Hydrostatic-pressure dependencies of deep impurity levels in zinc-blende semiconductors

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The derivatives with respect to hydrostatic pressure are predicted for deep levels associated with *s*- and *p*-bonded impurities in Si, Ge, AlP, AlAs, AlSb, GaP, GaAs, GaSb, InP, InAs, InSb, and ZnSe. It is shown that by combining data, both for deep levels and for their hydrostatic-pressure derivatives, with theory it is often possible to determine (i) the site of the impurity, (ii) the symmetry of the deep level, and (iii) a quite small number of substitutional *s*- and *p*-bonded impurities that could be responsible for the data. We use this method to argue that the deep levels observed by Aladashvili *et al.* in InSb to lie in the interval between 0.1 and 0.15 eV above the valence-band maximum are probably A_1-symmetric levels associated with C_{In} and/or antisite Sb_{In} (or levels associated with defect complexes involving these defects).

I. INTRODUCTION

Several years ago, deep levels were defined as impurity states in semiconductors whose energies were more than 0.1 eV from a nearby band edge—namely levels that were not thermally ionized at room temperature. More recently this definition has been revised as a result of the recognition that deep levels can, when perturbed, cease being energetically deep in the gap and can actually pass into a band where they become resonances. The current definition of a deep level is one that is caused by the central-cell potential of the defect.[1] In fact, all *s*- and *p*-bonded substitutional impurities in zinc-blende semiconductors produce typically four such deep levels in the vicinity of the fundamental band gap: one *s*-like (A_1 symmetric) and one triply degenerate *p*-like (T_2) level. These deep levels, more often than not, are resonances that lie outside the band gap, and hence are not "deep" by the old definition.

Despite the fact that various theories of deep levels have been developed,[2-4] beginning with the classical paper by Lannoo and Lenglart on the levels associated with the Si vacancy,[5] the theories generally have not been capable of identifying a particular impurity from the energies of its observed deep levels in the fundamental band gap. This is due only in part to the fact that the best theories of deep levels have theoretical uncertainties of a few tenths of an eV for their level predictions.

Ren *et al.*[6] following the "deep-level pinning" ideas of Hjalmarson *et al.*[2], showed for substitutional *s*- and *p*-bonded point defects on a site that all deep levels in the band gap with a particular symmetry have almost the same wave function—independent of the defect (see Fig. 1). This notion was confirmed experimentally by various electron-nucleon double resonance (ENDOR) measurements of deep-level wave functions in semiconductors.[7,8] Thus, no experiment that probes only the valence electronic properties of a deep level is capable of easily identifying the impurity responsible for the level: it is necessary to probe the nucleus [e.g., with ENDOR (Ref. 7)] or the core [e.g., with extended x-ray-absorption fine structure (EXAFS) (Ref. 9)] to achieve such a unique identification.

The situation has been further complicated due to the demonstration by Sankey *et al.*[10] that extended substitutional defects often have almost the same deep-level energies as their constituent isolated impurities. Thus analyses of observed energy levels are unlikely to reveal even if the defect producing the level is a point defect. (This complication is also a simplification, because it means that theoretically one need consider only isolated defects, since defect complexes have, to a good approximation, spectra which are the sums of their constituents' spectra.)

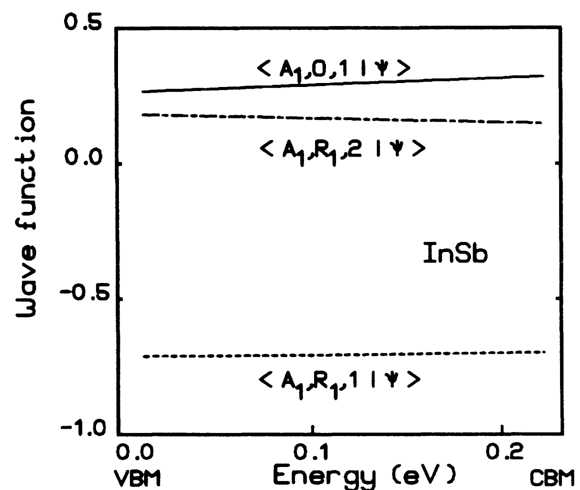

FIG. 1. Indium-site substitutional defect wave functions in InSb are shown as functions of deep energy level E. The on-site wave function $\langle A_1,0,1 \mid \psi \rangle$ in the notation of Ref. 6 and first-shell wave functions $\langle A_1,\mathbf{R}_1,1 \mid \psi \rangle$ [inward-directed hybrids (Ref. 6)] and $\langle A_1,\mathbf{R}_1,2 \mid \psi \rangle$ [outward-directed hybrids (Ref. 6)] are shown by solid, dashed, and dashed-dotted lines, respectively. All these curves are nearly flat and show that the deep defect wave functions depend very little on their energy levels.

