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Native defects in a $(GaP)_1/(InP)_1$ strained-layer superlattice: local electronic structure and diffusion mechanism

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Abstract. The local electronic structure of intrinsic defects, including antisites, interstitials, vacancies and complexes with themselves or with Si impurities, in a $(GaP)_1/(InP)_1$ (001) strained-layer superlattice determined by the Keating model, is calculated using a developed recursion method. Besides the localized states obtained, attention is paid to the electronic occupancy on various defects. A general consequence of describing the influence of isolated defects on the electron distribution of their neighbours is given. It is found that the charged state of an atom will be changed when it becomes an antisite. A closely bound (I_P–P_{III}) (III ≡ Ga or In) pair, formed by coulombic interaction, will induce some states in energy gap. No evidence is found anywhere of EL2-like behaviour in this system. Some novel diffusion mechanisms, based on I_P and V_P complex formation and dissociation, are presented.

1. Introduction

The foreign impurities and intrinsic defects in a matched GaAs/AlAs superlattice have been extensively studied in numerous calculations with varying degrees of sophistication [1–11], of which we have presented the electronic structures of antisite, interstitial, vacancy, and complexes of these, by using a recursion method with tight-binding models [10, 11]. The success in explaining some experimental observations [12] has proved that the procedure developed to study small amounts of intrinsic defects in multilayer systems is a viable tool in avoiding the computational impediment required by a general band-structure method based on Bloch's theorem.

The advances in modern growth techniques with good control of epitaxial crystal structures have caused considerable interest in new varieties of artificial superlattices fabricated from mismatched semiconductor materials [13–15]. One typical example is the GaP/InP strained-layer superlattice (SLS), in which the lattice mismatch is larger than 7%. Very recently, the structural and electronic properties of a GaP/InP SLS have been studied by several groups [16–19]. However, to our knowledge, no detailed reports are available on native defects in the mismatched superlattice. The present study was motivated by the interest in this kind of problem in the GaP/InP system, because

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understanding the characteristics of intrinsic defects is a key step in the device application, especially for multilayer structures.

We shall study antisites, interstitials, vacancies and complexes formed by themselves or with impurities in a GaP/InP SLS. Although the interaction between the P_{Ga} antisite and foreign impurities [20–22], and the chemical trends in the formation [23] in bulk GaP have received considerable experimental and theoretical attention, many important issues still require further discussion. In fact, some defect-related properties, e.g. the charged state, will be changed by the influence of the strain in a mismatched superlattice. These questions can be answered in terms of the calculated electronic structures, which are the characteristic functions for many physical properties of native defects.

It should be noted that the system that we are faced with now is more complicated than a lattice-matched GaAs/AlAs superlattice. First, we must consider the structural stability of GaP/InP SLS. Without this discussion, all calculations may lead us to obtain incorrect results. Keating [24] introduced a useful method for describing the elastic energy of covalent crystals with a zincblende structure, which has been extended to the case with more than two kinds of atom in a unit cell by Pedersen [25] and us [19]. From our results, it is found that the bond length deviations of the stable $(GaP)_1/(InP)_1$ SLS, obtained by the Keating model, from their bulk values are in good agreement with first-principles total energy calculations.

In section 2, after a brief description of the stable $(GaP)_1/(InP)_1$ (001) SLS determined by the Keating potential and the recursion method used in the calculation, all possible models of intrinsic defects and complexes of these or with Si impurities are set up in a cluster with 10 000 atoms as an imitation of a real case. The local electronic structures of isolated defects are given in section 3, where the influence on the electronic distribution is also discussed. Two typical interstitial–antisite pairs I_P–P_{Ga} and I_P–P_{In} are studied in section 4, in order to investigate whether or not an EL2-like defect exists in the GaP/InP system. Section 5 shows the description of self-diffusion and impurity diffusion mechanisms. A summary of our results is given in section 6.

