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Theoretical study of native defects and impurities in InP

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A study is made of the trends in the deep levels, formation energies, and abundances of native defects and impurities in InP. We predict deep-level positions and equilibrium abundances for the eight native tetrahedral point defects. These consist of two vacancies, two antisites, and the two native atoms at both nonequivalent tetrahedral interstitial sites. The effects on native defects of electron irradiation and the introduction of common dopants Zn and S in InP are also investigated. The theoretical studies are done within the local-density approximation using a recently developed parameter-free self-consistent pseudopotential and pseudoatomic orbital scheme.

I. INTRODUCTION

Characterizing the electronic, diffusive, and annealing properties of III-V compound semiconductors to determine their feasibility for the development of optoelectronic devices has become a subject of intense interest in recent years. Currently much attention is being focused on the semiconductor InP which appears to be promising for solar-cell use. InP has a direct band gap of nearly optimum energy (1.4 eV) and is experimentally found to be both highly efficient and resistant to radiation damage. Solar efficiencies around 17% have been achieved in InP making the material's efficiency comparable to that of GaAs. Unlike GaAs or most other III-V compounds, however, Yamaguchi *et al.*[1] found that defects induced in InP by electron irradiation appear to anneal away at room temperatures restoring much of the material's solar-cell properties.

The issue of radiation damage as well as many other problems in InP and other semiconductors are intimately related to the nature of the defects present in the material. Within the last few years, significant experimental effort has been spent in an attempt to identify the nature of the defects present in InP. Techniques such as electron paramagnetic resonance[2,3] (EPR) and deep-level transient spectroscopy[4] (DLTS) have provided some clues into the nature of the electronic states present in the material, but these techniques do not measure the underlying atomic source of these states directly. In III-V compound semiconductors such as InP the problem of identifying these defects and their effect on the properties of the material is also complicated by the multiplicity of possible defect types. Determination of the defects present in a material usually requires extensive comparisons between experimental observations and theoretical predictions. Although a few empirical studies have been done on defects in InP,[5,6] almost no extensive *ab initio* theoretical studies have been carried out for this material. In view of its possible technological uses, it is therefore worthwhile to preform a study of its basic properties in relation to defects. Such fundamental questions as the location of defect levels in the gap, the identity of the major native defects, and the effect of impurity incorporation on the crystal under various stoichiometric conditions have not been answered.

In this paper we began a theoretical study of the nature of native point defects and impurity incorporation in InP. We find the large mass and size difference between In and P leads to many unusual and interesting properties in InP. We predict deep-level positions, formation energies, and relative abundances of tetrahedrally coordinated native point defects under stoichiometric and nonstoichiometric conditions. Lower symmetry defects, such as hexagonal-site interstitials, might also be important for some charge states but were not considered here since they are normally higher in energy than the tetrahedral-site defects. The question of self-compensation and radiation resistance in InP will also be examined in light of the predicted defect formation energies and charge states. Finally, we will consider the influence of the impurities Zn and S on the electronic properties of InP and on the native defect abundances.

II. METHOD

The method used to calculate the defect levels and total energies is based on the Hohenberg-Kohn-Sham local-density approximation (LDA) and uses Hamann-Schlüter-Chiang–type[7] pseudopotentials. The Ceperley-Alder[8] exchange-correlation potential is used as parametrized by Perdew and Zunger.[9] Instead of the conventional plane-wave basis functions, here we use a basis of pseudoatomic orbitals supplemented with only a few low-energy plane waves. This keeps the size of the Hamiltonian matrix (which must be diagonalized) small. The Bloch wave function is thus written as

$$\psi_{\mathbf{k}}(\mathbf{r})=\sum_{\mu} a_k(\mu)\Phi_{\mu}(\mathbf{k},\mathbf{r})+\sum_{\mathbf{g}} b_k(\mathbf{g})(1/\Omega)e^{i(\mathbf{k}+\mathbf{g})\cdot\mathbf{r}} , \quad (1)$$

where the first term represents the localized orbital wave-function component and the last term represents a small free-electron-like contribution to the wave function. The Bloch-like basis states for state μ (μ being a collective label which includes both position and orbital type) are written in the usual tight-binding form:

$$\Phi_\mu(\mathbf{k},\mathbf{r}) = \sum_{l} e^{i\mathbf{k}\cdot(l+\tau)} \Phi_\mu^{\mathrm{PAO}}(\mathbf{r}-l-\tau)\ , \tag{2}$$