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This insensitivity of deep impurity levels to the impurity raises the question of how much information can be gleaned from simple electronic measurements of deep levels, such as measurements of their energies and pressure derivatives.[11–13] In this paper, we show that (if we limit ourselves to *s*- and *p*-bonded substitutional impurities in zinc-blende semiconductors) combined measurements of a deep level and its change with hydrostatic pressure can usually determine both the symmetry of the level and the site (anion or cation site) of its parent impurity. Furthermore, we also show that the number of candidates for producing a particular deep level in the band gap can be reduced in number to only a few—and that this can be done even for impurities in a small-band-gap semiconductor such as InSb, whose (low-temperature) band gap of 0.23 eV is smaller than the uncertainty in most theories.

II. THEORY

Our theoretical approach is based on the model of electronic structure of Vogl *et al.*,[14] the theory of deep levels of Hjalmarson *et al.*,[2] and the work of Ren *et al.*[11] on pressure effects. We note that Ren's basic approach to pressure effects on deep levels in GaAs led to the targeting several years ago of oxygen and the antisite defect as possible constituents of the defect $EL2$— and that the role of the antisite defect is now generally acknowledged, while some (but not all) authors continue to believe that oxygen is also a constituent of $EL2$. Thus the basic theoretical approach of Ren *et al.* has a history of success, and we use that approach here for deep levels in other zinc-blende semiconductors.

The deep levels E are obtained by solving the secular determinant

$$\det[1-G_0(E)V]=0 .$$

Here, $G_0(E)$ is the Green's function, which is real in the fundamental energy band gap

$$G_0=(E-H_0)^{-1} .$$

The host Hamiltonian H_0 is taken to be the nearest-neighbor empirical tight-binding model of Vogl *et al.*[14] which is a ten-band model capable of describing both the chemistry of sp^3 bonding and the indirect-gap energy band structure of semiconductors such as Si and GaP, by virtue of its five-orbital sp^3s^* basis centered on each site. Expressed formally in terms of Löwdin orbitals[15] $|n,b,\mathbf{R}\rangle$ centered at the atom in unit cell $\mathbf{R}$ at site b (b denotes anion or cation) the Bloch-like tight-binding basis states are

$$|n,b,\mathbf{k}\rangle=N^{-1/2}\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}|n,b,\mathbf{R}\rangle .$$

Here, n runs over s, s^*, and the three p states. In this basis, the host Hamiltonian is a 10×10 matrix for each wave vector $\mathbf{k}$ (see Refs. 14 and 16). By diagonalizing this matrix and obtaining its eigenvalues $E(\mathbf{k},\lambda)$, namely the band structure, and its eigenvectors $|\mathbf{k},\lambda\rangle$, namely the Bloch states, one can construct the Green's-function operator

$$G_0(E)=\sum_{\mathbf{k},\lambda}(|\mathbf{k},\lambda\rangle\langle\mathbf{k},\lambda|)/[E-E(\mathbf{k},\lambda)] .$$

The defect-potential matrix V is taken to be diagonal and centered solely on the impurity site in the Löwdin basis; this approximation is now well established, and corresponds to neglecting lattice relaxation around the impurity.[2] Coulombic charge-state splittings[17] are also neglected. Since any underlying theory for predicting the deep levels of a given impurity is only accurate to a few tenths of an eV, the omission of lattice relaxation and charge-state splittings does not appreciably increase the theoretical uncertainty. Following Hjalmarson *et al.*,[2] we approximate the diagonal matrix elements of V on the impurity site as

TABLE I. Exponents $\eta_{l,l'}$ $(l,l'=s,p,s^*)$ for the bond-length dependencies of the nearest-neighbor matrix elements. Exponents η are obtained by fitting the observed pressure dependencies (Table II) of the direct band gaps at Γ, L, and X, and the indirect gaps from L and X, to the valence-band maximum, using the least-squares method.

	$\eta_{s,s}$	$\eta_{s,p}$	$\eta_{x,x}$	$\eta_{x,y}$	$\eta_{s^*,p}$
Si	3.000	1.600	3.825	2.600	3.327
Ge	4.400	2.400	2.300	2.500	3.982
AlP	2.386	1.637	1.521	1.247	2.486
AlAs	3.205	1.656	2.398	1.706	3.214
AlSb	2.553	4.249	1.192	3.272	4.469
GaP	3.697	2.804	1.630	2.795	2.841
GaAs	4.144	2.341	2.220	2.596	2.665
GaSb	4.044	2.013	1.634	2.281	1.245
InP	3.100	4.443	3.049	2.366	1.207
InAs	2.539	2.812	3.757	2.825	3.014
InSb	4.012	2.987	2.533	2.751	3.134
ZnSe	1.874	1.185	1.838	1.330	3.185

TABLE II. Pressure coefficients of zinc-blende semiconductors (in meV/kbar).

