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Effect of pressure on the Fermi surface and band structure of InBi†

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Measurements have been made of the pressure dependence of a number of cross-sectional areas of the Fermi surface of InBi. A relativistic orthogonalized-plane-wave band calculation has been made as a function of the various parameters which as calculated does not agree with the published experimental Fermi surface. A band model is proposed which accounts for the accepted Fermi surface of InBi. This band picture is found to be consistent with the measured pressure behavior of the Fermi surface and accounts in a qualitative fashion for the anomalies in the pressure dependence of the elastic constants and in the temperature dependence of the NMR.

I. INTRODUCTION

The fact that InBi crystallizes in a tetragonal ($B10$) structure and is a semimetal, as opposed to the usual situation in the III-V one-to-one compounds which are cubic semiconductors, has prompted a good deal of study. Of particular interest is the possible interrelation between the anomalous crystal structure of this compound and its electronic structure and properties. The Fermi surface of this material has a rather long and confusing history. InBi was the first intermetallic compound in which direct Fermi-surface data, via de Haas–van Alphen (dHvA) oscillations in the magnetic susceptibility, were obtained. This initial study by Thorsen and Berlincourt[1] used pulsed-field dHvA techniques. Torque and further pulsed-field studies were subsequently reported by Saito[2] and Beck *et al.*,[3] respectively. A substantial amount of cross-sectional area data was obtained by ultrasonic and field-modulation dHvA techniques by Shapira *et al.*[4] The results of these various measurements were only in qualitative agreement.

Some improvement in reconciling the various Fermi-surface data was achieved by Meyer *et al.*[5] who argued quite convincingly that spurious signals could be obtained in what were thought to be single crystals of InBi from oriented inclusions of In_2Bi and/or In_5Bi_3. These conclusions were based upon detection of superconducting transitions at the literature values for these two compounds[6,7] (InBi is not superconducting above 0.5 K).[7] The resulting interpretation of Meyer *et al.* was that the Fermi surface of InBi consisted of two sets of nearly ellipsoidal sheets with a 2 : 1 volume ratio. Using the notation of Saito[2] and of Shapira *et al.*,[4] the largest sheet is ellipsoidal and oriented along [001] and is associated with the γ oscillations. The β oscillations are associated with a sheet with one-half the volume and are also oriented along [001]. Meyer *et al.* ignored very prominent low-frequency oscillations detected in torque,[2] pulsed-field,[3] and field-modulation[4] studies. The α oscillations correspond to a roughly ellipsoid sheet oriented along [001] with a volume of approximately 10^{-3} that of the γ's. The ζ sheet is roughly five times as large as the α's and is probably an ellipsoid oriented along [100].

The situation with respect to pressure studies of InBi is no less confusing. Bridgman observed a change in slope of resistance versus pressure near 15 kbar.[8] Gordon and Deaton[9] reported that there was no volume discontinuity or phase change in InBi to 30 kbar. This is to be contrasted with complicated phase behavior with pressure on either side of 1 : 1 In to Bi ratio.[9] Rapoport *et al.*[10] recently reported a jump in the resistance with pressure near 19 kbar which they attribute to a first-order crystallographic transition. This interpretation has been rendered suspect by subsequent measurements of the elastic constants of single-crystal InBi by Fritz[11] to pressures of 24 kbar in a hydrostatic medium. This study indicates that there are broad anomalies in several of the acoustic-mode velocities near 14 kbar but that no first-order transitions occur up to 24 kbar.

