Native defects in the $Al_xGa_{1-x}Sb$ alloy semiconductor

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Defect concentrations in $Al_xGa_{1-x}Sb$ which is in equilibrium with a liquid phase are calculated. When the liquid phase is Ga rich, a Ga antisite (Ga_{Sb}^{2-}) or an Al antisite (Al_{Sb}^{2-}) is dominant, and the concentrations of vacancies are much smaller than the antisite concentrations. Ga_{Sb}^{2-} is dominant in GaSb equilibrated with a Sb-rich solution, but the concentration of Sb antisites comes close to that of Ga_{Sb}^{2-} as temperature is lowered. For x larger than 0.6, a group-III vacancy is the predominant defect in the case of Sb-rich solutions. Calculated net acceptor concentrations agree well with those determined experimentally. A complex defect composed of Ga_{Sb} and a Ga vacancy, which have been taken as the dominant residual acceptor, is expected to be negligible.

I. INTRODUCTION

It has been considered that $Al_xGa_{1-x}Sb$ is a suitable material for optoelectronic devices. It has a direct band structure when x is smaller than 0.2 and the band-gap energy of this composition region corresponds to the wavelength region of 1.2–1.7 μm. However, in most cases, the InGaAsP alloy is used for devices of this wavelength region, and $Al_xGa_{1-x}Sb$ is scarcely used. This is because we do not have enough knowledge to control its physical properties. GaSb grown from a stoichiometric melt or by liquid-phase epitaxy (LPE) shows a p-type conduction without intentional doping. The p-type conduction has been considered to be due to native defects and not due to impurities.[1-5] However, the dominant native defect has not been conclusively identified. From various experimental results, it has been confirmed that the residual acceptor is related to deficiency of Sb in the solid. An Sb vacancy can be immediately ruled out as the residual acceptor, because an anion vacancy usually acts as a donor.[6] Effer proposed that the residual acceptor is a Ga antisite Ga_{Sb}.[2] On the other hand, Van Maaren suggested that it is a complex defect composed of a Ga vacancy V_{Ga} and Ga_{Sb},[3] and this model has been accepted to some extent.[4,5] However, an argument against this model was given by Kröger[7]: since both Ga_{Sb} and V_{Ga} act as an acceptor, they should not form a complex but repel each other because of the Coulomb force.

Electrical and optical characteristics of the residual acceptor are not completely understood. However, it is now generally agreed that the residual acceptor is a double acceptor, i.e., doubly ionizable.[8-15] In fact, there is clear evidence that the acceptor is doubly ionizable; strong luminescence due to electron transition from the conduction band to the residual neutral acceptor is observed from melt-grown undoped GaSb, but this luminescence peak completely disappears by donor doping.[16,17] This fact cannot be explained by the single-acceptor model but by the double-acceptor model. When the acceptors are doubly ionizable, they are ionized doubly in n-type materials and thus the transition from the conduction band to the neutral acceptor is very difficult to observe. The first ionization energy is measured to be about 30 meV and the second energy 70–100 meV.

In this study, we carry out a thermodynamic calculation of native defect concentrations in $Al_xGa_{1-x}Sb$ alloys. Our theoretical model is extended from that of Van Vechten.[18] The most important feature of his theory is that antisites as well as vacancies are taken as dominant defects. In some thermodynamic models, only vacancies are considered and antisites are neglected.[19] Later, Blom showed using the theory of Van Vechten that the number of antisites is much larger than that of vacancies in GaAs grown from Ga-rich liquid solutions.[20] He also calculated the defect concentrations in $Al_xGa_{1-x}As$ ternary alloys. However, his model for ternary alloys does not seem sound in some aspects, as discussed in our previous paper.[21] Recently, Edelin and Mathiot calculated defect concentrations in GaSb using their own model.[22] Their results indicate that the Ga antisite is the predominant defect.

In the previous paper, we presented a formalism of calculation of defect concentrations in III-V ternary alloys grown from liquid phase.[21] The formalism is applied to $Al_xGa_{1-x}Sb$ in this study, and dependence of defect concentrations on temperature and Al composition is investigated. Effects of impurity doping are also discussed. $Al_xGa_{1-x}Sb$ is grown from both Ga- and Sb-rich liquid solutions. Thus, the defect concentrations in crystals grown from Ga-rich solutions and those in crystals grown from Sb-rich ones are both calculated and compared with each other.

