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# Calculation of the Soft X-Ray *K*-Emission and Absorption Spectra of Metallic Li

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To test the possibility that the premature peaking of the Li *K* emission spectrum might arise from one-electron band effects, and alternatively, to provide a starting point for various screening model estimates, we have calculated the one-electron emission and absorption densities of metallic Li by the augmented-plane-wave method. Eigenenergies and wave functions were evaluated at many general points in the Brillouin zone as well as symmetry points. No early peaking was found in the emission density. We note, however, that by applying Overhauser's estimate of inner level broadening by the phonon field to the one-electron densities, a good fit to the experimental data can be obtained. At present, there is no basis for claiming uniqueness for this agreement.

## I. INTRODUCTION

THE soft x-ray emission spectrum of metallic Li has attracted much theoretical attention, because of its premature peak about 0.6 eV below the 50% point of the high-energy emission edge, as shown in Fig. 1.[1] While band theory has had some noteworthy successes in predicting properties of Li metal (the Knight shift,[2] for example, and the cohesive energy,[3] among others[4]), the soft x-ray emission band profile has remained a puzzle. Band theoretical calculations at points of high symmetry[5] indicate that the Fermi energy lies below the energy of zone face contact, and that the $p$ admixture of the eigenfunctions (only this component is sampled by the $s$-like inner level) increases monotonically through the filled part of the band.[6] Thus, one expects the $K$ spectrum to peak within $kT$ (0.03 eV) of the emission edge, not well below it.

In view of the agreement between band theory and experiment cited above, it is reasonable to look for an explanation peculiar to the x-ray emission process itself. With this in mind, a number of authors[7–9] have invoked collective effects, the general argument being that screening of the inner vacancy produces a resonant enhancement of the transition probability below the Fermi level. In more recent calculations of the soft x-ray transition probability of the interacting electron gas, there is some apparent division of opinion. The work of Hedin[10] and Rystephanick and Carbotte[11]

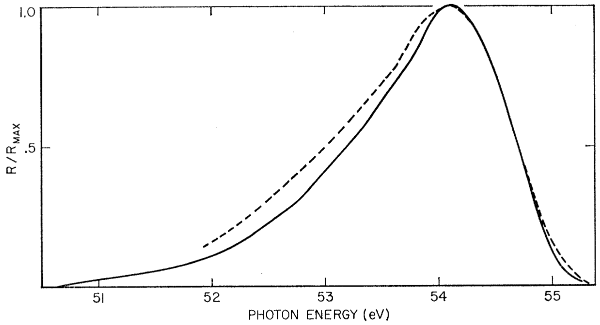

FIG. 1. The measured Li emission profile of Tomboulian and Bedo (Ref. 1), solid curve, compared with profile calculated in this work, dashed curve.

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[1] D. H. Tomboulian and D. E. Bedo, Phys. Rev. **109**, 35 (1958).

[2] R. A. Moore and S. H. Vosko, Can. J. Phys. **46**, 1425 (1968).

[3] W. E. Rudge, Massachusetts Institute of Technology Quarterly Progress Report No. 69, p. 53, 1968 (unpublished); Phys. Rev. **181**, 1024 (1969).

[4] F. S. Ham, Phys. Rev. **128**, 2524 (1962).

[5] F. S. Ham, Phys. Rev. **128**, 82 (1962).

[6] This point is supported by the experimental Knight-shift results. See Ref. 2.

[7] H. Jones and B. Schiff, Proc. Phys. Soc. (London) **A67**, 217 (1954).

[8] D. A. Goodings, Proc. Phys. Soc. (London) **86**, 75 (1965).

[9] F. K. Allotey Phys. Rev. **157**, 467 (1967).

[10] L. Hedin, Solid State Commun. **5**, 451 (1967); and in *Proceedings of the Glasgow Conference on Soft X-Ray Spectrometry and the Band Structure of Metals and Alloys*, edited by D. J. Fabian (Academic Press Inc., New York, 1968).

[11] R. G. Rystephanik and J. P. Carbotte, Phys. Rev. **166**, 607 (1968).

indicates a degree of energy-dependent enhancement, but no obvious peaking. However, solutions of the appropriate integral equations have not yet been obtained. Nozières and de Dominicis,[12] on the other hand, predict that near the Fermi energy, the spectral intensity may be either enhanced or diminished, depending on the phase shifts of the Bloch functions near the vacancy and the orbital symmetry of the vacancy. Ausman and Glick[13] have estimated the phase shifts for a Li $K$ hole and from them predict a diminution of intensity near the Fermi level. The effect is qualitatively correct, but detailed numerical comparison between experimental and theoretical emission and absorption profiles have not been made. Pursuing another possibility, Stott and March[14] argued from calculations based on estimates of the Li conduction-band momentum eigenfunction that the one-electron transition probability itself peaks below the Fermi energy. A more exact calculation of the $K$ transition probability in the one-electron approximation is therefore desirable, both as a check of the latter possibility, and as an essential starting point for estimates of the former sort, if numerical comparison with experiment is sought.