where the pseudo-atomic-orbitals (PAO's), $\Phi_\mu^{\mathrm{PAO}}(r)$, are constructed directly from the corresponding pseudopotential and fitted to Slater-type functions for computational convenience. The evaluation of the periodic potential, charge density, and total energies is efficiently performed by Fourier transforming the Bloch functions and working in the formalism of plane waves. We use a kinetic-energy cutoff of 20 eV for the low-energy plane-wave basis and expand the PAO's in plane waves up to a kinetic energy of 110 eV. We find that this mixed-basis method generally produces errors of a few tenths of an eV which is comparable to the more conventional plane-wave-only pseudopotential method. The calculations are done fully self-consistently within the pseudopotential framework of Ihm *et al.*[10] The pseudopotentials are constructed from the *s* and *p* valence states and the excited *d* state of the atoms and fit to the Bachelet *et al.* analytic form.[11] Further details on the use of PAO's can be found in previous work by Jansen and Sankey.[12] The highest closed-shell *d* state for In (4*d*) may be important for some applications, but its neglect here was considered justifiable since formation energies vary on the scale of several eV's. Generally, the emphasis here will be on properties associated with energies varying on the eV scale.

III. BULK PROPERTIES

Before embarking on the calculation of defect energies we first look at bulk properties of the material. Of fundamental importance is the band structure. We compare in Fig. 1 the band structure of InP using sp^3 PAO's only [Fig. 1(a)] and sp^3 PAO's supplemented with a few low-energy plane waves [Fig. 1(b)] to those computed using the conventional plane-wave-only method which is rigorously complete. We find that even with just sp^3 orbitals alone the valence bands are already quite well represented [see Fig. 1(a)]. In fact, the lowest-lying conduction band is also quite accurate near the conduction-band minimum (at point Γ) but diverges appreciably from the plane-wave results near the *X* point and other regions of the Brillouin zone. If just a few plane waves are added to the basis [Fig. 1(b)] we find these low-lying conduction bands are significantly improved and the valence bands are virtually identical to the plane-wave results. Due to the use of the LDA our computed gap (1.1 eV) is smaller than the experimental energy gap (1.4 eV).

In addition to eigenvalues (band structure), the PAO method also allows for accurate determination of total energies. For the lattice constant and bulk modulus, which depend on total energies, we obtain 5.71 Å and 84 GPa, respectively, compared to the respective experimental values of 5.87 Å and 71 GPa.[13] These results for the lattice constant and bulk modulus appear slightly less accurate than is typically found in semiconductors due probably to the neglect of the 4*d* electrons in the In pseudopotential. Nevertheless, we do not expect these errors, which derive from total-energy variations on the meV scale, to upset the orderings of the dominant defect abundances which are derived from defect formation energies varying on a scale of several eV. For the defect calculation we have used the experimental lattice constant.

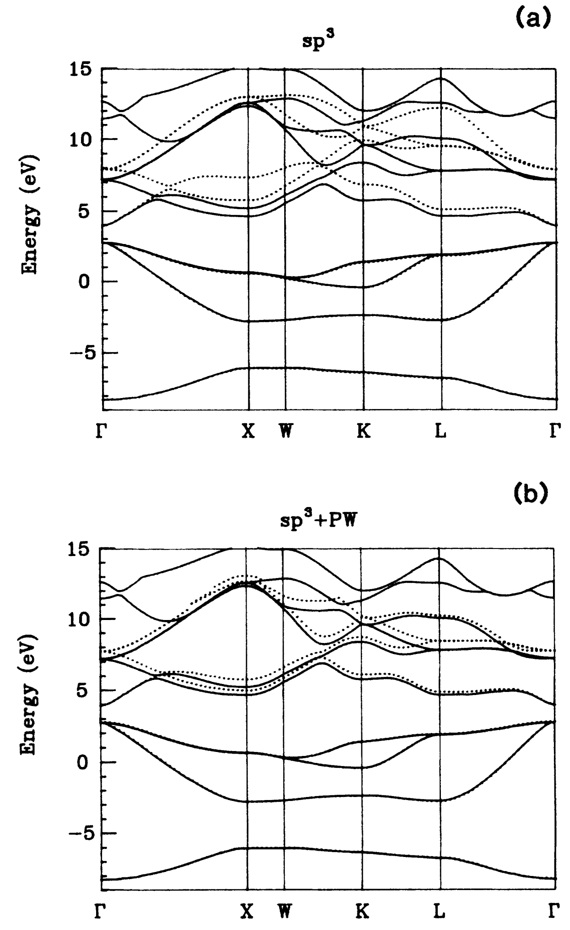

FIG. 1. Band structure of InP for (a) sp^3 orbitals only (dotted lines) vs plane waves (solid lines) and (b) sp^3+PW vs PW. The charge density used in the Hamiltonian is self-consistently determined independently for each basis. No shifts of any kind were made in the bands.

