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Electronic structure and binding energy of the $\mathrm{As_{Ga}}$-As_i pair in GaAs: EL2 and the mobility of interstitial arsenic

G. A. Baraff and M. Schluter
AT&T Bell Laboratories, Murray Hill, New Jersey 07974-2070

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The binding energy and electronic structure of the $\mathrm{As_{Ga}}$-As_i defect pair in GaAs has been calculated using the self-consistent Green's-function technique. The arsenic interstitial ion was placed along a [111] antibonding direction relative to the arsenic antisite ion. At a separation of one bond length, we find that As_i is bound in *n*-type material and unbound in *p*-type. The relative stability of the interstitial defect in the two T_d sites (at a distance of one and two bond lengths from $\mathrm{As_{Ga}}$) also depends on the Fermi energy. These calculations raise questions about, and propose a definitive test for, a recent microscopic model of the structure of EL2.

I. INTRODUCTION

The search for the structure of EL2—a native, metastable defect giving rise to an important midgap level in gallium arsenide[1]—continues. The experimental consensus is the EL2 involves an antisite defect: Its EPR spectrum in that ground configuration is remarkably close to that of the isolated $\mathrm{As_{Ga}}$ antisite,[2] although in some work, an associated gallium vacancy has been reported.[3] Less is known about the structure of EL2 in the metastable configuration that it can reach after optical absorption. This is because the metastable configuration gives rise neither to levels in the gap nor to an EPR spectrum. Since no studies have yet proposed a plausible mechanism by which optical absorption at the isolated antisite can produce the observed metastability, it is speculated that the antisite is present as part of a complex of two or more elementary native defects. Many such models have been proposed,[4–9] most relying on significant atomic displacement near the defect when a transition between the ground configuration and the metastable occurs.

Models involving a vacancy or an interstitial are particularly appealing because both contain especially weak or missing bonds, allowing larger atomic motion in response to a change in electronic state such as optical absorption might produce.

We have earlier calculated the properties of the $\mathrm{As_{Ga}}$-V_{As} nearest-neighbor pair.[6] We found that, in spite of many EL2-like features, it differed from EL2 in having its EPR-active wave function resemble that of the arsenic vacancy, not that of the arsenic antisite. That is, we found that too closely bound a complex destroyed the antisitelike character of the EPR-active wave function.

Recently, von Bardeleben *et al.*[10,11] proposed a heuristic yet microscopic model of EL2 which does seem to account for much of what is known experimentally. Their model is that EL2 consists of the arsenic antisite with an interstitial arsenic atom nearby. In the ground-state configuration, the interstitial atom is sufficiently distant that the nearly isolated antisite is seen. In the metastable configuration, the interstitial moves in close enough that the antisite is no longer identifiable. Additional support for this model is provided in electron-nuclear double resonance (ENDOR) measurements by Spaeth.[12] These are consistent with an arsenic interstitial along the (111) axis from the antisite at a distance of the order of two bond lengths. The levels and the EPR spectrum of the isolated arsenic interstitial have never been seen, so their absence from the experimental signature of the EL2 ground state is not unexpected. However, one of the key conclusions of the present study is that *if* EL2 is this interacting pair with the interstitial where Spaeth's work suggests it should be, then the isolated interstitial levels should have been seen as part of the EL2 ground state. The question of whether or not they have been observed is an open one perhaps, but its answer is essential to the validity of the model.

In the present paper, we present the results of self-consistent Green's-function calculations of the electronic structure and binding energy of the $\mathrm{As_{Ga}}$-As_i pair. Of the two possible locations allowed for the interstitial by the ENDOR measurements, the one in the *antibonding* direction is the one on the shortest migration path to the antisite. Such a path starts at the T_d symmetry site with four arsenic nearest neighbors (a site we shall henceforth designate as T), passes through the puckered hexagon of three arsenics and three galliums (a site we shall henceforth designate as H) and ends near the T_d symmetry location surrounded by four gallium sites (a location we shall henceforth designate as T^*). One of these four gallium sites is now occupied by the $\mathrm{As_{Ga}}$ antisite.

At a separation of two bond lengths, the defects can be assumed not to interact with each other chemically. Their electronic structure is derivable from that of the isolated defects with the help of a simple model we have devised for this purpose. For closer distances, we have carried out Green's-function calculations with the interstitial along the antibonding direction at one bond length distance (the T^* site) and at 1.5 bond length distance (the H site). These calculations motivate and justify the model we devised for use at two bond lengths separation (the T site). The results of these calculations raise some pointed questions about the model proposed for EL2, and suggest a definitive test of it.

In Sec. II, we shall describe briefly some of the details of the Green's-function calculation. Following that, in Sec. III, we review what we have earlier calculated for the electronic structure of the isolated $\mathrm{As}_{\mathrm{Ga}}$,[13,14] and also for the isolated arsenic interstitial[14] at both sites of T_d symmetry (T and T^*), in an otherwise perfect crystal. We review the experimental information about the location of the antisite levels,[2,15] and compare these with what we have calculated. From that comparison, we suggest a level structure for the interstitial (none of which has yet been observed) which is lower in the gap than our earlier calculations[14] had placed it.

In Sec. IV, we present our model of the weakly interacting defects. We deduce the level structure and excitation energies it predicts. From these we can show how the optical excitation lowers the barrier between the neutral ground-state configuration and the neutral metastable configuration of the pair. In Sec. V, we present the results of the Green's-function calculations of the defect pair with the interstitial at T^* and at H. In Sec. VI, we synthesize the results of the calculations presented in Secs. IV and V into a scenario describing the electronic excitation and lattice relaxation expected for the defect pair. We compare this scenario to the experimental properties of EL2. Although this comparison is very encouraging and provides some support for the model of von Bardeleben *et al.*,[10,11] there are still some points for which we cannot at this time provide convincing theoretical justification and some for which genuine problems remain.

II. GREEN'S-FUNCTION CALCULATION: DETAILS

The calculations are done in the Green's-function scheme as described in Ref. 16, with the use of local density theory, the Ceperly-Alder form of the exchange correlation energy, and first-principles pseudopotentials of the Hamann-Schlüter-Chang type.[17] The Green's function used here, with the C_{3v} symmetry appropriate to the antisite-interstitial defect pairs, extends over 30 lattice sites and carries eight Gaussian orbitals per site. This function space is identical to the one used in Refs. 6 and 18. The 30 lattice sites are chosen such that the two defects, all of their nearest neighbors, and all atoms bonded to these nearest neighbors, are included in spatial region treated as the defect. As discussed in Ref. 18, the eight Gaussian orbital set gives less accurate local-density-approximation (LDA) bandstructures; i.e., the gaps are wider and *no* scissors correction is needed ($\Delta=0$). Total energy differences are meaningful only if energies evaluated within the same orbital set are compared. Thus binding energies and migration barriers are evaluated using this C_{3v} Green's function. Formation energies, however, have to be evaluated by using the highly converged results for single site defects[14] as reference. As in Ref. 14 we have not taken lattice relaxations into account explicitly. We expect them to affect our results, e.g., barriers, to less than ~ 0.5 eV and we shall therefore focus on properties unaffected by this uncertainty.