In the next section, we describe the calculation procedure of the defect concentrations. In Sec. III, the calculations are given and compared with the experimental results. Finally, the origin of the native acceptor in $Al_xGa_{1-x}Sb$ is discussed in Sec. IV.

II. CALCULATION PROCEDURE

Since we have already described the model of the defect thermodynamics in III-V alloys in detail,[21] the calculation

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procedure is described only briefly in this paper. Vacancies and antisites are considered as dominant defects, and the solid phase is assumed to be in equilibrium with a liquid phase. The reactions to be considered are as follows:

$$\mathrm{Ga}_l = \mathrm{Ga}_{\mathrm{III}} + V^x_{\mathrm{Sb}}, \quad (1)$$

$$\mathrm{Al}_l = \mathrm{Al}_{\mathrm{III}} + V^x_{\mathrm{Sb}}, \quad (2)$$

$$\mathrm{Sb}_l = \mathrm{Sb}_{\mathrm{Sb}} + V^x_{\mathrm{III}}, \quad (3)$$

$$V^x_{\mathrm{III}} = V^{+}_{\mathrm{III}} + h^{+}, \quad (4)$$

$$V^x_{\mathrm{Sb}} = V^{-}_{\mathrm{Sb}} + e^{-}, \quad (5)$$

$$\mathrm{Ga}_l = V^x_{\mathrm{III}} + \mathrm{Ga}^{2-}_{\mathrm{Sb}} + 2h^{+}, \quad (6)$$

$$\mathrm{Al}_l = V^x_{\mathrm{III}} + \mathrm{Al}^{2-}_{\mathrm{Sb}} + 2h^{+}, \quad (7)$$

$$\mathrm{Sb}_l = \mathrm{Sb}^{2+}_{\mathrm{III}} + V^x_{\mathrm{Sb}} + 2e^{-}, \quad (8)$$

where the subscripts l, III, and Sb represent a liquid phase, a group-III lattice site, and a group-V lattice site, respectively. The superscripts represent charge states: x is for a neutral state. e^- and h^+ are an electron and a hole, respectively.

In addition to the above reactions of defect formations, the following reactions of compound formation are considered:

$$\mathrm{Ga}_l + \mathrm{Sb}_l = \mathrm{Ga}_{\mathrm{III}} + \mathrm{Sb}_{\mathrm{Sb}}\,(\mathrm{GaSb}), \quad (9)$$

$$\mathrm{Al}_l + \mathrm{Sb}_l = \mathrm{Al}_{\mathrm{III}} + \mathrm{Sb}_{\mathrm{Sb}}\,(\mathrm{AlSb}). \quad (10)$$

The calculation procedure is as follows: From the equilibrium condition of the above reactions, all of the charged defect concentrations are expressed as functions of the electron concentration n. Then, they are substituted into the equation of the charge neutrality condition, and n is calculated numerically. Once n is obtained, the defect concentrations are calculated easily.

The enthalpies of vacancy formations used here were calculated by Van Vechten on the basis of his macroscopic cavity model.[23] In his model, the formation enthalpy of a vacancy is mainly the surface energy of a cavity (= vacancy). The formation enthalpy of V^x_{Sb} is larger than that of V^x_{Ga} or V^x_{Al}, because the covalent radius of Sb is larger than those of Ga and Al. The enthalpies of antisite-pair formations were calculated using the Pauling table of the elemental electronegativities.[18,24] Here we assume that the enthalpy is the same for both group-III and group-V antisites: The excess enthalpy is due to core potential and size difference between group-III and group-V atoms and thus similar for both types of antisites. The values of the enthalpies and entropies of defect formations are listed in Table I. The enthalpies of ionization of vacancies are assumed to be 20% of the band-gap energy.[18] The table also shows temperatures and entropies of fusion of the compounds,[25] from which the equilibrium constants of reactions (9) and (10) are obtained. In our calculation, the liquid phase is assumed to be a regular solution. In fact, this assumption is not always reasonable for Sb-rich solutions: the eutectic point of Sb and GaSb is about 590 °C, and the regular solution model is invalid below and near the eutectic point. However, we assume that Sb does not solidify even at temperatures below the eutectic point in order to clarify the difference in defect concentrations between solids grown from Ga-rich solutions and those grown from Sb-rich ones.

