The bandgap energy of the dilute bismuth $\text{GaBi}_x\text{Sb}_{1-x}$ alloy depending on temperature

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The bandgap energy of the dilute bismuth $\text{GaBi}_x\text{Sb}_{1-x}$ alloy vs. temperature is investigated in this study. Its reduced temperature-sensitiveness is because of the localized character of the valence band states (VBS). In order to describe the reduced temperature-sensitiveness of the bandgap energy, a new term including localized energy is added to Varshni's equation. It is found that the localized energy exhibits an increasing trend as the bismuth fraction increases, which indicates that the localized character of the VBS becomes strong with the increasing bismuth fraction. It is also found that the influence of the bismuth fraction on the temperature dependence of the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$ is smaller than that of $\text{GaBi}_x\text{As}_{1-x}$. In addition, the element indium is undoubtedly a good candidate to lessen the bismuth fraction to realize that the spin-orbit-splitting (SOP) energy surpasses the bandgap energy in $\text{GaBi}_x\text{Sb}_{1-x}$.

Keywords: $\text{GaBi}_x\text{Sb}_{1-x}$, bismuth impurity level, bandgap energy, Sb-rich

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1. Introduction

The group III-V-Bi alloys have been extensively investigated for their unique physical properties. These properties include the significant bismuth-induced bandgap reduction [1], the relative immunity of the bandgap with temperature [2], and the rapid increase of the spin-orbit-splitting (SOP) energy [3]. Such properties make III-V-Bi semiconductors suitable for optoelectronic devices which operate in the near-infrared and mid-infrared ranges. In recent years, much attention has been shifted toward $\text{GaBi}_x\text{Sb}_{1-x}$ after the in-depth and widespread research on $\text{GaBi}_x\text{As}_{1-x}$ and $\text{InBi}_x\text{As}_{1-x}$.

At present, several groups have studied the bandgap energy of the Sb-rich $\text{GaBi}_x\text{Sb}_{1-x}$ alloy vs. composition. Rajpalke et al. [4] synthesized the $\text{GaBi}_x\text{Sb}_{1-x}$ alloy with bismuth fraction up to 0.05 and found that the bandgap reduction was 36 meV/%Bi. Their absorption spectra studies at room temperature showed that the bandgap reduction was greater than the result predicted by

the virtual crystal approximation (VCA) [5]. Afterward, they synthesized the $\text{GaBi}_x\text{Sb}_{1-x}$ alloy with bismuth fraction up to 0.096 and proposed that a combination of the valence band anticrossing (VBAC) model with the VCA could be available to estimate the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$ with bismuth fraction <0.1 [6]. Delorme et al. [7] synthesized the $\text{GaBi}_x\text{Sb}_{1-x}$ alloy with bismuth fraction up to 0.14, which made it possible to study the composition dependence of the bandgap energy in a wider composition range. Polak et al. [8] considered that $\text{GaBi}_x\text{Sb}_{1-x}$ should not be attributed to the highly mismatched alloy as the atomic size mismatch and the difference in electronegativity between antimony and bismuth atoms were quite small. They proposed that the quadratic equation with a bowing term might be more suitable for depicting the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$ than the combination of the VBAC model with the VCA. The bowing coefficient acquired by Polak et al. [9] was about 1.0 eV. The research on the bandgap energy of the dilute bismuth $\text{GaBi}_x\text{Sb}_{1-x}$ vs. temperature has also been carried out. Kopaczek et al. [10] measured the bandgap

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shift of $\text{GaBi}_x\text{Sb}_{1-x}$ with temperature by photoreflectance (PR). It was shown experimentally that the difference of the bandgap energy depending on temperature between $\text{GaBi}_x\text{Sb}_{1-x}$ and GaSb was so slight that the bandgap shift of $\text{GaBi}_x\text{Sb}_{1-x}$ with temperature was almost equal to that of GaSb in the same temperature range, which seemed that incorporating bismuth atoms in GaSb did not reduce the temperature-sensitiveness of the bandgap energy. They further found that the temperature dependence of photoluminescence (PL) peaks was almost equal to that of the bandgap energy determined by PR [11]. Yoshida et al. [2] found that the incorporation of the bismuth fraction in the III–V semiconductors could result in the temperature-insensitiveness of the bandgap energy. The different results mean that it is necessary to further ascertain whether the incorporation of the bismuth fraction in GaSb can reduce the temperature-sensitiveness of the bandgap energy. In this work, the following three issues are taken as the main research points. (1) Whether can the bismuth incorporation reduce the temperature-sensitiveness of the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$? (2) If the bismuth fraction can reduce its temperature-sensitiveness, why does Kopaczek et al. [10] consider that the similar behavior is not shown in their results? (3) How can we describe the reduced temperature dependence of the bandgap energy of the dilute bismuth $\text{GaBi}_x\text{Sb}_{1-x}$.