Semiconductor	dE_Γ/dp	dE_L/dp	dE_X/dp	$dE_{L\Gamma}/dp$	$dE_{X\Gamma}/dp$
Si	1.0	6.2	3.0	5.5[a]	−1.5
Ge	14.2	7.8	5.5	5.0	−1.5
AlP	11.8[b]	5.21[b]	−0.62[b]	4.36[b]	−2.2[b]
AlAs	12.6[b]	6.27[b]	0.58[b]	4.82[b]	−2.5[b]
AlSb	9.00	7.5[a]	4.0[a]	6.4[a]	−1.5
GaP	10.5	5.8	1.8[a]	2.1[a]	−1.1
GaAs	10.7	5.0	4.6[a]	5.5[a]	−1.5[a]
GaSb	14.7	7.5	6.0	5.0	−1.5[c]
InP	8.5	7.5[a]	4.6[a]	6.8[a]	1.8[a]
InAs	10.15	7.0	3.5[a]	4.8[a]	−0.02[a]
InSb	15.5	8.5	6.0	8.3[a]	−1.1[c]
ZnSe	7.0	2.5[a]	−0.3[a]	1.4[a]	−2.0[a]

[a]Reference 20.
[b]R.-D. Hong, S. Lee, and J. D. Dow (unpublished).
[c]Reference 21. All other experimental values are those cited in Ref. 20.

$$V_s=\beta_s(w_s(\text{impurity})-w_s(\text{host}))\ ,$$

$$V_p=\beta_p(w_p(\text{impurity})-w_p(\text{host}))\ ,$$

and

$$V_{s^*}=0\ ,$$

where the energies w_l ($l=s$ or p) are atomic-orbital energies in the solid,[14] and β_s and β_p are constants (0.8 and 0.6, respectively[2]). These approximations to the defect-potential matrix of a specific impurity, V, are needed to associate a particular deep-level energy E or pressure derivative dE/dp with the impurity. They are not necessary to obtain a relationship between dE/dp and E, however, because this relationship depends only on the existence of such a matrix V, not on our ability to accurately predict the numerical values of its matrix elements.

Hydrostatic pressure does not affect the defect potential within the context of the Hjalmarson model, because the defect potential does not depend on the bond length. It does alter the off-diagonal two-center matrix elements of the host Hamiltonian H_0, however, because these matrix elements depend on the bond length d:

$$H_{l,l'}=H^0_{l,l'}(d_0/d)^{\eta_{l,l'}}\ .$$

Here, $H^0_{l,l'}$ and $H_{l,l'}$ ($l,l'=s$, p, and s^*) are the off-diagonal matrix elements corresponding to the bond lengths d_0 and d, respectively; d_0 is the zero-pressure bond length; the finite-pressure bond length d is obtained from the hydrostatic pressure p by using Murnaghan's[18] equation of state

$$p=[B_0/(dB_0/dp)][(d_0/d)^{3\,dB_0/dp}-1]\ ;$$

and $\eta_{l,l'}$ are exponents with values near 2, according to both Harrison[19] and Vogl *et al.*[14] We have obtained, by trial and error, sets of exponents $\eta_{l,l'}$ that reproduce rather well the observed deformation potentials or hydrostatic-pressure derivatives of the band gaps at Γ, X, and L symmetry points of the Brillouin zone. The exponents $\eta_{l,l'}$ are presented in Table I, and the experimental pressure coefficients used to determine them are given in Table II.[20,21]

III. RESULTS

For the tetrahedral (T_d) symmetry of zinc-blende semiconductors, the secular determinant reduces to two scalar equations, one for s-like A_1-symmetry deep levels,

$$(V_s)^{-1}=\sum_{\mathbf{k},\lambda}|\langle s,b,\mathbf{0}|\mathbf{k},\lambda\rangle|^2/[E-E(\mathbf{k},\lambda)]\ ,$$

and another for p-like T_2 levels,

$$(V_p)^{-1}=\sum_{\mathbf{k},\lambda}|\langle p,b,\mathbf{0}|\mathbf{k},\lambda\rangle|^2/[E-E(\mathbf{k},\lambda)]\ .$$

We evaluate the sums using the special-points method[22] for fixed E, and then graphically determine the defect potentials V that produce a level at that energy. This process is repeated for the pressurized semiconductor to obtain dE/dp versus V also. Then the defect potential V is eliminated to yield dE/dp as a function of E.