A final addition to this complex picture are the anomalies in the nuclear-magnetic-resonance spectrum reported by Setty and Mungurwadi.[12] These investigators reported a change in sign of the ^{115}In Knight shift at 230 K and a disappearance of the quadrupolar splitting and thus the electric field gradient at the In site at about 170 K. The change in sign of the Knight shift is similar to the situation in $AuGa_2$ referred to as "the $AuGa_2$ dilemma."[13] Anomalies in $AuGa_2$ but not in its isomorphous cogeners $AuIn_2$ and $AuAl_2$ could be explained by a band-structure picture[14] in which a peak in the density of states of $AuGa_2$, associated with the flat band giving rise to the second band-hole sheet, was sampled with temperatures above

~100 K or pushed through the Fermi level with a pressure of 7 kbar at 1 K. This electron transition[15] picture gives a satisfactory semiquantitative explanation for a large body of NMR, superconducting transition temperature, and Fermi surface data.[16]

The apparent similarity of the temperature anomalies in the NMR data between InBi and $AuGa_2$ and the confusing pressure behavior of InBi prompted us to undertake band-structure and Fermi-surface studies as a function of interatomic spacing. Such studies[17,18] have been useful in unraveling details of the electronic structure previously, and it was hoped that some clarification of the situation in InBi could be achieved.

In Sec. II we describe our band theoretical approach, the experimental procedure is outlined in Sec. III, and we discuss our results in Sec. IV.

II. THEORETICAL

The calculations to be described are all relativistic-orthogonalized-plane-wave calculations.[19] The crystal potential model uses superimposed self-consistent-field relativistic free-atom *potentials*. The Kohn-Sham-Gasper ($\alpha = \frac{2}{3}$) version of the Hartree-Fock-Slater free-electron exchange is employed. The lattice constants used were $c/a = 0.9546$, $a = 5.000$ Å, $u = 0.393$. Since the band structure we find is not consistent with the conclusions of Meyer *et al.*[5] a variety of checks were carried out. Convergence was verified by varying the number of plane waves employed. (Except for these tests the number used was about 200.) The c/a and u parameters were varied independently to rule out undue sensitivity of key features of the band structure to the error we might be making by using room-temperature parameters in the absence of 4-K numbers. Typical changes in the band structure were only 0.02 eV/% with a maximum variation near the Fermi energy ~0.1 eV/%. Several key symmetry points were calculated using $\alpha = 1$ (Slater exchange). Again, there were no drastic changes. If the results were particularly sensitive to details of the potential model, we would expect it to show up as α is varied, as was the case in such materials as Ge,[20] GaP,[21] and Mg_2Si.[22] In the absence of sensitivity to α we also expect that a model based on overlapping free-atom charge densities would not produce very different results.

The point of concern perhaps should be the lower symmetry. As is well known if the potential in a cubic crystal is expanded in spherical harmonics about an atomic site (of cubic symmetry), the second term to enter is $l = 4$ so that the spherical approximation is very good. However, in this tetragonal $B10$ structure, the second term allowed on a Bi site is $l = 1$. We certainly do not make a muffin-tin approximation. The potential used has non-spherical contributions on the Bi site to the extent that the In potentials overlap the Bi site, but the free-atom Bi potential used is required to be spherically symmetric. The error in neglecting an $l = 1$ potential contribution would affect states with different l character on Bi sites differently, but we have no easy measure of how large the effects are.

Since the calculated bands were rather complicated along the Λ and Σ axes, the bands on these axes were also obtained without spin-orbit splittings. The various band crossings allowed by single group symmetry do in fact account straightforwardly for all of the various wiggles observed.

For comparison, we also calculated InBi in the zinc-blende (ZnS) structure which is typical of lighter III-IV compounds. The resulting energy band structure is shown in Fig. 1. It differs from familiar cubic III-V's in that the In s band instead of being above the top of the Bi p complex is almost 2 eV below. This hypothetical structure is a semimetal with band overlap between L and Γ. It might be expected to be unstable against a Jahn-Teller rhombohedral distortion, but that certainly does not explain why the actual structure is tetragonal. The band overlap shown in this ZnS structure is consistent with the trends found in lighter III-V's where the band gap narrows with increasing atomic number.