2. Defect models in a stable structure

The stability of a (001)-oriented $(GaP)_1/(InP)_1$ SLS has been studied by the Keating method. In the case when there are more than two kinds of atom in a unit cell, a general formula for elastic energy of a system is written as

$$E = \sum \alpha(ss')[X_{ss'} \cdot X_{ss'} - (b_s + b_{s'})^2]^2$$
$$+ \sum \beta(ss's'')[X_{ss'} \cdot X_{ss''} + \tfrac{1}{8}(b_s + b_{s'})(b_s + b_{s''})]^2$$

where b_s is the covalent radius of atom s, and $X_{ss'} = X_s - X_{s'}$ is the position vector between atoms s and s'. In this performance, the bond stretching α and bond bending β force constants in the interface region are assumed to be the arithmetic mean of those of the two bulk materials [26]. By minimizing the elastic energy, we obtain the in-growth direction lattice constant $a_{\parallel} = 5.7292$ Å and the in-plane lattice constant $a_{\perp} = 5.6086$ Å for a stable $(GaP)_1/(InP)_1$ (001) SLS. In this structure, the InP sublattice is expanded in the Z-axis growth direction and contracted in the X–Y plane, and a contrary process happens in the GaP sublattice.

The recursion method [27] used is a well known approach for calculating the electronic structure of materials. In a chain model, the basis functions can be written by a

recursion relation. In our performance, we adopt Harrison's [28] parameters to set up the Hamiltonian of the system within tight-binding formalism. The validity of our calculation procedure has been confirmed by the results from self-consistent full-potential linearized augmented-plane-wave and self-consistent pseudopotential calculations [9]. By checking the convergence through calculations truncated at different recurrence chain lengths, we have found that $L = 30$ is satisfactory for the problem. Before considering in more depth the presence of different defects, the detailed calculations of the electronic structures of a stable GaP/InP SLS determined by the Keating model have been given in [19] by us, in which the strain influence was also discussed.

The recursion method is especially suitable for finding local details of point defects contained in crystals. In spite of the accurate results obtained through some band-structure calculation methods for specific cases, so far these discussions have only addressed bulk materials for the intractable computational requirement, especially in superlattices.

A symbol B_C is used to represent an antisite defect when a B atom is on a C site, and V_B represents a vacancy defect when a B atom is removed from the lattice site. Because of the reduced symmetry of the superlattice, there are three different cases for an interstitial in a $(GaP)_1/(InP)_1$ (001) SLS. The symbol $I_B(2)$ represents a B interstitial in the centre of the tetragonal unit cell, which is similar to that shown in figure 2(*a*) of [23] and is just at the interface. The others, $I_B(1)$ and $I_B(3)$, represent a B atom along $[\bar{1}\bar{1}\bar{1}]$ and $[1\bar{1}1]$ directions in the GaP and InP layers, respectively. The nearest neighbours of the $I_B(2)$ interstitial are two In and two Ga atoms, and these of both $I_B(1)$ and $I_B(3)$ are four P atoms. In our calculation, we assume an isolated defect or a complexed pair of defects in a cluster containing about 10 000 atoms as an imitation of a real case.

3. Local electronic structure of an isolated defect

3.1. Antisite

First, we discuss a group III antisite in a $(GaP)_1/(InP)_1$ (001) SLS. Figure 1 shows the local density of states (LDOS) and partial density of states (PDOS) of an In_P defect, where the broken curves which serve as references are the results of a normal In atom. It is found that the LDOS of an In_P antisite shifts towards the high-energy region. (Note that the zero of energy scale is at infinite distance.) The induced defect state, which is mainly contributed by p partial waves, is localized at $E_v + 0.020$ Ryd. A similar case is obtained for a Ga_P antisite, where the corresponding state is at $E_v + 0.022$ Ryd.

A contrary process happens for a group V antisite, in which the LDOS shifts towards the low-energy region (see for example figure 2). The LDOS shape is similar to that of an n-type doping Si impurity [19]. The donor-like levels, which originate from s partial waves, are at $E_c - 0.056$ Ryd and -0.067 Ryd for P_{In} and P_{Ga}, respectively. By comparison with the results of a GaAs/AlAs superlattice [10], we find that the local environment of antisites are very similar in the two multilayer systems.

