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Arsenic interstitials and interstitial complexes in low-temperature grown GaAs

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First-principles molecular-dynamics calculations have been used to calculate the formation energy of the lowest-energy As interstitial configuration relative to the formation energies of As antisites and Ga vacancies in As-rich GaAs, and to identify and study the properties of energetically favorable complexes containing one As antisite and one As interstitial. It is suggested that the electronic and optical properties of the antisite-interstitial complexes match the properties of the defects responsible for the dominant donor band in some samples grown around 350 °C. [S0163-1829(97)07424-9]

I. INTRODUCTION

There has been great recent interest in understanding the properties of low-temperature-grown (LT) GaAs: i.e., GaAs grown by molecular-beam epitaxy (MBE) at substrate temperatures of 200–400 °C, generally followed by annealing at a higher temperature. It has been shown that this process can produce buffer layers for semiconductor devices of unusually high resistivity, leading to substantial improvements in device performance.[1–2] Due to the extremely fast (subpicosecond) carrier lifetimes which can be achieved in this material, together with a high carrier mobility and a high dielectric breakdown strength, LT GaAs can also be used to make high-speed and high-voltage photoconductive switches and fast, high-sensitivity, wide bandwidth photodetectors.[3]

LT GaAs is grown under As-rich conditions, resulting in up to 1.5% excess As or more in the lattice.[4] This excess As must be accommodated in the as-grown material by point defects such as As antisites, As interstitials, Ga vacancies, and complexes involving these defects. The first point defect to be identified in LT GaAs was the arsenic antisite. Signals corresponding to substantial quantities of As antisites have been seen both in EPR (Ref. 5) and in absorption experiments[6,7] on LT GaAs, although these experiments cannot determine whether the As antisites are isolated, or whether they occur primarily in complexes with other point defects. Some of the antisites observed in LT GaAs are photoquenchable, like the isolated As antisite:[8,9] when exposed to light with an energy of about 1.1 eV, they lose their characteristic EPR and absorption signals. Other antisites observed in LT GaAs are nonphotoquenchable. Although the numbers cited for different samples and different growth conditions vary, the total measured concentration of As antisites generally leaves a considerable fraction of the reported deviation from stoichiometry in LT GaAs unaccounted for.

The location of the excess As which is not observed as As antisites is controversial. Slow positron annihilation studies[10] have been used to demonstrate the existence of Ga vacancies in LT GaAs, and both rapid diffusion[11] and ion channeling[12] experiments have been cited as evidence of the existence of As interstitials in LT GaAs. However, these experiments do not provide such an unambiguous, quantitative measure of the concentrations of Ga vacancies and As interstitials as the EPR and absorption experiments do for As antisites. Again, as for the As antisites, the experiments which have been cited as evidence for Ga vacancies and As interstitials cannot determine whether these defects are present primarily as isolated defects, or in complexes with other defects.

In addition to the controversy over relative concentrations of the important point defects and defect complexes in LT GaAs, there is also still controversy over the specific contributions of the point defects, which are present in as-grown LT GaAs in extremely high concentrations, and the As precipitates, which are present in material annealed at temperatures around 600 °C or above, in determining the properties of LT GaAs. To further complicate the situation, optimization of LT GaAs for different applications requires varying both the growth temperature and postgrowth processing, which may lead to precipitate-dominated material in some cases and material dominated by the residual point defects in other cases, as well as to different relative concentrations of the various point defects and defect complexes. Although it will not solve all the controversies, achieving a better understanding of the most numerous point defects in as-grown LT GaAs is an essential first step toward a full understanding of this material.

We have used first-principles molecular-dynamics methods to calculate the formation energy of the lowest-energy As interstitial configuration relative to the formation energies of As antisites and Ga vacancies in As-rich GaAs, and to identify and study the properties of energetically favorable complexes containing one As antisite and one As interstitial. In Sec. II, the calculations of the relative formation energies of As interstitials, As antisites, and Ga vacancies in As-rich GaAs are presented, and the implications for the relative concentrations of various point defects are discussed. In Sec. III,

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the results of the calculations on interstitial-antisite complexes are presented. Conclusions are summarized in Sec. IV.