2. Physical model and discussion

Figure 1 shows the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$ vs. temperature determined by PR [10]. The decline of the bandgap energy with elevating temperature is on account of the band shrinking effect. We know that elevating temperature can enlarge the volume of the samples. At the same time, elevating temperature can make the bond length getting longer. The longer bond length can result in the weaker $s-s$ coupling effect [12]. It can also result in a weaker $p-p$ coupling effect [13]. Usually, the weakened $s-s$ coupling effect lowers the Γ conduction band minimum (CBM) of GaSb while the weakened $p-p$ coupling effect raises the Γ valence band maximum

(VBM) of GaSb. Therefore, the bandgap energy has a tendency to decrease with elevating temperature.

Fig. 1. Dependence of the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$ on temperature. The experimental values are from Kopaczek et al. [10].

Fig. 2. The bandgap shift of the $\text{GaBi}_x\text{Sb}_{1-x}$ alloys when the temperature is changed from 15 K to 290 K.

In order to compare the bandgap shifts of $\text{GaBi}_x\text{Sb}_{1-x}$ with different bismuth fractions in the same temperature range, we handle the data in Figure 1 and acquire the bandgap shift in the temperature range from 15 K to 270 K for the four samples. The results are displayed in Figure 2. As shown in Figure 2, the bandgap shift with temperature decreases with increasing bismuth fraction, which indicates that the temperature-sensitiveness

of the bandgap energy is reduced. The reduced temperature-sensitiveness of the bandgap energy can be attributed to that of the Γ VBM for $\text{GaBi}_x\text{Sb}_{1-x}$. The following evidence support this opinion: (1) The bismuth impurity level in GaSb is a localized level and it locates below the Γ VBM of GaSb. The bismuth impurity level has an impact on the Γ VBM of $\text{GaBi}_x\text{Sb}_{1-x}$. As the Γ VBM of $\text{GaBi}_x\text{Sb}_{1-x}$ is influenced by the localized bismuth impurity level, its temperature-sensitiveness ought to be reduced. (2) For $\text{GaBi}_x\text{As}_{1-x}$, the reduced temperature-sensitiveness of the bandgap energy is because of the decreased temperature-sensitiveness of the Γ VBM [14]. Fitouri et al. [15] found that the localized state originated from the Bi clusters. As the Bi clusters introduce the localized energy levels near the valence band (VB) of the host material, the investigation done by Fitouri et al. [15] supports that the reduced temperature-sensitiveness of the bandgap energy is due to the decreased temperature-sensitiveness of the Γ VBM. Since $\text{GaBi}_x\text{Sb}_{1-x}$ resembles $\text{GaBi}_x\text{As}_{1-x}$, the reduced temperature-sensitiveness of the bandgap energy for $\text{GaBi}_x\text{Sb}_{1-x}$ should be also because of the reduced temperature-sensitiveness of the Γ VBM. (3) Zhao et al. [16] found that the reported Γ VBM of $\text{GaBi}_x\text{Sb}_{1-x}$ depending on composition was quite weak in the Sb-rich range. The weak composition dependence demonstrates that the Γ VBM manifests a localized character conspicuously. Generally, if the Γ VBM is localized, its temperature-sensitiveness should be reduced.

It is worth noting that although the bismuth fraction can influence the temperature-sensitiveness of the Γ VBM for $\text{GaBi}_x\text{Sb}_{1-x}$, the bandgap energy of the dilute bismuth $\text{GaBi}_x\text{Sb}_{1-x}$ alloy still displays a temperature dependence which resembles that of GaSb, implying that the effect of the bismuth fraction is limited. It is intriguing that why the influence of the bismuth fraction on the temperature-sensitiveness of the Γ VBM for $\text{GaBi}_x\text{Sb}_{1-x}$ is limited. It is relevant to the location and the localized extent of the bismuth impurity level. We know that the energy distance from the bismuth impurity level to the Γ VBM of GaSb is large. Under this condition, the effect of the localized bismuth impurity level on the Γ VBM

of $\text{GaBi}_x\text{Sb}_{1-x}$ cannot be significant. Besides, the atomic size mismatch and the difference in electronegativity between bismuth and antimony atoms are not large. For this reason, the localized extent of the bismuth impurity level in GaSb is not so strong as that in GaAs. This should be another reason that the impact of the bismuth impurity level on the temperature-sensitiveness of the Γ VBM for $\text{GaBi}_x\text{Sb}_{1-x}$ is limited. In accordance with the above analysis, the bandgap energy *vs.* temperature is primarily dominated by the host material GaSb.