It should be emphasized that there are two levels of approximation in the theory for the defect-potential matrix V: (i) the diagonal form (with arbitrary matrix elements V_s and V_p) which is the only approximation entering into the determination of dE/dp as a function of E, and introduces a small theoretical uncertainty of $\simeq 0.5$ meV/kbar into dE/dp;[11] and (ii) the expressions of V_s and V_p in terms of atomic energies, which are necessary to associate a deep level E with a particular impurity (or defect potential) and introduce an uncertainty in E of about $\simeq 0.3$ eV. Thus, the uncertainty in dE/dp as a function of V, which is the combination of these two uncertainties, is considerably larger than the uncertainty in dE/dp as a function of E (by typically a factor of 4, as can be deduced, for ex-

ample, from Fig. 2). Thus, although the uncertainty in E *for a particular defect* is comparable with the band gap of InSb and the uncertainty in dE/dp for that defect is a significant fraction of the predicted range of possible values for dE/dp, the uncertainty in dE/dp *for a particular level* E is considerably smaller, and so that relationship can be used to determine the symmetry of the deep level and the site of its parent impurity, even though unambiguous determination of the defect, namely, highly accurate determination of $E(V)$, is not possible. Here we exploit this fact and note that similar elimination of the defect potential from the theory of ENDOR and ESR spectra of deep levels produced successful and accurate theories.[6]

The theoretical uncertainty of $\simeq 0.5$ meV/kbar in dE/dp was first arrived at[11] by varying the major elements of the theory, such as the tight-binding matrix elements and exponents η, over the range of reasonable possibilities. It has been borne out by experiments for the A_1 deep level of a N impurity on an anion site in GaP (Refs. 12 and 23) and in GaAs (Ref. 24), which have exhibited the predicted pressure coefficients dE/dp. The theory can rather accurately predict a derivative dE/dp associated with a deep level E, even though it cannot accurately assign an impurity to a given energy.

Since the relationship dE/dp versus E depends on the site of the impurity and the symmetry of its deep level, comparison of data for dE/dp and E with theory can yield the site of the impurity and the symmetry of its deep level. Once the site and the symmetry are known, the number of candidates for producing such a level E (to within a few tenths of an eV) is greatly reduced.

We illustrate this point for deep levels in InSb, a material whose band gap is smaller than the theoretical uncertainty. The predicted pressure derivatives dE/dp are given in Fig. 2 as functions of the deep-level energies E. (The estimated theoretical uncertainty in dE/dp is roughly 0.5 meV/kbar.) The impurities associated theoretically with the deep levels E are also displayed on each curve—although this association is limited by a few-tenths-of-an-eV theoretical uncertainty in the energy E of the deep level associated with a specific impurity. Therefore we have shown on the sides of the figure those impurities (including the vacancy, denoted Va) that might have deep levels in the band gap if the theory's deep-level predictions were altered by 0.3 eV. We have considered as impurities the atoms from columns IIB and III–VIII of the Periodic Table, as well as Li, Na, K, Rb, Be, and Mg.

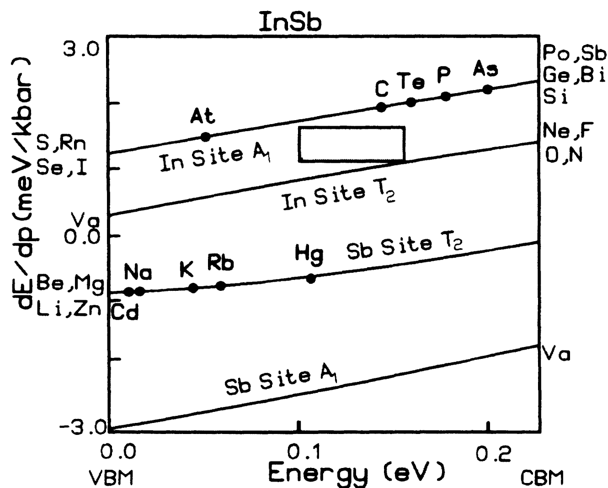

FIG. 2. Pressure coefficients dE/dp in meV/kbar for deep defect levels in InSb as functions of their energies E (in eV) in the band gap. The predicted values of dE/dp and E for specific impurities on particular sites are indicated by circles. On the sides of the figure are impurities expected to produce deep levels in the host bands, but within 0.3 eV of the gap. The boxed, shaded region corresponds to data of Aladashvili *et al.* (Ref. 25).

To illustrate how the theory can be applied to identify deep impurities, consider the deep levels observed by Aladashvili *et al.*[25] near 0.15 eV in InSb, with pressure derivatives of ~ 1 meV/kbar. These levels (see Fig. 2) correspond to either In-site T_2 levels or In-site A_1 levels within the uncertainty of 0.5 meV/kbar. However, no In-site T_2 levels lie at such energies, to within ± 0.3 eV, indicating that the only candidates from the set of s- and p-bonded substitutional impurities for producing these levels are the In-site A_1 levels: S, Rn, Se, I, At, C, Te, P, As, Po, Sb, Ge, Bi, and Si. Thus we have reduced the possibilities to some impurities from Columns IV, V, and VI of the Periodic Table on the In site, producing A_1-symmetric levels.