II. RELATIVE TOTAL ENERGIES OF POINT DEFECTS

Due to computational limitations, the earliest first-principles theoretical work[13–15] on As interstitials in GaAs considered only tetrahedral configurations, where the extra atom occupies the largest empty space in the lattice, so that minimal distortion of the surrounding lattice is required. Tetrahedral As interstitials in GaAs were found to have high formation energies, and were therefore predicted to be much less numerous than antisites and vacancies in As-rich GaAs.[13,15] In addition, tetrahedral As interstitials were found to be donors,[13–15] so that they could not compensate the As antisites, which are also donors. These results suggested that the dominant acceptors in LT GaAs must be Ga vacancies. However, recent work on several semiconductor systems has shown that in many cases a relatively complicated configuration, such as a bond-centered or split interstitial configuration, is the most energetically favorable.[16] Later theoretical work on interstitials in GaAs (Ref. 17) showed that the lowest-energy configurations for both donor and acceptor As interstitials are not tetrahedral, but split interstitial configurations. In fact, according to the results of ion channeling experiments which preceded publication of these calculations, roughly 60% of the excess As in LT GaAs grown at 200 °C was reported to be occupying a split interstitial configuration centered on an As site.[12]

We have used first-principles molecular-dynamics calculations to investigate how much the formation energy of an As interstitial is reduced when it is allowed to move from the tetrahedral configuration into the lowest energy split interstitial configuration. We used the Sankey-Niklewski method,[18] which is based on density functional theory in the local-density approximation (LDA), and uses norm-conserving pseudopotentials.[19] This method is implemented in terms of a basis of pseudoatomic orbitals, and uses the Harris-Foulkes energy functional,[20,21] which has been shown to give results similar to self-consistent Sankey-Niklewski calculations for GaAs.[22] We have used the Ceperley-Alder form[23] as parametrized by Perdew and Zunger[24] for the exchange-correlation potentials, and we used cubic supercells containing 65 atoms. With this size of cell, total energies were found to be calculated sufficiently accurately using one special *k* point. The electronic defect levels reported are the levels obtained for the special *k* point.

The As split interstitial which is preferred for neutral and negatively charged states is a (110) split interstitial, centered on an As site.[17] Since this interstitial is an acceptor, it should be the most numerous As interstitial in LT GaAs, which tends to be *n* type in its as-grown state. We find that this split interstitial is 4.0 eV lower in energy, in the neutral charge state, than the neutral tetrahedral As interstitial with As nearest neighbors, which was the lowest-energy As interstitial investigated in Ref. 15, where relative formation energies of tetrahedral As interstitials, As antisites, and Ga vacancies in As-rich GaAs were reported.

Comparison of the formation energies of defects involving different numbers of excess As atoms in As-rich GaAs requires an accurate calculation of the formation energy of bulk GaAs, relative to pure Ga and As. Although our pseudoatomic orbital methods give quite accurate results for calculations of semiconductor properties, including the relative formation energies of different configurations of a particular defect in the semiconductor, these methods are less accurate than the plane-wave methods of Ref. 15 for calculating the energy of pure, metallic phases. Therefore, in order to compare the formation energies of the lowest-energy As split interstitials, As antisites, and Ga vacancies in As-rich GaAs, we will use some of the results of Ref. 15.

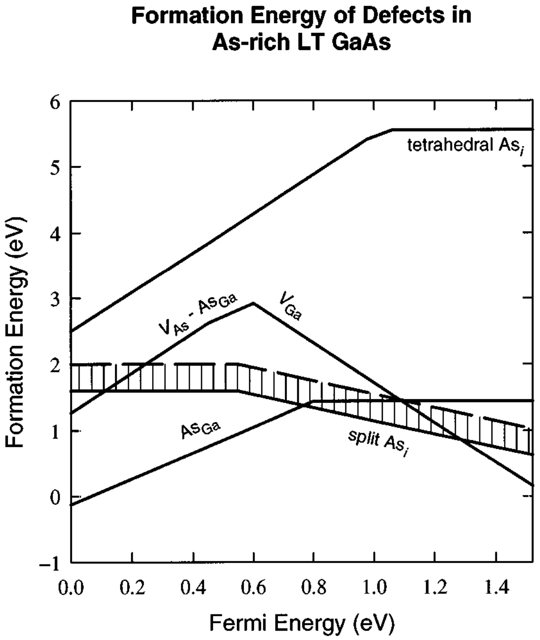

FIG. 1. Formation energy of defects in As-rich GaAs, for Fermi energies ranging from the valence-band edge to the conduction-band edge.