It is reported that the BAC model can give a good description for the bandgap energy of the dilute nitride alloys ($\text{GaN}_x\text{As}_{1-x}$ [17] and $\text{GaN}_x\text{P}_{1-x}$ [18]) and the dilute oxygen alloys ($\text{ZnO}_x\text{Se}_{1-x}$ [19]) depending on temperature. After fitting the experimental bandgap energy depending on temperature using the BAC model, we can obtain that the nitride impurity level depending on temperature is quite weak [17]. We can also obtain that the oxygen impurity level depending on temperature is weak [20]. Both the results show that the nitride impurity and the oxygen impurity levels are localized, which demonstrates that the results acquired by investigating the temperature dependence of the bandgap energy are consistent with those acquired by investigating the composition dependence of the bandgap energy. However, when the BAC model is adopted to give a depiction for the bandgap energy of the dilute bismuth $\text{GaBi}_x\text{As}_{1-x}$ alloy *vs.* temperature, the acquired bismuth level depending on temperature is strong [21]. As the bismuth level is localized, its temperature dependence should not be strong, which means that the BAC model is not suitable for giving a description for the bandgap energy of the dilute bismuth $\text{GaBi}_x\text{As}_{1-x}$ alloy *vs.* temperature. Since $\text{GaBi}_x\text{Sb}_{1-x}$ is quite similar to $\text{GaBi}_x\text{As}_{1-x}$, the BAC model should not be suitable for giving a depiction for the bandgap energy of the dilute bismuth $\text{GaBi}_x\text{Sb}_{1-x}$ alloy *vs.* temperature, either. In order to prove this opinion, we employ the combination of the valence BAC model with the VCA reported by Zhao et al. [16] to describe the temperature dependence of the bandgap energy of $\text{GaBi}_{0.042}\text{Sb}_{0.958}$. It is obtained that the temperature coefficient of the bismuth level can be larger than that of the bandgap energy of GaSb. We know

that the decreased temperature coefficient of the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$ is because of the localized character of the valence band states (VBS). For this reason, the bismuth impurity level in the valence BAC model is localized, which means that its temperature coefficient is not large.

In general, Varshni's equation can be employed to depict the variation of the bandgap energy of GaSb with temperature [22].

$$E_{g,\text{GaSb}}(T) = E_{g,\text{GaSb}}(0) - \frac{\gamma_{\text{GaSb}} T^2}{T + \theta_{\text{GaSb}}}. \quad (1)$$

where $E_{g,\text{GaSb}}(0)$ denotes the bandgap energy of GaSb at 0 K. γ_{GaSb} and θ_{GaSb} are the so-called Varshni parameters. Usually, θ_{GaSb} represents the Debye temperature of GaSb. The reported Debye temperature of GaSb is 266 K [23] so $\theta_{\text{GaSb}} = 266$ K is adopted.

Although the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$ vs. temperature can also be estimated by Varshni's equation, no parameter in Varshni's equation gives a description for the localized character of the VB. In order to solve this problem, we plan to employ Varshni's equation to depict the bandgap energy of GaSb vs. temperature. After the incorporation of the bismuth fraction in GaSb, a term $\Delta(T)$ should be brought in to depict the reduced temperature-sensitiveness of the bandgap energy for $\text{GaBi}_x\text{Sb}_{1-x}$. Considering the impact of the bismuth fraction on the bandgap energy at 0 K, $E_{g,\text{GaSb}}(0)$ in Varshni's equation ought to be replaced by $E_{g,\text{GaBiSb}}(0)$. Varshni's equation can be modified as below after introducing $\Delta(T)$ and replacing $E_{g,\text{GaSb}}(0)$ by $E_{g,\text{GaBiSb}}(0)$.

