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ons, Inc., New York, 196
Phys. Letters 10, 203 (1965
D. Lang, Phys. Rev. 15
659 (1967).

TABLE VI. Deformation potentials (in eV) of the transitions at L.

Deformation potentials	Experiment			Theory		
	Present paper	Zallen[a]		Present paper	DFJ[b]	Jacobs[c]
$(L_2' - E_F)/\partial e_{yz}$	-72 ± 12			-56		
$(L_2' - E_F)/\partial e^d$	-9.6 ± 1.5	9.7 ± 2.0			-5.1	
$(L_{2'} - L_1{}^u)/\partial e$	-1.1 ± 0.1	Absolute value <1.3			-0.8	
$(L_{2'} - L_1{}^u)/\partial e$					-5.9	-4.1

[a] Reference 47.
[a] Reference 43.
[a] Reference 48.
$e = \Delta V/V$ is the relative change of the volume V.

the form given by Cohen and Mueller.[35] Using symmetrized plane waves as well as symmetrized tight-binding functions, we can write down the eigenvalues of L_2' and of $L_3{}^{u,l}$ immediately:

$$L_2' = k^2 - V_{111}, \qquad (7)$$

$$L_3{}^{l,u} = E_d + \pi - \delta \pm [(\pi - \delta)^2 + 4.5(-\sigma + \delta)^2]^{1/2}. \qquad (8)$$

The vector k is that of the L point, V_{111} is a pseudopotential form factor, E_d gives the position of the d bands above Γ_1, and $\sigma \equiv (dd\sigma)$, $\pi \equiv (dd\pi)$, and $\delta \equiv (dd\delta)$ are the two-center tight-binding integrals defined by Slater and Koster.[36] The two L_1 levels are obtained from the secular equation

$$\begin{vmatrix} H_{\Phi\Phi} - E & H_{\Phi d} \\ H_{d\Phi} & H_{dd} - E \end{vmatrix} = 0. \qquad (9)$$

The function d is a tight-binding Bloch sum symmetrized to L_1 and Φ is a plane wave symmetrized to L_1 and orthogonalized to d,

$$\Phi = (\varphi - b_d d)/C. \qquad (10)$$

The abbreviations used in Eq. (10) are

$$\varphi = (2/V)^{1/2} \cos(k \cdot r), \qquad (11)$$

$$b_d = \langle \varphi | d \rangle, \qquad (12)$$

$$C^2 = 1 - b_d{}^2. \qquad (13)$$

The matrix elements of Eq. (9) are

$$H_{dd} = E_d - 4(\pi - \delta), \qquad (14)$$

$$H_{\Phi d} = (H_{\varphi d} - b_d H_{dd})/C, \qquad (15)$$

$$H_{\Phi\Phi} = (k^2 + V_{111} + V_{\varphi\varphi}{}^{(2)} + b_d{}^2 H_{dd} - 2b_d H_{\varphi d})/C^2. \qquad (16)$$

We calculated b_d and the tight-binding integrals using the atomic wave function and the atomic potential calculated by Hartree and Hartree[37] and parametrized

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[35] M. H. Cohen and F. M. Mueller, in *Atomic and Electronic Structure of Metals* (American Society for Metals, Metals Park, Ohio, 1967), p. 61.
[36] J. C. Slater and G. F. Koster, Phys. Rev. 94, 1498 (1954).
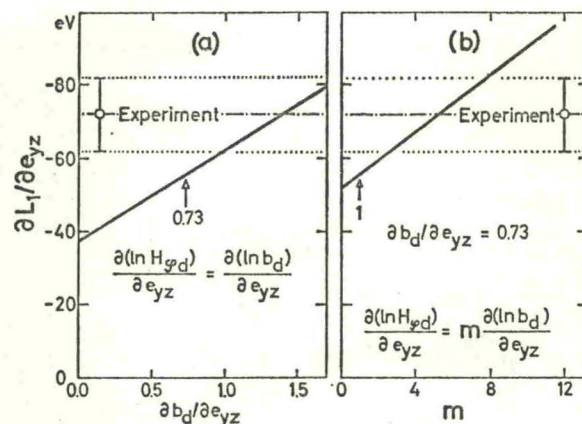[37] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) A157, 490 (1936).

FIG. 13. The dependence of the shear strain deformation potential $\partial L_1/\partial e_{yz}$ on the strain coefficient of the orthogonality integral b_d [part (a) of the figure] and on the strain coefficient of the hybridization $H_{\varphi d}$ [part (b) of the figure]. The value $\partial b_d/\partial e_{yz} = 0.73$ was calculated using atomic d functions.

by Fletcher and Wohlfahrth.[38] The numerical values are given in Table V. The tight binding integrals agree with those calculated by Fletcher and Wohlfahrth. The value of the orthogonalization integral b_d given by Mueller[34] is 16% lower than the one reported here.

A first-principles calculation of the quantities E_d, $H_{\varphi d}$, and $\Delta V_{\varphi\varphi}{}^{(2)}$ is extremely difficult and will not be attempted here. Instead, we determine them from the eigenvalues of Fig. 9,[13,14] using the calculated values of b_d and of the tight-binding integrals. In particular, the value of the hybridization integral $H_{\varphi d}$ is evaluated from the difference between H_{dd} (the eigenvalue of $L_1{}^d$, neglecting hybridization) and $L_1{}^d$. E_d is calculated from $L_3 - \Gamma_1$ using Eq. (8). ($L_3{}^u - L_3{}^l$ given by this equation agrees with the value taken from Fig. 9. One would expect this, since these bands have no interaction with the sp bands.) The form factor V_{111} given by Eq. (7) is also taken from the calculated band structure.

$\Delta V_{\varphi\varphi}{}^{(2)}$ is the matrix element of the crystal potential, calculated with the $l = 2$ component of φ. It was introduced in the model Hamiltonian[35] following a suggestion by Heine.[39] Its numerical value (calculated using the $L_1 - L_1{}^d$ gap of Fig. 9) is small, namely, -0.75 eV. Neglecting $\Delta V_{\varphi\varphi}{}^{(2)}$ gives $L_1 - L_1{}^d = 9.85$ eV using Eq. (9), which is only 0.60 eV higher than the value of Fig. 9. $\Delta V_{\varphi\varphi}{}^{(2)}$ will be neglected in the following. The zero-strain values of V_{111}, $H_{\varphi d}$, and E_d are listed in Table V.

The tight-binding parameters for changed nearest-neighbor distances were calculated in the same way as for the distance in the unstrained crystal. For trigonal distortion (Table I) and levels with k parallel to [111], the strain coefficient of H_{dd} is (R is the nearest-neighbor

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[38] G. C. Fletcher and E. P. Wohlfahrth, Phil. Mag. 42, 106 (1951).
[39] V. Heine, Phys. Rev. 153, 673 (1967).