The electronic occupancy (EO) and valence (in parentheses) of all possible antisites in a stable $(GaP)_1/(InP)_1$ SLS are listed in table 1. It is interesting to find that the ionicity of a group III or V atom will be changed when it becomes an antisite. For example, the valence of a Ga atom is $+0.34$, while it is -0.68 for a Ga_P antisite. It is important to discuss the self-diffusion procedure in the GaP/InP system. Besides, the electrons on a Ga-related antisite are a little more than that on an In-related antisite.

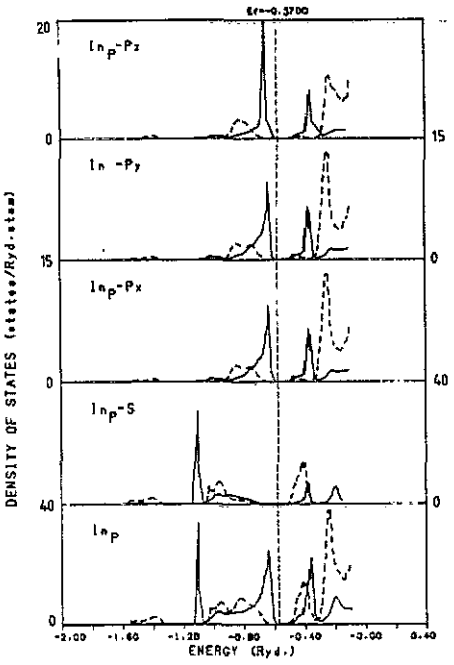

Figure 1. LDOS and PDOS of an antisite In_P, where the corresponding results (----) for a normal In atom serve as reference.

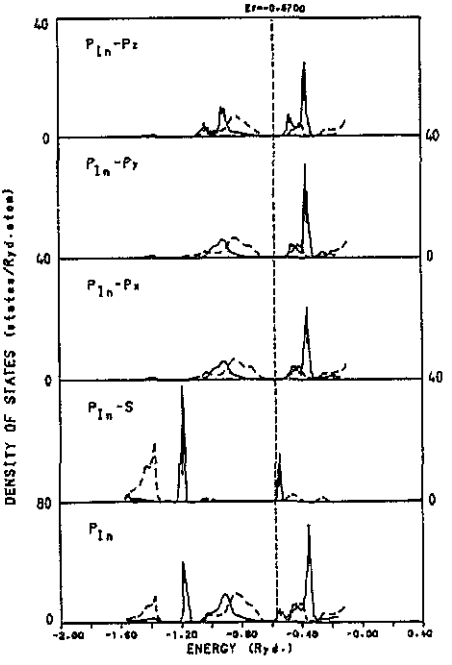

Figure 2. LDOS and PDOS of an antisite P_{In}, where the results (----) for a normal P atom serve as reference.

Table 1. The EO and valence (in parentheses) of antisite defects in a stable (001)-oriented $(GaP)_1/(InP)_1$ SLS.

	EO			TEO
Antisite	S	P_x	P_y	P_z	
P_{In}	1.802	0.863	0.863	0.883	4.411 (0.589)
P_{Ga}	1.672	0.865	0.865	0.851	4.253 (0.747)
In_P	1.337	0.705	0.709	0.713	3.465 (−0.465)
Ga_P	1.449	0.739	0.741	0.749	3.679 (−0.679)

3.2. Interstitial

Figure 3 shows the local electronic structures of a Ga interstitial in an InP layer, and its influence on a neighbouring P atom. The p partial waves across the Fermi level (E_F = −0.5700 Ryd) form unbonding states of an $I_{Ga}(1)$ defect. Compared with a normal P atom, the main influence of the $I_{Ga}(1)$ interstitial is on the conduction band, while the valence band shape is well conserved. The decrease in the bottom of the conduction band is about 0.01 Ryd. The same result as for the GaAs/AlAs superlattice is obtained, i.e. that all possible group-III interstitials are donor-like defects.

