Burstein-Moss shift in impurity-compensated bulk $\text{Ga}_{1-x}\text{In}_x\text{Sb}$ substrates

R. Pino, Y. Ko, and P. S. Dutta
Department of Electrical, Computer, and Systems Engineering, Center for Integrated Electronics, Rensselaer Polytechnic Institute, Troy, New York 12180

Shekhar Guha
Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, Ohio 45433

Leonel P. Gonzalez
Air Force Research Laboratory, Materials and Manufacturing Directorate, Anteon Corporation, Dayton, Ohio 45433

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The optical and electrical properties of tellurium- (Te) compensated $\text{Ga}_{1-x}\text{In}_x\text{Sb}$ bulk crystals with alloy compositions ranging from $x=0.37$ to $x=0.98$ have been investigated. It has been observed that the Burstein-Moss shift plays an important role in the optical properties of $\text{Ga}_{1-x}\text{In}_x\text{Sb}$ crystals for the alloy compositions greater than $x=0.5$ and net donor concentrations in the $2.9 \times 10^{17}$ to $2.6 \times 10^{18}$ cm$^{-3}$ range at 300 K. A good agreement has been obtained between the theory and experimental observations. Furthermore, electrical characterizations at 300 and 77 K show that Te compensates the native defects in $\text{Ga}_{1-x}\text{In}_x\text{Sb}$, irrespective of the alloy composition. © 2004 American Institute of Physics. [DOI: 10.1063/1.1796538]

I. INTRODUCTION

The III-V ternary alloy system GaSb–InSb with a band gap in the range of 0.73–0.17 eV (Ref. 1) is a promising candidate for future lasers and photodetectors beyond 2 $\mu$m and high efficiency thermophotovoltaic cells operating in conjunction with the low-temperature black body sources.\textsuperscript{2,3}

As we know, for semiconductor materials and devices, impurity doping plays a significant role on the electrical and optical characteristics. However, very little knowledge exists on this material system. The present work was aimed at investigating the optical and electrical properties of the Te-doped $\text{Ga}_{1-x}\text{In}_x\text{Sb}$ bulk crystals with alloy compositions ranging from $x=0.37$ to $x=0.98$.

II. EXPERIMENT

Tellurium- (Te) compensated $\text{Ga}_{1-x}\text{In}_x\text{Sb}$ bulk crystals were grown via the vertical Bridgman method in a single-zone furnace from the Mellen Corporation in an argon ambient at 1 atm pressure. For a charge synthesis, 7N pure Ga and In and 6N pure Te and Sb were used, as-received without any chemical treatment. A directional solidification was conducted in flat-bottom silica crucibles of 2-in. diameter with 2-in. diameter annealed at 500 °C for 1–2 min. The samples used in our measurements were taken from the region of the ingot reached outside the hot zone of the furnace, the crystal was cooled to room temperature over a period of 12 h by appropriately programming the furnace temperature-time profile.

After the growth process, the ingots were sliced perpendicular to the growth axis to extract wafers. The wafers were lapped and polished on both sides with commercial slurries to achieve mirror-shining surfaces. Lapping was performed with a 17.5 $\mu$m alumina slurry on a glass plate. Polishing was performed using a 1 $\mu$m alumina slurry on a nylon pad and 0.1 $\mu$m alumina slurry on a velvet pad. The final wafer thickness was approximately 630 $\mu$m. The composition of each sample was obtained via electron probe microanalysis (EPMA) using a JEOL-733 electron microprobe. The optical transmission properties were obtained using a Thermo Nicolet Fourier transform infrared (FTIR) spectrometer at 300 K. The electrical characterizations were obtained using a commercial EGK HEM-2000 Hall-effect measurement system setup at 300 and 77 K ($0.5 \times 0.5$ cm$^2$ average sample size). The ohmic contacts to the samples were provided by an indium annealed at 500 °C for 1–2 min. The samples used in our measurements were taken from the region of the 2-in-diameter wafer lying halfway between the center and the edge along the radial direction.