Reported here are APW (augmented-plane-wave) calculations for the first band of metallic Li. A fine $k$-space mesh, including many general points in the zone, has been used. Wave functions were extracted, and the one-electron $K$ emission and absorption transition probabilities, as well as the state density, evaluated. No evidence of transition probability peaking below $E_F$ was found. Because of the broad width of the observed emission and absorption edges, and their strong overlap, the strength of various broadening mechanisms and their effects on the one-electron transition densities were estimated. It was found that the observed emission and absorption spectra can be fitted fairly well by folding a phonon broadened inner level smearing function into the calculated transition densities. The theoretical expression for this broadening function, due to Overhauser,[15] has not yet been subjected to systematic experimental test. In view of this, the numerical success achieved cannot be regarded as unique.

## II. BAND CALCULATIONS

Slater's APW method[16,17] was employed to estimate eigenvalues and eigenfunctions for the first band of metallic Li over a cubic mesh of 506 points in 1/48 of the bcc Brillouin zone, including 204 general points. The muffin-tin form of the Wigner-Seitz potential tabulated by Kohn and Rostoker[18] was used, with their assumed lattice constant, $a=6.5183$ a.u. Eight orbital angular momenta and 27 reciprocal-lattice vectors were employed in the basis set. Calculations were done for all first band energies $\leq -4$ eV (absolute energy), a value above the energy of zone fact contact, permitting estimates of the $K$ absorption discontinuity to be made. Eigenvalues were converged to less than $10^{-3}$ eV.

To estimate the $K$-emission density $R_K(E)$ (proportional to the spontaneous photon flux/unit energy/sr), histograms of bar width $\Delta E$ were constructed, $R_K$ being assigned values

$$R_K(E_i)=\sum_{\mathbf{k}} w(\mathbf{k})\left(\frac{E(\mathbf{k})-E_c}{E(\Gamma_1)-E_c}\right)^3 \times|\langle\psi(\mathbf{k},E)|\mathbf{r}|\psi_{1S}\rangle|^2 g(E,\mathbf{k})$$

at each mesh point $E_i<E_F$. $E(\Gamma_1)$ is the energy at the bottom of the band, and $E_c$ is the core level energy. The quantity $g(E,\mathbf{k})$ is 1 if

$$E_i-\tfrac{1}{2}\Delta E\leq E(\mathbf{k})<E_i+\tfrac{1}{2}\Delta E\,,$$

and zero otherwise. The weight function is

$$w(\mathbf{k})=2n(\mathbf{k})d(E,\mathbf{k})/\sum_{\mathbf{k}} n(\mathbf{k})\,,$$

where $n(\mathbf{k})$ is the number of points in the star of $\mathbf{k}$, $d$ is the degeneracy of the state with energy $E(\mathbf{k})$, and 2 is the spin degeneracy. The calculated density curves of Fig. 2 were constructed by averaging 10 histograms, with bar width 0.2 eV, and origin successively shifted by 0.02 eV. For the absorption density $A_K(E)$ the exponent in the energy factor is reduced to 1, and the range of energy is $E_i>E_F$. The state density is gotten by summing $w(\mathbf{k})g(E)$ alone.[19]

A one-center estimate of the matrix element was made for each $E(\mathbf{k})$ from the normalized band wave function and the Li $1s$ orbital tabulated by Herman and Skillman.[20] A one-center approximation should be quite good for the x-ray emission process, in view of the negligible overlap of inner shell electron wave functions and consequent near infinite hole effective mass. The

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[12] P. Nozières and C. T. de Dominicis, Phys. Rev. **178**, 1097 (1969).

[13] G. A. Ausman and A. J. Glick, Phys. Rev. **183**, 687 (1969).

