TABLE V. Matrix elements and strain coefficient of matrix elements which were used to calculate the deformation potentials at L.

Orthogonality matrix element	Tight-binding integrals	Pseudopotential	Hybridization	Zero of d bands above Γ_1
$b_d=-0.366$	$\sigma=-0.332$ eV $\pi=+0.180$ eV $\delta=-0.027$ eV	$V_{111}=0.29$ eV	$H_{\varphi d}=1.32$ eV	$E_d=5.75$ eV
$\partial b_d/\partial e_{yz}=0.73$[a] $k\partial(\ln b_d)/\partial(3k)=0.332$	$R\partial(\ln\sigma)/\partial R=-5.5$[b] $R\partial(\ln\pi)/\partial R=-6.9$ $R\partial(\ln\delta)/\partial R=-8.0$	$\partial V_{111}/\partial e_{yz}=-3.85$ eV[a] $\partial V_{111}/\partial e=-0.93$ eV[c]	d	e

[a] The strain tensor for trigonal distortion is given in Table I. [b] R is the nearest-neighbor distance. [c] $e=\Delta V/V$ is the relative change of the volume. [d] See Text and Figs. 13 and 14. [e] See Table VII.

longer distinguish between the energy shift of the 2.1-eV edge and the change of the $E_F-L_3^u$ separation. The numerical value is $\partial(E_F-L_3^u)/\partial e=-(1.1\pm0.1)$ eV, where $e=\Delta V/V$ denotes the relative change of the volume.

The $X_5\to X_4'$ transition contributes only a small fraction of the total ϵ_2 at 3.9 eV. It is impossible to get reliable values of $d\epsilon_2/d(\hbar\omega)$ appropriate to this fraction of ϵ_2. We do not attempt to calculate the shear-strain deformation potential of this transition; instead, we simply show that it will produce a negative $W_{11}-W_{12}$ below the energy of the critical point. The level X_4' has free-electron character; it does not interact with the d bands because of symmetry (Fig. 9). Its eigenvalue is k^2 ($\mathbf{k}=\mathbf{X}$, in atomic units), neglecting a small pseudopotential form factor. The shear coefficient for $\mathbf{k}$ perpendicular to z (stress axis, see Table I) is $\partial(\ln k^2)/\partial e_{zz}=+1$. The shear coefficient of the X_5 level, which has tight binding character, will be small compared to that of k^2. Thus the sign of the change in $X_4'-X_5$ is given by the change of k^2. For light polarized parallel to z only those transitions of $X_5\to X_4'$ with $\mathbf{k}$ perpendicular to z contribute according to the selection rules (these are strictly valid only for the X point and zero spin-orbit splitting, but they will hold approximately). Thus, the M_1 c.p. shifts to higher energies for positive e_{zz}, producing negative values for $W_{11}-W_{12}$ below 4.0 eV, as observed.

The $\text{FS}\to L_1$ transition has been found to be responsible for the large values of W_{44} and $W_{11}+2W_{12}$ at 4.3 eV and for the edge in ϵ_2 at this energy. Because of the strong localization of this transition the deformation potentials derived from W_{ij} will be close to those of the transition with $\mathbf{k}=\mathbf{L}$. Transitions connected with M_1 and M_2 singularities in J which are not modified by the Fermi energy will behave differently, because they are only moderately localized, as discussed in the Introduction. The deformation potentials of transitions with different $\mathbf{k}$ will generally be different. Indeed, Brust and Liu[31] have shown recently that the deformation potential of the transition with $\mathbf{k}$ of the saddlepoint and the energy shift per strain of the corresponding structure in the optical spectrum can differ significantly.

The background slope of ϵ_2 at 4.3 eV due to transitions other than $\text{FS}\to L_1$ cannot be determined rigorously. We use the slope of ϵ_2 at 4.05 eV, which is -0.5/eV (Fig. 12). The similarity of $W_{11}+2W_{12}$ and W_{44} around 4.3 eV shows that changes of M and J which can be large for shear strain only do not contribute significantly to W_{44}. Furthermore, W_{ij} has its maximum where the slope of ϵ_2 is largest and where the contribution of this transition to the total ϵ_2 is still small. If present, changes of J and M would have the largest effect on W_{44} at the maximum contribution of $L_2'\to L_1$ to ϵ_2. Thus neglecting changes of M and J is justified here. This also justifies the analysis of the previous sections, where we considered the effect of shear strain on the $\mathbf{k}$ degeneracy only.

Without spin, the $L_2'\to L_1$ selection rules are $M_{z'}\neq0$, $M_{x'}=M_{y'}=0$, where $\mathbf{k}=\mathbf{L}$ is parallel to z' (z'= stress axis, Table I). With spin, these rules will still be approximately valid ($|M_{x'}|^2\ll|M_{z'}|^2$). The selection rules for $\mathbf{k}\neq\mathbf{L}$ will be different from the ones given above, even without spin. The strong localization of the transitions in $\mathbf{k}$ space assures that this deviation is small. The shear coefficient of the transition will be calculated neglecting the deviations from the selection rules given above.

The deformation potentials determined from experiment and evaluated using the assumption discussed above are $\partial(L_1-E_F)/\partial e=(-9.6\pm1.5)$ eV and $\partial(L_1-E_F)/\partial e_{yz}=(-72\pm12)$ eV for $\mathbf{k}$ parallel [111]. The largest uncertainty in these coefficients is due to the background slope in ϵ_2 (the values given earlier[12] are 8% higher because the background slope used was -0.3/eV instead of -0.5/eV used here).

Theory of the Deformation Potentials at L

The theoretical estimate of the deformation potentials of the $\text{FS}\to L_1$ transitions given earlier[12] neglected the plane-wave admixture to the wave function of the d state L_{1d}, i.e., d-sp hybridization. The treatment outlined below includes the hybridization.

We use the model Hamiltonian developed by Saffren,[32] Ehrenreich and co-workers,[33] and Mueller[34]

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