IV. DEFECT DEEP LEVELS AND FORMATION ENERGIES

We now study native point defects in the material using supercells of 32 atoms plus the defect. In the calculation of the defect energies the sp^3 basis would probably be sufficient for our purposes here. However, since a few plane waves (up to kinetic energy 20 eV) made some improvement in the bands and changed the computational effort only minimally, we decided to include a few low-energy plane waves in the basis as well for additional variational freedom. No relaxation about the defects was included in this study since these effects are generally small compared with formation energy differences. Of course, for some cases relaxation effects may become important, but here we will focus on results which are not strongly sensitive to small energy differences.

The formation energies are derived from total supercell energy differences and depend on the Fermi level.[14,15] There is an arbitrary constant in the formation energies due to the fact that no solid-state reaction exists which produces only one defect in a multiatom material. We have fixed this constant by setting the two vacancy formation energies equal to each other in their zero charge state: $\varepsilon(V_{\mathrm{P}}^0)=\varepsilon(V_{\mathrm{In}}^0)$. Although the choice is arbitrary, this convention often leads to the appealing condition that the dominant defect at stoichiometry is simply the defect with the lowest formation energy.

A. Vacancies

The formation energies for two native vacancy point defects in InP are shown in Fig. 2. The phosphorus-site vacancy defect, V_{P}, forms an A_1-symmetric state below the valence-band edge and a T_2-symmetric state resonant with the conduction bands. The removal of a phosphorous atom provides the crystal with three excess electrons which may be thought of as coming from an unpaired In atom. Two of these electrons are trapped by the A_1 state while the remaining electron acts as a donor. Thus, the V_{P} defect is predicted to have a $+1$ charge state for Fermi levels in the gap. Such a charge state was examined using electron paramagnetic resonance by von Bardeleben[3] recently and attributed to the V_{P} defect, though no level position was given.

The In-site vacancy defect, V_{In}, acts strikingly different from the V_{P} defect in InP. We find V_{In} forms an A_1 state below the valence-band edge and a T_2-symmetric triply degenerate *acceptor* state deep within the band-gap region. As the Fermi level changes from *p*-type to *n*-type material the T_2 state changes its occupancy giving rise to charge states of from -1 to -3. Thus, formation energies for the V_{In} defect vary dramatically in going from *n*-type to *p*-type material. The transition state energies from the nth to the $(n+1)$th charge state shown in the figure are defined relative to the valence-band edge E_V by

$$\varepsilon_{TS}^{n/(n+1)}=E_S(n)-E_S(n+1)-E_V\ , \tag{3}$$

where $E_S(m)$ is the supercell energy with m electrons placed in a uniform background to preserve charge neutrality. For negatively charged states excess electrons in the system are put into gap states.

B. Antisites

The two antisite formation energies are shown in Fig. 3. The most outstanding feature in the plot is that the $\mathrm{P_{In}}$ antisite is significantly lower in energy than the $\mathrm{In_P}$ antisite for any Fermi level. Thus, $\mathrm{P_{In}}$ antisites should be more abundant than $\mathrm{In_P}$ antisites in stoichiometric material. The $\mathrm{In_P}$ antisite forms an A_1 state well below the valence-band edge and a T_2 state in the gap which can be occupied with up to six electrons giving rise to charge states of from $+3$ to -2 in the gap region. The $\mathrm{P_{In}}$ antisite forms an A_1 state within the gap which assumes charge states from $+2$ to 0 as the Fermi level rises, and a T_2 state resonant with the conduction band. The $\mathrm{P_{In}}$ antisite has been studied using EPR by Kennedy and Wilsey.[2] The experimental results indicate a $+1/+2$ transition level appears in the gap region in agreement with our predictions though the level may be somewhat higher in energy than predicted here. Further studies including relaxation and perhaps the inclusion of the 4*d* pseudopotential for In may be useful in resolving the small discrepancy in the level position.