[14] M. J. Stott and N. H. March, Phys. Letters **23**, 408 (1968); and in *Proceedings of the Glasgow Conference on Soft X-Ray Spectrometry and the Band Structure of Metals and Alloys*, edited by D. J. Fabian (Academic Press Inc., New York, 1968). N. H. March (private communication) states that a good bit of their information on the momentum eigenfunction is based on analysis of the emission spectrum. If their point of view is correct, and we must stress that it is a logical alternative to the viewpoint taken here, then the Wigner-Seitz potential is incorrect. Calculations of other physical properties of Li metal from their momentum eigenfunction have not yet been made. Comparison of such predictions with those cited in Refs. 2–4 should shed light on this issue.

[15] A. W. Overhauser (private communication). For a discussion, see Sec. III.

[16] J. C. Slater, Phys. Rev. **51**, 151 (1937).

[17] T. Loucks, *Augmented Plane Wave Method* (W. A. Benjamin, Inc., New York, 1967).

[18] W. Kohn and N. Rostoker, Phys. Rev. **94**, 1111 (1954).

[19] An earlier calculation over a 64-point mesh in 1/48 of the zone displayed large fluctuations in $R_K$ and the state density, and incidentally, a large peak below $E_F$ which reproduced experiment. These have largely been smoothed out with the fine mesh, but some statistical fluctuations evidently remain.

[20] F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Inc., Englewood Cliffs, N. J., 1963).

integrals were carried out only over the APW sphere (radius equal $\frac{1}{2}$ the nearest-neighbor distance). The error resulting from this truncation was checked at a number of points by approximating the integral over the region between the APW sphere and the Wigner-Seitz cell boundary with an integral over a spherical shell bounded by the APW and Wigner-Seitz spheres (the latter a sphere centered on the Wigner-Seitz cell, with the same volume). The maximum error indicated is no more than 3%, a result to be expected from the fact that the calculations show the average probability of a band electron being found outside the APW sphere is 0.32, while for a 1*s* atomic electron it is 0.04.

Solutions of the Wigner-Seitz potential have been carried out by many workers and by many different techniques, generally at points of high symmetry, or including at most a few general points. The results for $E(\mathbf{k})$ at symmetry points in the present work are in excellent agreement with those of Ham[5] for the same lattice constant. The state density of Li calculated here agrees with his, justifying his interpolation procedure. More recently, Rudge[3] has constructed self-consistent potentials for metallic Li, using the Slater local exchange potential, with coefficients 1 and $\frac{2}{3}$. His bands are some what narrower than those calculated from the Wigner-Seitz potential, and lie slightly higher in absolute energy. No large differences are seen, however; wave-function symmetries are the same throughout the first band, and the Fermi surface resists contact with the zone face. The Wigner-Seitz potential, therefore, appears adequate for the purposes of this work.

## III. COMPARISON WITH EXPERIMENT

The calculated emission density and mean transition probability (obtained by dividing the emission density by the state density) shown in Fig. 2 display no sign of early peaking. But inspection of the experimental emission edge of Fig. 1, and the absorption edge determined by Skinner and Johnston,[21] shown in Fig. 3, shows that they are both quite broad, and overlap strongly. Because of this, it seems worthwhile to assess the strength of various broadening mechanisms and their effect on the one-electron emission and transition densities. The following conclusions were drawn. The Fermi distribution function has far too narrow an edge. The radiative lifetime of the $K$-shell vacancy was estimated from first-order perturbation theory by integrating over the $K$ transition probability calculated in this work, and found to be about $10^{-8}$ sec, resulting in a radiative $K$ level width of about $10^{-6}$ eV. The effect of the natural isotopic abundance was estimated, and found to result in a spread of less than $10^{-3}$ eV. This work, and that of Rudge,[3] indicates that overlap broadening of the $K$ state is negligible. Phonon broadening of the conduction-band states should also be negligible.[22]

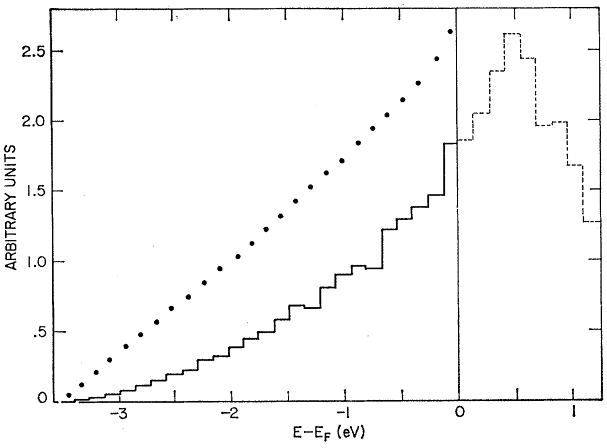

FIG. 2. The calculated soft x-ray transition densities: (a) emission, solid lines, $E<E_F$; (b) absorption, dashed lines, $E>E_F$; (c) dotted curve, calculated mean of the emission transition probability, obtained by dividing the emission-transition density by the state density. Ordinate scale in arbitrary units.