TABLE I. Enthalpies and entropies of defect formations in GaSb and AlSb (see Refs. 18 and 23). Temperatures and entropies of fusion are also shown. H is given in eV and S in k (the Boltzmann constant).

	GaSb		AlSb	
	H	S	H	S
V^x_{III}	2.03	1.1	2.30	1.1
V^x_{Sb}	2.56	1.1	2.81	1.1
$\mathrm{III}^{2-}_{\mathrm{Sb}}$	0.27	0	0.48	0
$\mathrm{Sb}^{2+}_{\mathrm{III}}$	0.27	0	0.48	0
T^F (K)	983		1338	
S^F	7.95		7.42	

III. NUMERICAL RESULTS

A. GaSb

Figure 1 shows temperature dependence of defect concentrations in GaSb. V_X (X = Ga, Sb) includes both of neutral and charged vacancies. In fact, almost all vacancies are ionized at temperatures above 300 °C, and the number of neutral vacancies is negligibly small. The antisite concentrations shown in Fig. 1(a) are much larger than the vacancy concentrations shown in Fig. 1(b).

Since the enthalpy of Sb-vacancy formation $H(V^x_{\mathrm{Sb}})$ is larger than $H(V^x_{\mathrm{Ga}})$, the number of V_{Ga} is larger than that of V_{Sb} even when the GaSb is in equilibrium with a Ga-rich solution. Because of the same reason, the number of $\mathrm{Ga}^{2-}_{\mathrm{Sb}}$ is larger than that of $\mathrm{Sb}^{2+}_{\mathrm{Ga}}$ at temperatures near the melting point; the enthalpy of reaction (8) is larger than that of reaction (6) because $H(V^x_{\mathrm{Sb}}) > H(V^x_{\mathrm{Ga}})$, and thus the defect formation through reaction (8) is difficult to activate. However, for the Sb-rich case, the concentration of $\mathrm{Ga}^{2-}_{\mathrm{Sb}}$ is smaller than that of $\mathrm{Sb}^{2+}_{\mathrm{Ga}}$ at temperatures lower than 530 °C. This is because the relative concentration of Ga in the liquid phase decreases rapidly and $\mathrm{Ga}^{2-}_{\mathrm{Sb}}$ formation through reaction (6) occurs less frequently, as the temperature is lowered. At low temperatures, GaSb grown from Sb-rich solutions is expected to be slightly Sb-rich.

The conduction is always p type in the case of Ga-rich solutions. The hole concentration at high temperatures is twice as large as the $\mathrm{Ga}^{2-}_{\mathrm{Sb}}$ concentration. At temperatures above 530 °C, GaSb grown from an Sb-rich solution is also p type, but the hole concentration is lower than in the Ga-rich case. The conduction type is converted from p to n in the case of Sb-rich solutions, when the temperature is lowered to below 530 °C. In fact, the eutectic point of Sb and GaSb is 590 °C, and thus we can say that GaSb grown from a liquid phase is always p type.

Figure 2 shows the solidus of GaSb. The existence region of GaSb is extended mainly into the Ga-rich region of the diagram. This is because $\mathrm{Ga}^{2-}_{\mathrm{Sb}}$ is created in a larger number than $\mathrm{Sb}^{2+}_{\mathrm{Ga}}$.