Two of these defects are very likely to be present in InSb: C and Sb. While C is very likely more soluble on the In site than Sb, the native antisite defect should also be easily formed. In this regard, we note that the concentration of antisite defects should be greatly increased by radiation damage, and so such studies of Aladashvili's deep levels should permit identification of the deep impurity, if it is indeed an antisite defect.

The observation of several deep levels near 0.1 eV probably is due either to the defects being clustered in complexes, or to there being different impurities, such as C and Sb with nearly equal deep-level energies.

In any case, this illustration for InSb shows how hydrostatic-pressure data, when combined with deep-level data, can determine the site of the impurity and the symmetry of the deep level, while simultaneously restricting the candidates for producing the deep level to a few impurities.

The predictions for deep impurities for other zinc-blende semiconductors are given in Figs. 3–13. For the most part we find dE/dp larger for cation-site levels than for anion-site levels, although this situation can be reversed for some (especially T_2 symmetric) levels if the levels are very near the conduction-band edge.

We can understand these calculated results qualitatively by using a defect-molecule model, as shown in Fig. 14. In Fig. 14(a) are shown the In and Sb atomic energy levels. After solid InSb is formed, the atomic energy levels become levels in the solid, as depicted in Fig. 14(b), and their ordering is different from in the free atoms, due to interaction between atoms. Under hydrostatic compres-

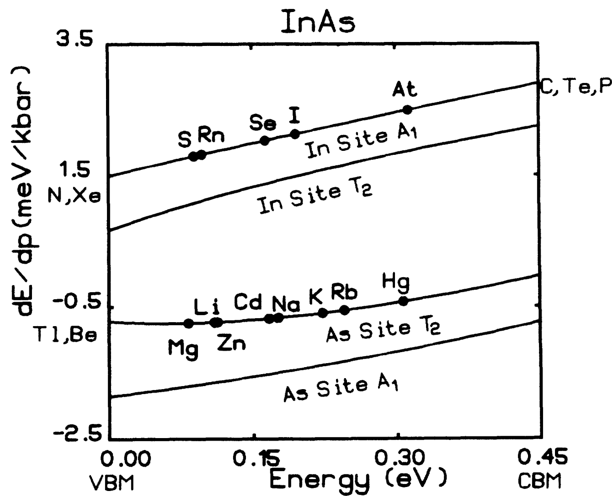

FIG. 3. Pressure coefficients dE/dp in meV/kbar for deep defect levels in InAs as functions of their energies E (in eV) in the band gap.

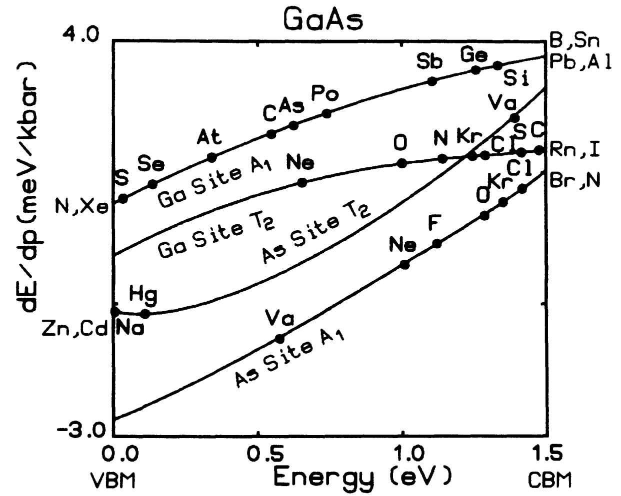

FIG. 6. Pressure coefficients dE/dp in meV/kbar for deep defect levels in GaAs as functions of their energies E (in eV) in the band gap.

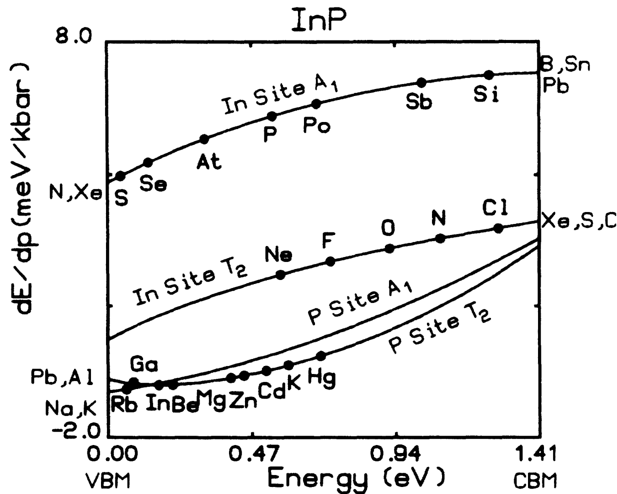

FIG. 4. Pressure coefficients dE/dp in meV/kbar for deep defect levels in InP as functions of their energies E (in eV) in the band gap.