$$E_{g,\text{GaBiSb}}(T) = E_{g,\text{GaBiSb}}(0) - \frac{\gamma_{\text{GaSb}} T^2}{T + \theta_{\text{GaSb}}} + \Delta(T), \quad (2)$$

where $E_{g,\text{GaBiSb}}(0)$ denotes the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$ at 0 K. As $\Delta(T)$ depicts the reduced temperature-sensitiveness of the bandgap energy and the bandgap energy vs. temperature is primarily dominated by the host material GaSb, it is better that $\Delta(T)$ adopts the similar form as $\frac{\gamma_{\text{GaSb}} T^2}{T + \theta_{\text{GaSb}}}$.

$$\Delta(T) \propto \frac{T^2}{T + \theta}. \quad (3)$$

The reduced temperature-sensitiveness of the bandgap energy is relevant to the bismuth fraction, so θ_{GaBi} should take the place of θ . In order to depict the localized character of the VB, an energy parameter σ is brought into $\Delta(T)$. Since the reduced temperature-sensitiveness of the bandgap energy is only on account of the localized character of the VBM, the parameter σ_{VBM} can describe the localized character of the VBM. After the above factors are taken into account, $E_{g,\text{GaBiSb}}(T)$ can be written as:

$$E_{g,\text{GaBiSb}}(T) = E_{g,\text{GaBiSb}}(0) - \gamma_{\text{GaSb}} \frac{T^2}{T + \theta_{\text{GaSb}}} + \frac{\sigma_{\text{VBM}}}{T_0} \frac{T^2}{T + \theta_{\text{GaBi}}}, \quad (4)$$

where σ_{VBM} is the localized energy to describe the localized character of the VB. T_0 is an empirical parameter. Its value can choose the highest temperature measured in the experiment. θ_{GaBi} is the Debye temperature of GaBi. Its value has not been reported at present. Based on the results by Varshni [22], the reported Debye temperature of GaX (X = N, P, As, Sb) decreases with an increasing atomic number of X. For this reason, it can be inferred that the Debye temperature of GaBi should be lower than that of GaSb. It is found that the Debye temperature of GaAs is approximate to that of InP. It is also found that the Debye temperature of GaSb is approximate to that of InAs. Based on this factor, it is predicted that the Debye temperature of GaBi should be approximate to that of InSb. We know that the reported Debye temperature θ_{InSb} is 203 K [22]. In this work, the adopted Debye temperature θ_{GaBi} is 200 K.

Eq. (2) is employed to fit the data measured in the experiment in Figure 1. The empirical parameter T_0 is set to be 290 K. Table 1 lists the acquired parameters in Eq. (2). One can see that the modified Varshni's equation can depict the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$ vs. temperature excellently. Besides, we can find the enlargement of the localized energy as the bismuth fraction increases, which indicates that the localized character of the

VB can be enhanced with the increase of the bismuth fraction.

Table 1. The parameters obtained in Eq. (2).

Bi fraction x	γ (meV/K)	$E_g(0)$ (eV)	σ (meV)
0	0.57	0.813	0
0.007	0.57	0.783	8.6
0.021	0.57	0.741	8.7
0.042	0.57	0.686	25.3

It is very interesting that why Kopaczek et al. did not give the opinion that the bismuth fraction can reduce the temperature-sensitiveness of the bandgap energy of $\text{GaBi}_x\text{Sb}_{1-x}$. We consider that it is due to two reasons. (1) The reduced temperature-sensitiveness of the bandgap energy for $\text{GaBi}_x\text{Sb}_{1-x}$ is much less evident than that for $\text{GaBi}_x\text{As}_{1-x}$, which leads to that the reduction of the temperature-sensitiveness of the bandgap energy for $\text{GaBi}_x\text{Sb}_{1-x}$ is easily left out. (2) In Kopaczek et al. [10], although the experimental bandgap energies depending on temperature for four samples are fitted with Varshni's equation, the Debye temperature in Varshni's equation are different, which leads to that the acquired temperature coefficient γ cannot be compared with each other directly. In fact, as all of the bismuth fractions for the four samples are very small, the difference in the Debye temperatures for the four samples should be quite slight. In the circumstances, we can use the same Debye temperature for the four samples. If the same Debye temperature is used for the four samples, it is easy to perceive that the temperature-sensitiveness of the bandgap energy for $\text{GaBi}_x\text{Sb}_{1-x}$ is reduced.