B. $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{Sb}$

Figure 3(a) shows the composition dependence of defect concentrations in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{Sb}$ in equilibrium with group-III-rich liquid solutions. The $\mathrm{III}^{2-}_{\mathrm{Sb}}$ concentration

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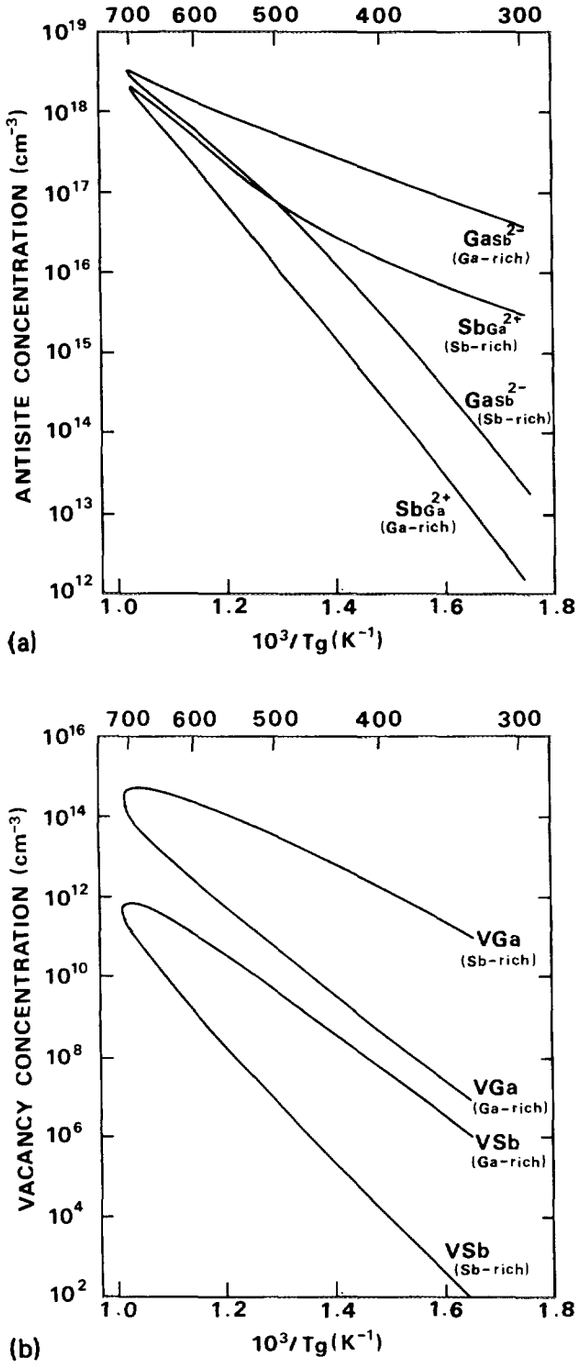

FIG. 1. Temperature dependence of defect concentrations in GaSb. (a) Antisites. (b) Vacancies.

shown in the figure is the sum of those of Ga_{Sb}^{2-} and Al_{Sb}^{2-}. As x increases, the antisite concentrations decrease, because an introduction of an atom with different valence causes a larger increase in the enthalpy with increasing band-gap energy. On the other hand, the vacancy concentrations remain nearly constant. This is due to the cancellation of various factors which influence the concentrations. For example, $H(V_{III}^{x})$ increases as x increases, but the enthalpy of incorporation of an Sb atom from the liquid phase becomes a larger negative

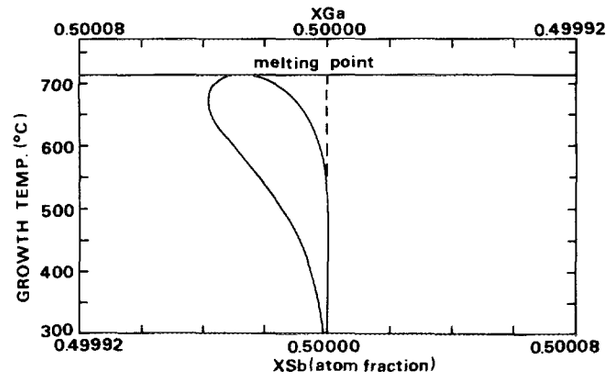

FIG. 2. Calculated solidus of GaSb.

value. Thus, the enthalpy of reaction (3), which is the sum of these two enthalpies, does not change considerably. Composition of the liquid phase also influences the defect concentrations. Al content in the liquid phase sharply increases with x in the composition range above 0.9. Then Al_{Sb}^{2-} increases through reaction (7) in this composition range.