III. REVIEW OF THE PROPERTIES OF THE ISOLATED DEFECTS

A. The isolated antisite

All calculations agree that an isolated anion antisite in a III-V compound semiconductor pulls down an A_1 symmetry state from the conduction band, forming a double donor with two levels, $(0/+)_a$ and $(+/2+)_a$, in the gap. The three charge states, $2+$, $1+$, and 0, result from an occupancy of 0, 1, and 2 electrons in the A_1 state. The difference in energy between these two levels is caused by interelectron repulsion and will be designated as U_a:

$$(0/+)_a-(+/2+)_a\equiv U_a \ . \qquad (3.1)$$

The first measurements[2] of these levels for $\mathrm{As}_{\mathrm{Ga}}$ in GaAs gave $(+/2+)=0.52$ eV and $(0/+)=0.75$ eV (both relative to the top of the valence band) and $U_a=0.23$ eV.

The first calculation of these levels by Bachelet *et al.*[13] found $(0/+)=1.10$ eV and $(+/2+)=0.83$ eV, giving $U=0.27$ eV. Those same calculations predicted a T_2 resonance in the conduction band and an A_1-T_2 splitting of 0.87 eV for $\mathrm{As}_{\mathrm{Ga}}{}^{0}$ (neutral) and 0.99 eV for $\mathrm{As}_{\mathrm{Ga}}{}^{2+}$ (charge $2+$) before Jahn-Teller and breathing relaxation occur. A subsequent calculation,[14] using a more accurate scheme for calculating the charge and for handling the Coulomb tails on the potential,[16] gave $(0/+)=1.50$ eV and $(+/2+)=1.25$ eV with $U_a=0.25$ eV, i.e., *worse* agreement on the levels and essentially no change in U_a. In both calculations,[13,14] we noted that the combination of local-density theory and first-principles pseudopotentials yielded gaps that were too small. We speculated that the empirical procedure we used to raise the conduction band and to correct the gap may incorrectly raise those levels which, like the antisite levels, are derived from conduction bands. There are reasons for suspecting that conduction-band-derived levels calculated in this way are systematically high, but that intradefect excitation energies and level spacings, such as U, are more accurate.

Experimental studies of optical transitions in EL2 have been interpreted as being the $A_1\rightarrow T_2$ transition of the $\mathrm{As}_{\mathrm{Ga}}$ antisite. They occur in the range 1.0—1.3 eV.[19–21] Interpreting the earliest data[22] in this way places the $A_1\rightarrow T_2$ transition at 1.18 eV, and gives 0.14 eV for the Jahn-Teller relaxation energy because the no-phonon transition occurs at 1.04 eV.

B. The isolated arsenic interstitial

Self-consistent Green's function calculation of As_i, the arsenic interstitial, have been carried out[14] with the interstitial at the T^* site (designated as T_{d2} in Ref. 14) and at the T site (designated at T_{d1} there). In both cases there was a state of T_2 symmetry pulled down from the conduction band into the gap and an A_1 state pulled down further, into the valence band. For the neutral defect, the T_2 gap state is occupied by three electrons. The calculated levels (one of which is not accurately placed in Fig. 1 of Ref. 14) are designated $(0/+)_i$, $(+/2+)_i$, and $(2+/3+)_i$. For T^*, they are at 1.30, 0.97, and 0.64 eV, respectively. For T, they are at 1.48, 1.15, and 0.82 eV, respectively, without Jahn-Teller relaxation. The intracenter U_i, the spacing between adjacent levels, is 0.33 eV, essentially independent of site T or T^*. There is no experimental information with which to compare.

It is interesting to note that, *as calculated*,[14] the antisite $(0/+)_a$ level and the T-site interstitial $(0/+)_i$ level are both at virtually the same energy. Both levels were pulled down from the conduction band. Presumably, both are too high relative to experiment. If we drop the calculated interstitial level structure by the amount needed to place the calculated antisite levels into agreement with experiment, acceptor levels $(-/0)_i$ and possibly even $(2-/-)_i$ will be pulled down into the gap. We shall include the possible existence of the single interstitial acceptor level $(-/0)_i$ as a feature of the model that follows.

IV. MODEL FOR DEFECTS IN WEAK INTERACTION

In order to describe the energy of the isolated antisite defect, we specify $N_A=0,1,2$, the occupation number for the A_1 state, and $N_T=0,1$, the occupation number for T_2 state. Although $N_T=2,3,\ldots,6$ are possible, the resulting states will decay so rapidly as to be ignorable at the outset. We expand the total energy of the isolated antisite in terms of these two variables, retaining terms up to second order,

$$E_a(N_A,N_T)=E_a^0+N_A\varepsilon_A+N_T\varepsilon_T+\tfrac{1}{2}(N_A^2U_A+2N_AN_TU_x+N_T^2U_T)\ .$$

The three U terms are basically measures of electron-electron repulsion. The A_1 and T_2 wave functions are not too dissimilar, being different symmetry combinations of antibonding (i.e., node carrying) charge densities in the four (111) *bonding* directions. For this reason, we set all the U terms equal to each other: $U_A=U_x=U_T=0.23$ eV, the experimental (and, to within 0.02 eV, our calculated) value. The additive energy E_a^0 plays no role: in all generality, we can set it to zero. Thus, the energy of the isolated antisite is

$$E_a(N_A,N_T)=N_A\varepsilon_A+N_T\varepsilon_T+\tfrac{1}{2}(N_A+N_T)^2U_a\ , \tag{4.1a}$$

$$U_a=0.23\text{ eV}\ . \tag{4.1b}$$

The levels of the isolated antisite (the energies required to add electrons to the defect from the top of the valence band) are by definition, given by

$$(+/2+)_a\equiv E_a(1,0)-E_a(0,0)=\varepsilon_A+\tfrac{1}{2}U_a\ , \tag{4.2a}$$

$$(0/+)_a\equiv E_a(2,0)-E_a(1,0)=\varepsilon_A+\tfrac{3}{2}U_a\ , \tag{4.2b}$$

from which we have $(0/+)_a-(+/2+)_a=U_a$, in agreement with (3.1).

There are also intracenter excitations. In the neutral state, we have

$$\varepsilon^0(A_1\to T_2)\equiv E_a(1,1)-E_a(2,0)=\varepsilon_T-\varepsilon_A\ , \tag{4.3a}$$

and in the charge 1 + state, we have

$$\varepsilon^{1+}(A_1\to T_2)=E_a(0,1)-E_a(1,0)=\varepsilon_T-\varepsilon_A\ . \tag{4.3b}$$

(The degeneracy between these two excitation energies is the result of our idealization that $U_A=U_x=U_T$).