C. Interstitials

Let us now consider the case of interstitial native point defects. These defects are of special interest since they are expected to be relatively mobile in a compound semiconductor and therefore will be of interest in understanding many diffusion properties of InP. Interstitials are

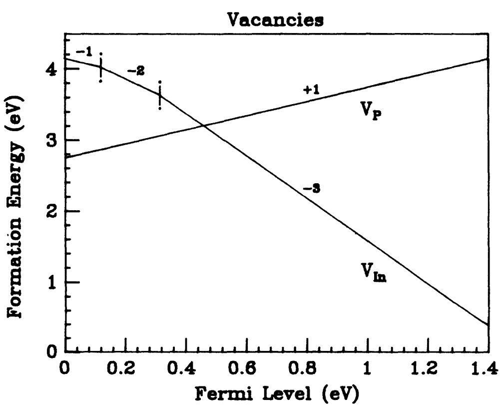

FIG. 2. Formation energies for the two vacancy point defects in InP as a function of Fermi level. V_{In} forms a triply degenerate T_2-symmetric gap state near the valence-band edge (the T_2 transition-state energies are indicated by vertical bars shouldered by dots). No gap states are present for V_{P}.

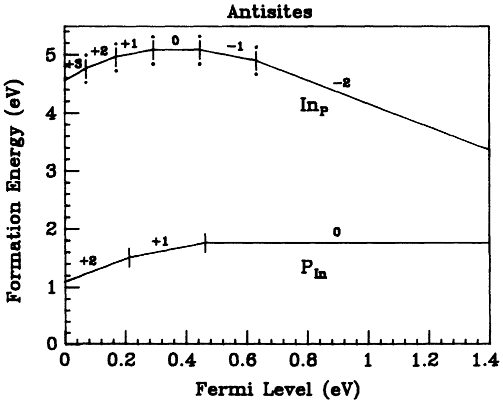

FIG. 3. Formation energies for the two antisite point defects in InP as a function of Fermi level. $\mathrm{P_{In}}$ forms a nondegenerate A_1-symmetric gap state (vertical bars), whereas $\mathrm{In_P}$ forms a triply degenerate T_2-symmetric gap state (vertical bars shouldered by dots).

also often generated in radiation-damaged materials. Interstitial phosphorous has been experimentally observed to form in InP under electron irradiation.[1,4]

As is typical for self-interstitials, we find that both In and P form donor-type interstitial defect (see Fig. 4). In fact, both In and P interstitials form triple donors in p-type InP. The anion, P, being the more electronegative species forms an A_1 state below the valence-band edge which consumes two of the five excess electrons from the interstitial P atom, and a triply degenerate T_2 state within the gap which may be singly, doubly, or triply occupied [Fig. 4(a)]. The cation, In, forms a nondegenerate A_1 gap state with occupancies of from 0 to 2 and a T_2 state resonant with the conduction bands [Fig. 4(b)]. It is interesting to observe that the lowest-energy interstitial site switches from T_A to T_C in going from p-type to n-type material for both interstitial atoms (though the difference is smaller than the error in our method in some cases). This possible switching of sites is unusual for III-V materials, and is similar to the case of Zn interstitials in the II-VI material ZnSe.[14] The analogy between ZnSe and InP may be pushed even further if one considers that in both of these materials cation interstitials are predicted to be the lowest-energy defects overall for p-type material.

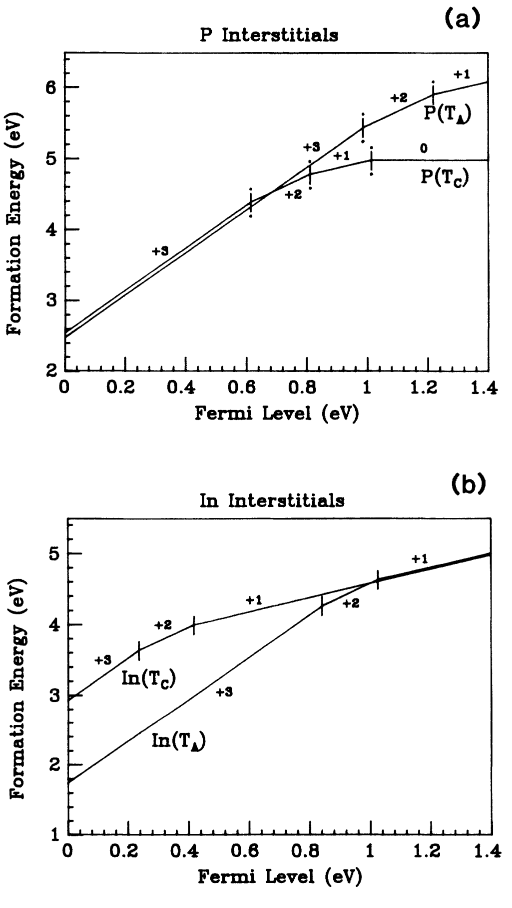

FIG. 4. As in Fig. 3, but for (a) P interstitials and (b) In interstitials.