Figure 1 shows the formation energies of tetrahedral As interstitials, As antisites, and Ga vacancies in As-rich GaAs, as a function of Fermi level, taken from information given in Ref. 15. The structural transformation of the Ga vacancy to an As antisite-As vacancy complex is shown, using information given in Ref. 25 and 26. We have added our results for the formation energy of the As split interstitial to this figure, by placing the neutral split interstitial formation energy 4.0 eV below the neutral tetrahedral interstitial formation energy. We note that our calculations compared the energy of the fully relaxed split interstitial to the energy of the unrelaxed tetrahedral interstitial, as the tetrahedral interstitial was found to be unstable in our calculation, and relaxed to a completely different configuration when given enough time. Since the results reported for the tetrahedral interstitial formation energy in Ref. 15 included a small amount of lattice relaxation, which may have lowered the reported energy somewhat below the formation energy for the unrelaxed tetrahedral interstitial, the solid line in Fig. 1 which is labeled as the formation energy of the split As interstitial is actually a lower bound for the formation energy. This line will be lower than the true formation energy of the split interstitial by an amount equal to the relaxation energy of the tetrahedral interstitial in Ref. 15. This relaxation energy is considerably less than 0.8 eV.[27] For the purposes of plotting, we have assumed that the formation energy of the split interstitial may be as much as 0.4 eV above the solid line which gives our initial estimate and the lower bound to the formation energy. Figure 1 therefore shows a possible energy range of 0.4 eV for the formation energy of the split interstitial.

Even with this rather generous error bar, we find that the formation energy of the As split interstitial is comparable to the formation energy of the As antisite for As-rich GaAs with a Fermi level near the middle of the gap. The As split interstitial formation energy is lower than the formation energy for Ga vacancies, suggesting that As interstitials may be more numerous than Ga vacancies in LT GaAs.

Although the $\langle 110 \rangle$ split interstitial configuration is expected to have the lowest formation energy in LT GaAs, there are several other configurations within half an eV of the lowest-energy configuration for As interstitials in all charge states.[17] This suggests that As interstitials may be able to move about quite freely, without having to go over large energy barriers, in agreement with experimental evidence that As interstitials diffuse rapidly in GaAs. Rapidly diffusing defects have been observed in LT GaAs, in concentrations comparable to or greater than concentrations of As antisites.[11] These defects have been identified as As interstitials,[11] since the activation energy for diffusion of these defects matches the activation energy for As interstitial diffusion deduced from other experiments on GaAs.[28]

Since As interstitials are expected to be quite mobile, they are likely to be able to move about as the material cools after growth, until they form a complex with another defect. In LT GaAs, the large deviation from stoichiometry ensures high concentrations of defects such as As antisites, which can attract and form complexes with acceptor As interstitials. Therefore, As interstitials may be present primarily in small clusters and complexes in this material. In order to identify the location of the excess As which is not observed as As antisites, it may therefore be helpful to identify low-energy complexes of As interstitials with other defects which are expected to be present in high concentrations in LT GaAs, study their properties, and look for evidence of their existence in LT GaAs grown under various conditions.

In fact, if we assume that there are significantly more As interstitials than Ga vacancies, there is additional experimental evidence that the excess As which is not accounted for by measured antisite concentrations is present primarily in the form of defect complexes, rather than isolated interstitials. This evidence comes from recent experimental analyses of the lattice dilation as a function of As antisite concentration,[29,30] which include the assumption that concentrations of Ga vacancies are significantly lower than concentrations of As antisites, so that lattice contraction due to the vacancies can be neglected. Although these analyses disagree over whether the As antisites represent the majority or merely a significant minority of the excess As, they agree that the lattice dilation contributed by As interstitials is less than might be expected. They conclude that either there are significantly fewer As interstitials than As antisites,[29] or the lattice dilation contributed by an As interstitial is smaller than the lattice dilation contributed by an As antisite.[30]

We find that the lowest-energy isolated As interstitial introduces slightly more lattice dilation than an isolated As antisite. In our 65-atom supercells, which are larger than the 32-atom supercells used by Chadi,[17] and therefore give a more accurate picture of the lattice dilation or contraction contributed by each defect, the average bond length from the As site occupied by a neutral, isolated split interstitial to its four-nearest neighbors is increased by almost 12% over the ideal bond length in GaAs, while the average bond length from the neutral, isolated As antisite to its nearest neighbors is increased by 9% over the ideal bond length. We find that the volume of the irregular tetrahedron containing the neutral, isolated As interstitial, whose vertices are the four-nearest neighbors of the interstitial, is increased 36% by the presence of the defect, while the volume of the tetrahedron containing the neutral, isolated As antisite, whose vertices are the four-nearest neighbors of the antisite, is increased by 29%. These results support the conclusion that interstitial-containing complexes, which can contribute a smaller amount of lattice dilation per excess As atom than isolated As interstitials, account for a large part of the excess As which is not observed as As antisites.