Tomboulian and Bedo[1] noted that a good fit to their emission spectrum could be obtained by folding a Gaussian smearing function of half-width at half-maximum of 0.35 eV into the $E^{3/2}$ profile expected from simple free-electron theory. This Gaussian edge shape suggests that phonon broadening of the inner level plays a role here. We therefore estimate the strength of such broadening, and its effect on absorption as well as the emission spectrum.

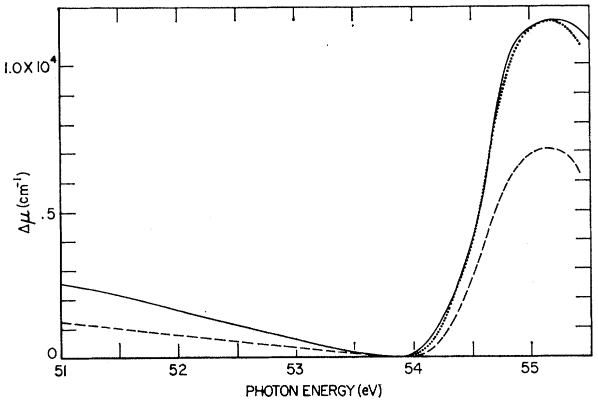

FIG. 3. The Li $K$-absorption profile; $\Delta\mu$ is the change in linear absorption coefficient $\mu$ across the edge; solid line, experiment, after Skinner and Johnston (Ref. 21); dashed curve, calculated in this work; dotted curve, calculated edge scaled to match measured curve at peak.

Overhauser[23] estimates the shift in energy of a

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[21] H. W. B. Skinner and J. E. Johnston, Proc. Roy. Soc. (London) **A161**, 420 (1937).

[22] A. Radkowsky, Phys. Rev. **73**, 749 (1948).

[23] A. W. Overhauser (private communication). If we assume the metal lattice to be a Debye solid, then we can write

$$\langle|eV|^2\rangle^{1/2}=(E_F{}^2k\Theta/6Mu^2)^{1/2}\times\left(1+8(T/\Theta)^3\int_0^{\Theta/T}dx\,x^3(e^x-1)^{-1}\right)^{1/2},$$

where $\Theta$ is the Debye temperature. The temperature-dependent term can be fitted quite well by $[1+(8T/3\Theta)^2]^{1/4}$. This latter expression differs from that quoted by Parratt [L. G. Parratt, Rev. Mod. Phys. **31**, 619 (1959)] only in the fractional exponent. The value $\frac{1}{8}$ given there is presumably a typographical error.

localized charge at a point $R$ in a simple metal as the dynamic change in potential energy, equal to the product of the deformation potential and the local, thermally fluctuating dilation:

$$eV(\mathbf{r})=\tfrac{2}{3}E_F\times i\sum_{\mathbf{q}}(\hbar q^2/2\rho\omega_q\Omega)^{1/2}a_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{R}}-a_{\mathbf{q}}^{\dagger}e^{-i\mathbf{q}\cdot\mathbf{R}},$$

where $a_{\mathbf{q}}^{\dagger}$ and $a_{\mathbf{q}}$ are the usual creation and annihilation operators, $\Omega$ is the volume of the sample, $\rho$ is the density, and $E_F$ is the Fermi energy. The sum is over all longitudinal phonon modes. Accordingly,

$$\langle|eV|^2\rangle=\sum_{\mathbf{q}}(4E_F{}^2/18\rho\Omega\omega_q)\langle(a_{\mathbf{q}}a_{\mathbf{q}}^{\dagger}+a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}})\rangle,$$

where only the diagonal terms of a double sum are kept, because terms like $e^{(i\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}}$ sum to zero. Also, terms with two creation or two annihilation operators have zero expectation value. Now $(a_{\mathbf{q}}a_{\mathbf{q}}^{\dagger}+a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}})=2n_{\mathbf{q}}+1$. Since the distribution of the dilation is Gaussian, so is the energy band smear, with half-width at half-maximum

$$\mathcal{W}=(2\ln 2)^{1/2}\langle|eV|^2\rangle=(8\ln 2E_F{}^2kT/9Mu^2)^{1/2},$$

where $M$ is the ionic mass, $k$ is Boltzman's constant, $u$ is the longitudinal sound velocity, and the following approximations have been made: $\omega_q\cong uq$, and $(\langle n_q\rangle+\frac{1}{2})\cong kT/h\omega q$. This expression yields a value of $\mathcal{W}=0.37$ eV for Li at 300 K.