It is found that the localized character of the VBS in $\text{GaBi}_x\text{Sb}_{1-x}$ is weaker than that in $\text{GaBi}_x\text{As}_{1-x}$. It is owing to three aspects. (1) The variation of the temperature can lead to the volume shrink effect. According to the reported volume deformation potential, we can estimate the influence of the volume shrink effect on the Γ CBM and the Γ VBM qualitatively. We find that the difference in the volume deformation potential for the bandgap between GaAs and GaSb is very slight. However, the volume deformation potential for the Γ CBM

state of GaAs is much smaller than that of GaSb so the volume deformation potential for the Γ VBM state of GaAs is much larger than that of GaSb. The localized effect of the bismuth impurity level primarily has an influence on the Γ VBM. It almost has no influence on the Γ CBM. In this case, the Γ VBM of $\text{GaBi}_x\text{Sb}_{1-x}$ depending on temperature should be less influenced by the bismuth impurity level than that of $\text{GaBi}_x\text{As}_{1-x}$, which leads to that the localized character of the VBS in $\text{GaBi}_x\text{Sb}_{1-x}$ is weaker than that in $\text{GaBi}_x\text{As}_{1-x}$. (2) The atomic size mismatch and the difference in electronegativity between bismuth and antimony atoms are smaller than those between bismuth and arsenic atoms. Under this condition, the localized effect of the bismuth impurity level in $\text{GaBi}_x\text{Sb}_{1-x}$ is weaker than that in $\text{GaBi}_x\text{As}_{1-x}$. Even if the energy distance from the localized bismuth impurity level to the Γ VBM of GaSb is equal to that from the bismuth impurity level to the Γ VBM of GaAs, the localized character of the VBS in $\text{GaBi}_x\text{Sb}_{1-x}$ should be weaker than that in $\text{GaBi}_x\text{As}_{1-x}$. (3) The energy distance from the localized bismuth impurity level to the Γ VBM of GaSb is much larger than that from the bismuth impurity level to the Γ VBM of GaAs. Usually, the larger the energy distance is, the smaller the influence of the localized bismuth impurity level is. For the above aspects, the localized character of the VBS in $\text{GaBi}_x\text{Sb}_{1-x}$ ought to be weaker than that in $\text{GaBi}_x\text{As}_{1-x}$.

Furthermore, if the bismuth fraction is sufficiently large, the bandgap energy in $\text{GaBi}_x\text{Sb}_{1-x}$ will be surpassed by the SOP energy [6]. As a matter of fact, it is quite difficult to synthesize the films of $\text{GaBi}_x\text{Sb}_{1-x}$ with large bismuth fractions. Is there a possibility for lessening the bismuth fraction via introducing another element in $\text{GaBi}_x\text{Sb}_{1-x}$ to realize that the SOP energy is larger than the bandgap energy? We hold the opinion that it is very likely if the right element is brought into. We know that if the introduced element is able to reduce the bandgap energy and does not lower the SOP energy, the bandgap energy can be overtaken by the SOP energy more easily. On the basis of the above analysis, it is inappropriate to introduce the elements aluminum, phosphorus, and arsenic. The reason is that the bandgap energy of

the alloy should be enlarged and its SOP energy will be lowered after introducing these elements as the bandgap energies of GaP, GaAs, and AlSb are larger while the SOP energies of GaP, GaAs, and AlSb are smaller than those of GaSb [24]. We notice that the bandgap energy of InSb is much smaller than that of GaSb. We also notice that the SOP energy of InSb is larger than that of GaSb [25], which shows that the element indium should be a good candidate because the bandgap energy of the alloy will be reduced and its SOP energy is not be lowered after this element is chosen.

3. Conclusion

In conclusion, the bandgap energy of the dilute bismuth $\text{GaBi}_x\text{Sb}_{1-x}$ alloy vs. temperature is studied. It is found that its reduced temperature-sensitiveness can be attributed to the localized character of the VBS. A new term including localized energy is added to Varshni's equation to describe the reduced temperature-sensitiveness of the bandgap energy. Results reveal that the localized energy increases with the increase of the bismuth fraction, which suggests that the localized character of the VBS becomes strong with the increasing bismuth fraction. Additionally, the element indium should be a good candidate to lessen the bismuth fraction to realize that the SOP energy surpasses the bandgap energy in $\text{GaBi}_x\text{Sb}_{1-x}$.

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