and $H_{\varphi d}$ in a fashion equivalent to that of Fig. 13. The dependence on $\partial(\ln E_d)/\partial e$ is also included [Fig. (14(b)].

In calculating the volume coefficient of E_F, we use the experimental value of $\partial(E_F-L_3^u)/\partial e$, the volume coefficient of E_d as calculated above, and Eq. (7), together with the strain coefficients of the tight binding parameters (Table V). The resulting value of $\partial(\ln E_F)/\partial e$ is given in Table VII.

Assuming no strain dependence of b_d and $H_{\varphi d}$ at all except for $\Omega^{-1/2}$), we find the theoretical values of $\partial L_1/\partial e_{yz}$ and $\partial(L_1-L_3^u)/\partial e$ to be 62 and 50% of the corresponding experimental numbers [Eqs. 13(a) and 14(a)], respectively. This part of the deformation potentials is mainly due to the strain dependence of k^2 and, for hydrostatic deformation, to the strain dependence of $\Omega^{-1/2}$.

Discussion

The preceding analysis dealt with the observed structure in W_{ij}. A legitimate question is whether the energy bands predict more structure than actually observed. Pure shear strain will produce a significant change in ϵ_2 only for strongly or moderately localized transitions. Moreover, even if the transitions are localized but have k vectors of low symmetry (i.e., neither parallel to [001] nor to [111]), there will be a signal for both trigonal and tetragonal strain (Table III) and the signal will tend to be small. Looking for localized Δ, X, Λ, and L singularities only, we expect the $X_5\rightarrow X_4'$ and the FS $\rightarrow L_1$ transitions to show up between 2 and 5.5 eV, as they do, i.e., the measurements are complete. On the other hand, hydrostatic strain will produce a signal for nonlocalized transitions too. Experimental examples are the maximum in $W_{11}+2W_{12}$ at 2.1 eV and the shoulder at 4.8 eV.

The energies of the identified transitions agree to within ± 0.1 eV with the corresponding difference of the eigenvalues, calculated with Chodorow's[26] potential. Band-structure calculations based on potentials different from that of Chodorow deviate from experiment by as much as 1.5 eV. Table VIII compares the energies of the experimentally observed transitions with predictions of different calculations.[13,14,42–44] There are other experimental results which agree most closely with the result of the $E(\mathbf{k})$ calculation based on Chodorow's potential, the most important of which is the area of the neck, measured with the de Haas–van Alphen effect. The experimental numbers which were re-examined recently[45,46] agree with the calculation[13,14,42] to within 11%. For calculations with other potentials one might not get contact of the Fermi surface with the [111] face of the BZ at all.[42]

TABLE VIII. Energies of observed transitions in eV.

Energy	Experiment	Chodorow[a]	l-dependent[b]	Watson[c]	Self-consistent[d]
$E_F-L_3^u$	2.1 ±0.1	2.1	2.3	1.6	3.2
$X_4'-X_5$	4.0 ±0.1	4.0	4.7	3.1	5.5
L_1-E_F	4.15±0.1	4.0	5.15	3.9	

[a] References 13 and 14.
[b] References 13.
[c] References 42 and 43.
[d] Table II of Ref. 44.

Thus, the experimental evidence for the superiority of the band structure calculated with Chodorow's potential is overwhelming. However, there is no theoretical formalism known today which tells us that we have to choose just this potential. For example, a self-consistent augmented-plane-wave calculation as the one reported by Snow and Waber[44] will agree with the experimental results once the exchange term is properly adjusted, but there is no theoretical justification for such an adjustment.

Zallen[47] measured the change of the reflectance with volume applying hydrostatic pressure directly to the crystal. His results are also listed in Table VI. He could quote only a lower limit for the deformation potential of the 2.1-edge. Our method is much more sensitive here because the large slope of the edge produces a large $\Delta\epsilon_2$ even for the small deformation potential. The two experiments are of comparable accuracy in terms of energy shifts for the 4.3-eV edge. The modulation experiment lost part of its advantage here because the slope is smaller and the slope of the background unknown. The results of the two measurements agree within the experimental error.

Objections might be raised against the procedure used here to calculate the deformation potentials. In particular, one ought to construct the tight-binding functions d from resonance functions rather than from atomic orbitals, as discussed by Heine.[39] However, this would have little effect on the d-sp overlap b_d, because the largest contribution to this integral comes from regions where the resonance function and the atomic d function are identical (the maximum of the integrand lies at 0.53 of the nearest-neighbor distance). The calculated strain coefficients of the tight-binding integrals σ, π, δ (Table V) are higher than predicted by Heine's theory, which would give $R\partial(\ln\beta)/\partial R=-5$ ($\beta=\sigma,\pi,\delta$), but their influence on the deformation potentials is small. Furthermore, it is not clear how the theory of Heine has to be modified if one abandons the muffin-tin approach, i.e., for overlapping potentials.

Two other calculations of the hydrostatic deformation potentials are known.[43,48] Both are listed in

[41] J. S. Faulkner, H. L. Davis, and H. W. Joy, Phys. Rev. 161, 656 (1967).
[42] H. L. Davis, J. S. Faulkner, and H. W. Joy, Phys. Rev. 167 601 (1968).
[43] E. C. Snow and J. T. Waber, Phys. Rev. 157, 570 (1967).
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[45] W. J. O'Sullivan and J. W. Schriber, Cryogenics 7, 118 (1967).
[47] R. Zallen, in *Colloquium on the Optical Properties and the Electronic Structure of Metals and Alloys, Paris 1965*, edited by F. Abelès (North-Holland Publishing Co., Amsterdam, 1966), p. 164.
[48] R. Jacobs (private communication).