III. INTERSTITIAL COMPLEXES

We have searched for the low-energy complexes containing one As interstitial and one As antisite by putting an As antisite beside an As interstitial, and allowing the complex to relax. Starting with the As interstitial in several different split interstitial configurations, as well as in tetrahedral, hexagonal, twofold-coordinated bridge-bond configurations, and slightly displaced from these positions, the complex generally undergoes a large transformation, ending close to one of two final configurations.

The lowest-energy complex consists of two As atoms sharing a vacant Ga site. This complex was suggested by Delerue, Lannoo, and Stievenard,[31] on the basis of physical considerations and tight-binding electronic structure calculations, as a candidate for the metastable state of the EL2 defect found in Czochralski-grown GaAs. This complex looks quite similar to the dominant acceptor split interstitial, except that the two As atoms of the complex share a Ga site, instead of an As site, so that the complex contributes a net increase of 3 to the excess of As atoms over Ga atoms, while the split interstitial only contributes one net excess As atom to the total deviation from stoichiometry. Because of the similarity to the split interstitial, we may call this complex a ‘‘split antisite.’’ It is shown in Fig. 2. For a detailed comparison, Table I gives the coordinates of the two atoms of the split defect and their four-nearest neighbors, for the dominant acceptor As split interstitial and the split antisite. The orientation of the split antisite obtained from the present first-principles molecular-dynamics calculations differs slightly from the orientation obtained from the simple valence force-field model of Delerue, Lannoo, and Stievenard; in Ref. 31, the two central atoms of the split antisite are displaced from each other along an axis equivalent to the $\langle 111 \rangle$ axis, while in Table I, the central atoms are displaced from each other approximately along the $\langle 120 \rangle$ axis.

Since the two As atoms forming the split antisite are each triply coordinated, this defect contains no As atoms which

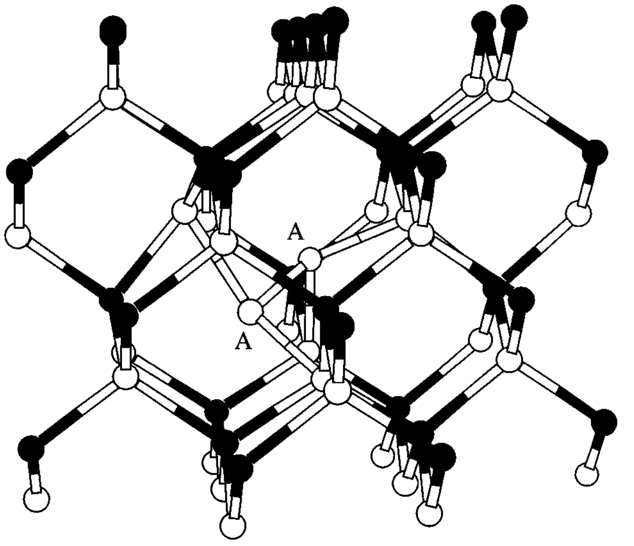

FIG. 2. Supercell containing the split As antisite. The Ga atoms are black, and the As atoms are white. The two As atoms forming the split antisite are labeled *A*.

are tetrahedrally bonded to four other As atoms. Therefore, the split antisite will not show up in EPR experiments as an As antisite. In addition, the split antisite has no electronic levels in the midgap region. Therefore, it will not have the characteristic strong absorption seen for the As antisite, which corresponds to an electronic transition from the midgap donor level of the antisite to a localized resonance in the conduction band.

The split antisite does have a donor level near the conduction-band edge, which can contribute one electron to the conduction band. According to the previous tight-binding calculations,[31] this donor level is above the conduction-band edge. However, we find that for a split antisite which has relaxed to its lowest-energy configuration, the donor level is 0.3 eV below the conduction band.

