SHALLOW DONOR GROUND STATE LEVELS IN Ge

	Table 1.		
Quantity	Value		Units
$\epsilon_{12}(L_1 - L_1)$.2.2*	*	_
$\epsilon_{13}(\Delta_1 - \Delta_1)_{//}$	1.6*		_
$\epsilon_{14}(\Delta_1 - \Delta_1)_{\perp}$	2.3*		-
$\epsilon_{15}(L_1 - \Delta_1)$	2.2*		-
U12	-0.184 [†]		meV
U_{13}	-0.512^{\dagger}		meV
U_{14}	-0.713^{\dagger}		meV
U_{15}	-0.472^{\dagger}		meV
$\left[E\left(T_{1}\right)-E\left(A_{1}\right)\right]L_{1}$	0.77^{+}		meV
$[E(T_1) - E(A_1)] \Delta_1$	3.86 [†]		meV
$[E(E) - E(T_1)] \Delta_1$	0.40 [†]		meV

* These values are deduced from Fig. 3 of Walter and Cohen.¹⁰

† Present work.

dielectric constant $\epsilon = \epsilon (\underline{k}_{0i} - \underline{k}_{0j} = \underline{q})$ has been taken into account following the results of Walter and Cohen. 10 The ellipsoidal shape of the equienergetic surfaces about the minima have been taken into account through an appropriate average of the longitudinal and transverse effective Bohr radii.9 The Bloch functions have been replaced with plane wave functions, a reasonable approximation for a slowly varying potential. The integration method was carried on with a delta function, as discussed by Callaway. 11 The values so obtained for U_{ij} are reported in Table 1 with the proper dielectric constant values used for calculations. The U_{ij} listed refer to the following interactions: U_{12} to $L_1 - L_1$, U_{13} to $\Delta_1 - \Delta_1$ (parallel valleys), U_{14} to $\Delta_1 - \Delta_1$ (perpendicular valleys), and U_{15} to $L_1 - \Delta_1$. The calculated values for the energy splittings between the T_1 and A_1 levels associated with the L_1 minima, and the T_1 and A_1 , and E and T_1 levels associated with the Δ_1 minima for Ge at atmospheric pressure are also reported in Table 1.

The effect of an applied hydrostatic pressure P was then included assuming a rigid shift in energy of the L_1 and Δ_1 minima with P, ¹² and a dielectric constant ϵ pressure independent. Using the pressure coefficients (respect to the valence band)



FIG. 1. Pressure dependence of the ground state levels for shallow donors in Ge (broken lines). Full lines exhibit the pressure dependence of the L_1 and Δ_1 minima. The energy is measured from the conduction band edge at atmospheric pressure. The insert evidences the anomalous pressure dependence of the binding energy of the 1 $s(A_1)$ level in the crossing region between L_1 and Δ_1 minima. The binding energy is measured from the conduction band edge at the given pressure.

 $dE(L_1)/dP = 5 \ 10^{-6} \ eV/atm$, and $dE(\Delta_1)/dP = -1.5 \ 10^{-6} \ eV/atm^{12}$ the new energy locations of L_1 and Δ_1 minima have been calculated. Accordingly the new solutions of the secular determinant (1) have been carried on.

Results are reported in Fig. 1, where the strong interaction between the two A_1 levels associated with the L_1 and Δ_1 minima respectively is evidenced, in accord with the non crossing rule.¹³ This effect is maximum when the L_1 and Δ_1 minima are approaching the same energy and causes the binding energy of the A_1 level to exhibit the anomalous