This model is too simple to include relaxation of the Jahn-Teller type after the T_2 level is occupied. In reality, the $A_1\to T_2$ excitation occurs over a band of energies. However, for simplicity, we shall choose $\varepsilon^0(A_1\to T_2)$ to reproduce the lowest energy in that band, the no-phonon transition energy. Therefore, we take the experimental value.

$$\varepsilon_T-\varepsilon_A=1.04\text{ eV}\ . \tag{4.3c}$$

Next we turn to a description of the isolated interstitial. We allow it to move along the antibonding (111) direction through any unit cell. At both the T site and the T^* sites in that cell, the system has T_d symmetry. We can describe the defect by specifying $N_T=2,3,4$, the occupation number for the T_2 state. (Again, the other possible occupation numbers, $N_T=0,1,5,6$, are energetically uninteresting here.) At positions along that line other than T^* and T, the symmetry drops to C_{3v}, and the T_2 state splits into an A and E. Between T and T^*, A drops and E rises about half as much. To describe this situation, we replace N_T by N_A+N_E, denoting how the electrons in the T_2 manifold are distributed between its A component and its E component.

At the position of interest for this study, the A manifold is lower in energy than the E and therefore, under the restriction $N_T=2,3,4$, we have $N_A=2$ and $N_E=0,1,2$. To describe the defect then, we need only to specify R, its position along the line, and N_E, the occupation of its E state.

Again, we expand the energy of the interstitial to second order in the occupation number

$$E_i(N_E,R)=E_i^0(R)+N_E\varepsilon_E(R)+\tfrac{1}{2}N_E^2U_E(R)\ . \tag{4.4}$$

In the restricted occupancy range, we have two levels for the isolated interstitial, namely,

$$(-/0)_i\equiv E_i(2,R)-E_i(1,R)=\varepsilon_E(R)+\tfrac{3}{2}U_E(R)\ , \tag{4.5a}$$

$$(0/+)_i=E_i(1,R)-E_i(0,R)=\varepsilon_E(R)+\tfrac{1}{2}U_E(R)\ , \tag{4.5b}$$

from which

$$U_i\equiv(-/0)_i-(0/+)_i=U_E(R)\ . \tag{4.5c}$$

Our calculation of the isolated interstitial at the T and T^* site gave $U_i=0.33$ eV, essentially site independent. We shall discard the possibility that U_i changes appreciably from this value at intermediate locations, such as H, where the environment is somewhat different than at T or T^*. Therefore we take $U_E(R)=0.33$ eV, independent of R. Equation (4.5) becomes

$$(-/0)_i=\varepsilon_E(R)+\tfrac{3}{2}U_i\ , \tag{4.6a}$$

$$(0/+)_i=\varepsilon_E(R)+\tfrac{1}{2}U_i\ , \tag{4.6b}$$

$$U_i=0.33\text{ eV}\ . \tag{4.6c}$$

Now let us consider the defects in interaction. The interaction energy depends on all the variables of the problem:

$$V_R = V(N_A, N_T, N_E, R) \ .$$

In the large-R limit, where the defects are too far apart to interact via rebonding or less strongly, via mutual polarization, the interaction energy must go to the Coulomb limit

$$V_{R\to\infty} = Q_i Q_a / \epsilon R \ ,$$

where Q_i and Q_a, the charge of the interstitial and of the antisite, are given by

$$Q_i = -(N_E - 1) \ , \qquad (4.7a)$$

$$Q_a = -(N_A + N_T - 2) \ . \qquad (4.7b)$$

Thus,

$$V_{R\to\infty} = (N_A + N_T - 2)(N_E + 1)/\epsilon R \ .$$

At smaller values of R, deviations from this form will set in. Our Green's-function calculations (Sec. V) show no serious chemical rebonding effects occurring at the H site, and so we feel confident in using the model at H, at T, and beyond. The total energy for the interacting defect pair, and its total charge $Q = Q_i + Q_a$, is therefore

$$\begin{aligned} E(N_A, N_T, N_E, R) = {} & N_A \varepsilon_A + N_T \varepsilon_T + \tfrac{1}{2}(N_A + N_E)^2 U_a \\ & + E_i^0(R) + N_E \varepsilon_E(R) + \tfrac{1}{2} N_E^2 U_i \\ & + (N_A + N_T - 2)(N_E - 1)/\epsilon R \ , \end{aligned} \qquad (4.8)$$

$$Q = -(N_A + N_T + N_E - 3) \ . \qquad (4.9)$$

For each total charge Q, these are several choices of occupation numbers possible from within the set $N_A = 0,1,2$; $N_T = 0,1$; and $N_E = 0,1,2$. One of these choices will yield the lowest energy, which is the ground state. The difference between this and the other energies gives various excitations of the system.

We start with the $+\,1$ charge state for which there are five possible sets of occupation numbers. We designate the energies as E_j^+. Each index j is associated with an occupation number set as described in Table I. The occupation and energies are also shown pictorially in Fig. 1. We evaluate the total energies in (4.8), and take their differences, using (4.2) and (4.5) to express these differences in the form

$$E_5^+ - E_2^+ = \varepsilon_T - \varepsilon_A \ , \qquad (4.10a)$$

$$E_4^+ - E_1^+ = \varepsilon_T - \varepsilon_A \ , \qquad (4.10b)$$

$$E_2^+ - E_1^+ = (0/+)_a - (0/+)_i \ , \qquad (4.10c)$$

$$E_3^+ - E_1^+ = (-/0)_i - (+/2+)_a - 2/\epsilon R \ . \qquad (4.10d)$$

Equations (4.10a) and (4.10b) show that neither $j=5$ nor $j=4$ can be the ground state. Of the remaining three possibilities, $j=1,2,3$, only $j=1$ will be EPR active. Since it is known that EL2 in its ground state of charge $1+$ exhibits an EPR spectrum, the defect pair can be EL2 only if E_1^+ is the ground state. Assuming that this is so, (4.10c) gives

$$(0/+)_a - (0/+)_i > 0 \ , \qquad (4.11a)$$

while (4.10d) gives

$$(-/0)_i > (+/2+)_a + 2/\epsilon R \ ,$$

which we can rearrange to

$$(0/+)_a - (0/+)_i < U_a + U_i - 2/\epsilon R \ . \qquad (4.11b)$$

Using a bond length of 2.45 Å and an $\varepsilon = 12.85$ (Ref. 23) we have $2/\epsilon R = 0.46$ eV at $R = 2$ bond lengths. Thus there is a very tight limit on these levels, namely

$$0 < (0/+)_a - (0/+)_i < 0.23 + 0.33 - 0.46 = 0.10 \text{ eV} \ . \qquad (4.12)$$

TABLE I. Occupation number values for the $1+$ charged defect pair.

J	N_A	N_T	N_E	Q_a	Q_i
1	1	0	1	$1+$	0
2	2	0	0	0	$1+$
3	0	0	2	$2+$	$1-$
4	0	1	1	$1+$	0
5	1	1	0	0	$1+$

Our earlier calculation of these levels[14] satisfies this constraint although, as we remarked earlier, the calculated antisite levels are much higher than the experimental values.

