	Zero of d bands above
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.32 eV	$E_d = 5.75$
	c

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ce, edited by W. A. Harris...
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Phys. Letters 10, 203 (1965...
D. Lang, Phys. Rev. 1...

659 (1967).

Table VI

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

Deformation potentials	Experiment Present paper	Zallen[a]	Theory 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	
$(L_1 - L_1^u)/\partial e$	-1.1 ± 0.1	Absolute value < 1.3		-0.8	
$(L_1 - L_1^u)/\partial e$				-5.9	-4.1

a Reference 47.
b Reference 43.
c Reference 48.
d $= \Delta V/V$ 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 $\mathbf{k}$ 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

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

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

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

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

[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).

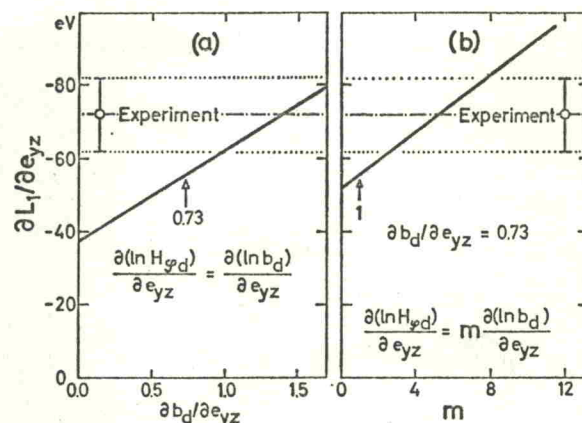[37] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) A157, 490 (1936).

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 $\mathbf{k}$ parallel to [111], the strain coefficient of H_{dd} is (R is the nearest-neighbor

[38] G. C. Fletcher and E. P. Wohlfahrth, Phil. Mag. 42, 106 (1951).

[39] V. Heine, Phys. Rev. 153, 673 (1967).