The first-principles binding energy of the neutral split antisite, relative to the uncharged, isolated split interstitial and the uncharged, isolated As antisite, is calculated to be 1.4 eV. Since the isolated antisite and isolated interstitial can lower their energies by exchanging an electron and becoming charged, the binding energy relative to the singly charged acceptor interstitial and the singly charged As antisite is lower. Using our calculated electronic levels gives a binding energy of 1.3 eV relative to the charged defect pair. However, some uncertainty arises from the fact that our calculations, using the LDA with a pseudoatomic orbital basis, give a band gap of 1.2 eV for GaAs, while the experimental gap at room temperature is 1.4 eV. If the acceptor level of the isolated split interstitial is assumed to be derived from valence-band states, the donor level of the isolated As antisite is assumed to be derived from conduction-band states, and the ''scissors'' operator is used to move the conduction-band-derived states up uniformly by 0.2 eV so as to reproduce the room-temperature experimental gap, we get a calculated binding energy of 1.1 eV for the split antisite, relative to the singly charged, isolated As antisite, and the singly charged, isolated acceptor interstitial.

The binding energy of the split antisite complex, calculated above, is not large. If the barriers to breakup of this complex are also not very large, the lifetime of this complex before breakup may be reasonably short. When the split antisite complex breaks up, it releases an interstitial and an antisite. Since the As interstitial is expected to be quite mobile, it may soon form a complex with another antisite.

Even though the split antisite complexes may be regularly breaking up and forming again, there should be a significantly higher concentration of split antisite complexes than isolated interstitials, as can be seen from the following order-of-magnitude arguments. We note that the point defects in as-grown LT GaAs have not achieved full equilibrium with the surroundings; there are nonequilibrium amounts of excess As in the material. However, if isolated As interstitials are present in the material as it cools down after growth or annealing, they should be mobile enough so that the concentrations of the interstitials and interstitial-containing complexes are at least in equilibrium with each other.

Neglecting small changes due to entropy factors, the concentrations of the split antisite complex, isolated antisite, and isolated interstitial must therefore satisfy the following relationship:

$$c_{\text{split antisite}} = c_i c_a \exp[E_b/(k_B T)],$$

TABLE I. The atomic coordinates for the (110) split As interstitial and the split As antisite, in the neutral charge state. The coordinates are given in units of the cubic lattice constant of GaAs, with the origin chosen to be at the point midway between the two As atoms of the split defect. The first two lines give the coordinates of the two As atoms forming the split defect, and the following four lines give the coordinates of the four-nearest neighbors of the defect. The four-nearest neighbors are Ga atoms for the split interstitial, and As atoms for the split antisite.

(110) split As interstitial	Split As antisite
As(0.1418,0.1583,0.0014)	As(0.0828,0.1953,0.0132)
As(−0.1418,−0.1583,−0.0014)	As(−0.0828,−0.1953,−0.0132)
Ga(0.2765,0.2907,0.3650)	As(0.3155,0.2329,0.3991)
Ga(−0.2960,−0.2937,0.3584)	As(−0.2388,−0.3308,0.3787)
Ga(−0.2683,0.2557,−0.1968)	As(−0.3008,0.2891,−0.2209)
Ga(0.2461,−0.2816,−0.2020)	As(0.2994,−0.3527,−0.1689)

where c_i is the fraction of As lattice sites which are occupied by an isolated, singly charged acceptor split interstitial, c_a is the fraction of Ga lattice sites which are occupied by an isolated, singly charged As antisite, $c_{\text{split antisite}}$ is the fraction of Ga lattice sites which are occupied by a neutral split antisite complex, E_b is the binding energy of the complex relative to the isolated defects, and k_BT is Boltzmann's constant times the absolute temperature. At room temperature and for a binding energy of 1.1 eV, the exponential factor $\approx 4\times 10^{18}$. Therefore, in order to be in equilibrium with concentrations $c_a \approx 5\times 10^{-8}$, corresponding to 10^{15} singly charged, isolated antisites/cm^3, and $c_i \approx 5\times 10^{-13}$, corresponding to 10^{10} isolated, singly charged, acceptor interstitials/cm^3, the concentration $c_{\text{split antisite}}$ would have to be about 10^{-1}, corresponding to 2×10^{21} neutral split antisites/cm^3. The concentration of charged split antisite complexes would be higher, for a Fermi level in the midgap region. Obviously, before such a high concentration of complexes could be formed, the concentration of isolated interstitials would be depleted to well below the concentration we have assumed. But this simple analysis shows that if the isolated interstitials are sufficiently mobile to come into equilibrium with the interstitial-containing complexes, then at any point in time most of the interstitials would be present in complexes, not as isolated interstitials.

