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Phil Won Yu
W.C. Mithel
M. G. Mier
S. S. Li
Weizhen Wang

Wright State University - Main Campus, weizhen.wang@wright.edu

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Evidence of intrinsic double acceptor in GaAs

Phil Won Yu
University Research Center, Wright State University, Dayton, Ohio 45435

W. C. Mitchel
Materials Laboratory, Wright–Patterson Air Force Base, Ohio 45433

M. G. Mier
Avionics Laboratory, Wright–Patterson Air Force Base, Ohio 45433

S. S. Li and W. L. Wang
Department of Electrical Engineering, University of Florida, Gainesville, Florida 32611

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Acceptor present in undoped p-type conducting GaAs have been studied with photoluminescence, temperature-dependent Hall measurements, deep level transient spectroscopy, and spark source mass spectrometry. It is shown that p-type conduction is due to the presence of the shallow acceptor CAs and the cation antisite double acceptor GaAs. The first and second ionization energies determined for GaAs are 77 and 230 meV from the valence-band edge.

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GaAs has been of great interest both because of its technological importance and its fundamental properties. The role of deep impurities and intrinsic defects as electrically active centers has long been known in GaAs. Recently, many studies have been made of intrinsic vacancies and antisite defects, formed due to stoichiometry deviation during crystal growth and electron or neutron irradiation. In particular, several works\(^5\)–\(^7\) show that the anion antisite AS\(_{Ga}\) is responsible for a main electron trap located at \(-0.75\) eV from the conduction band (commonly known as EL2).

Recently, we have identified\(^5\) an acceptor level located at 77 meV from the valence-band edge present in liquid encapsulated Czochralski (LEC) grown materials. The acceptor is present both in p-type conducting and n-type seminsulating crystals grown from Ga-rich melts. The 77-meV acceptor was attributed to a center involving a cation antisite double acceptor GaAs on the basis of the background impurities, crystal growth in Ga-rich melts, and the presence of near-intrinsic emissions corresponding to antisite defects.\(^7\)

In this letter we present the result of studies on acceptors present in undoped bulk p-type materials. The experimental methods employed are photoluminescence (PL), temperature-dependent Hall measurements (TDH), deep level transient spectroscopy (DLTS), and spark source mass spectrometry (SSMS). The results show that all observed acceptors including the 77-meV acceptor can be attributed to the presence of CAs and the double acceptor GaAs.

Two wafers of p-type conducting crystals grown by LEC method were chosen for this study. PL excitation was made with a 647.1-nm line of a Kr laser with a maximum intensity of \(~400\) mW. A van der Pauw configuration was employed for TDH measurements. Ohmic contacts were made by evaporation of Ag-Mn alloy and an Al-Schottky barrier structure was used for DLTS and capacitance-voltage (C-V) measurements. SSMS was performed with liquid-helium cryopumping in the source region and 170 °C bakeout processing before analysis in order to reduce the background impurities such as C and O.

SSMS shows that the main background impurities are C and B. The concentration of B for sample A is \(4 \times 10^{16}\) cm\(^{-3}\) whereas sample B shows a surface contamination in the range \(4 \times 10^{15} - 4 \times 10^{16}\) cm\(^{-3}\). The concentration of C is listed in Table I. Other impurities are not our concern simply because the concentration is much less than \(4 \times 10^{15}\) cm\(^{-3}\).

![Image](https://example.com/image.png)

**Table I.** Detailed physical parameters obtained with four different experimental techniques (energy in meV and concentration in cm\(^{-3}\)).

<table>
<thead>
<tr>
<th>Sample</th>
<th>Method Parameters</th>
<th>C(_{As})</th>
<th>Ga(_{As})</th>
<th>Ga(_{As})</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SSMS C</td>
<td>(4 \times 10^{15}) (Total)</td>
<td>77</td>
<td>230</td>
</tr>
<tr>
<td>A</td>
<td>PL (E_A)</td>
<td>6</td>
<td>80</td>
<td></td>
</tr>
<tr>
<td></td>
<td>DLTS (E_A)</td>
<td>(4.1 \times 10^{15})</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Hall (E_A)</td>
<td>7</td>
<td>199</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(N_{A})</td>
<td>5.8 (\times 10^{15}) (Total Ga(_{As}))</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(N_{D})</td>
<td>1.0 (\times 10^{15}) (Total donor)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(N_{D})</td>
<td>9.7 (\times 10^{15}) (Total donor)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>SSMS C</td>
<td>(4 \times 10^{15}) (Total)</td>
<td>77</td>
<td>230</td>
</tr>
<tr>
<td></td>
<td>PL (E_A)</td>
<td>6</td>
<td>80</td>
<td></td>
</tr>
<tr>
<td></td>
<td>DLTS (E_A)</td>
<td>(2.4 \times 10^{16})</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Hall (E_A)</td>
<td>66</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(N_{A})</td>
<td>4.4 (\times 10^{16}) (Total Ga(_{As}))</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(N_{D})</td>
<td>7.3 (\times 10^{15}) (Total donor)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