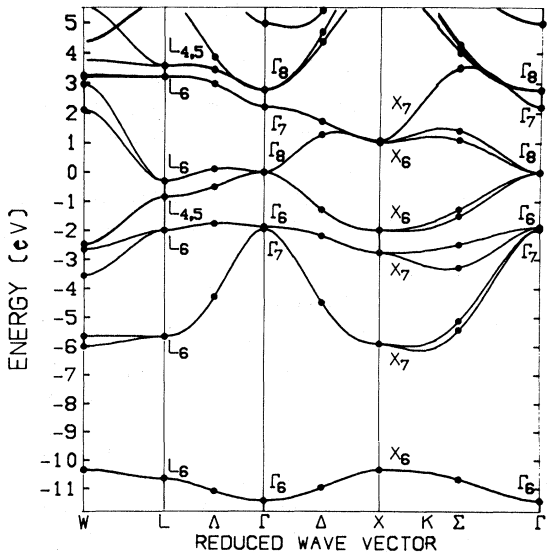

FIG. 1. Calculated energy bands for InBi in the zinc-blende structure. This crystal structure is *not* observed for InBi although it is typical for other III-V materials. The Fermi energy is at -0.1 eV.

III. EXPERIMENTAL

Samples were cut into right-circular cylinders ~2 mm diam × 4 mm in length from an ingot grown from 99.999+% starting material (Johnson and Matthey) by the Bridgman technique. The materials were held ~18 h in the molten state in the cleaned fused silica crucible to ensure homogeneity, and grown at a rate of 5 mm/h. de Haas-van Alphen oscillations were detected using the field-modulation technique in a 55-kG superconducting solenoid usually near 1.1 K. Pressure derivatives were obtained by either the fluid-helium phase-shift method or by measurement of the dHvA frequency as a function of pressures to 4 kbar generated in solid He. In several cases both techniques were found to agree to within experimental uncertainties. These experimental techniques have been discussed in detail in previous reports[18,23] so will not be repeated here.

Because of the findings of Meyer *et al.* indicating InBi crystals could have oriented crystallites of other compounds of Bi and In, we have made some attempts to determine to what extent we are dealing with the one-to-one compound. We have looked for superconducting transitions in our samples near 4.1 or 5.6 K, the literature values for In_5Bi_3 and In_2Bi, respectively.[6,7] Our sensitivity is such that we should be able to detect $\lesssim 0.5\%$ of the sample volume if it were to become superconducting. We find no indication whatsoever for a transition corresponding to In_5Bi_3, but a contribution to the susceptibility was detected over a broad temperature range from 5 to 8 K which might be attributed to ~1% of the sample being In_2Bi.

IV. RESULTS AND DISCUSSION

The results of our pressure studies of the Fermi surface of InBi are summarized in Table I. The orbit nomenclature in Table I and throughout our discussion is that of Shapira *et al.*[4] The pressure derivatives are large and of both positive and negative sign, which is perhaps not too surprising in view of the large anisotropy in the compressiblity and the semimetallic nature of the material. Of most interest and potential, from the standpoint of trying to understand the anomalies in the electronic properties, are the behaviors of the α cross section for $\vec{H}\|[001]$ and of the ζ cross section for $\vec{H}\|[100]$. Figure 2 shows some of our data for the α cross section and the extrapolation to the pressure P_c at which we would expect the cross section to disappear resulting in an electron transition or Lifshitz transition.[15] As mentioned in Sec. I, such transitions have been used to explain anomalies similar to those observed in the NMR properties of InBi.

The important question of the presence of inclusions of In_2Bi and/or In_5Bi_3 raised by Meyers *et al.* must be addressed. This is particularly true with respect to the α and ζ oscillations, which are associated with the smallest sheets reported, but which Meyers *et al.* unfortunately ignored. Our search for superconductivity as mentioned above appears to rule out the occurrence of In_5Bi_3 of sufficient amount to give rise to the extremely large amplitude α oscillations. We cannot completely rule out the possibility of a small amount of the order of 1% In_2Bi on this basis. Anderson and Chung[24] have reported dHvA results on this material. It seems quite likely from their results that the δ oscillations for $\vec{H}\|[001]$, reported by several investigators, do indeed correspond to the strongest oscillations observed in In_2Bi. We have not detected these oscillations in our samples so con-

TABLE I. Pressure derivatives $d\ln F/dp \equiv [F(P) - F(P=0)]/F(P=0)\Delta P$. Orbit nomenclature is that of Ref. 4.