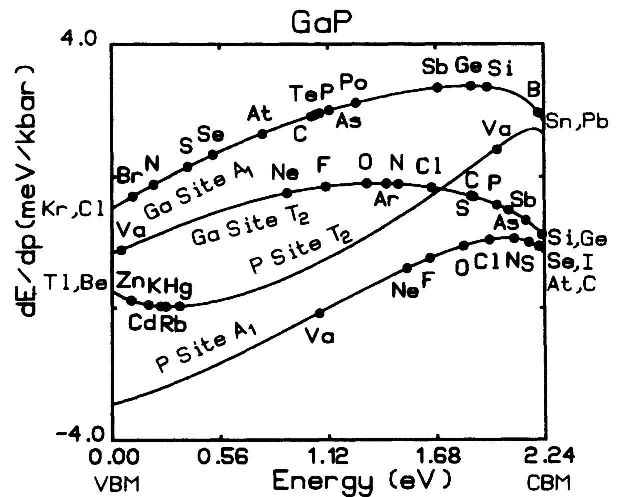

FIG. 7. Pressure coefficients dE/dp in meV/kbar for deep defect levels in GaP as functions of their energies E (in eV) in the band gap.

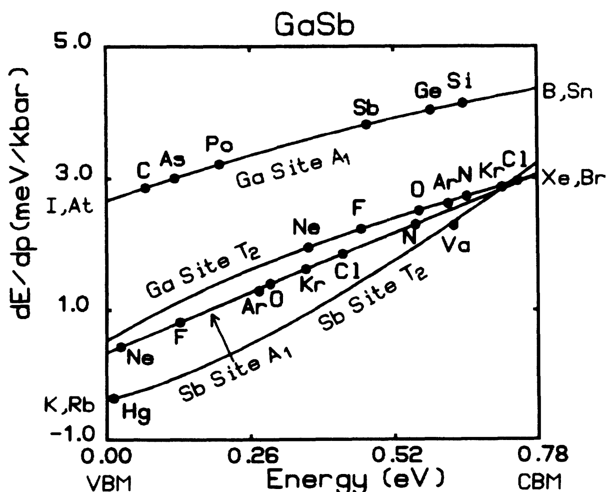

FIG. 5. Pressure coefficients dE/dp in meV/kbar for deep defect levels in GaSb as functions of their energies E (in eV) in the band gap.

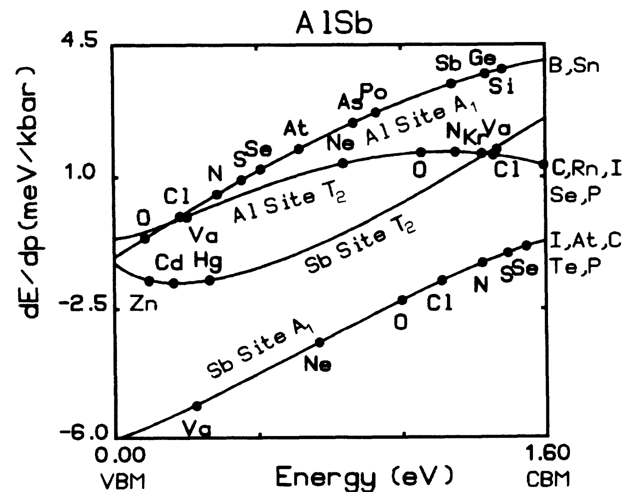

FIG. 8. Pressure coefficients dE/dp in meV/kbar for deep defect levels in AlSb as functions of their energies E (in eV) in the band gap.

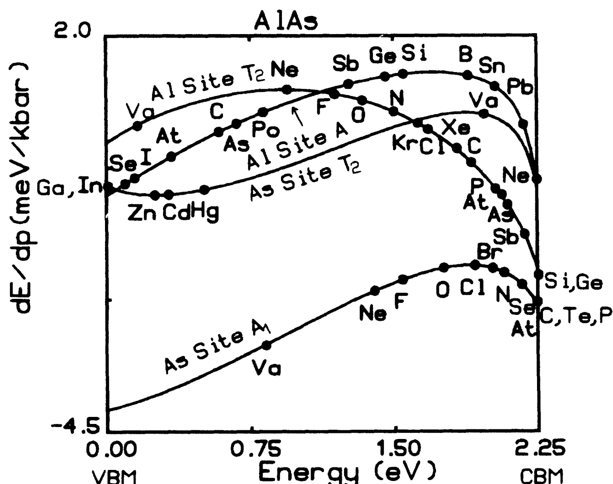

FIG. 9. Pressure coefficients dE/dp in meV/kbar for deep defect levels in AlAs as functions of their energies E (in eV) in the band gap.