The calculations of group V interstitials are given in figure 4. A P interstitial mainly affects the valence band of its neighbours, but the shift of the top is not as significant as

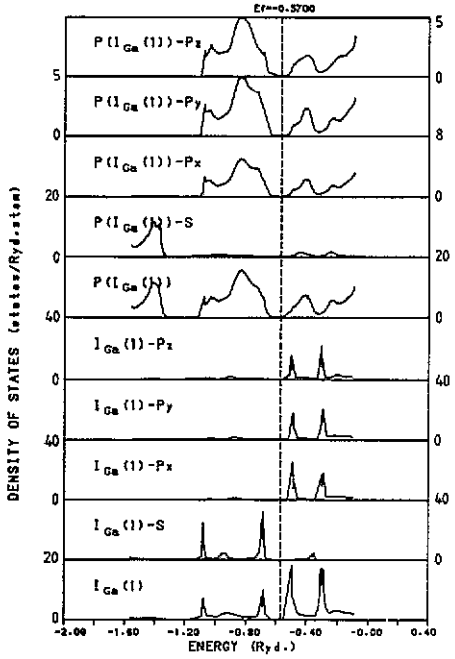

Figure 3. LDOS and PDOS of an interstitial $I_{Ga}(1)$ in an InP layer and its neighbouring P atom.

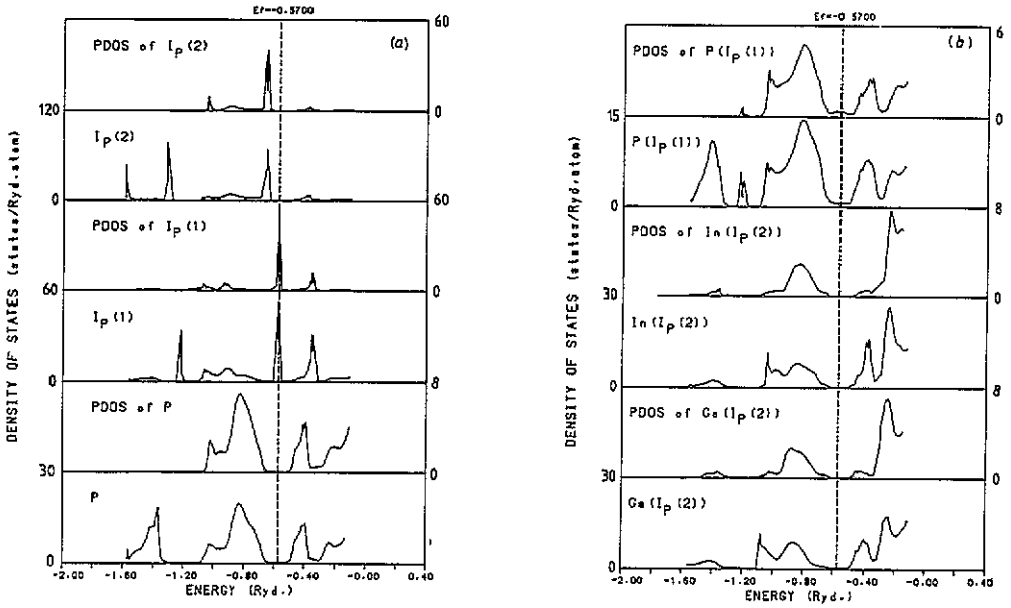

Figure 4. LDOS and PDOS of (*a*) group V interstitials and (*b*) their neighbours.

that of the conduction band bottom. An important fact is found, for the first time, that $I_P(j)$ ($j = 1, 2, 3$) are anions in a $(GaP)_1/(InP)_1$ SLS. It is different from a group V interstitial in a GaAs/AlAs superlattice. The change in the charged state of a group V

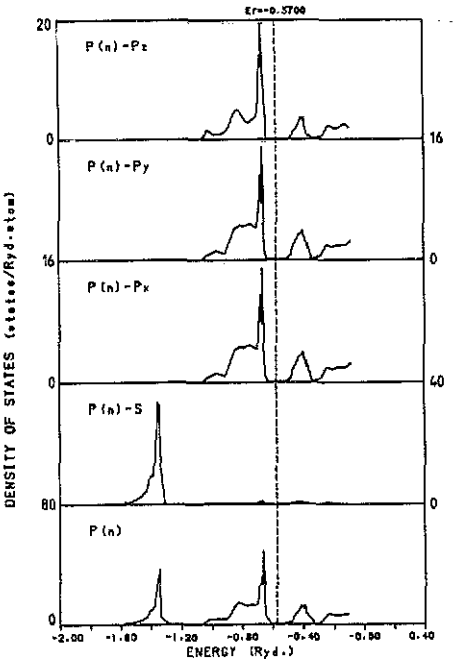

Figure 5. LDOS and PDOS of a P atom near the Ga vacancy.

