Calculation Method for the Bandgap of Antimonide Based Multicomponent Alloys

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As the most important material parameter of semiconductor, bandgap is necessary to be investigated to meet the design requirements of the high-performance optoelectronic devices. A new method of is proposed to calibrate the bandgap of antimonide based multi-component alloys with considering the effect of spin-orbit splitting of bands and the doublet degeneracy of valance band on the bandgaps of Sb-containing materials. A correction factor is introduced in the conventional calculation, and the spin-orbit splitting method is proposed. Besides, the \( \text{In}_{x}\text{Ga}_{1-x}\text{As}_{y}\text{Sb}_{1-y} \) films with different compositions are grown on GaSb substrates by molecular beam epitaxy, and the corresponding bandgaps are obtained by photoluminescence to test the accuracy and reliability of this new method. An error rate analysis reveals that the \( \alpha \) calculated by the spin–orbit splitting correction method is decreased to 2%, almost one order of magnitude smaller than the Moon method, which means that the new method can calculate the antimonide multicomponent more accurately with some applicability. This work can give a reasonable interpretation for the reported results and beneficial to tailor the antimonides properties and optoelectronic devices.

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1. Introduction

The III–V semiconductor material system (GaIn)(AsSb) establishes a firm platform for optoelectronic devices operating near the mid-infrared spectral range (2–3 µm). The devices based on the antimonides have been intensively developed in recent years with the potential applications in a wide variety of areas such as material processing, secure free-space communication, infrared countermeasures, and atmospheric pollution monitoring [1–3].

The bandgap of multicomponent materials are the basement to research the structural design and fabrication of high-performance Sb-containing optoelectronic device. It can be obtained from the photon luminescence spectroscopy, infrared absorption spectroscopy, the cyclotron resonance experiments etc., which are difficult and complicated [4–6]. For the numerical techniques and analysis, the research on the materials bandgap developed slowly in the past decades and the correlative reports are very few. At the present, the Moon method proposed in 1974 is still the major way in the structure design and simulation, which has a low precision and cannot satisfy the modern optoelectronic apparatus requirements [7, 8].

In this paper, the band structure of antimonide based multicomponent materials are systematically investigated. The spin–orbit splitting correction method is presented in the calibration of the antimonide materials bandgap by considering the effect of spin–orbit splitting off bands and degeneracy of valence band on the band structure. In order to confirm the validity and practicability of new method, the \( \text{In}_{x}\text{Ga}_{1-x}\text{As}_{y}\text{Sb}_{1-y} \) films with different compositions are grown on GaSb substrates by molecular beam epitaxy (MBE), and the corresponding bandgaps are obtained by photoluminescence (PL).

2. Theoretical analysis

Antimonide based multicomponent alloys mainly refer to the Sb-containing binary, ternary and quaternary compounds, consisting of the III-group elements (Ga, In, Al, etc.) and V-group elements (As, Sb, etc.). Compared with the single-component semiconductor materials, the calibration of multicomponent alloys parameters is more complicated and difficult, which is usually derived with the binary or ternary compounds parameters. Taking \( \text{In}_{x}\text{Ga}_{1-x}\text{As}_{y}\text{Sb}_{1-y} \) as an example, the schematic diagram of calibrating quaternary semiconductor material parameters are shown in Fig. 1.

![Fig. 1. Relationship between the parameters of binary, ternary, quaternary antimonides semiconductor compounds.](image-url)
pute the bandgap of semiconductor materials. The main idea of the method is dividing the quaternary antimonide into four binary related materials. InGaAs, GaSb, GaAs, and InSb. The bandgap of InGaAsSb, for example, is considered as an aggregation of InAs, GaSb, GaAs, and InSb. The bandgap of InGaAsSb is decided in the following formula: 

\[ E_g^{InGaAsSb} = xyE_g^{InAs} + (1-x)(1-y)E_g^{GaSb} \]

\[ + x(1-x)\Delta xyE_g^{GaAs} + (1-x)(1-y)\Delta E_g^{GaSb} \]

\[ -x(1-x)yC_r^{InGaSb} - (x(1-x))\Delta C_r^{GaSb} \]

\[ -xy(1-y)E_g^{GaSb} - (1-y)(y)\Delta C_r^{GaSb} \].

