Gallium antimonide (GaSb)

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Abstract

Although GaSb has not been widely utilized in technological applications, its energy band structure does allow various interesting physical experiments to be performed on intervalley transfer mechanisms and thus the nature of L and X energetic minima in the Ga series of III-V semiconductor compounds can be clarified.
1 Crystalline structure

The crystal lattice of CaSb belongs to the zinc blende lattice and is constituted by two \textit{fcc} sublattices formed by atoms Ga and Sb. The density of the crystal is 5.61 g · cm\(^{-3}\) and the lattice constant \(a_0 = 6.09593 \; \text{Å} \) \cite{1} and the melting point \(T = 985 \; \text{K} \) \cite{2} and Debye temperature \(\theta_D = 266 \; \text{K} \).

The zinc blende structure of GaSb is based on the diamond lattice but the two different atoms in primitive cell. The two \textit{fcc} sublattices can be defined by basic translational vectors: \(a_o/2(1,1,0), a_o/2(0,1,1), a_o/2(1,0,1)\) and are displaced by vector \(d=a_o/4(1,1,1)\) with respect to one another. The bonding forces in such semiconductor compounds are partially covalent and partially ionic. Although the zinc blende structure is closely related to the diamond structure, there is an important difference between the two: the diamond lattice has a center of inversion midway between two atoms in primitive cell, whereas the zinc blende lattice does not. This has implications for the nonlinear optical properties of GaSb: only crystals lacking a center of inversion can be strongly nonlinear\cite{4}. Besides the translations there are 24 symmetry operations of the group \(T_d\) which transform the zinc blende lattice into itself. Since the translational symmetry of the lattice is that of the \textit{fcc} sublattices, the values of the wave vector \(k\) on which energies and wave functions depend can be defined within a volume of reciprocal space which is obtained by bisecting with perpendicular planes the reciprocal lattice of basic vectors \(2n/a_o(1,1,1), 2n/a_o(1,1,1), 2n/a_o(1,1,1)\), where \(n\) - integer number. The points of high symmetry \(\Gamma [k=0], L[k=2n/a_o(1/2,1/2,1/2)], X[k=2n/a_o(1,0,0)]\) are represented in the Fig.2 along with the lines \(\Lambda\) and \(\Delta\) which connect \(\Gamma\) with \(L\) and \(X\). There are three \(X\) - points and four \(L\) - points. The path from the center of zone \(\Gamma\) to the points of high symmetry is very significant for description of the band structure of the crystal. The reduced zone (first Brillouin zone) is displayed in Fig.2. and the symmetry point and symmetry lines are indicated \cite{1}.

![Figure 1: Crystalline structure of GaSb.\cite{2}](image1)

![Figure 2: First Brillouin zone \cite{1}.](image2)
2 Energy band structure

The conduction band in CaSb is characterized by three sets of minima the lowest minima at $\Gamma$, slightly higher minima at the L - points at the surface of the Brillouin zone and even higher minima at the X - points. The valence band has the structure common to all zincblende semiconductors (Fig. 3.).

Figure 3: Band structure of GaSb obtained with a non-local pseudopotential calculation [2].

In the direct band material such as GaSb the position of minima at X and L can be determined by Hall effect and by study of the pressure dependence of resistivity. The measurements of ultraviolet reflectivity helps to determine the band gaps.

3 Elastic constants and lattice dynamics in GaSb

Below the experimentally measured elastic constants are presented (Table 1.). The values of elastic constants were determined on the base of measurements of transit time pulses of 30 $MHz$ longitudinal and transverse ultrasonic waves in sulfur doped $n$ type single crystals of GaSb down to 4.2 K [7]. A pulse echo-overlap method was used to measure the transit times of $2 \sim \mu$sec wide pulses of longitudinal and transverse ultrasonic waves in samples to which the appropriate quartz transducers were bounded. The velocity of each type of ultrasonic wave was deduced from the measured transit time and the sample length. The elastic constants were, in turn, deduced from the velocities $v$ and the sample density $\rho$. The relations used to obtained the elastic constants from the velocities are:

\[
\rho v^2_{[110],[\bar{1}10]} = \frac{1}{2} \cdot (c_{11} + c_{12} + 2c_{44}),
\]

(1)

\[
\rho v^2_{[110],[\bar{1}10]} = \frac{1}{2} \cdot (c_{11} - c_{12}),
\]