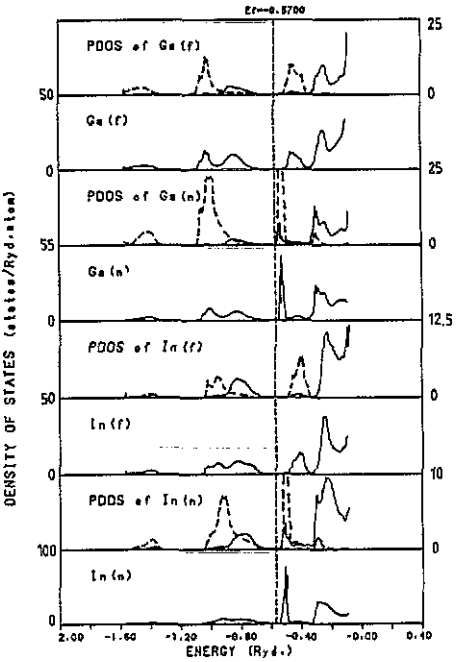

Figure 6. Influence of a P vacancy on its neighbours, where n or f represents an atom near to or far from the vacancy: ——, s partial waves.

interstitial may be due to the influence of strain on the electronic structure of a mismatched superlattice.

3.3. Vacancy

In the same way as for other defects discussed above, there will be some new localized states in the energy gap with the presence of a vacancy. Figure 5 shows the LDOS and PDOS of a P(n) atom which is located near to a gallium vacancy. The shift of the LDOS peak of the highest valence band is about 0.17 Ryd towards the Fermi level, while the position of the conduction band peak does not change by comparison with that of a normal P atom. It is found that the main influence of a group III vacancy is on the p states of its neighbours. The V_{In}-related shift is 0.16 Ryd. From the calculation of the electron distribution, we find that there is a negative centre around a group III vacancy.

When a P vacancy appeared at the interface, the local electronic structure is as drawn in figure 6, where some results of the atoms Ga(f) and In(f) far from the defect are also given as references. In this case, we find that a P vacancy affects not only the p electron distribution of its neighbours, but also the *s* electron distribution. The LDOS peak shifts of the lowest conduction band are 0.10 Ryd and 0.07 Ryd for In(n) and Ga(n) atoms, respectively. Because of the different ionicities between Ga–P and In–P bonds, a local interface field is set up, which will induce a slight shift in the charge distribution into the InP layer.

Table 2. The influence of intrinsic and foreign defects on the TEO and valence (in parentheses) of their nearest neighbours in a $(GaP)_1/(InP)_1$ SLS.

Isolated defect	TEO on nearest-neighbour atom		
	P	Ga	In
P_{In}	5.156 (−0.156)		
P_{Ga}	5.225 (−0.225)		
In_P		2.858 (0.142)	2.748 (0.252)
Ga_P		2.832 (0.168)	2.729 (0.271)
V_P		2.299 (0.701)	2.032 (0.969)
V_{In}	5.897 (−0.897)		
V_{Ga}	5.964 (−0.964)		
$I_P(1)$	5.356 (−0.356)		
$I_P(2)$		2.778 (0.222)	2.522 (0.478)
$I_P(3)$	5.247 (−0.247)		
$I_{In}(1)$	5.435 (−0.435)		
$I_{In}(2)$		2.574 (0.426)	2.735 (0.265)
$I_{In}(3)$	5.323 (−0.323)		
$I_{Ga}(1)$	5.430 (−0.430)		
$I_{Ga}(2)$		2.898 (0.102)	2.575 (0.425)
$I_{Ga}(3)$	5.401 (−0.401)		
Si_P		2.821 (0.179)	2.577 (0.423)
Si_{In}	5.352 (−0.352)		
Si_{Ga}	5.326 (−0.326)		
	5.465 (−0.465)	2.664 (0.336)	2.406 (0.594)