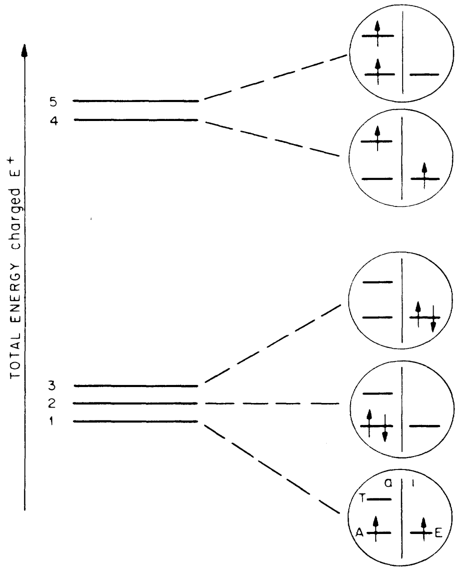

FIG. 1. Occupancies and total energies for the $\mathrm{As_{Ga}}$-As_i defect pair in the state of overall charge $+\,1$. The total energies are deduced from the occupancies using the total energies given by the expression 4.8 and the *assumption* that if the pair is indeed EL2, the ground state must be EPR active.

It is interesting to note that the two unpaired electrons for the $j=1$ ground state will give rise to two EPR spectra. One will be that of $\mathrm{As_{Ga}}^+$. The other is linked to As_i. It will show a *very* small central hyperfine interaction because the E state has a node on the arsenic interstitial. It will show four arsenic ligands at one bond length distance. Such as spectrum might be mistaken for a gallium vacancy.[24] The pair $\mathrm{As_{Ga}}$-$\mathrm{V_{Ga}}$ has been reported in EPR spectra by Goltzene *et al.*[3] in neutron irradiated material.

Now we consider the neutral states of the pair. There are again five possible occupations. We designate the resulting energies as E_j^0. Each index j is associated with a set of occupation numbers according to Table II. Figure 2 summarizes this information pictorially. The energy differences are now

$$E_5^0-E_2^0=\varepsilon_T-\varepsilon_A\ , \tag{4.13a}$$

$$E_3^0-E_1^0=\varepsilon_T-\varepsilon_A\ , \tag{4.13b}$$

$$E_2^0-E_1^0=U_i-\frac{1}{\epsilon R}-[(0/+)_a-(0/+)_i]\ , \tag{4.13c}$$

$$E_3^0-E_4^0=\frac{1}{\epsilon R}-U_a-[(0/+)_a-(0/+)_i]\ . \tag{4.13d}$$

All the quantities on the right of (4.13) have been previously evaluated, and we deduce that E_1^0 and E_2^0 are close in energy (within 0.1 eV) and low, while E_3^0, E_4^0, and E_5^0 are also close in energy, and high.

Of the two possible ground states ($j=1$ and $j=2$), one, $j=2$, will exhibit the $\mathrm{As_{Ga}}^+$ EPR spectrum. However, the $\mathrm{As_{Ga}}^+$ EPR spectrum does *not* appear for the neutral EL2 defect. If the pair is EL2, then $j=1$ must be the ground state. Returning to (4.13c), this requires that

$$[(0/+)_a-(0/+)_i]<U_i-1/\epsilon R=0.33-0.23$$
$$=0.10\ \mathrm{eV}\ . \tag{4.14}$$

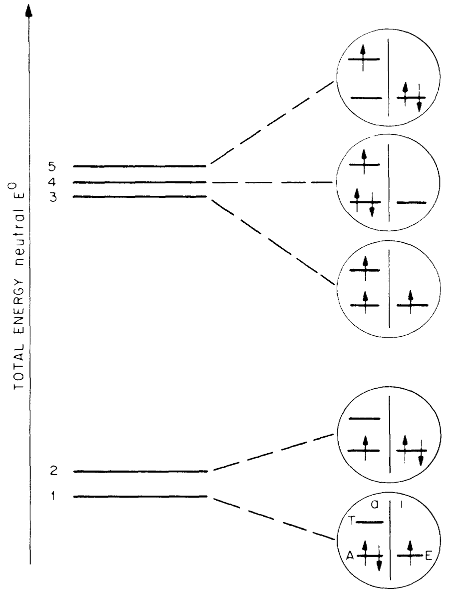

FIG. 2. Same as Fig. 1 but for the neutral state of the pair, which has no unpaired electron on the antisite.

TABLE II. Occupation number values for the neutral defect pair.

J	N_A	N_T	N_E	Q_a	Q_i
1	2	0	1	0	0
2	1	0	2	1+	1−
3	1	1	1	0	0
4	2	1	0	1−	1+
5	0	1	2	1+	1−

The condition (4.14) is independent of the condition (4.12), although if (4.12) is satisfied, (4.14) will be also.

Now let us list the various excitations out of E_1^0, ranking them in the order of their likely importance.

(1) $E_1^0\to E_3^0$ at 1.04 eV. As shown by Fig. 2, this is the $A_1\to T_2$ transition of the neutral antisite, with the neutral interstitial playing no role. It is optically allowed. The two wave functions of the antisite overlap strongly.

(2) $E_1^0\to E_2^0$ at ≈ 0.1 eV. This is a charge transfer excitation resulting in $\mathrm{As_{Ga}}^+$ and $\mathrm{As}_i{}^-$. It is inhibited by the small overlap between the A_1 antisite wave function and the rather distant interstitial E wave function. It is a less likely transition than $E_1^0\to E_3^0$. The near degeneracy of E_1^0 and E_2^0 suggests that in a multielectron calculation, there might be an appreciable amount of E_2^0 mixed into the ground state. Such a mixing might provide the attraction needed to bind this pair of defects, but we put this suggestion forth only as a speculation.

(3) $E_1^0\to E_4^0$ at ≈ 1.1 eV. This a charge-transfer excitation resulting in $\mathrm{As_{Ga}}^-$ and $\mathrm{As_I}{}^+$—a dipole in the opposite sense from the previous one. It is inhibited both by small wave-function overlap (although the T_2-E overlap is slightly greater than the A_1-E overlap because T_2 is a resonance while the A_1 is a true bound state) and the need for a photon to supply the energy.

(4) $E_1^0\to E_5^0\approx 1.1$ eV. This is the least likely of all. It has charge transfer, needs a photon, and in addition, it is a two electron transition.

In addition to these, the E_1^0 ground state can be ionized to one of the states in the $Q=1+$ manifold plus an electron in the conduction bond.

We now enumerate the various decay possibilities for the E_3^0 excited state which results from the $A_1\to T_2$ transition at the neutral antisite, the only strong transition of the four.

(1) $E_3^0\to E_1^0$. This would be the radiative transition back to the ground state, and is expected to be strong.

(2) $E_3^0\to(\mathrm{As_{Ga}}+\mathrm{As}_i)^++e^-$. As a resonance in the conduction band, the $A_1\to T_2$ transition is sufficiently long lived that individual phonon peaks can be resolved.[22] Nonetheless, as a resonance, there is finite probability for the electron to leave the defect and enter the conduction band where subsequent scatter can relax its energy down to the band minimum.