V. DEFECT EQUILIBRIA

Once the formation energies are known the equilibrium defect concentrations can be solved for through a statistical-mechanical procedure involving mass-action equations for the possible defect reactions in the crystal.[14] The concentration of defect type X is defined as $[X]=N_X/N_L$, where N_X and N_L are the number of X-type defects and lattice sites, respectively. The defect concentrations are interrelated through products of Boltzmann factors and depend on several variables including temperature, Fermi level, and stoichiometry. Since defect concentrations depend exponentially on formation energies, there is no hope of predicting accurate absolute concentrations. Here we will be content to predict relative trends in the defect concentrations as a function of these variables.

Of primary importance is the stoichiometry parameter, which is defined as $S=(N_{\rm P}-N_{\rm In})/N_L$, and can be expressed in terms of the individual defect concentrations as

$$S=2([{\rm P_{In}}]-[{\rm In_P}])+([V_{\rm In}]-[V_{\rm P}])+([{\rm P}_i]-[{\rm In}_i]) . \tag{4}$$

[If impurities are present this expression is modified by the additional term $([X_{\rm In}]-[X_{\rm P}])$, where X is the impurity atom.] For particular cases, at low temperatures normally only a few defects are important and the stoichiometric constraint can be significantly simplified. Let us now examine the two important cases of p-type and n-type InP.

A. *p* type

For the case of p-type InP we predict the dominant stoichiometric defects are $\rm P_{In}$ and $\rm In_\mathit{i}$ (See Fig. 5, $i=T_A$ interstitial site). At low temperatures the remaining defects will have negligible concentrations by comparison. The governing reaction in p-type material is then

$${\rm P_P}+2{\rm In_{In}}\leftrightarrow{\rm P_{In}}+2{\rm In}_i$$

and the stoichiometric constraint [Eq. (4)] reduces to $S\sim2[{\rm P_{In}}]-[{\rm In}_i]$. Accordingly, at stoichiometry ($S=0$) the material contains twice as many $\rm In_\mathit{i}$ interstitial atoms as $\rm P_{In}$ antisites. High excesses of P lead to a reduction of the $\rm In_\mathit{i}$ intersititals and the $\rm P_{In}$ antisite becomes the only important defect. Likewise, excess In leads to a reduction of the $\rm P_{In}$ antisite concentration and an increase in the $\rm In_\mathit{i}$ interstitial concentration.

The concentration of the dominant defect at stoichiometry can be written

$$[{\rm In}(T_A)]_{S=0}=\exp(-\beta E_0) ,$$

where $\beta=1/k_BT$. The parameter E_0 is then related simply to defect concentrations and is useful in that it varies over only a few eV and not exponentially as the concentrations do. From mass-action and the stoichiometric constraint we find in p-type material E_0 is given in terms of the defect formation energies ε_μ (where μ is the Fermi level) by

$$E_0(p\text{-type})\approx\tfrac{1}{3}[\varepsilon_\mu(\mathrm{P_{In}})+2\varepsilon_\mu(\mathrm{In}_i)-\beta^{-1}\ln 2] \;.$$

From the formation energies with $\mu=0$ we find $E_0(p\text{-type})=1.5$ eV with $\beta=7\ \mathrm{eV}^{-1}$.

It is interesting to compare our predictions for InP with those of GaAs.[14,15] The results for p-type InP are markedly different from those for p-type GaAs where interstitials were not found to be equilibrium defects. The In_i defect is a triple donor and the $\mathrm{P_{In}}$ defect is a double donor so that each reaction

$$\mathrm{P_P}+2\mathrm{In_{In}}\rightarrow\mathrm{P_{In}}+2\mathrm{In}_i$$

produces eight compensating donor electrons. In contrast to this, in p-type GaAs a relatively high value was found for E_0 ($E_0=2.3$ eV) (Ref. 14) and the governing reaction

$$\mathrm{Ga_{Ga}}+\mathrm{As_{As}}\rightarrow\mathrm{As_{Ga}}+\mathrm{Ga_{As}}$$

only produced two donors. Among other things, these results indicate that significantly more self-compensation by native defects should be expected in p-type InP than is predicted in p-type GaAs.