For $Al_xGa_{1-x}Sb$ in equilibrium with Sb-rich solutions, the number of antisites monotonously decreases even at compositions above 0.9, as shown in Fig. 3(b). The drastic change in the liquid composition does not occur in the case of Sb-rich solutions. The number of III_{Sb}^{2-} is larger than that of Sb_{III}^{2+} for $x<0.2$, but the converse is true for $x>0.2$. As x increases, the solubility of the group-III elements in the liquid Sb decreases and the liquid becomes more Sb rich. Consequently, Sb_{III}^{2+} increases compared with III_{Sb}^{2-}, and the solid also becomes more Sb rich.

Temperature dependence of the defect concentrations at each composition is similar to that shown in Fig. 1.

C. Comparison with experimental results

The net acceptor concentration $N_A - N_D$ is calculated from the defect concentrations and compared with the C-V data reported recently.[26,27] At low Al composition, where vacancy concentrations are negligibly small, $N_A - N_D = 2N([III_{Sb}^{2-}] - [Sb_{III}^{2+}])$. Here N is the total number of atoms and $[X]$ is the relative concentration of a defect X. Figure 4 shows the calculated and measured net acceptor concentrations. The open circles represent the net acceptor concentrations in $Al_{0.1}Ga_{0.9}Sb$ grown from Ga-rich solutions, and the filled circles represent those in GaSb grown from Sb-rich solutions. Our calculation does not include any fitting procedure, and the parameters used are all taken from the literature. Nevertheless, the agreement between theoretical and experimental values is very good. This shows that the model is appropriate and the theoretical results are qualitatively correct. In the case of Sb-rich solutions, $N_A - N_D$ decreases rapidly near temperatures of 600 °C because of the compensation of Ga_{Sb}^{2-} by Sb_{Ga}^{2+}; the number of Sb_{Ga}^{2+} is close to that of Ga_{Sb}^{2-} as shown in Fig. 1(b).

Al composition dependence of the acceptor concentration has not been reported. However, we found that the intensity of luminescence due to the residual acceptors de-

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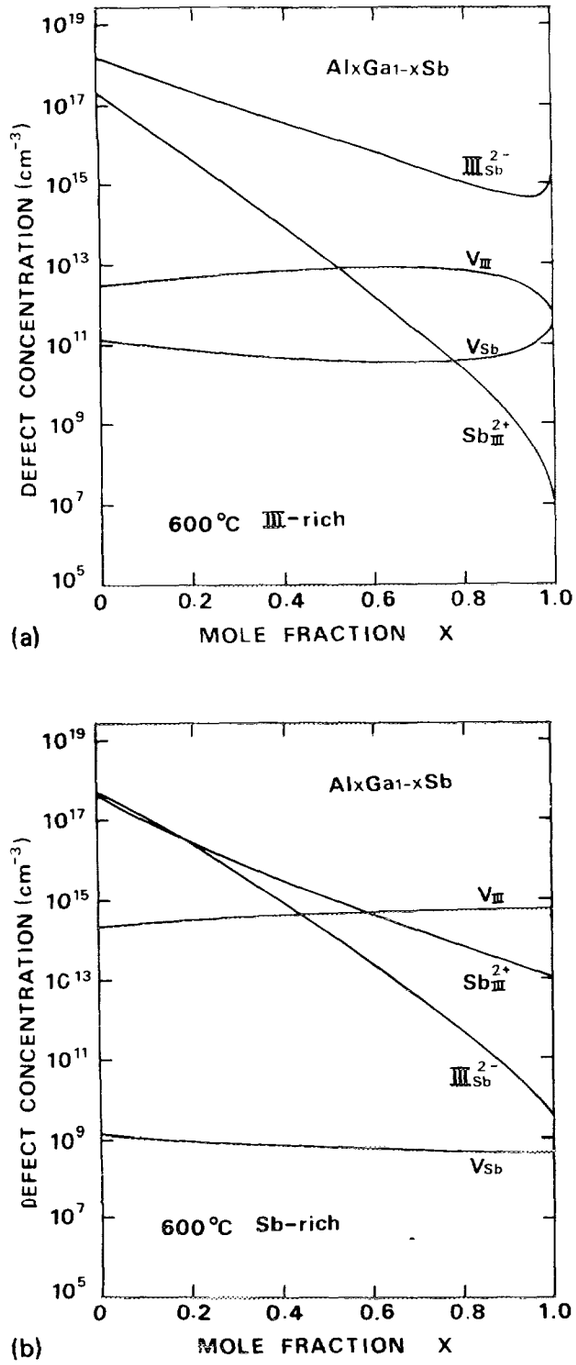

FIG. 3. Composition dependence of defect concentrations in $Al_xGa_{1-x}Sb$. (a) Group-III-rich liquid solution. (b) Sb-rich liquid solution.