(3) $E_3^0\to E_4^0$. This is a one-electron charge transfer, resulting in $\mathrm{As_{Ga}}^-$ and $\mathrm{As}_i{}^+$. It is inhibited by small wave

function overlap, but it is nearly a zero energy transition, which helps it. [According to Eq. (4.13d), and the numbers we have obtained for the terms on the right, $E_3^0 \rightarrow E_4^0$ is not a decay, it is very low energy excitation. The model contains approximations, however, and the relative ordering of two levels this close can really not be definitively stated. We must therefore consider this decay as a possibility instead of firmly ruling it out.]

(4) $E_3^0 \rightarrow E_5^0$. This is also a nearly zero energy, one electron charge transfer, so the above discussion applies. The only difference is that the charge transfer occurs in the opposite direction, giving $\mathrm{As_{Ga}}^+$ and $\mathrm{As}_i{}^-$.

(5) $E_3^0 \rightarrow E_2^0$. This is the least likely decay, involving as it does, both charge transfer and a mechanism to dispose of about 1 eV.

There are several intra-center decay processes available to E_4^0 and E_5^0, in the event that either is reached as a result of E_3^0 decay.

$E_5^0 \rightarrow E_2^0$ is the $T_2 \rightarrow A_1$ transition at the $(\mathrm{As_{Ga}})^+$ and is strongly allowed. The other decay channel, $E_5^0 \rightarrow E_1^0$ is exceedingly slow, involving two electron transitions, one of which is a charge transfer, and the need, moreover to dispose of 1.1 eV.

$E_4^0 \rightarrow E_1^0$ involves charge transfer of one electron and disposal of 1.1 eV, and so is likely to be slow. $E_4^0 \rightarrow E_2^0$ involves transfer of two electrons and will be slower still. We conclude that if E_4^0 is reached via decay of E_3^0 it will be long lived. However, if the interstitial migrates to T^*, wave-function overlaps will be much greater and the electronically excited states would then decay to their electronic ground state.

Having obtained the excitation energies and decay schemes for the neutral defect, we turn now to other charge states. The intent here is solely to identify the ground-state configurations, so that we may calculate the levels in the gap. Therefore, we consider the three possibilities for the $Q = 2+$ charge state of the pair, as given by Table III,and the three possibilities for the $Q = 1-$ state of the pair, as given by Table IV. The energies are denoted E_j^{2+} and E_j^-, respectively. By using (4.8) to evaluate energy differences, we find that $j = 1$ is the ground state for the $2+$ charged pair and that $j = 2$ is the ground state for the $1-$ charged-state pair.

For the four charge states of the pair, the four ground-state energies are E_1^{2+}, E_1^+, E_1^0, and E_2^-. The differences between them are, by definition, the levels of the pair, i.e., the energy needed to add an electron from the valence band to the pair. These levels are indicated in Fig. 3:

$$(+/2+)_p \equiv E_1^+ - E_1^{2+} = (0/+)_i - 1/\epsilon R \ , \tag{4.15a}$$

$$(0/+)_p \equiv E_1^0 - E_1^+ = (0/+)_a \ , \tag{4.15b}$$

TABLE III. Occupation numbers for the 2 + charged defect pair.

J	N_A	N_T	N_E	Q_a	Q_i
1	1	0	0	1+	1+
2	0	1	0	1+	1+
3	0	0	1	2+	0

TABLE IV. Occupation numbers for the 1 − charged defect pair.

J	N_A	N_T	N_E	Q_a	Q_i
1	2	1	1	1−	0
2	2	0	2	0	1−
3	1	1	2	0	1−

$$(-/0)_p = E_2^- - E_1^0 = (-/0)_i \ . \tag{4.15c}$$

Starting with the 2 + state $(\mathrm{As_{Ga}}^+ : \mathrm{As}_i{}^+)$ the first electron is captured by the interstitial, resulting in $(\mathrm{As_{Ga}}^+ : \mathrm{As}_i{}^0)$. The second electron is captured by the antisite giving $(\mathrm{As_{Ga}}^0 : \mathrm{As}_i{}^0)$ and the last electron is captured again by the interstitial, giving $(\mathrm{As_{Ga}}^0 : \mathrm{As}_i{}^-)$. It is an interesting coincidence that, due to the accidental equality between U_a and $1/\epsilon R$, if (4.12) is true, the $(+/2+)_p$ energy, which can be expressed as

$$(+/2+)_p = (+/2+)_a + U_a - 1/\epsilon R - [(0/+)_a - (0/+)_i]$$

is very close to the isolated antisite $(+/2+)_a$ level.

We now consider the possibility that the interstitial at the T site migrates to the T^* site, encountering an energy barrier at the H site enroute. In so far as this defect pair is to be a model for EL2, the question to be addressed is, "How does the optical absorption at 1.1 eV help the neutral defect over the barrer?"

For the neutral defect pair, we found that the ground-state energy was $E_1^0(R)$. (We now make the position dependence explicit.) The ground-state barrier for the neutral system is denoted B. Setting $R = 1.5$ bond lengths (H), or two bond lengths (T), we have, by definition, that

$$B = E_1^0(H) - E_1^0(T) \ .$$

The barrier for the neutral system in the electronically excited state j $(=2,3,4,5)$ is

$$B_j \equiv E_j^0(H) - E_j^0(T) \equiv B + \Delta B_j$$

and so the amount by which the barrier height has been changed is

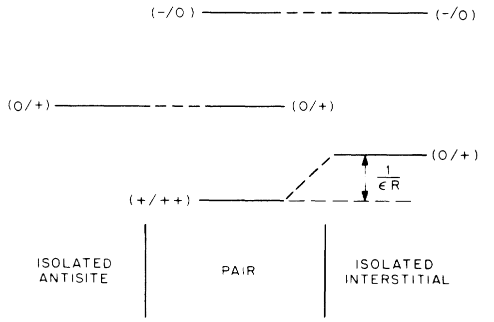

FIG. 3. Levels for the defect pair with the interstitial at T. This is supposed to be the ground-state configuration for EL2. The relationship between these levels and those of the isolated defects is shown.

$$\Delta B_j=[E_j^0(H)-E_1^0(H)]-[E_j^0(T)-E_1^0(T)] . \qquad (4.16)$$

We evaluate this using the energy expression (4.8) and the occupation numbers given in Table II, with the result that

$$\Delta B_2=+\Delta E_m-\Delta E_c , \qquad (4.17a)$$

$$\Delta B_3=0 , \qquad (4.17b)$$

$$\Delta B_4=-\Delta E_m-\Delta E_c , \qquad (4.17c)$$

$$\Delta B_5=+\Delta E_m-\Delta E_c , \qquad (4.17d)$$

where

$$\Delta E_m \equiv \varepsilon_E(H)-\varepsilon_E(T) \approx 0.4 \text{ eV} \qquad (4.18a)$$

as estimated from our Green's-function calculations and

$$\Delta E_c \equiv (1/\epsilon R)_H-(1/\epsilon R)_T=0.08 \text{ eV} . \qquad (4.18b)$$