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\textsuperscript{a)Author to whom correspondence should be addressed; electronic mail: dutap@rpi.edu}
III. RESULTS AND DISCUSSION

The EPMA results are shown in Fig. 1. At approximately 1 mm of growth, in the first to freeze region of the ingot, the alloy composition corresponds to Ga$_{0.63}$In$_{0.37}$Sb as expected from the pseudobinary phase diagram$^8$ for a starting melt composition of $x=0.75$, Ga$_{0.25}$In$_{0.75}$Sb. At approximately 4.5 mm of growth, the ingot showed a composition of about Ga$_{0.57}$In$_{0.43}$Sb, and subsequently, the alloy composition in the solid increased to reach a composition of Ga$_{0.02}$In$_{0.98}$Sb at approximately 19 mm of growth, in the last to freeze region of the ingot. Profiling of selected wafers showed a maximum radial composition variation between 2% and 3% of InSb. Figure 1 also shows a steplike shape as the alloy composition varies from 0 to 20 mm along the growth direction. This characteristic-growth behavior can be attributed to a constitutional supercooling during growth due to the increasing indium concentration at the solid-liquid interface$^9$ as well as to the low-temperature gradient and high growth rate imposed by the growth parameters mentioned previously.

Figure 2 shows the band gap obtained from the FTIR transmission measurements as well as the calculated from the EPMA data by using Eq. (1), which describes the band gap for Ga$_{1-x}$In$_x$Sb as a function of mole fraction, $x$, where $E_{G(GaSb)}$ and $E_{G(InSb)}$ are the band gaps of GaSb (0.726 eV) and InSb (0.17 eV),$^{10}$ respectively, and $C$ is the optical bowing parameter (0.415 eV).$^{11}$

$$E_{G[(GaSb)_{1-x}(InSb)_{x}]} = (1 - x)E_{G(GaSb)} + xE_{G(InSb)} - x(1 - x)C. \tag{1}$$

Figure 2 also includes the theoretically predicted band offset, taking into account the well-known Burstein-Moss shift.$^{12}$ It is observed that for concentrations less than $x=0.5$ the agreement between the band edges obtained from the EPMA and FTIR measurements is quite good. However, for concentrations higher than $x=0.5$, there is an increasing difference between the two measured band edges. The largest band edge-offset of 0.15 eV occurs in the last to freeze region of the ingot for a solid composition that corresponds to Ga$_{0.02}$In$_{0.98}$Sb. This band-edge offset may be directly related to the well-known Burstein-Moss shift.$^{12}$ The Burstein-Moss shift is related to the impurity concentration in the material as well as to the magnitude of the charge-carriers effective mass.$^{12}$ For example, impurities in InSb could cause the observed optical gap to vary as much as 0.21 eV depending on the impurity concentration in the material.$^{13}$ The measurement of the transport properties helps in ascertaining the Burstein-Moss shift in various materials.

Figure 3 shows the carrier concentration (a), electron mobility (b), and resistivity (c) versus alloy composition, $x$, in the solid at 77 and 300 K. It is observed that both the electron carrier concentration and mobility increase with increasing alloy composition, $x$, at 77 and 300 K. It has been shown that Te compensates native defects in GaSb, which give rise to an increase in the mobility with an increasing carrier concentration.$^{14,15}$ This particular type of variation of
mobility with a carrier concentration has been attributed to the dominance of impurity scattering under the conditions of high compensation. Furthermore, the increase of composition, $x$, in the solid would tend to lower the electron effective mass, because electrons in InSb have a much higher mobility than in GaSb. From Figs. 3(a) and 3(b), it is observed that, indeed, the electron effective mass must be decreasing with increasing composition because both the electron mobility and concentration are increasing with composition, $x$. Therefore, as the carrier concentration and mobility increase with increasing composition, $x$, it is expected that the resistivity will decrease with increasing composition as can be observed in Fig. 3(c). From this information, we can conclude that the electrical characteristics, which give rise to the Burstein-Moss shift, are being exhibited by most of the samples, in particular, the samples with a high composition, $x$. Therefore, we should be able to theoretically predict the magnitude of the band offset by using the model described by Burstein.