Since the split antisite will not be visible as an antisite in EPR or absorption experiments, it can contribute to the excess As which is not accounted for by the antisites. The amount of lattice strain contributed per excess As atom is lower for the split antisite complex than for the isolated split interstitial, in agreement with the experimental evidence that the net lattice dilation contributed by the excess As which is not seen as antisites is small. We find that the volume of the irregular tetrahedron containing the split antisite, whose vertices are the four-nearest neighbors of the defect, is increased by 61% by the presence of the defect. Since the split antisite introduces a deviation from stoichiometry equivalent to three excess As atoms, it increases the volume surrounding its lattice site by 20% per excess As, while the isolated As interstitial increases the volume surrounding its lattice site by 36% per excess As.

The other low-energy complex of an As interstitial and an As antisite, which we have described previously,[32,33] contains a minimally distorted As antisite, with a split interstitial as one of its nearest neighbors. The electronic band structure of this complex contains an antisite-derived level in the midgap region and an antisite-derived resonance in the conduction band.[33] Therefore, this complex will have the EPR and absorption signatures characteristic of an As antisite. However, since it contains an interstitial as well, it contributes one extra As to the excess As which is not accounted for by the measured concentrations of As antisites.

This nearest-neighbor complex, like the split antisite, has a low binding energy. Its binding energy relative to the isolated, singly charged antisite and the isolated, singly charged acceptor interstitial is 0.5 eV.[32] If the barriers to the breakup of this complex, and to transformation between the split antisite and the nearest-neighbor complex, are similar in magnitude to the binding energies, it seems likely that both the split antisite and the nearest-neighbor complex are continuously forming, breaking up, and transforming into each other, even at room temperature. This means that at any given time there will be substantial concentrations of the split antisite, the nearest-neighbor complex, and various configurations in between. Since the nearest-neighbor complex has a donor level about 0.5 eV below the conduction band[32] and the split antisite has a donor level about 0.3 eV below the conduction band, we might expect that defect configurations intermediate between these two complexes would have donor levels intermediate between these donor levels. Therefore, rather than two separate defect levels corresponding to the split antisite and the nearest-neighbor complex, complexes consisting of an As interstitial and an As antisite may be responsible for a band of electronic states, roughly between 0.3 and 0.5 eV below the conduction band.

Recent experiments have identified a donor band which appears to be due to defects with properties similar to the properties of the antisite-interstitial complexes.[34] This band lies between 0.3 and 0.5 eV below the conduction band, in good agreement with the calculated energies for the band due to antisite-interstitial complexes. Like the defects responsible for the 0.3–0.5 eV donor band, the nearest-neighbor complex has the EPR and absorption signatures characteristic of an As antisite.[32,33] Like the defects responsible for this band, and unlike the isolated antisite, the antisite-interstitial complex is unphotoquenchable.[32,33]

The 0.3–0.5 eV band is the dominant donor band in some samples grown around 350 °C.[34] In fact, we have previously predicted that the excess As might be expected to be present in low-energy complexes, including antisite-interstitial complexes, rather than in configurations dictated by the kinetics of growth, in LT GaAs grown around 400 °C. This is because the anomalously large lattice strain present in LT GaAs disappears in LT GaAs which has been grown or annealed around 400 °C, indicating that at this temperature, the excess As is sufficiently mobile that it can move into low-energy configurations, involving less lattice strain.

IV. CONCLUSIONS

The (110) As split interstitial, which is the lowest-energy configuration for As interstitials in LT GaAs, and acts as an acceptor, is found to have a formation energy comparable to the formation energy of an As antisite, and less than the formation energy of a Ga vacancy, in As-rich GaAs with a Fermi level in the midgap region. This suggests that As interstitials may be more numerous than Ga vacancies in LT GaAs. Since As interstitials are expected to be quite mobile, they are likely to be present predominantly in interstitial-containing complexes, rather than as isolated interstitials.

We have found two low-energy complexes containing an As interstitial and an As antisite. The lowest-energy antisite-interstitial complex, which may be called a ''split antisite,'' will not be seen as an antisite in EPR or absorption experiments. This complex contributes less lattice dilation per excess As atom than an isolated interstitial, in agreement with experimental evidence that the excess As which is not accounted for by measured antisite concentrations contributes only a small amount to the net lattice dilation. The binding energy of the split antisite, and the binding energy of the nearest-neighbor interstitial-antisite complex, which has been discussed previously,[32,33] are low, suggesting that these complexes may be continuously forming, breaking up, and transforming into each other. Therefore, these interstitial-antisite complexes may be responsible for a donor band, instead of two separate donor levels. Our results suggest that the properties of these antisite-interstitial complexes match the properties of the defects responsible for the dominant donor band in some samples grown around 350 °C.[34]

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