Here, \( E_g \) is the bandgap of binary semiconductor materials, \( C_r \) is the bowing parameters of \( \Gamma \) bands in ternary compounds. The related concrete parameters are shown in Tables I and II.

### Table I

| Binary material | \( E_g \) | \( \Delta \) |
|-----------------|----------|-----------|
| InAs           | 0.359    | 0.38      |
| InSb           | 0.17     | 0.81      |
| GaAs           | 1.43     | 0.34      |
| GaSb           | 0.72     | 0.82      |

### Table II

| Ternary material | \( \Gamma \) | \( X \) | \( L \) | \( \Delta \) |
|------------------|-------------|--------|--------|----------|
| InGaAs          | 0.6         | 1.4    | 0.72   | 0.2      |
| InGaSb          | 0.42        | 0.33   | 0.38   | 0.1      |
| GaAsSb          | 1.2         | 1.09   | 1.09   | 1.61     |
| InSb            | 0.58        | 0.59   | 0.57   | 1.2      |

The structural diagram of InGaAsSb is indicated in Fig. 2. For InGaAsSb, the conduction band includes \( \Gamma \) band, \( X \) band, and \( L \) band, while the valence band has light hole band, heavy hole band, and splitting-off band. By definition, the bandgap is equal to the energy difference between the bottom of conduction band and the top of valence band. Both of the above two points is set in the valley of \( \Gamma \) band for InGaAsSb, so the bowing parameters that the Moon method used is the \( \Gamma \) band.

However, by comparing the material parameters in Table I, it can be identified that the bandgaps of most splitting off bands are greater than \( \Gamma \) bands, which means the effects of split off band on the bandgap cannot be ignored and the bowing parameters of splitting-off band should also be used in the bandgap calibration. Besides, because the tops of heavy hole band and light hole band are coincident at the highest point of valence band, the degeneracy of valence band should be another key element to the structure of antimonides.

In order to obtain the more precise bandgap of InGaAsSb in theory, a spin–orbit splitting correction factor \( \tau \) is introduced in the calibration for the unique band structure of InGaAsSb.

![Fig. 2. Diagram of InGaAsSb band structure.](image)

\[ t = \frac{1}{2} \left[ x(1-x)\Delta \Gamma xyE_g^{GaAs} + x(1-x)(1-y)\Delta E_g^{GaSb} \right. \]

\[ -x(1-x)y\Delta C_r^{InGaSb} - (x(1-x))(1-y)\Delta C_r^{GaSb} \]

\[ -xy(1-y)\Delta E_g^{GaSb} - (1-y)(y)\Delta C_r^{GaSb} \].

### 3. Results and discussion

In order to validate the theoretical results, the InGaAsSb thin films are grown on GaSb substrates by DCA P600 MBE system, and the experimental values of antimonide bandgaps are obtained by photoluminescence. Figure 3 shows the PL spectra of InGaAsSb and InGaSb calibrated by the Moon method and the spin–orbit splitting method are indicated in Table III. Compared with the experimental values, the relative error \( \alpha \) of calibration results using different methods is obtained by the following formula:

\[ \alpha = \frac{| \text{theoretical value} - \text{experimental value} |}{\text{experimental value}} \times 100\%. \]
From Table III, it can be seen that the bandgap calibrated by the spin–orbit splitting method is closer to the experimental values, the relative error $\alpha$ is reduced by almost 7 times, which suggests that the new method is superior to the common Moon method for antimonide based multicomponent alloys precisely. This work can give a reasonable interpretation for the reported results and beneficial to tailor the antimonide property and photonics devices.

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