B. *n* type

The dominant equilibrium defects in n-type InP are predicted to be the V_{In} and $\mathrm{In_P}$. If the concentration of all other defects are considered negligible, then by conservation of atoms we see that the governing reaction for this system is $\mathrm{In_{In}}\leftrightarrow 2V_{\mathrm{In}}+\mathrm{In_P}$ and the stoichiometric constraint is $S=[V_{\mathrm{In}}]-2[\mathrm{In_P}]$. Thus, excess P creates more V_{In} vacancies and excess In produces more $\mathrm{In_P}$ antisites. From Figs. 2 and 3 we see the V_{In} is a triple ac-

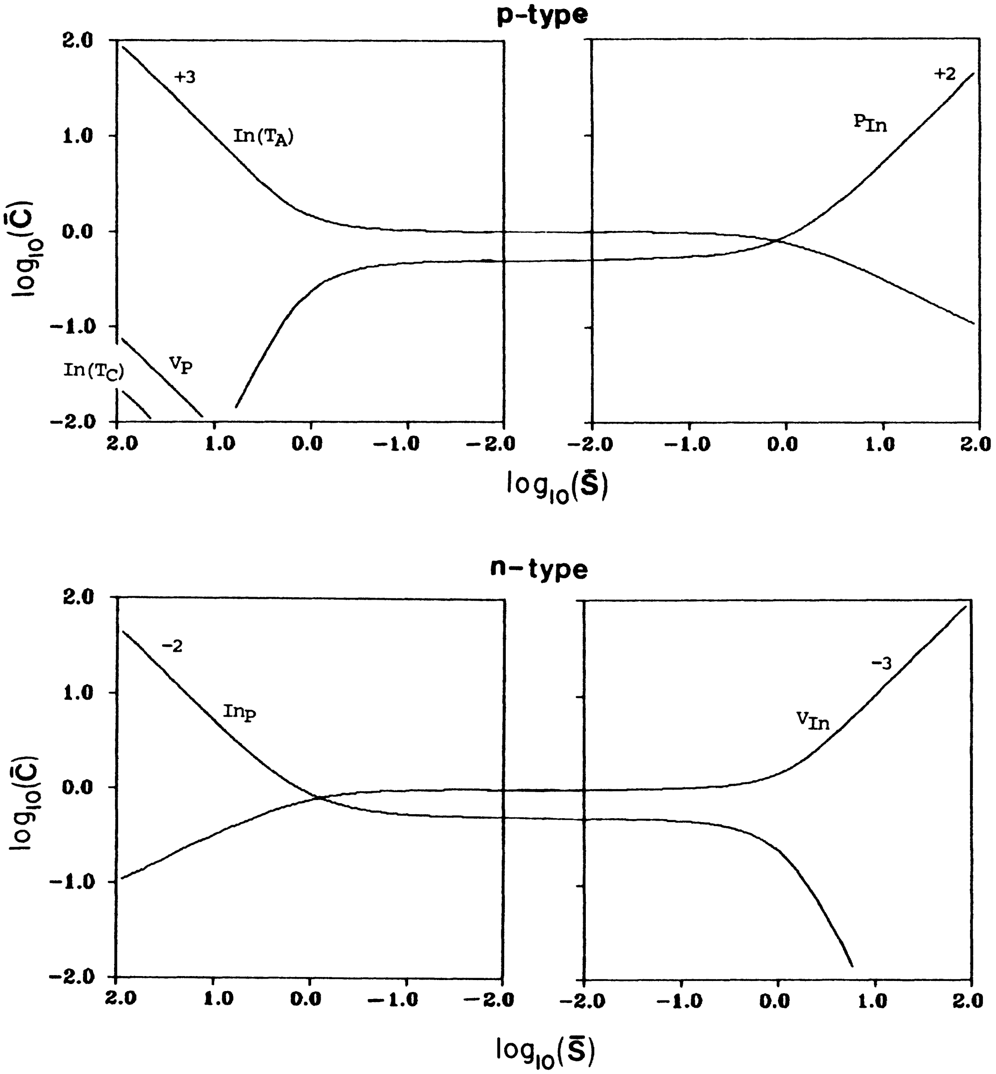

FIG. 5. Native defect concentration as a function of stoichiometry for p- and n-type InP. The right panel is for positive stoichiometry S (excess P) and the left panel is for negative stoichiometry S (excess In). The center point between panels corresponds to perfect stoichiometry ($S=0$). Only the major defects appear in the graph, the remaining defects having concentrations which would appear below the plot window shown. The bar above S and C indicates that these quantities are in units of the dominant defect concentration at stoichiometry.

ceptor and the In_P is a double acceptor in n-type InP so that eight holes are produced by the governing reaction. At stoichiometry, the dominant defect concentration is given by

$$[V_{\rm In}]_{S=0}=\exp(-\beta E_0)\ ,$$

with

$$E_0(n\text{-type})=\tfrac{1}{3}[2\varepsilon_\mu(V_{\rm In})+\varepsilon_\mu({\rm In_P})-\beta^{-1}\ln 2]_{\mu=1.4}$$
$$=1.3\ {\rm eV}\ .$$

Thus, as in p-type material, the system may have significant self-compensation effects in n-type InP. The n-type InP defects found here are identical to the analogous defects previously found for n-type GaAs.[14]

VI. RADIATION RESISTANCE

Much of the recent interest in InP has stemmed from the discovery that it is highly radiation resistant. Room-temperature annealing of radiation-induced defects in InP found by Yamaguchi *et al.*[1] is somewhat surprising in view of the fact that no such room-temperature annealing effects are observed in the chemically similar material GaAs. To explore possible mechanisms behind radiation resistance in InP it is imperative to examine the nature of the material's point defects. A consideration of the difference between defect energetics in GaAs and InP should be helpful in shedding light on this problem.