In the three excited states for which $\Delta B_j \neq 0$, the excited state E_j^0 is one in which a charge transfer has occurred, just as Samuelson and Omling[25] had suggested might happen after the initial optical excitation. The term ΔE_c is the barrier lowering caused by the attraction between the charged defects. However, even if one reduces the value of ε at H (arguing that the screening becomes less at small distances) so as to make the Coulomb lowering larger, the Coulomb term is still small compared to ΔE_m. ΔE_m arises from the charge-state dependence of the barrier for interstitial migration, an effect which is present even in the infinite crystal. This can be understood as follows: The $T \rightarrow H \rightarrow T^*$ migration of As_i in the infinite crystal and $T \rightarrow H \rightarrow T$ migration of the self-interstitial in silicon[26] are qualitatively similar. In both cases, there is a T_2 state high in the gap. This state splits into an A component which drops, and an E component which rises, as the interstitial reaches the H point. Whatever barrier exists with no electrons on the defect is lowered by the presence of the first electron, and is lowered even further by the presence of the second. (Both of these go into the A state which drops as the barrier is approached.) However, placing a third electron on the defect starts to raise the barrier again, because the E state that it occupies rises as the barrier is approached. Thus, $\text{Si}_i{}^0$ in silicon and $\text{As}_i{}^+$ in As_{Ga}, both of which have two electrons in the A state, have the lowest barriers. The migration barrier for $\text{As}_i{}^0$ exceeds that of $\text{As}_i{}^+$ by exactly ΔE_m.

Now to return to (4.17): The interstitial in the ground state $j=1$ migrates as the neutral species $\text{As}_i{}^0$ with one electron in the E state. In the excited states $j=2$ and $j=5$, it migrates as $\text{As}_i{}^-$. The extra electron in the E state raises the barrier by ΔE_m. In the excited state $j=4$, it migrates as $\text{As}_i{}^+$, with a barrier that is ΔE_m lower. Thus, one of the four excited states, $j=4$, does have a lowered barrier and the lowering is of the order of 0.5 eV.

It is obvious that the optical excitation $E_1^0 \rightarrow E_3^0$ occurs on the antisite creating a hole on the A level. This lowers the barrier only if the long-lived state E_4^0 can be reached from E_3^0 (i.e., by charge transfer from the interstitial to fill the hole.) As was remarked earlier, the simple model here *barely* fails to place E_4^0 below E_3^0. We regard the above scenario as a likely answer to the question of how excitation at the antisite lowers the barrier for interstitial migration. It does so by creating a hole to which the interstitial can lose an electron at no energy cost and thus cross the barrier as the positively charged species.

We turn now to the results of Green's-function calculations.

V. GREEN'S-FUNCTION CALCULATION: RESULTS

Even at the small separation of one bond length, the electronic structure of the defect pair is a recognizable combination of the states of the two noninteracting defects. With each isolated defect in a site of T_d symmetry, there are two wave functions in the gap, the antisite A_1 and the interstitial T_2. The corresponding interstitial A_1 state, well below the T_2, is a valence-band resonance that plays no role other than to hold two of the five electrons needed for the neutral arsenic.

In the C_{3v} symmetry of the defect pair, the T_2 splits into an A and an E. This A and the antisite A_1 form bonding and antibonding combinations. The E state is noninteracting.

Calculations using the C_{3v} symmetry wave function with the interstitial at the T^* site give the eigenvalues listed below. (These eigenvalues are not the same as levels. Levels can be obtained from eigenvalues calculated using half-integer, rather than integer, values of the occupation numbers.) The isolated $\text{As}_{\text{Ga}}{}^+$ eigenvalue is at 1.15 eV. The isolated $\text{As}_i{}^0$ eigenvalue is at 1.14 eV. For the defects interacting, the bonding and antibonding states of the $(\text{As}_{\text{Ga}}-\text{As}_i)^+$ pair are at 0.55 and 1.37 eV, a splitting of 0.82 eV. The average energy of the bonding and antibonding pair is 0.96 eV, lower by 0.18 eV than the average energy of the infinitely separated pair. The E state of the interacting pair is at 0.81 eV, lower by 0.33 eV than the T_2 eigenvalue of the isolated $\text{As}_i{}^0$. There are no unpaired electrons here and no EPR signal, as there was when the interstitial was at T.

Putting an additional electron in to get $(\text{As}_{\text{Ga}}+\text{As}_i)^0$ raises the bonding A eigenvalue by 0.43 to 0.98 eV and raises the E eigenvalue by 0.56 to 1.36 eV. However, the unpaired electron goes into the E state, which is entirely As_i. This level structure therefore gives no occupancy at which an As_{Ga}-like EPR signal can be seen. This is in agreement with the proposed EL2 model where the interstitial close to the antisite is the metastable state of EL2, which experimentally has no EPR spectrum.

The calculated level structure here does pose a problem for the EL2 model in that this defect certainly has a $(0/+)$ level in the gap. As calculated, there will also be a $(+/2+)$ level in the gap. However, if the entire level structure is lowered (on the assumption that local density theory has again put the levels too high), then this $(+/2+)$ level might disappear, but a $(-/0)$ level (the filling of the fourth E state) will certainly then be present. In either case, there are levels in the gap associated with this configuration whereas experimentally, the EL2 metastable has none. If the EL2 model of von Bardeleben *et al.*[10] is correct, the interstitial arsenic must choose another location near the antisite, one where all the levels are swept out of the gap. We do not know if such a position exists.

We now turn to the binding energy of this defect pair with the interstitial at T^*: This was calculated by comparing the total energy of the three defects, namely the isolated $\mathrm{As_{Ga}}$, the isolated As_i, and the pair. The difference is the binding energy, counted as positive if the pair is of lower energy than the sum of the separated defects. The binding energy is Fermi-level dependent, because the transition from interacting defects to separated defects involves transfer of electrons between the defects and a Fermi reservoir. As is shown in Fig. 4, the pair is bound in n-type material and unbound in p type. At some intermediate value of μ, the binding energy might be only slightly negative, as is appropriate for a metastable situation. However, the remark cannot be regarded as a comment on the proposed EL2 model because, as we noted earlier, the presence of levels in the gap rules out this geometry as a description of the EL2 metastable configuration. If the levels are swept out of the gap in the new geometry, the μ dependence of binding energy may be quite different from what is found here.

We now consider the interstitial at the H site. The isolated interstitial is already at a site of C_{3v} symmetry, with its T_2 level split into an A, which should be low, and an E, which should be above the original T_2. Again the A and the antisite A_1 form bonding and antibonding combinations. Due to the greater separation, the added splitting will be much less and the separation will be determined more by the position of the noninteracting states. Again, the E will not have a state with which to interact.

Calculations using the C_{3v} symmetry Green's function give the eigenvalues listed below for the charge state $1+$. The bonding state, which is all interstitial A_1, is at 0.32 eV, the E state, which is also all interstitial, is at 1.54 eV. The original T_2 state, if the A had dropped twice as far as the E had risen, would have been at 1.05 eV, which is 0.09 eV lower than for the isolated defect. That is, the proximity lowering of the E state is reduced from 0.33 eV at T^* to 0.09 here, while the crystal field splitting has raised the E state by 0.41 eV. The agreement here reinforces the description of the two defects as being almost independent at the H site separation.