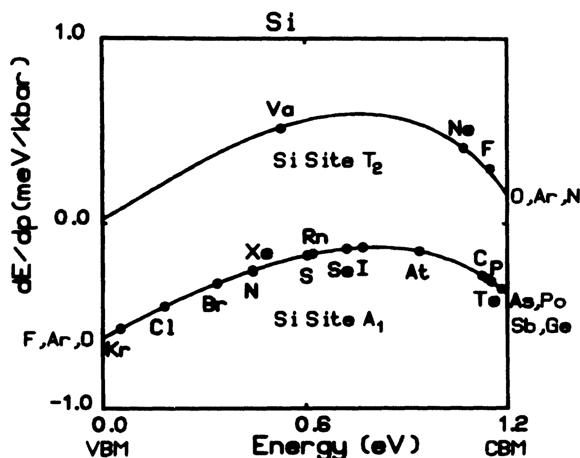

FIG. 12. Pressure coefficients dE/dp in meV/kbar for deep defect levels in Si as functions of their energies E (in eV) in the band gap.

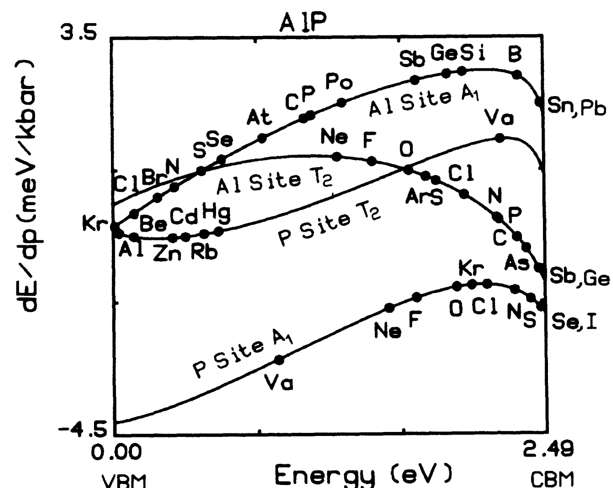

FIG. 10. Pressure coefficients dE/dp in meV/kbar for deep defect levels in AlP as functions of their energies E (in eV) in the band gap.

sion, the interaction between atoms increases, and the levels shift as shown by arrows in Fig. 14(b). (In the solid, these energy levels are energy levels of a defect molecule consisting of one atom and its four nearest neighbors—and so the levels should be thought of qualitatively as representing the center of gravity of the corresponding partial densities of states.) The In T_2 level must move up in energy and the Sb A_1 level must go down, due to level repulsion. The nearest-neighbor coupling dictates that level repulsion cause the In A_1 level to move up—in the opposite direction of Sb A_1. Similarly, the Sb T_2 level moves to lower energy. Since the valence-band maximum has predominantly Sb T_2 character and is taken to be the zero of energy, the pressure

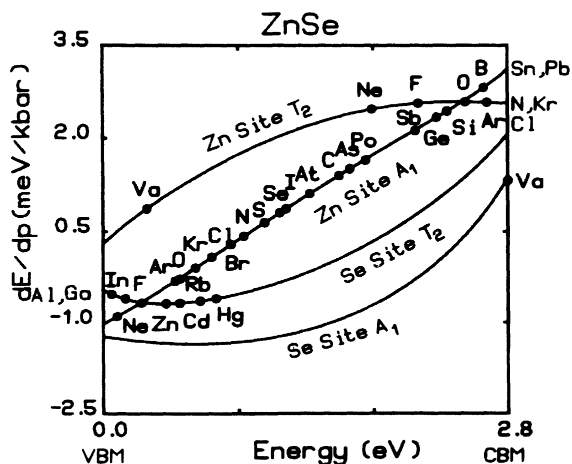

FIG. 11. Pressure coefficients dE/dp in meV/kbar for deep defect levels in ZnSe as functions of their energies E (in eV) in the band gap.

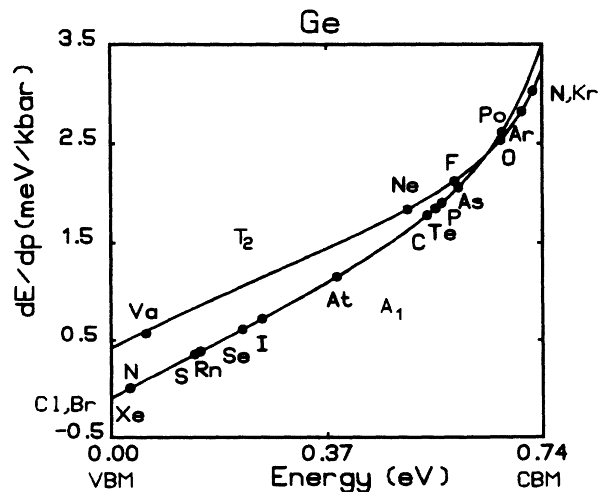

FIG. 13. Pressure coefficients dE/dp in meV/kbar for deep defect levels in Ge as functions of their energies E (in eV) in the band gap.