Under high-energy electron bombardment one must momentarily abandon the assumption of equilibrium and consider probable kinetic processes between the bombarding electrons and the atoms in the crystal. The primary reaction occurring in the crystal upon electron irradiation will be the creation of vacancy-interstitial pairs. If these pairs are well separated (i.e., the interstitial is not near the vacancy) they cannot recombine immediately and thus simple nonequilibrium point defects will be introduced into the crystal. From (nonrelativistic) energy and momentum conservation requirements for displaced atom X, we find the threshold energy $E_{\rm th}(X)$ for this primary reaction will be roughly proportional to the mass ratio M_X/m, where m is the electron mass and M_X is the mass of the displaced atom, times the reaction energy associated with the creation of the defect pair, $E_{\rm pair}(X)$:

$$E_{\rm th}(X)\sim(M_X/m)E_{\rm pair}(X)\ . \tag{5}$$

For well-separated defects the pair energy, $E_{\rm pair}(X)$, can be taken as the sum of the interstitial and vacancy formation energies for atom X:

$$E_{\rm pair}(X)=\varepsilon_\mu(V_X)+\varepsilon_\mu(X_i)\ . \tag{6}$$

This approximation neglects interstitial migrational energies, but these are generally small compared with the formation energies. Thus, in this simple analysis we are only considering gross energy differences (~ 1 eV or more) between GaAs and InP which tend to drive atomic diffusion and annealing behavior in these materials.

In InP the pair-energy term generally favors the formation of defects involving In, especially for n-type InP. However, this pair-energy difference is more than compensated for by the large mass disparity between In and P which promotes the formation of defects involving P. Thus, for InP we have $E_{\rm th}({\rm In})>E_{\rm th}({\rm P})$, so that *anion*-derived defects are predicted to form more readily under lower-energy (~ 100 keV) electron irradiation consistent with experimental observations.[1,4] In contrast to this, for GaAs both the pair energy and mass difference between Ga and As terms favor the reaction involving the Ga atoms (namely ${\rm Ga_{Ga}}\rightarrow V_{\rm Ga}+{\rm Ga}_i$). That is, in GaAs we find $E_{\rm th}({\rm Ga})<E_{\rm th}({\rm As})$, favoring the formation of *cation*-derived defects.

For both materials, cation-derived defects are largely favored over anion defects under *equilibrium* conditions. If migration barrier differences between InP and GaAs are not large, this suggests that the defects created through electron irradiation in InP (anion defects) may anneal away more readily than those in GaAs (cation defects). Of course, quantitative predictions of annealing rates will, at the very least, require extremely accurate calculations of both formation energies and migration barriers. Nevertheless, this simple analysis, which avoids details of the kinetic processes involved in diffusion, may at least provide a qualitative interpretation of the observed radiation resistance of InP.

VII. S AND Zn IMPURITIES

Two common dopants for n-type and p-type InP are S and Zn, respectively. Let us then look at the effect these impurities have on the properties of InP. In particular, we predict the site they should occupy under various conditions and consider how these impurities might affect the crystal's electrical behavior, and native defect abundances. Both impurity atoms are represented using ground-state valence s and p pseudopotentials and exicted-state d pseudopotentials, as was done for the bulk atoms.

In Fig. 6 we plot the impurity formation energies for each of the four different sites the impurities can occupy (two substitutional sites and two tetrahedral interstitial sites). Although these impurities tend to drive the crystal either n type or p type, we have plotted the formation energies for all Fermi level positions in the gap. The arbitrary zero of energy for the impurities is fixed here by the condition $\varepsilon(X^0_{\rm In})+\varepsilon(X^0_{\rm P})=0$, relating the zero-charge-state substitutional defect formation energies for impurity X.