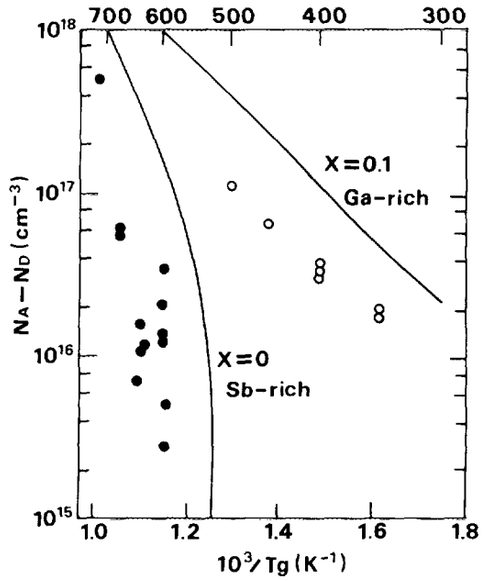

FIG. 4. Comparison between calculated and measured net acceptor concentrations. The open circles show those in $Al_{0.1}Ga_{0.9}Sb$ grown from Ga-rich solutions and the filled circles in GaSb grown from Sb-rich solutions (see Refs. 26 and 27).

creases with increasing Al composition. This tendency agrees with the results shown in Fig. 3. Details of the experimental results were published elsewhere.[28]

IV. DISCUSSION

First, we estimate the number of the complex defect $Ga_{Sb}V_{Ga}$, which is sometimes taken as the dominant defect. Complex defects are not taken into account in our model. However, the calculated concentrations of the point defects will not be changed much, even when we take complex defects into account since the numbers of antisites and vacancies are mainly determined by the condition of equilibrium between the solid and the outside phase. In order to estimate the complex concentration from the calculated point defect concentrations, we consider the following reaction in GaSb:

$$Ga_{Sb}^{2} + V_{Ga}^{x} = (Ga_{Sb}V_{Ga})^{2} ,$$

$$[(Ga_{Sb}V_{Ga})^{2}] = [Ga_{Sb}^{2}][V_{Ga}^{x}]\exp(H'/kT), \qquad (11)$$

where H' is the binding energy of Ga_{Sb}^{2} and V_{Ga}^{x} and k the Boltzmann constant. The number of V_{Ga} is much larger than that of V_{Ga}^{x}, but V_{Ga} and Ga_{Sb}^{2} repel each other because of the Coulomb force. On the other hand, the above reaction will be energetically favorable, i.e., $H' > 0$ because the association will reduce the excess chemical and strain energies of the defects. At $T = 500$ °C, for example, the concentration of V_{Ga}^{x} is 6×10^{8} cm^{-3} and thus the relative concentration $[V_{Ga}^{x}]$ is 3×10^{-14} in the case of Ga-rich solutions, according to our calculation results. Hence, H' needs to be more than 2 eV for $[(Ga_{Sb}V_{Ga})^{2}]$ to exceed $[Ga_{Sb}^{2}]$. H' of 2 eV is about the same as $H(V_{Ga}^{x})$ and seven times greater than $H(Ga_{Sb}^{2})$. H' cannot be that large. Even if we assume that $H' = H(Ga_{Sb}^{2})$, i.e., that no chemical energy is required to convert Ga—Sb bonds to Ga—Ga bonds in the vicinity of a V_{Ga}, $[(Ga_{Sb}V_{Ga})^{2}]$ is still much smaller than $[Ga_{Sb}^{2}]$. Therefore, $(Ga_{Sb}V_{Ga})^{2}$ is expected to be negligible compared with Ga_{Sb}^{2}.