Field direction	Frequency (MG)	Orbit	$d\ln F/dp$ (%/kbar)
[001]	0.137	α	$-8+1$ [a]
			-8.3 ± 0.6 [b]
	3.19	β	$0.3\ (\pm0.1)$ [a]
			$0.3\ (\pm0.1)$ [b]
	7.78	γ	$0.03\ (\pm0.02)$ [a]
[100]	11.08	γ	$0.3\ (\pm0.1)$ [a]
	0.63	ζ	$9\ (\pm3)$ [a]
17 deg. from [110] in (001)	3.8	ϵ	$1\ (\pm0.5)$ [a]

[a] Fluid He phase shift.
[b] Solid He to 4 kbar.

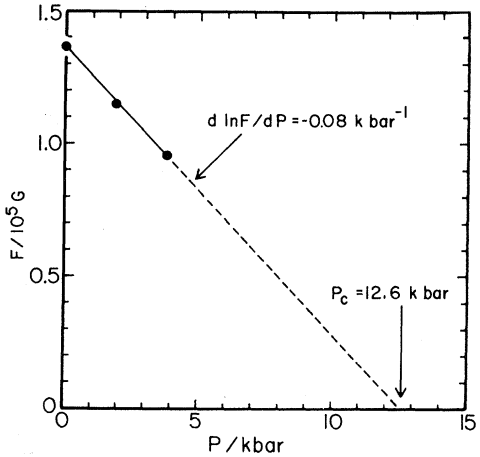

FIG. 2. Pressure dependence of the α frequency (1.38×10^5 G) for $\vec{H}\|[001]$. Data were obtained to ~4 kbar in solid He at ~1.1 K. The dashed curve is a straight-line extrapolation to zero frequency.

clude that we have a negligible amount of In_2Bi in our sample.

A final possibility, particularly in view of the predeliction of this material to crystallize out In-rich compounds, is that one could have effects from free Bi. It is well known that Bi gives rise to very strong dHvA signals and that the cross sections giving rise to these signals are decreasing rapidly in size with pressure.[25] Furthermore, thin films of Bi are known[26] to have T_c values of the order of 6–7 K which could possibly account for the broad "transition" we observe in the 5–8-K range. We do *not* believe that the α's can be attributed to Bi inclusions because the high-amplitude Bi frequencies are much lower in frequency $[(1.5-6.8)\times 10^4 G]$ than that observed for the α's.

The α oscillations were observed by Saito,[2] Beck *et al.*,[3] and by Shapira[4] *et al.* in a variety of samples. The ζ and α frequencies were observed to change in opposite directions with different sample preparations by Shapira *et al.*[4] indicating that they correspond to carriers of opposite signs. We conclude that the α and ζ oscillations are due to InBi.

The calculated band structure for InBi is shown in Fig. 3. The circles are calculated ROPW points and the lines are smooth curves connecting the points which satisfy the compatibility rules. The approximate Fermi energy is indicated at about −0.4 eV. Looking at Fig. 3, we can see that the calculated Fermi surface consists of at least three pieces, an electron surface at Z and hole surfaces at Γ and on the Σ axis. (See Fig. 4 for the location of the various symmetry points in the Brillouin zone for the simple tetragonal lattice.) There are also several other places where the overlap of bands with the Fermi energy is within our calculational uncertainty. This calculated Fermi surface is not compatible with the experimentally known information about the Fermi surface. Meyer *et al.* observe two sheets with a two-to-one volume ratio. InBi is a semimetal and must have the same number of holes and electrons (except for slight differences due to variations from stoichiometry or impurities). Thus unless there is a significant contribution from another piece of Fermi surface, the smaller of the sheets must have a multiplicity of twice that of the larger. Both Γ and Z have multiplicity 1 and the Σ axis has multiplicity 4. The calculated shape of the pieces at Γ and Z are compatible with the β and γ oscillations, respectively, but the multiplicity is wrong to achieve compensation with just these pieces. On the other hand, it is very unlikely that the calculated piece on the Σ axis could be the right size for compensation and have not been observed. (The calculated pieces are ellipsoidal with major axes along [110].) The simple picture[5] of two pieces with a multiplicity ratio of 2 places very tight limitations on the possibilities. It requires either that one piece be on the Λ axis (not centered on Γ or Z) or that the β piece be located on a low-symmetry axis or plane. We rule out X, M, A, and R, since states in any of those locations are degenerate and any Fermi surface associated with them must in fact consist of nested pieces. The only axis with multiplicity of 2 is the Λ axis. Since the multiplicity associated with Γ and Z is one and with various symmetry axes is 4($\Gamma-X$, $\Gamma-M$, $Z-R$, and $X-R$, for example),