The S impurity atoms are found to prefer the P site to the In site and by a large amount [Fig. 6(a)]. Small variations in native stoichiometry are not expected to change this result. We find S_P produces no deep traps so that the excess valence electron of S on the P site is free to roam the crystal as a donor electron. Thus, S should be a good single-donor n-type dopant atom in InP. Since S occupies the P site, the incorporation of S into InP has the same effect on the *native* defect abundances as an excess of P atoms. In Fig. 6(b) we show the formation energies for Zn impurities. We expect Zn to be a p-type dopant occupying the In site. Our results indicate that ${\rm Zn_{In}}$ is indeed the lowest-energy impurity defect in InP and acts

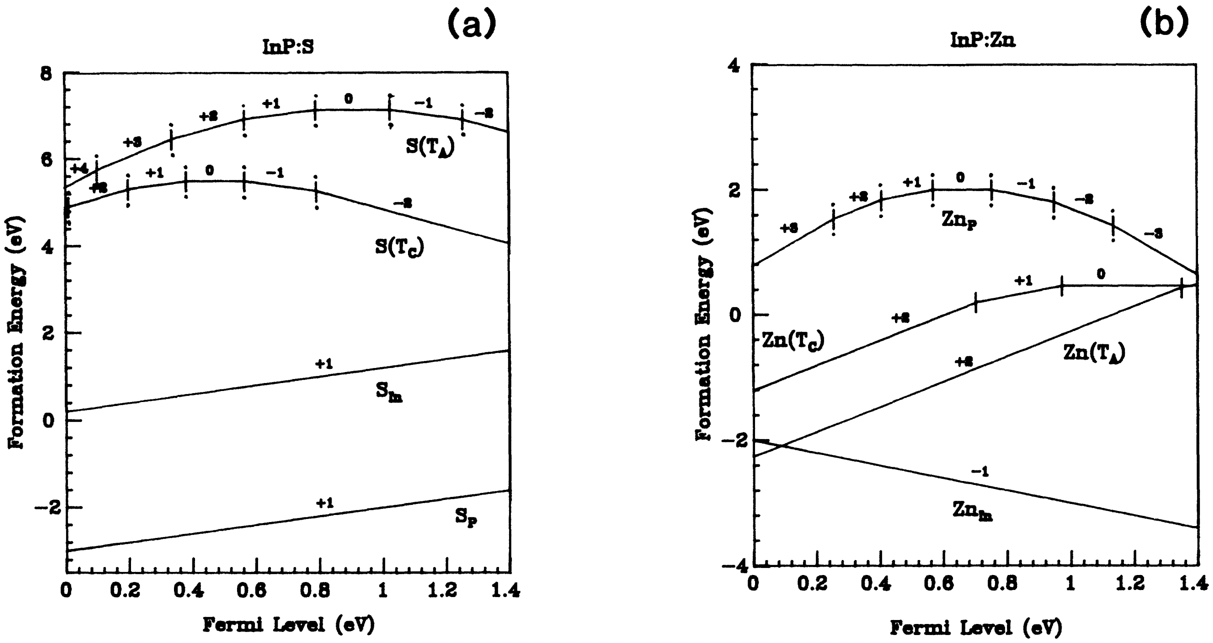

FIG. 6. Transition states and formation energies for substitutional and interstitial (a) S and (b) Zn impurities in InP. The A_1 transition states are indicated by single vertical bars while T_2 states are represented by vertical bars shouldered by dots. Notice the close competition between interstitial and substitutional Zn in *p*-type material (b).

as a single acceptor. As the material becomes *p* type, however, we see that interstitial Zn becomes important. Since these interstitial Zn are double donors they may act to destroy the *p*-type. When the Fermi level is near the valence-band edge we predict a competition will exist between the $\mathrm{Zn_{In}}$ defects which drive the system *p* type and the Zn_i defects which drive it away from *p* type. Thus, under complete equilibrium conditions we predict Zn incorporation may not produce good *p*-type material due to the action of interstititial Zn donors. Both the interstitial site and the substitutional site should be important when the material approaches *p* type.

VIII. CONCLUSION

An extensive theoretical study has been made of native and impurity point defects in InP. Deep-level positions and formation energies were predicted using a first-principles pseudopotential and pseudo-atomic-orbital technique. Using a statistical-mechanical procedure the equilibrium defect concentrations were also predicted and the factors that influence defect formation were analyzed. We have also used the defect formation energies to address the question of radiation resistance in InP. We predict moderate energy electron irradiation favors the production of P interstitials and P-site vacancies which are high-energy defects. Last, the effects of Zn and S impurities in InP were studied for both *n*-type and *p*-type doping. We find that an interesting bistability occurs for Zn incorporation in *p*-type InP, where the Zn is equally likely to go either interstitial or form $\mathrm{Zn_{In}}$ substitutional defects.

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