3.4. Influence on valence electron distribution

As a sensitive sign for discussing the influence of isolated native defects on the electronic structure of a crystal, the total electronic occupancy (TEO) and valence (in parentheses) of an atom near to these defects in a $(GaP)_1/(InP)_1$ (001) SLS are given in table 2. The corresponding results for a Si impurity in the light-doping case are also listed, where we use Si_C for a Si dopant on a C site. In the last row of the table, we show the TEO of an atom in an ideal $(GaP)_1/(InP)_1$ SLS without defects.

First of all, we confirm that the presence of a point defect does not change the charged state of its neighbour atoms; it only affects the distribution of valence electrons on them. In general, because of the strong interaction between a broken bond with other hybrid bonds on the same atom, the influence of a vacancy is more significant than other defects. For example, the TEO change of a P atom made by a nearby V_{Ga} or V_{In} defect is 9% or 8%, while other influences on the same atom are within 4%. In some cases the influence of an interstitial is almost as important as a vacancy. For example, the increasing TEO of an In atom made by an $I_{In}(2)$ defect is 14%, while its decrease due to a V_P vacancy is 16%. This is because the interstitial has also changed the atomic configuration. The influence of an isolated defect on the electron distribution of its neighbours can be summarized in the following sequence: vacancy, the same kind of interstitial, antisite, and Si impurity. This trend may hold true in other III–V semiconductor materials, which is useful for analysing the effect of an isolated defect.

4. I_P–P_{Ga} and I_P–P_{In} complexes

Is there an EL2-like defect in the GaP/InP system? This is a very interesting question for much effort [29–31] has been made to investigate this pair in the GaAs system. From

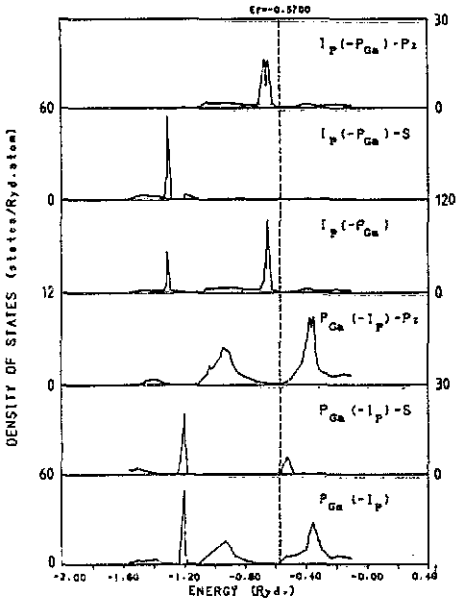

Figure 7. Local electronic structure of an I_P–P_{Ga} *complex.*

Table 3. The EO and valence (in parentheses) of a defect in I_P–P_{Ga} and I_P–P_{In} complexes.

	EO				TEO
	S	P_x	P_y	P_z	
$I_P(-P_{Ga})$	1.852	1.415	1.414	1.410	6.091 (−1.091)
$P_{Ga}(-I_P)$	1.628	0.895	0.896	0.888	4.307 (0.693)
$I_P(-P_{In})$	1.852	1.410	1.410	1.402	6.073 (−1.073)
$P_{In}(-I_P)$	1.748	0.895	0.895	0.906	4.444 (0.556)