(2)

\[
\rho v^2_{[100],[\bar{1}00]} = c_{44}.
\]

(3)

<table>
<thead>
<tr>
<th>Elastic moduli ($10^{11}$dyn/cm$^2$)</th>
<th>$T=296$ K, $\rho = 5.619$ g/cm$^3$</th>
<th>$T=77$ K, $\rho = 5.638$ g/cm$^3$</th>
<th>$T=4$ K, $\rho = 5.638$ g/cm$^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{11}$</td>
<td>8.834</td>
<td>9.052</td>
<td>9.082</td>
</tr>
<tr>
<td>$c_{12}$</td>
<td>4.023</td>
<td>4.113</td>
<td>4.131</td>
</tr>
<tr>
<td>$c_{44}$</td>
<td>4.322</td>
<td>4.435</td>
<td>4.447</td>
</tr>
</tbody>
</table>

Table 1. Elastic constants for GaSb [7].
4 Dispersion of acoustic waves

The acoustical (A) and optical (O) modes of transverse (T) and longitudinal (L) branches of the phonon dispersion curves which were measured on the base of inelastic neutron scattering experiments are presented on the figure below. Three different directions of the wave propagation have been investigated. $\xi = a_0 k / 2 \pi$, where $a_0$ crystal constant = 6.0959 Å[7]. The measurements were conducted at room temperature on a single crystal of undoped GaSb.

![Dispersion curves](image)

Figure 4: Phonon dispersion curves in GaSb crystal [8].

The above frequency dispersion data were used to calculate the lattice contribution to the heat capacity $C_v$ (Fig. 5.) and the Debye temperature $\theta_D$. The temperature dependence of both the heat capacitance and Debye temperature are presented on the Fig. 5. The results obtained are in good accordance with those theoretically calculated.

![Heat capacity and Debye temperature](image)

Figure 5: Temperature dependence of heat capacitance $C_v$ and Debye temperature $\theta_D$ in GaSb, measured and calculated [8].

5 Transport properties

By transport properties we mean the response of the electrons to applied forces. The proper approach to the problem of electronic motion in a periodic lattice would be to solve the time dependent Schrödinger equations. It's known that the electrons moving in a perfect periodic potential with no applied forces has a constant velocity and is not scattered by the atoms of the crystal. Only crystal imperfections serve to scatter electrons. In order to get correct equations of motions we have to take into account the "effective masses" of electrons. Effective mass is one of the important concepts in the analysis of semiconductors, in the theory of scattering. The important point is that an electron in a periodic potential is accelerated relative to the lattice in an applied electric or magnetic field as if the mass
of electron were equal to an effective mass which differs from the mass of free electron [4]. In GaSb the conduction band lowest valley occurs at the same $k$ value as the valence band maximum (for instance $k=0$). It means that GaSb belongs to a direct gap semiconductors. The curvatures (or effective masses) of valence and conduction band edges are another important features of transport properties of GaSb is illustrated in Fig. 6.

![Figure 6: Effective masses in the energetic valleys of GaSb [5].](image)

The large curvature of the band structure in $\Gamma$ valley results in a low effective mass and corresponding high mobility of the conduction electrons. High electron mobility is used to good purpose in galvanomagnetic devices, based on either the Hall effect (proportional to $\mu$, electron mobility) or magnetoresistance (proportional to $\mu^2$). The high mobility also implies that conduction electrons acquire a high drift momentum in an electric field and hence there is strong energy transfer to the electron assembly leading to pronounced “hot electron” effects [4]. Although the $\Gamma$ valley is spherically symmetrical in the energy bands of GaSb there is an essential deviation from the simple relation:

$$E = \frac{\hbar^2 k^2}{2m_e^*}$$

between the energy $E$ and the electronic crystal momentum $\hbar k$ ($m_e^*$ being the effective mass of carriers in the $\Gamma$ valley). The deviation arises from the interaction of the conduction band with the nearest valence band and given via $(kp)$ perturbation method by formula:

$$\frac{m}{m_e^*} = 1 + \frac{P^2}{3} \left( \frac{2}{E_g} \right) + \frac{1}{E_g + \Delta},$$

where $m$ is free electron mass, $E_g$ is the fundamental band gap, and $\Delta$ is the valence band spin orbit splitting. For GaSb, the experimental parameters $m_e^* = 0.041m$ ($\Gamma$ valley), $E_g = 0.726$ eV, $\Delta = 0.80$ eV. The effective masses of electrons (in units of $m$) are presented in Table. 2 [2].