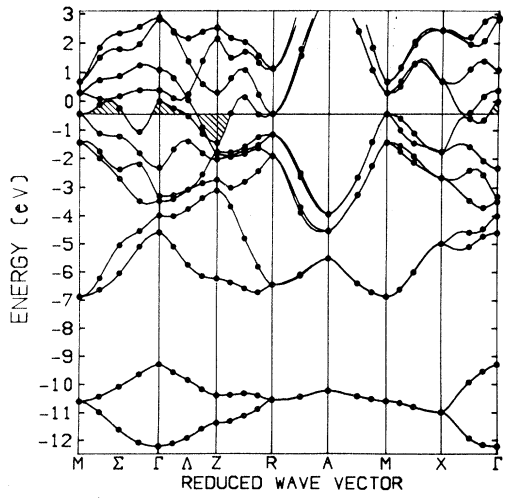

FIG. 3. Calculated energy band structure of InBi. Approximate Fermi energy is −0.4 eV. The points shown are calculated relativistic orthogonalized-plane-wave results. The lines are smooth curves through the points. This band structure leads to a Fermi surface that is incompatible with experiment (see text).

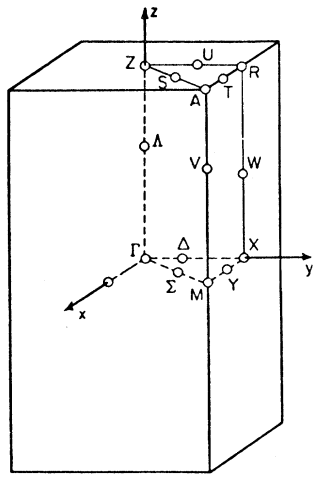

FIG. 4. Brillouin zone for the simple tetragonal lattice.

a 2 to 1 ratio or a 4 to 2 ratio with pieces at any of these locations requires one piece be a Λ axis piece. The Γ-A and Γ-R axes, as well as planes containing these axes, do have multiplicity 8 so that a piece located at one of these relatively low-symmetry locations could be part of an 8 to 4 ratio. However, it would be surprising if such a low-symmetry piece were the source of the β oscillations which Meyer *et al.*[5] found to have constant frequency in the (001) plane. From the band-structure calculation, we are most confident that the electron piece at Z exists. It would require an adjustment of at least 1.5 eV to get rid of this piece. This seems outside of uncertainties involved. Also, there seems little likelihood that a [110] oriented ellipsoid large enough to complete compensation would not have been observed. So we will treat the Σ axis piece as another that comes within uncertainty of the Fermi energy.

If we assume that the electron piece at Z is correct, we can consider two possible situations which could resolve our disagreement with the experimental result. We will assume the electron piece corresponds to the γ oscillation and associate the β oscillation with the holes. Then one possibility is that there is some third piece of Fermi surface that together with the β and γ sheets satisfies compensation. The α and ζ volumes are small enough to be neglected in this consideration. A possible candidate might be the ϵ oscillations reported by several investigators and which we have also observed. Meyer *et al.*[5] argued convincingly against this on the basis of the relative amplitudes of the ϵ (and δ) to the β and γ oscillations in different samples. The arguments of Meyer *et al.* concerning the ϵ and δ oscillations and their assignment to inclusions of In_2Bi and/or In_5Bi_3 are compelling, particularly in view of the good agreement for the δ's with the In_2Bi results of Anderson and Chung.[24]