the valence of an isolated defect discussed in section 3, we find that I_P and P_{III} (III ≡ Ga or In) have charged states of opposite sign. It is different from I_{As} and As_{Ga} in bulk GaAs and the GaAs/AlAs superlattice, where they are both donor-like defects. Accompanied by a negative Ga_{As} defect, a loosely bound complex I_{As}–As_{Ga} at a distance about 1.5–2 bonds lengths is formed, which leads to the EL2 phenomenon in GaAs [29, 30]. In a GaP/InP SLS, a closely bound I_P^-–P_{III}^+ pair at a bond length can be formed by coulombic attraction. Figure 7 shows the LDOS and PDOS of the I_P–P_{Ga} complex, where I_P lies along a $[\bar{1}\,\bar{1}\,\bar{1}]$ antibonding direction. It is clear that there are some defect-related states in the energy gap of the $(GaP)_1/(InP)_1$ (001) SLS. They are at $E_v + 0.001$ Ryd and $E_c - 0.024$ Ryd, contributed by p partial waves of I_P and s partial waves of P_{Ga}, respectively. These can be observed by optical experiments. Therefore, it is reasonable to believe that an EL2-like absence may not occur in a GaP/InP SLS. So far, we have not found any experimental report about EL2 phenomenon even in bulk GaP material.

The EO and valence of a defect in the I_P–P_{Ga} and I_P–P_{In} complexes are given in table 3, from which we find that the electrons on the s state of an I_P interstitial are close to that

Table 4. The characteristics of intrinsic defects in a stable (001)-oriented $(GaP)_1/(InP)_1$ SLS. $I_i(2)$ ($i \equiv$ Ga, In or P) represents an interstitial in the centre of the tetragonal unit cell; $I_i(1)$ and $I_i(3)$ are interstitials that lie along $[\bar{1}\,1\,\bar{1}]$ and $[1\bar{1}1]$ antibonding direction in the InP and GaP layers, respectively.

Intrinsic defect	Cation	Anion
Interstitial	$I_{Ga}(1)$, $I_{Ga}(2)$, $I_{Ga}(3)$, $I_{In}(1)$, $I_{In}(2)$, $I_{In}(3)$	$I_P(1)$, $I_P(2)$, $I_P(3)$
Antisite	P_{Ga}, P_{In}	Ga_P, In_P
Vacancy	V_P	V_{Ga}, V_{In}

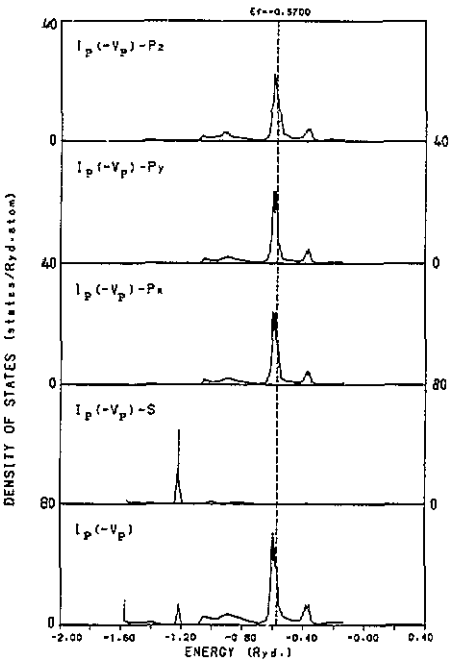

Figure 8. LDOS and PDOS of an I_P interstitial in the I_P–V_P pair.

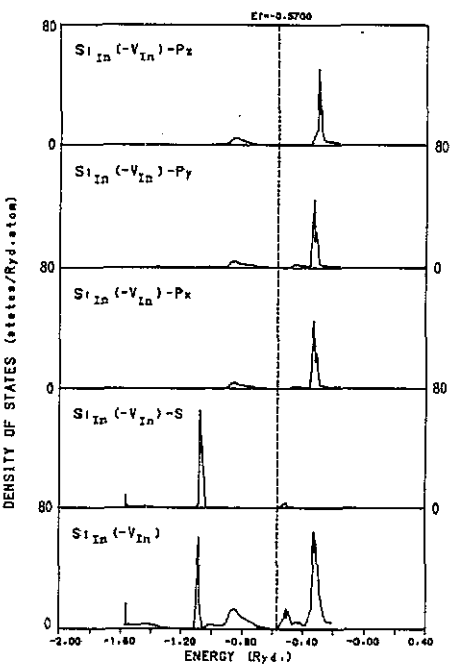

Figure 9. LDOS and PDOS of a Si_{In} donor in the Si_{In}–V_{In} pair.

on a p state. The TEO of an I_P is 6.09 (or 6.07), while for an I_{As} in a GaAs/AlAs superlattice it is about 4.58. This means that a group V interstitial in the GaP/InP system will have one or two electrons more than that in the GaAs/AlAs superlattice.