<table>
<thead>
<tr>
<th>Valley</th>
<th>$\Gamma$ valley</th>
<th>L valley</th>
<th>X valley</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_e^*$</td>
<td>0.041</td>
<td>0.11</td>
<td>0.22</td>
</tr>
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</table>

Table 2. Effective masses of electrons in energetic valleys of GaSb.

6 Carrier mobility

The carrier mobility $\mu$ defined as the magnitude of carrier drift velocity $v$ per unit electric field $E$, may be expressed in terms of the carrier relaxation time $\tau$ for various scattering
processes in the form [5]:

$$\mu = \frac{v}{\mathcal{E}} = \frac{q\tau}{m^*},$$

(6)

where \( m^* \) - conductivity effective mass. The effective masses of electrons \( m_n^* \) and holes \( m_p^* \) in semiconductors can be determined by cyclotron resonance [9]. The electrical conductivity \( \sigma \) in the presence of both electrons and holes is given by the sum of separate contributions:

$$\sigma = q(n\mu_e + p\mu_h),$$

(7)

where \( n,p \) - concentration of electrons and holes [4]. The typical value of \( \mu_e \) and \( \mu_h \) for GaSb is given in Table 3. For intrinsic semiconductor GaSb the concentration of electrons and holes are equal \( n=p \). This permits us to write the \( dc \) conductivity in the following form [5]:

$$\sigma = 2q\left(\frac{kT}{2\pi\hbar^2}\right)^{3/2}(m_e m_h)^{3/4} \exp\left\{-\frac{E_g}{kT}\right\} \cdot (\mu_e + \mu_h).$$

(8)

By using the temperature dependence of carrier mobility we can determine the energy gap \( E_g \) of GaSb. The temperature dependence of \( \mu_e \) and \( \mu_h \) for GaSb is well studied [2]. GaSb possesses the cubic zincblende structure and a direct energy gap. However, the four equivalent \( L_{1c} \) minima lie energetically very near the lowest conduction band minimum ( \( \sim 0.07 \text{ eV} \) above \( \Gamma_{1c} \)), so that most electrons populate \( L_{1c} \) at room temperature. Because of this complicated transport situation, and because of the relatively small energy gap \( 0.0726 \text{ eV} \) at \( \Gamma \), GaSb has not been widely utilized in technological applications. Nevertheless, the band structure of GaSb does allow various interesting physical experiments to be performed on inter-valley transfer mechanisms and the nature of \( L_{1c} \) and \( X_{1c} \) minima in the Ga series of III-V crystals[5].

GaSb has direct energy gap and low electron effective mass and due to this a high electron mobility. For the \( n \)-type GaSb all three conduction bands with minima situated at \( L \) and \( X \) contribute to entire conductivity. \( X \) band contributes to conductivity mostly above 180 \(^\circ\)C. The mobilities of electrons and holes in the sample of GaSb with concentration of \( n = 1.49 \times 10^{18} \text{ cm}^{-3} \) at room temperature are presented in the following table.

<table>
<thead>
<tr>
<th>Electron mobility ( \mu_e (\text{cm}^2/\text{V} \cdot \text{s}) )</th>
<th>Hole mobility ( \mu_h (\text{cm}^2/\text{V} \cdot \text{s}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3750 (( \Gamma ) minima)</td>
<td>680</td>
</tr>
<tr>
<td>482 (( L ) minima)</td>
<td>2500 (77 K)</td>
</tr>
<tr>
<td>107 (( X ) minima)</td>
<td></td>
</tr>
</tbody>
</table>

Table 3. Electron and hole mobilities in GaSb[2].

## 7 Conclusions

The band structure, effective masses, valence crystal binding and transport properties are the most important features which describe the general nature of the GaSb semiconductor compound. The increased interest to this material may be explained by the unique feature of GaSb very narrow energy gaps, high mobility, and small effective masses of carriers and due to this the possibilities of practical applications in high frequency semiconductor devices.
(Gunn diode). There is also considerable scientific interest in all mixed III-V compounds of Ga series. The continuous variability of parameters in such kinds of materials makes possible the design of a material with virtually any gap width within the given range. The designability of such materials is especially useful for infrared or optical devices in which operation over particular wavelength ranges is required, such as in infrared sensors and injection lasers[3].

References