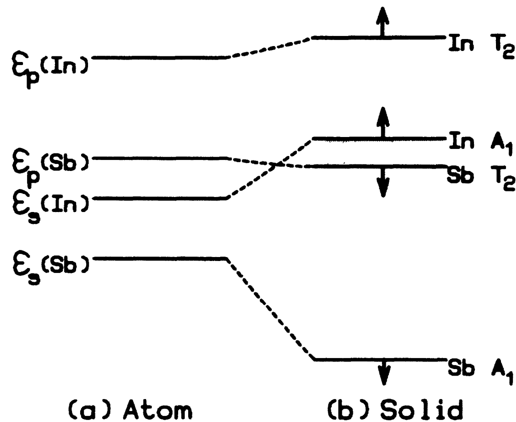

FIG. 14. Defect-molecule model for InSb. (a) Atomic energy levels (s and p orbitals) for In and Sb. (b) In the zinc-blende crystal symmetry, the atomic energy levels form singlet A_1 levels and triplet T_2 levels. The shaded region is approximately the band gap of InSb. The arrows indicate the expected directions of movement of these host levels (and the impurity levels derived from them) when hydrostatic compression is applied to the InSb crystal.

coefficient of the Sb T_2 levels are small in magnitude. The In-site A_1-symmetric impurity levels in the band gap have a larger pressure dependence than In-site T_2 levels, because the A_1 host levels are closer to the gap and hence repel impurity levels more. These general rules normally govern the pressure dependencies of the deep impurity levels—although they are sufficiently qualitative in character that exceptions to them are to be expected.

In summary, we have predicted the hydrostatic-pressure dependencies of deep levels in 12 semiconductors and have shown how pressure data can be analyzed to yield the site of the deep impurity, the symmetry of the deep level, and either the impurity itself or a handful of candidates likely to be the impurity responsible for the deep level.

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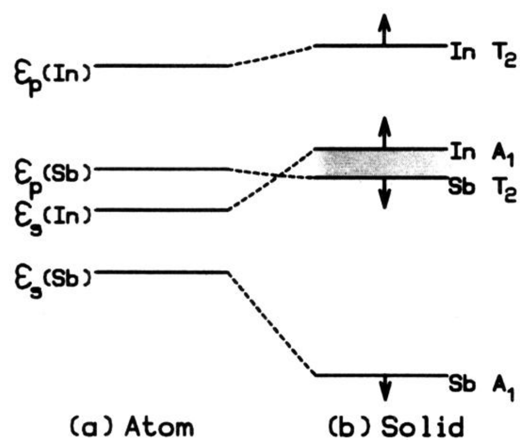

FIG. 14. Defect-molecule model for InSb. (a) Atomic energy levels (s and p orbitals) for In and Sb. (b) In the zinc-blende crystal symmetry, the atomic energy levels form singlet A_1 levels and triplet T_2 levels. The shaded region is approximately the band gap of InSb. The arrows indicate the expected directions of movement of these host levels (and the impurity levels derived from them) when hydrostatic compression is applied to the InSb crystal.

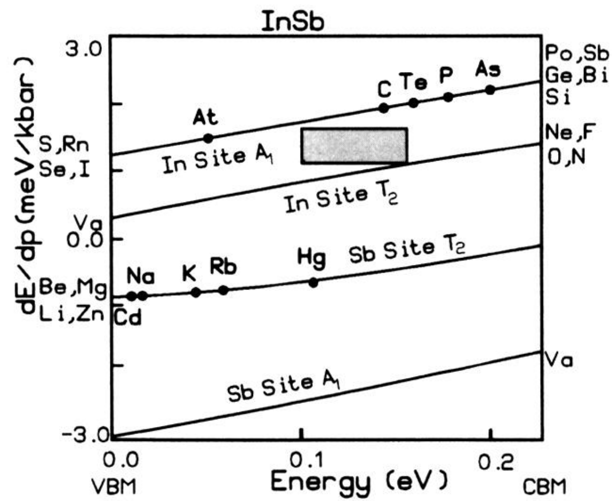

FIG. 2. Pressure coefficients dE/dp in meV/kbar for deep defect levels in InSb as functions of their energies E (in eV) in the band gap. The predicted values of dE/dp and E for specific impurities on particular sites are indicated by circles. On the sides of the figure are impurities expected to produce deep levels in the host bands, but within 0.3 eV of the gap. The boxed, shaded region corresponds to data of Aladashvili *et al.* (Ref. 25).