5. Self-diffusion and impurity diffusion

Study of the kinetic properties of a crystal shows that self-diffusion and impurity diffusion processes occur through some mobile Frenkel complexes. These defect pairs are formed

by coulombic interaction, directly or indirectly. In order to discuss the diffusion mechanisms in a $(GaP)_1/(InP)_1$ SLS, the characteristics of all isolated intrinsic defects are given in table 4.

Self-diffusion through the superlattice is associated with the movement of vacancies and interstitials, in which they jump from one equilibrium position to a neighbouring position. From the results shown in table 4, we can find some similar processes for a group III intrinsic defect in the present SLS as in the GaAs/AlAs superlattice [10]. It is interesting to note that I_P and V_P are also in oppositely charged states, which are different from I_{As} and V_{As} in the GaAs/AlAs superlattice, where they are both donor-like defects. Therefore, the general self-diffusion paths, which are suited not only to a group III defect but also to a group V defect in the GaP/InP SLS, can be described as

$$V \leftrightarrow V + (I' + V') \leftrightarrow (V + I') + V' \leftrightarrow V'$$

or

$$I \leftrightarrow I + (V' + I') \leftrightarrow (I + V') + I' \leftrightarrow I'.$$

This means that the opportunity for the self-diffusion process increases in the GaP/InP system. Figure 8 shows the local electronic structure of a P interstitial in the I_P–V_P pair. Besides the V_P vacancy, this I_P has three other nearest P atoms.

Based on the calculation of the defect-related charged states, impurity diffusion can be discussed by correlation effects. The significant complexes that control the impurity diffusion mechanism are

$$Si_{III}^{+} + V_{III}^{-} \leftrightarrow (Si_{III}^{+} - V_{III}^{-}) \qquad (III \equiv Ga \text{ or } In)$$

in the n-type doping structure, and

$$Si_P^{-} + V_P^{+} \leftrightarrow (Si_P^{-} - V_P^{+})$$

in p-type doping. These complexes are thought to be mobile species, while the isolated Si_{III}(III ≡ Ga or In) and Si_P defects will be immobile. The LDOS and PDOS of the Si_{In} defect in the Si_{In}–V_{In} pair are given in figure 9. The related impurity level is at $E_c - 0.007$ Ryd, which mainly originates from an s partial wave.

6. Summary

We have tried to produce a comprehensive picture of foreign impurity Si and intrinsic defects P_{Ga}, P_{In}, Ga_P, In_P, V_P, V_{Ga}, V_{In}, $I_P(j)$, $I_{Ga}(j)$ and $I_{In}(j)$ (where $j = 1, 2, 3$) in a stable (001)-oriented $(GaP)_1/(InP)_1$ SLS. The calculation of localized states and EOS of various defects show their characteristics directly. It is found that the charged state of an atom will be changed when it becomes an antisite. The influence of an isolated defect on the electron distribution of its neighbours is in the following sequence: vacancy, the same kind of interstitial, antisite and Si impurity. This may be rather a general consequence. Based on the charged states of intrinsic defects listed in table 4, a closely bound I_P–P_{III} (III ≡ Ga or In) pair has been proved to exist in the GaP/InP system. It will induce some related states in the energy gap, which can be observed by optical experiments. Therefore, no evidence has been found anywhere of EL2-like behaviour in this superlattice. Some new favourable self-diffusion and impurity diffusion processes, which did not occur in the GaAs/AlAs superlattice, are proposed for the first time.

The structural parameters of the $(GaP)_1/(InP)_1$ (001) SLS determined by the Keating model are in good agreement with first-principles total energy calculations. The recursion procedure developed for semiconductor superlattices proves to be a practical method for discussing small amounts of defects in these systems, which avoids the computational impediment required by a band-structure calculation based on Bloch's theorem.

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