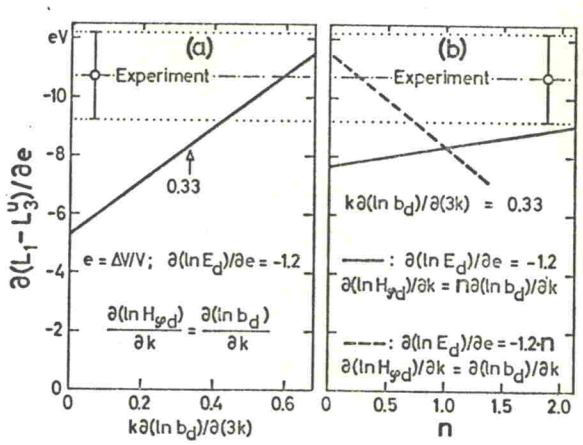

FIG. 14. The dependence of the volume deformation potential $\partial(L_1-L_3^u)/\partial e$ on the strain coefficients of b_d and $H_{\varphi d}$ plotted in a way similar to that of Fig. 13. In addition, the dependence on the volume coefficient of E_d is given [dashed curve in part (b) of the figure].

distance)

$$\partial H_{dd}/\partial e_{yz}=-[12\sigma-8\pi+4\delta+R\partial(3\sigma+4\pi+5\delta)/\partial R]. \quad (17)$$

The strain dependence of V_{111} is calculated using a simple model potential.[40] It is constructed from a bare ion potential which is zero inside the core region ($r<r_c$) and equal to the Coulomb potential of a single positive charge outside ($-2/r$ in atomic units). Its Fourier transform is divided by ϵ_q, the static Hartree dielectric function for free electrons,[41] to give the form factor

$$V_q=-8(\cos qr_c)/(\epsilon_q\Omega q^2), \quad (18)$$

where Ω is the volume of the unit cell. The value of r_c (0.23 of the nearest-neighbor distance) is determined by V_{111} of Table V; it is regarded as a constant in calculating the strain coefficients of V_{111} from Eq. (18). The values of the overlap integral b_d for the deformed crystal are calculated in the same way as b_d for zero strain. All strain coefficients discussed above are listed in Table V.

The calculation of the deformation potentials requires additional knowledge, namely, the strain coefficients of $H_{\varphi d}$, E_d, and E_F. The effect of pure trigonal shear strain will be considered first. In this case, there is no change of E_d and E_F linear in the strain components: The center of gravity of originally degenerate levels remains unchanged to first order; this causes E_d and E_F to be constant, too. As a consequence,

$$\partial(L_1-E_F)/\partial e_{yz}=\partial L_1/\partial e_{yz}. \quad (19)$$

A rigorous calculation of $\partial H_{\varphi d}/\partial e_{yz}$ would be even more difficult than the calculation of $H_{\varphi d}$ itself. We therefore simply assume the relative change of b_d and $H_{\varphi d}$ to

[40] N. W. Ashcroft, Phys. Letters 23, 48 (1966).
[41] W. A. Harrison, in *Frontiers in Physics*, edited by D. Pines (W. A. Benjamin, Inc., New York, 1966), p. 49.

TABLE VII. Volume coefficients of the Fermi energy and of the position of the d bands.

Volume coefficients[a]	Present paper	Derived from dHvA[b]	DFJ[c]
$\partial(\ln E_d)/\partial e$	-1.2 ± 0.5		-0.85
$\partial(\ln E_F)/\partial e$	-1.1 ± 0.3	-0.73	-0.86

[a] Γ_1 is the zero of energy and $e=\Delta V/V$ is the relative change of the volume V.
[b] Reference 50.
[c] Reference 43.

be identical,

$$\partial(\ln H_{\varphi d})/\partial e_{yz}=\partial(\ln b_d)/\partial e_{yz}. \quad (20)$$

Equation (20) completes the list of strain coefficients which are needed to calculate $\partial L_1/\partial e_{yz}$. Its numerical value (listed in Table VI) is 24% lower than the one determined from the experiments.

Figure 13 illustrates how the theoretical coefficient $\partial L_1/\partial e_{yz}$ changes when changing the assumptions specified above. Figure 13(a) gives the dependence on $\partial b_d/\partial e_{yz}$ assuming Eq. (20) to be valid. Figure 13(b) shows the variation with $\partial(\ln H_{\varphi d})/\partial e_{yz}$ using $\partial b_d/\partial e_{yz}=0.73$ as calculated from atomic d functions.[37]

Two volume deformation potentials $\partial(E_F-L_3^u)/\partial e$ (determined from the edge at 2.1 eV) and $\partial(L_1-E_F)/\partial e$ (from the edge at 4.3 eV) are used to calculate the volume coefficients of E_d and E_F relative to Γ_1. This can be done more accurately than the large experimental error of the L_1-E_F deformation potential might suggest. Recalling that the error is due to the uncertainty in the appropriate slope of ϵ_2, we note that the relative deviation of the experimental value from the true value is approximately equal for the volume and the shear strain deformation potentials.

Summing the two experimental volume deformation potentials eliminates E_F; the sum $\partial(L_1-L_3^u)/\partial e$ can be used to determine $\partial(\ln E_d)/\partial e$. In doing so, we always treat the normalization factor $\Omega^{-1/2}$ of b_d and $H_{\varphi d}$ explicitly and assume

$$\partial(\ln H_{\varphi d})/\partial k=\partial(\ln b_d)/\partial k, \quad (21)$$

which is the equivalent of Eq. (20). There are several choices on how to proceed. One possibility is to use the coefficient $\partial(\ln b_d)/\partial k$ as calculated with atomic d functions and a value for $\partial(L_1-L_3^u)/\partial e$ which is 24% smaller than the experimental one. Another choice would be to increase $\partial(\ln b_d)/\partial e_{yz}$ until the theoretical value of $\partial L_1/\partial e_{yz}$ matches the experimental one [Fig. 13(a)], to increase $\partial(\ln b_d)/\partial k$ by the same factor, and to use the experimental value of $\partial(L_1-L_3^u)/\partial e$. The volume coefficient of E_d turns out to be the same in both cases, proving that it does not depend drastically on the strain coefficients of b_d and $H_{\varphi d}$. Its numerical value is listed in Table VII. In Fig. 14, $\partial(L_1-L_3^u)/\partial e$ is plotted as a function of the strain coefficients of b_d