In Fig. 3, we have plotted the result of folding a Gaussian with $\mathcal{W}=0.3$ eV with the calculated absorption density. The photon energy scale for the calculated profile was established by matching the calculated and observed peaks in energy. The valence-band absorption background was estimated from Walter's[24] semiempirical formula. The calculated change in the linear absorption coefficient across the edge is $0.72\times10^4$ cm$^{-1}$, while the measured value is $1.15\times10^4$ cm$^{-1}$. Also shown is the calculated edge scaled to match the measured edge at the peak. The edge shape agreement is rather good, and we shall comment on the amplitude discrepancy in the next section.

If this approach is valid, an appropriate Gaussian smearing function should be folded into the $K$-emission density. The experimental Li profile of Fig. 1 was taken at $T=435$°K.[25] Assuming the temperature dependence of the expression for $\mathcal{W}$ to be correct yields an estimate of $\mathcal{W}=0.42$ at 435°K. The appropriately folded result is compared with the experimental result in Fig. 1. Agreement in the region of the peak and high-energy edge is quite good, but between the peak and the bottom of the band, the calculated curve lies somewhat above the experimental profile. The calculated emission curve is not arbitrarily positioned in Fig. 3. The photon energy scale assignment made in fitting the absorption curve was used. Thus, the calculation accurately predicts the observed separation in energy of the emission and absorption peaks.

The Tomboulian-Bedo result was selected for this comparison because we judge it to be undistorted by self-absorption. While not reporting them here, we have made estimates of the effects of self-absorption, as determined by x-ray take-off angle and the energy and angle of incidence of the exciting electron beam, on the Li emission profile. In particular, the "metallic" high-energy edge reported by Crisp and Williams[26] (at 4.0-keV excitation potential, electron beam impinging at 90° to the target surface with take-off angle about 15°) appears to be the result of self-absorption. This consideration points up the danger of trying to assess the strength of broadening mechanisms from emission spectra, and, unfortunately, the impossibility of investigating the validity of Overhauser's phonon broadening expression from presently available soft x-ray data.

At room temperature, the Overhauser expression predicts inner level half-widths of 0.37, 0.25, and 0.16 eV for Li, Na, and K, respectively. The observed emission edges of Na[27] $L_{2,3}$ and K[28] $M_{2,3}$ are not only narrower than that of Li, but much narrower than these estimates suggest. However, as noted above, self-absorption can sharpen an observed emission edge appreciably. A careful search of the literature for pertinent alkali metal data, to which the theory should be most applicable, showed that, save for Li, no emission spectrum which could be safely judged free of self-absorption, and no absorption data at all, are available. We must also bear in mind that Overhauser's expression is a first estimate. A more exact treatment may, for instance, show dependence on the orbital character and/or range of the inner level vacancy. It is also worth noting that comparison of measured and calculated low-temperature specific heats of Li and Na indicate that the phonon enhancement for Li is twice as large as for Na. According to Martin,[29] the experimental specific-heat ratio $C/C_0$ for Li exceeds the band-theory estimate by 0.24, while for Na, the excess is 0.12. This is at least suggestive that the phonon field may play a stronger role in inner level broadening in Li than in Na.

## IV. DISCUSSION AND CONCLUSIONS

For reasons discussed above, the premature peak in the $K$-emission spectrum of Li metal is *not* accountable on the basis of one-electron transition probabilities calculated from currently available crystal potentials,

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[24] B. Walter, Fortsch. Roentgen **35**, 1308 (1927), quoted by A. H. Compton and S. K. Allison, *X-Rays in Theory and Experiment* (D. Van Nostrand, Inc., New York, 1935), p. 537.

[25] Some adjustment of the photon energy scale of the Tomboulian-Bedo spectral profile has been made. Comparison of published data by Skinner (Ref. 27) and Tomboulian [Ref. 1, and also W. M. Cady and D. H. Tomboulian, Phys. Rev. **59**, 381 (1941)] shows Tomboulian's photon energy values to be consistently about 0.1 eV lower than Skinner's. Accordingly, the Bedo-Tomboulian curve has been shifted up in energy by 0.1 eV.