The second possibility (still assuming γ is at Z and that the Σ axis intersection is not involved) is that the β's are not at Γ but are associated with another intersection of the bands with the Fermi level. Since the piece at Z is an electron piece, we seek a hole piece. In Fig. 3 we note several regions of k space where bands come within calculational uncertainty of the Fermi energy. However, there is only one place to put the β's and achieve compensation on the Λ axis. Let us examine what would be required to place the hole piece on the Λ axis and hence satisfy the simple picture of Meyer *et al.* The relevant band structure results from including interactions (including spin orbit) among three free-electron bands—a pair of crossing Λ_1's whose large repulsion and hence splitting is evident in Fig. 3 and a Λ_5 which under spin-orbit interaction splits into one band which does not interact with the Λ_1's and one that does. The multiple-band crossings (of the free-electron bands) within uncertainty of the Fermi energy means that relatively minor band shifts can alter the shapes of the resulting bands significantly. All states in this region of k and energy have Bi p character but only some (Λ_1 derived) have Bi s. Perhaps the error in the s bands with respect to the p bands introduced by using a spherical Bi potential in the calculation is significant.

Having assigned the β's to the Λ axis, to complete the picture we must locate the α and ζ pieces. We assign the ζ to the intersection of the band at R with the Fermi level. We choose this intersection rather than one of the others because it probably has the right shape and it has a high density of In s-like states as will be discussed later. (The Δ axis intersection would be almost as good a choice—right orientation and pressure dependence, but not as much In-s character.)

Having made the ζ's electrons, we want the α's to be holes. The Σ axis piece is unacceptable because of orientation. The point M is unacceptable based on both shape and pressure derivatives. (The band at M moves up with pressure by far the fastest of any near Fermi energy feature.) We thus fall back to further complication of the Λ axis.

The α's need to be located at Γ. Thus the Λ axis band shown in Fig. 3 as part of the piece at Γ must develop a kink so that it crosses the Fermi energy three times instead of once between Z and Γ. The proposed band model is shown schematically in Fig. 5.

This band picture has several attractive features: (i) This is virtually the only place the β's can be and achieve compensation. This then agrees with the conclusions of Meyer *et al.*[5] concerning the δ and ϵ oscillations whose amplitudes

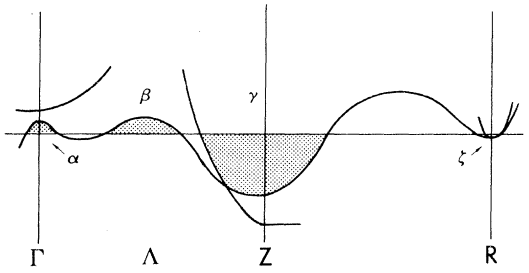

FIG. 5. Schematic energy band model of InBi. Bands not shown are assumed to not cross the Fermi energy. The effect of pressure is to increase the overlap of the bands at Λ and Z but with a net shift of the center of gravity and therefore E_F to higher energy. This decreases the overlap at Γ and increases it at R.

seem to vary enormously relative to the γ's and β's in different samples. (ii) This assignment makes the signs of the α and ζ carriers opposite (the former are holes, the latter electrons). This agrees with the finding of Shapira *et al.*[4] that these two sheets change size in opposite directions between different sample preparations. This is presumably due to a shift in the Fermi level due to impurities. (iii) The orientation dependence of the pockets of Fermi surface is qualitatively correct for each of the sheets.

Now we will test the ability of this picture to account for our pressure data. Because of the large anisotropy in the linear compressibilities[27] (the compressibility in the c direction is ~10 times that in the basal plane), the main effect of hydrostatic pressure is to decrease c/a. The effect of pressure on the atomic positional parameter u is as yet not measured, but our calculations showed that the Fermi surface was relatively insensitive to variations of this parameter.