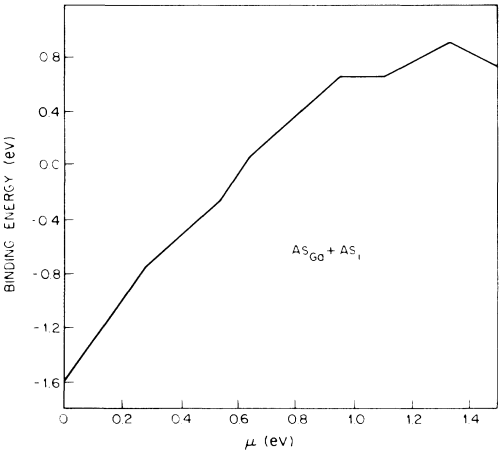

FIG. 4. Binding energy of the defect pair with the interstitial at the T^* site. The pair is bound (positive binding energy) in n-type material but unbound in p type.

The occupancy at H is unusual, in that there is an occupied eigenvalue (the E) above one (the A state at 1.37 eV) that could hold another electron. It turns out that the two states—the antisite A and the interstitital E—are close enough energetically and separated enough spatially that if we put the E electron on the A state, the antisite A eigenvalue goes up because of the change in potential there, while the interstitial A and E eigenvalue drop. This leaves the empty E below A. In either case, we have an unoccupied state below a full one. We have encountered this same problem and discussed the solution in studying the divacancy in GaAs.[18]

The total energy of the pair is now much greater than that of isolated defects, no matter what the Fermi energy. Therefore the H position is, at best, near a barrier for the interstitial migration.

In order to estimate the binding energy of the pair with the interstitial at the T site, we use the formation energy calculation from Ref. 14 to obtain the energy difference between an isolated interstitial at a T site and an isolated interstitial at a T^* site in an otherwise perfect crystal. Since the zero reference for binding energy is an isolated antisite plus an isolated interstitial in a distant T^* site, and since, according to the model of Sec. IV, the only interaction between the defects at this separation is Coulom-

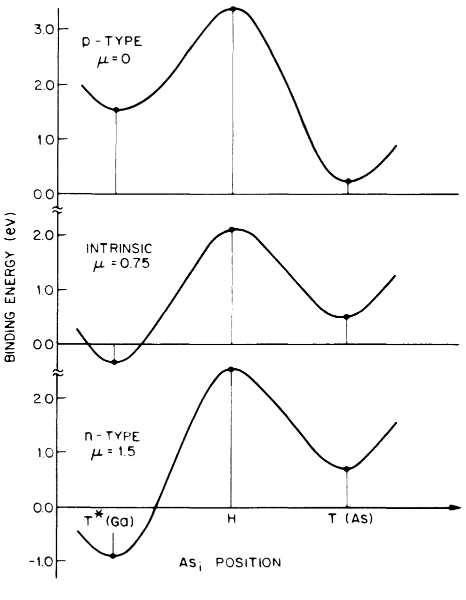

FIG. 5. Fermi level dependence of the calculated total energy. Within the local-density approximation, the pair is never stable with the interstitial at T. However, the binding needed to keep the interstitial at T might appear in a calculation in which correlation is included, because there is a very low energy charge-transfer state present which, within LDA, plays no role but which, in a multiconfiguration calculation, might lower the energy.

bic, we can obtain the binding energy we need.

The three binding energies, at the T^* site, at the H site, and at the T site, are plotted for $U=0$, 0.75, and 1.5 eV in Fig. 5, where a smooth curve has been interpolated through to show what these curves imply for binding and migration of the interstitial. There is no atomic relaxation, either due to size mismatch or atomic distortion, included in these values. Our experience with the silicon self-interstitial suggests that the barrier at H would be lower by about 0.5 eV if atomic relaxation had been taken into account. The problem that Fig. 5 poses for the defect pair model of EL2 is that it does not lead to binding at the T site. That is, although the EL2 metastable (the interstitial somewhere near the T^* site) can be bound in n-type material, there is no reason why the EL2 ground state (the interstitial near the T site) will stay bound within the local-density approximation. (We have offered, in Sec. IV, a reason why a multielectron calculation might give binding at T.)

VI. EL2 SCENARIOS AND SUMMARY

Let us first summarize our findings to this point, and then we shall discuss what support and problems they pose for the ($\mathrm{As_{Ga}}$-As_i) pair model for EL2.

Some of what we have found depends on detailed energy and level calculations. Some depends on the symmetries, degeneracies, and splittings of states in the gap. Some depends upon the idea that the interstitial-antisite interaction already is in its large separation limit at two bond lengths distance. Some depends on the assumption that the model is correct; that the ground state of EL2 is the pair with the interstitial near the T site. Of these four bases, the second is the best established and the first is the least. The last is the one to be tested.

The most important conclusion based on symmetry and degeneracy considerations alone is that isolated As_i migration through the infinite crystal along the channel $T\rightarrow H\rightarrow T^*\rightarrow H\rightarrow T$ is charge-state dependent, with the barrier increasing through the sequence $\mathrm{As}_i{}^+,\mathrm{As}_i{}^0,\mathrm{As}_i{}^{2+}\approx\mathrm{As}_i{}^-$. Our calculations suggest that the barrier increases by about 0.4 eV at each step. Our calculations also suggest that at the stable sites, the levels $(-/0)_i$, $(0/+)_i$, and $(+/2+)_i$ are in normal order and spaced by about 0.33 eV. These two conclusions taken together have implications regarding the conditions under which the arsenic interstitial will be a fast diffuser. These implication may be important in explaining the formation and annealing of the $\mathrm{As_{Ga}}$ antisite and of EL2, whatever it turns out to be.[27–31]

If EL2 is the $\mathrm{As_{Ga}}$-As_i pair, then, as shown in Sec. IV and Fig. 3, the isolated $(0/+)_i$ interstitial level must lie very close below the isolated $(0/+)_a$ antisite level. This fixes the position of the ladder of interstitial levels such that the $\mathrm{As_{Ga}}^+$ is the stable state for Fermi energy μ in the range $0.3<\mu<0.75$ [i.e., from $(0/+)_a=0.75$ eV to $U_i+0.10=0.43$ eV below $(0/+)_a$]. This range suggests that the barrier 0.5 ± 0.1 eV measured by Stievenard *et al.*[30] for the arsenic interstitial in p-type GaAs refers to the $\mathrm{As}_i{}^{2+}$ state. Our estimate of about 0.8 eV barrier raising along the sequence $\mathrm{As}_i{}^+,\mathrm{As}_i{}^0,\mathrm{As}_i{}^{2+}$ suggests that there is a very small (if any) barrier to $\mathrm{As}_i{}^+$ migration.