The Burstein-Moss shift depends greatly on the effective mass of the carriers. Therefore, we should try to approximate the electron effective mass in our Ga$_{1-x}$In$_x$Sb samples from the measured electrical properties. The Drude model says that the electron mobility can be expressed as $\mu = e \tau/m_e$, where $\mu$ is the electron mobility, $e$ is the electron charge, $\tau$ is the electron charge mobility, and $m_e$ is the effective mass of the electron. Solving for $m_e$, we get an equation relating the electron effective mass and the mobility of the material

$$m_e = \frac{e \tau}{\mu}. \quad (2)$$

In addition, assuming that the variation of $\tau$ with a doping concentration and chemical composition to be negligible at 300 K, the ratio of the actual electron effective mass, $m_e$, to the intrinsic electron effective mass, $m_i$, should be given by

$$\frac{m_e}{m_i} = \frac{e \tau/m_e}{e \tau/m_i} = \frac{\mu_i}{\mu_e} = \frac{\text{Intrinsic electron mobility}}{\text{Measured electron mobility}}. \quad (3)$$

where $\mu_e$ is the effective electron mobility due to the native defects and impurity effects. Miki et al. and Kawashima and Kataoka showed that the electron mobility in Ga$_{1-x}$In$_x$Sb varied linearly with composition, $x$. Therefore, taking the theoretical intrinsic electron mobility values for GaSb (3000 cm$^2$/V s) and InSb (77000 cm$^2$/V s) from Ref. 10, we can obtain a linear relation for mobility as a function of composition, $x$, for Ga$_{1-x}$In$_x$Sb

$$\mu_e = 74000x + 3000 \text{ cm}^2/\text{V s}. \quad (4)$$

The relations for the intrinsic effective mass for the holes and electrons in Ga$_{1-x}$In$_x$Sb were taken from Ref. 10 and shown in Eq. (5), where $m_i^e$ is the intrinsic electron effective mass, $m_{hh}$ is the heavy hole mass, $m_{lh}$ is the light hole mass, and $m_e$ is the electron rest mass.

$$m_i^e = \frac{0.015 + 0.01 \times (1 - x) + 0.025 \times (1 - x)^2}{m_i}. \quad (5)$$

Then, the expected electron effective mass due to the native defects and impurities in the material can therefore be approximated by

$$m_e = \frac{\mu_e^i}{\mu_e} \times (0.015 + 0.01 \times (1 - x) \quad (6)$$

+ $0.025 \times (1 - x)^2)m_i$. \quad (6)

From the hole mass relations in Eq. (5), the hole effective mass can be expressed as follows:

$$m_h = [(m_{lh})^{3/2} + (m_{hh})^{3/2}]^{2/3}. \quad (7)$$

In this treatment, it is assumed that the hole effective mass remains constant regardless of the doping concentration, as given by Eq. (7). The Burstein-Moss shift can be shown to be equal to

$$\Delta E_G = \left(\frac{1}{1 + \frac{m_e}{m_h}}\right) \times 2kT \times \ln \left(\frac{n}{N_c N_v}\right) + 4kT, \quad (8)$$

where $n$ is the measured electron carrier concentration, $N_c = 2(2m_e/kT)^{3/2}$ and $N_v = 2(2m_h/kT)^{1/2}$ are the effective density of conduction and valence-band states, $k$ is the Boltzmann’s constant, $T$ is the temperature in degree Kelvin, and $h$ is the Planck’s constant, respectively. Finally, the band-effective gap can be calculated as the sum of the expected Burstein-Moss shift [Eq. (8)] plus the intrinsic band gap given by Eq. (1) as follows:

$$E_G = \Delta E_G + E_G[(\text{GaSb})_{1-x}((\text{InSb})_x)]. \quad (9)$$

Figure 2 shows the plot of Eq. (9) along with the band edges obtained from the EPMA and FTIR data as a function of the sample composition, $x$. The figure shows a good agreement between the theoretically predicted band-edge offset explained by the Burstein-Moss shift and that obtained from the optical measurements. A better agreement between the theory and experiment may be achieved if (1) the variation of the hole effective mass and the average collision time, $\tau$, with a carrier concentration and alloy composition and (2) a better approximation to the linear variation of the intrinsic electron mobility with the alloy composition can be taken into account.

IV. CONCLUSION

It has been demonstrated that the Burstein-Moss shift plays an important role in the optical properties of Te-compensated Ga$_{1-x}$In$_x$Sb alloys. Also, electrical characterizations show that Te compensates the native defects in Ga$_{1-x}$In$_x$Sb, irrespective of the alloy composition. The optical band offset from the Burstein-Moss shift occurs at doping concentrations beyond mid-10$^{17}$ cm$^{-3}$.

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