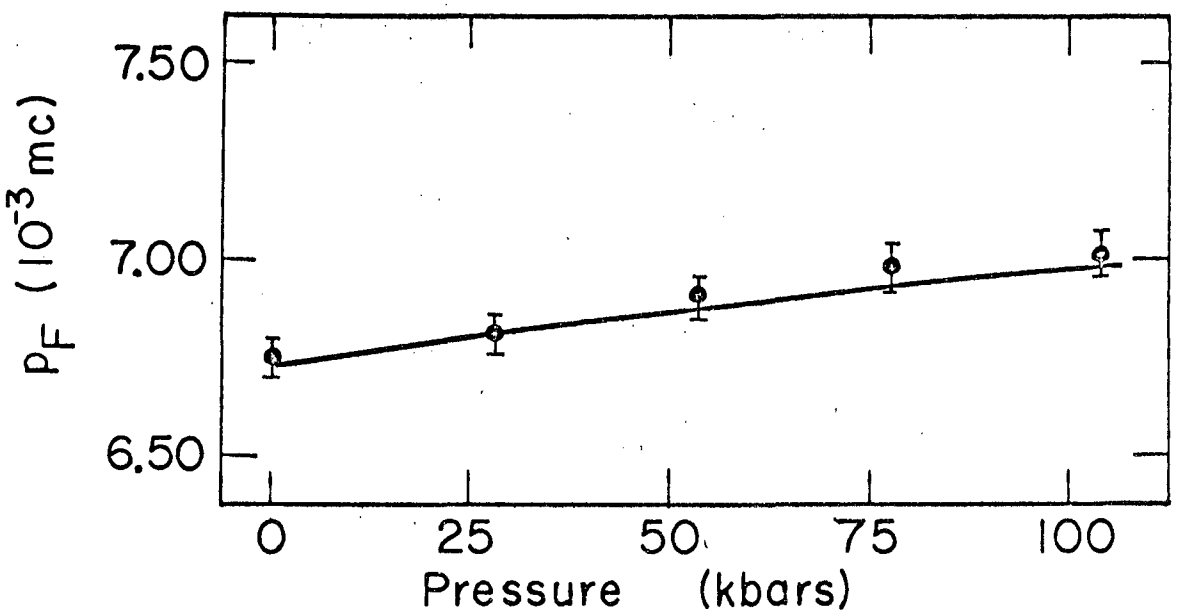

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Fig. 2 The Fermi momentum of aluminum as a function of pressure. The line is that predicted by the free electron model.

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