If the $\mathrm{As_{Ga}}$-As_i pair is EL2 so that the $(0/+)_i$ and $(0/+)_a$ levels are much closer than the spacing between isolated levels of either defect, then there is no Fermi energy at which the two defects are oppositely charged. Coulomb attraction cannot be the reason that the mobile interstitial seeks out the antisite neighborhood, and there is need to explain the formation of the stable EL2. In Sec. IV, we speculated that the near degeneracy of two low-energy states might, in a more sophisticated many-electron multiconfiguration calculation, provide the needed binding but we offered no evidence to support that speculation.

In Sec. IV we did suggest a reasonable mechanism by which the optical excitation at the antisite helps the interstitial across the barrier. The basic reason was that *after* optical excitation, there was a charge-transfer transition which brought the neutral pair to the state $(\mathrm{As_{Ga}}^- + \mathrm{As}_i{}^+)^0$, after which the interstitial could migrate as $\mathrm{As}_i{}^+$, with virtually no barrier.

It must be noted that $\mathrm{As_{Ga}}^-$ in isolation will decay immediately to the conduction band: The energy difference between $\mathrm{As}_i{}^-$ and $\mathrm{As}_i{}^0+E_g$, evaluated using (4.1) and (4.2), is

$$\begin{aligned} E_a(N_A=2,N_T=1)-[E_a(N_A=2,N_T=0)+E_g] &= \varepsilon_T+5/2U_a-E_g \\ &= (0/+)_a+\varepsilon_T-\varepsilon_A+U_a-E_g \ . \end{aligned} \tag{6.1}$$

Using the values $(0/+)_a=0.75$ eV, $\varepsilon_T-\varepsilon_A=1.04$ eV, $U_a=0.23$ eV, and $E_g=1.52$ eV, the last election is 0.50 eV above the conduction-band minimum. This is degenerate with the large density of states in the X and L conduction band valleys of GaAs and therefore decay is rapid.

On the other hand, as part of the $(\mathrm{As_{Ga}}^- + \mathrm{As}_i{}^+)^0$ complex, the decay energy, using (4.8), is

$$\begin{aligned} &E(N_A=2,N_T=1,N_E=1) \\ &\quad -[E(N_A=2,N_T=0,N_E=1)-E_g] \\ &\quad =\varepsilon_T+\tfrac{5}{2}U_a-E_g-1/\varepsilon R \ , \end{aligned} \tag{6.2}$$

i.e., lower than (6.1) by $1/\epsilon R=0.23$ eV. This leaves the electron only 0.27 eV above the conduction-band minimum. It is now degenerate only with the small density of states in the Γ valley and its lifetime against decay is very much larger.

If EL2 is the ($\mathrm{As_{Ga}}$-As_i) pair, then, as we showed in Sec. IV, the pair has an acceptor level $(-0/)_p$ which is like the acceptor level of the isolated interstitial $(-/0)_i$. Our *calculations*[14] give an interstitial level structure which is too high for $(-/0)_i$ to be in the gap. However, if EL2 is the pair, then we can evaluate the interstitial acceptor level as

$$\begin{aligned} (-/0)_p=(-/0)_i &= (0/+)_i+U_i \\ &= (0/+)_a \\ &\quad -[(0/+)_a-(0/+)_i]+U_i \ , \end{aligned} \tag{6.3}$$

i.e., somewhere between 0.23 and 0.33 eV above the main

$(0/+)_a$ EL2 donor level. We should broaden these limits somewhat; say to 0.23 and 0.5 eV above the donor level, to allow for the approximations we have made. One of these is our neglect of Jahn-Teller relaxation of the interstitial, which would effectively raise U_i. However, the main point is that there *must* be an acceptor level existent. We are not aware of such a level. Until it is found, there is a serious problem for the identification of EL2 with the pair, and the search for this level is the definitive test we propose for the model.

Finally, let us summarize the EL2 scenario which our analysis suggests, an analysis which is based on assuming the truth of the (As_{Ga}-As_i) pair model for EL2. As shown in Fig. 6, the configuration and electronic ground state for the neutral pair is with the neutral interstitial at the T site and the neutral As_{Ga} at its usual location in its electronic ground state. The electronic state, as in Fig. 2, is E_1^0. Absorption of a photon at the antisite takes the system to electronic state E_3^0. Most of the time, E_3^0 decays back to E_1^0 and the interstitial stays at T because the barriers in E_1^0 and E_3^0 are equal, and are too high to surmount. However, there is a small probability of a charge-transfer transition from E_3^0 to E_4^0, where the E electron on As_i fills the hole in the As_{Ga} A_1 state caused by the $A_1 \rightarrow T_2$ excitation. The barrier is lower in the state E_4^0 because the As_i can migrate as As_i^+, a state in which there may be virtually no barrier. In addition, there is a small additional Coulomb attraction, as suggested by Samuelson and Omling.[25]

Once across the barrier at H, the interstitial is closer to the antisite and their wave functions overlap more. The electronically excited state E_4^0, whose long life was caused by poor wave-function overlap, is now expected to decay rapidly, leaving the system in whatever electronic ground state is appropriate for the interstitial near T^*. If this is to be the metastable configuration, its total energy must be higher than it is at T, and we have drawn it this way in Fig. 6.

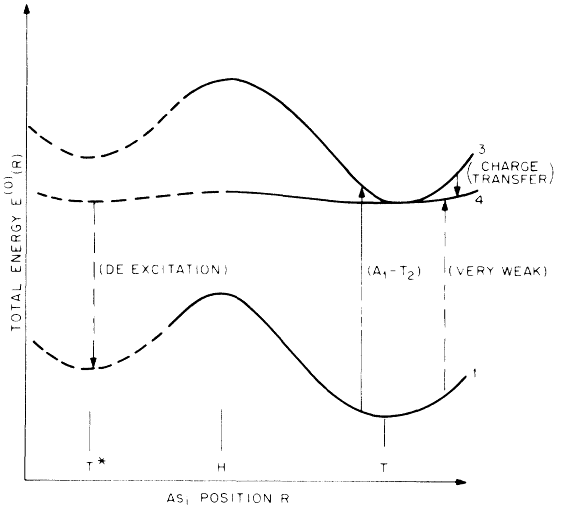

FIG. 6. Scenario showing the sequence of states encountered in the optically driven transition of the interstitial at T to the interstitial near T^*.

Our Green's-function calculations with the interstitial at T^* indicates that in addition to the electronic ground state for the neutral pair, other (charged) ground states are present, so there should be levels in the gap. This is a contradiction to the experimental situation, where the metastable has no levels in the gap. Therefore, either the pair model is wrong or the interstitial ends up in some *other* location close to the antisite where all the levels are driven out of the gap, if such other locations exist.

Because the interstitial at T^* cannot be the metastable EL2, and because we have no calculations which tell us what the metastable configuration actually is, we cannot present a scenario for the return from the metastable configuration to the ground configuration. However, even without information about the metastable configuration, we have been able to show that EL2 in its ground state must have an acceptor level located from 0.2 to 0.5 eV above its main donor level if the pair model is to be correct.

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