The reaction of the complex formation may occur during the cooling of the solid from the growth temperature. In this case, the number of $(Ga_{Sb}V_{Ga})^{2}$ cannot exceed the number of V_{Ga}. In any case, the complex defect is not considered to be dominant. As Edelin and Mathiot pointed out, the

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experimental observations which have been considered to indicate the existence of the complex can be equally well interpreted assuming that the dominant defect is a simple antisite.[22] In fact, the experimental results do not positively show the existence of the complex; rather, they indicate only that the dominant defect is a defect other than a single vacancy.

The energy level of a single acceptor or donor can be estimated by the hydrogen atom model based on the effective-mass approximation. Similarly, the energy levels of a simple antisite in III-V compounds may be estimated by the He atom model. Using the values of the hole effective-mass ratio of 0.4 and the relative dielectric constant of 15.7, the first ionization energy is estimated to be 37 meV and the second 88 meV for an effective-mass double acceptor in GaSb. The experimentally observed first ionization energy of the residual acceptor in GaSb is in the range between 25 and 35 meV, and the second energy between 70 and 100 meV.[2,10,11,12,15] Thus, the results of the He atom model agree well with the experimental data. Of course, the effective-mass approximation is not valid when the radius of the orbital of a trapped carrier is small compared with the lattice constant. The expected radius of the orbital of a hole trapped at a double acceptor is about 10 Å, half that of the hydrogenic orbital, and thus the validity of the He atom model cannot be readily established. Nevertheless, the success of the He atom model will suggest that the residual acceptor is a rather simple defect. This also supports the assignment of the residual acceptor to a simple antisite.

When GaSb is converted to n type by donor doping, Ga antisites are doubly ionized even at low temperatures. Thus, only the second ionization level is observed by the luminescence measurements of n-type GaSb. For n-type GaSb grown at the melting temperature, the band-edge emission is not observed, and only the emission due to the transition from the conduction band to the second ionization level is observed.[16,17] On the other hand, the band-edge emission as well as the emission associated with the first ionization level are observed from the melt-grown p-type GaSb. This indicates that the number of the residual acceptor increases because of the donor doping. The effect of an impurity doping is easily taken into account in the present calculation. It can be shown that the acceptor-type defects such as Ga_{Sb}^{2-} are greatly increased by a donor doping through the self-compensation mechanism. However, when we use the parameters shown in Table I, the self-compensation effect is overestimated: it needs donor atoms of more than 10^{20} cm^{-3} to convert GaSb to n type at the melting point. If we increase $H(Ga_{Sb}^{2-})$ and $H(Sb_{Ga}^{2+})$ by 0.2 eV, then the concentration of donor atoms required for the type conversion is about 10^{19} cm^{-3}, a reasonable number. In the case of the undoped GaSb, the agreement with the experimental data shown in Fig. 4 becomes better owing to this correction in $H(Ga_{Sb}^{2-})$ and $H(Sb_{Ga}^{2+})$. Hence, the enthalpies of antisite formation estimated by Van Vechten will be too small.

Edelin and Mathiot calculated defect concentrations in GaSb.[22] They also took Ga_{Sb}^{2-} to be a dominant defect. There are two free parameters in their model, and Edelin *et al.* determined them by fitting the results to experimental data. The major difference between their model and our model is that they neglect the existence of Sb antisites even for the crystal grown from Sb-rich solutions. According to our calculation results, Sb_{Ga}^{2+} grows significant as temperature is lowered in the case of Sb-rich solutions.

For further studies, the calculation will be extended to the case of solid-vapor equilibrium and quantitative estimate of complex defect concentrations.

V. SUMMARY

We have calculated defect concentrations in $Al_xGa_{1-x}Sb$ which is in equilibrium with a liquid phase. In the case of Ga-rich liquid solutions, Ga_{Sb}^{2-} or Al_{Sb}^{2-} is a dominant defect, and the concentrations of vacancies are much smaller than the antisite concentrations. Ga_{Sb}^{2-} is dominant in GaSb equilibrated with an Sb-rich solution, too, but Sb_{Ga}^{2+} begins to dominate as temperature is lowered. Calculated net acceptor concentrations agree well with those determined experimentally. The concentration of a complex defect $Ga_{Sb}V_{Ga}$ is expected to be negligibly small compared with antisite concentrations.

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