[26] R. S. Crisp and S. E. Williams, Phil. Mag. **5**, 525 (1960).

[27] H. W. B. Skinner, Phil. Trans. Roy. Soc. (London) **A239**, 95 (1940).

[28] R. S. Crisp, Phil. Mag. **5**, 1161 (1960).

[29] D. L. Martin, Phys. Rev. **124**, 438 (1961).

yet such potentials yield fair estimates of other physical properties of this material. This situation has naturally led to attempts to explain the phenomenon in terms of the nature of the x-ray emission process itself, screening models being particularly attractive in this regard.

In the hope of clarifying the situation to some degree, we have estimated the effects of various spectral broadening mechanisms on the one-electron emission and absorption densities, and found that reasonable agreement with experiment can be achieved by folding a phonon broadened inner level smearing function into these transition densities. In particular, the broad, overlapping emission and absorption edges are fitted well, and the observed energy separation between the emission and first absorption peaks is correctly predicted. Such agreement strongly suggests that phonon broadening plays an important role in the Li spectra. However, presently available soft x-ray data shed no reliable light on the general validity of the theoretical expression for the phonon broadening function. While the Ausman-Glick estimate of the Nozières–de Dominicis effect on the Li $K$-emission spectrum yields a prepeaking, no detailed numerical comparison of theory and experiment has yet been made. It is perhaps worth noting that the residual discrepancies between the present calculations and experiment suggest energy-dependent enhancement of the spectra, increasing with electron energy. To see this, note that the measured absorption edge jump significantly exceeds the calculated jump. Also, if such an enhancement factor were applied to the calculated emission spectrum, and the two curves compared by normalizing at peak intensity, the enhanced curve would appear narrower than the unenhanced.

## ACKNOWLEDGMENTS

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# Galvanomagnetic Studies of Sn-Doped Bi. II. Negative Fermi Energies

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Studies of the Shubnikov–de Haas effect and the Hall effect in single crystals of bismuth doped with tin are extended to excess hole concentration beyond $2\times10^{18}$ cm$^{-3}$, the upper limit achieved in earlier reported work. For dopings greater than about $3\times10^{18}$ cm$^{-3}$, the Fermi level lies below the bottom of the $L$-point conduction band, so that the Fermi energy measured from this band edge is negative. The passage of the Fermi level into the forbidden gap at the $L$ point is accompanied by the disappearance of electron quantum oscillations and by a decrease by two orders of magnitude in the magnetoresistance at 4.2°K. At about $5\times10^{18}$ excess holes/cm$^3$, a large magnetoresistance effect reappears, and low-field quantum oscillations, which are attributed to light holes at the $L$ point, are observed. The dependence of the light-hole periods on magnetic field orientation suggests that the longitudinal mass is smaller for $L$-point holes $[L_a(3)]$ than for electrons $[L_s(3)]$, as is predicted by Golin's band-structure calculation. $T$-point hole oscillations are observed for excess hole concentrations up to $10^{19}$ cm$^{-3}$ and measurements have been extended to fields of 90 kOe to study their anisotropy. The anisotropy is consistent with a $T$-point hole surface which is a prolate ellipsoid of revolution for excess hole concentrations up to $3\times10^{18}$ cm$^{-3}$, but the surface becomes less prolate as tin is added. Data on this surface are compared with the predictions of a six-band $\mathbf{k}\cdot\boldsymbol{\pi}$ calculation derived from Golin's pseudopotential theory, using the matrix elements at $T$ which he calculated; good agreement is obtained. It is pointed out that the analysis of band nonparabolicity in an earlier paper which makes use of the Abrikosov-Falkovski dispersion relation underestimates the magnitude of the $T_{45}^-(1)$-$T_6^+(3)$ direct gap at $T$. On the basis of the six-band model, the observed nonparabolicity is found to be consistent with the gap estimated by Golin.

## I. INTRODUCTION

In an earlier publication[1] (henceforth referred to as I) studies of the Shubnikov–de Haas effect in single crystals of bismuth doped with tin were reported. Attention in I was confined to samples in which the Fermi level was lowered by doping into the region, ~25–28 meV wide, between the Fermi level of pure bismuth and the edge of the $L$-point conduction band. In this paper we report the extension of this work to higher tin concentrations. The Fermi level can now drop into the gap at the $L$ point, so that the Fermi energy measured from the conduction-band edge is negative. At slightly higher dopings, the Fermi level enters the valence band at the $L$ point.

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[1] R. T. Bate and N. G. Einspruch, Phys. Rev. **153**, 796 (1967).