The bands along Λ near the Fermi energy were found to move upward in energy with respect to the rest of the bands with decreasing c/a (i.e., with pressure). This means that in order to maintain compensation, the Fermi level must rise also. The bottom of the electron band at Z goes down, hence the overlap is calculated to increase. The fractional change in the α's and ζ's due to the change in Fermi level will be larger due to their smaller size. The agreement of our model with the pressure results is excellent at least in a qualitative sense. The next question is whether this model can explain the anomalies reported as a function of temperature and pressure for InBi.

Fritz has recently published[11] studies of the pressure dependence of the elastic constants of InBi at room temperature which show anomalies at pressures of ~14 kbar. It is very tempting to attribute this behavior to the disappearance of the sheet of Fermi surface associated with the α's which should occur near 12 kbar (see Fig. 2). At room temperature we would expect the effect related to this electron transition to begin at a somewhat lower pressure and to be smeared out.

At first glance one might expect to be able to attribute the anomalous behavior of the Knight shift to thermal sampling of this same sheet in direct analogy to what was done in $AuGa_2$. Closer inspection, however, indicates that this line of reasoning is not fruitful. We require an *increase* of s character as the temperature is raised while our model would indicate that the sheet was decreasing in size since c/a is decreasing.[12] While this might be overcompensated by the thermal sampling as it is in $AuGa_2$, then the Knight shift would tend (as it does in $AuGa_2$) to saturate as the temperature is raised rather than continuing to rise. Furthermore, the bands at Γ are not particularly rich in In s character. On the other hand, the band at R is predominantly In s-like and furthermore is found to be anomalously flat so that in spite of its small size this sheet might be expected to give rise to a rather large In s density of states. This sheet will increase in overlap with the Fermi level as the temperature increases (c/a decreases) so this appears to be an attractive explanation for the Knight shift anomaly.

The situation with respect to the disappearance of the NQR and thus the electric field gradient is much less clear. Setty and Munguruadi[12] attempt to correlate this effect with the quantity $(1-c/a)$. This is, however, incorrect, as c/a equal to 1 in this structure does *not* result in a cubic environment even locally for the In nucleus, and furthermore the u parameter must be considered. (The cubic CsCl structure is obtained for $c/a=\frac{1}{2}\sqrt{2}$ and $u=\frac{1}{2}$.) The situation when $4u\ c/a=\sqrt{2}$ will result in a tetrahedral environment of *nearest neighbors* Bi. It is not apparent that this requirement is met either as a function of temperature. It is more likely that a detailed balance between conduction electron and point-charge effects gives rise to these effects and that our picture is not sufficiently detailed to address this feature.

V. SUMMARY

We have presented measurements of Fermi-surface cross sections and band calculations as a function of pressure or interatomic spacing. The first-cut band picture does not agree with the presently accepted experimental Fermi surface. We have suggested a tentative model based on a modified band picture in which bands are shifted with respect to the Fermi-level small amounts within the calculational uncertainty. This modified band picture accounts nicely for the experimental Fermi surface with respect to compensation of holes and electrons and the general orientation features. This picture gives a correct account of the pressure behavior of the four observed sheets of the Fermi surface as far as the signs and rough relative magnitudes of the pressure derivatives are concerned. We can account in a qualitative manner for the anomalies in the elastic properties by associating these effects with an electron transition which will occur near 12 kbar at 4 K as the α sheet of the Fermi surface disappears.

The anomalies in the In NMR properties can reasonably be assigned to the movement with c/a of an electron pocket at the point R in the Brillouin zone which our calculations indicate possesses a substantial amount of In s character.

We conclude that the band picture which we have developed is capable of explaining a good deal of the available Fermi surface data and can account for a number of the anomalous pressure and temperature dependent phenomena reported for InBi.

It must be emphasized that the picture we present while plausible, may not be unique. InBi is a semimetal so that much of the overlap of the bands at the Fermi level is near the calculational uncertainties involved. In point of fact, most band descriptions for semimetals involve parametrized band pictures. Further detailed experimental work will probably be required to better ascertain the utility of our model.

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