532 Appl. Phys. Lett. 41(6), 15 September 1982 0003-6951/82/060532-03$01.00 © 1982 American Institute of Physics
The near-intrinsic region emission $E_{in}$, GaAs-related emission at 1.493 eV and the emissions at 1.441 and 1.284 eV due to GaAs and GaAs$_2$, respectively, are seen. The apparent activation energy was obtained by the usual relation obtained from the temperature correction of the hole capture cross section was made by the capture cross-section $\sigma_p$ vs $1/T$ relation. The obtained value of the apparent activation energy is 130 meV from the valence band. The activation energy of the major hole trap is 80 meV after the temperature correction of 50 meV of capture cross section (the obtained value of $\sigma_p$ is $7.1 \times 10^{-15} \text{ cm}^2$). Therefore, it is evident that this trap at 80 meV is the same center observed as the 1.441-eV emission under photoexcitation. The density of the hole trap determined by $N_T = (N_A - N_p)2\Delta C/C$ under a complete filling condition is given in Table I.

Hole concentration $p$ vs $1/T$ relation obtained from sample A is shown in Fig. 3 (similar Hall data were presented by other workers elsewhere). The hole concentration was calculated with the Hall factor being unity. Figure 3 shows two saturation regions in $p$ vs $1/T$ relation. This indicates the presence of three acceptor levels. However, sample B shows only one saturation in the temperature range of our measurements due to a higher concentration of second acceptor.

Now, let us consider the nature of the antisite double acceptor GaAs$_2$. Recent calculation by Louis and Vergès shows that possible bound states of antisite defects in GaAs are $A_1$ and $T_2$ states. The $T_2$ state has threefold orbital degeneracy and twofold spin degeneracy. In particular, the neutral state of GaAs$_2$ is the $T_2$ state occupied by four electrons. Therefore, neutral, singly, and doubly charged states (GaAs$_0$, GaAs$_1$, and GaAs$_2$) can exist for GaAs$_2$. Following the usual notion we call the degeneracy factors corresponding to GaAs$_0$, GaAs$_1$, and GaAs$_2$ state respectively $g_{Ga0}$, $g_{Ga1}$, and $g_{Ga2}$. The value of degeneracy factors depends on the splitting of the $T_2$ state due to Jahn–Teller distortion. However, no splitting of the $T_2$ state is likely with the expectation of a very weak Jahn–Teller distortion as in the case of the effective-mass acceptors. The values of $g_{Ga0}$, $g_{Ga1}$, and $g_{Ga2}$ are 15, 6, and 1 under no splitting of the $T_2$ state, respectively.

We analyze the Hall data with two acceptors C$_A$ and GaAs$_2$. A charge neutrality condition for $p$-type sample can be given as follows:

$$p + N_D = N_C + N_{Ga} + 2N_{Ga}^-,$$  \hspace{1cm} (1)

$$N_C = \frac{N_C}{(1 + g_{Ga}/g_{Ga1})N_v} \exp(E_{Ga}/kT),$$ \hspace{1cm} (2)

$$N_{Ga}^- = N_{Ga} \left[ 1 + \frac{g_{Ga0}}{g_{Ga1}} \frac{p}{N_v} \exp \left( \frac{E_{Ga1}}{kT} \right) \right].$$

FIG. 1. $T = 4.2$-K PL characteristics of a $p$-type sample (sample A). The near-intrinsic region emission $E_{in}$, GaAs-related emission at 1.493 eV and the emissions at 1.441 and 1.284 eV due to GaAs and GaAs$_2$, respectively, are seen.

FIG. 2. Hole concentration $p$ vs $10^3/T$ for a $p$-type sample (sample A).

FIG. 3. Hole concentration $p$ vs $10^3/T$ for a $p$-type sample (sample A).
\[ N_2^{Ga} = N_{Ga} \left[ 1 + \frac{g_{Ga0}}{g_{Ga2}} \left( \frac{p}{N_e} \right)^2 \exp \left( \frac{E_{Ga0} + E_{Ga2}}{kT} \right) \right]^{-1} \]
\[ N_2^{Ga} = N_{Ga} \left[ 1 + \frac{g_{Ga0}}{g_{Ga2}} \left( \frac{p}{N_e} \right) \exp \left( \frac{E_{Ga0}}{kT} \right) \right]^{-1} \]

where \( N_c \) is the total CAs acceptors, \( N_{Ga} \) is the total number of Ga\(\text{As} \), \( N_e \) is the density of state in the valence band, and \( N_D \) is the total donors. \( E_{Ca}, E_{Ga0}, \) and \( E_{Ga2} \) are the activation energies attributable to CAs, Ga\(\text{As}\)/Ga\(\text{As}\), and Ga\(\text{As}\)/Ga\(\text{As}\) respectively. Ga\(\text{As}\)/Ga\(\text{As}\) and Ga\(\text{As}\)/Ga\(\text{As}\) mean the first and second ionization states of the double acceptor Ga\(\text{As}\).

As a good approximation of Eq. (1) we use the following equation:
\[ p + N_D = N_c + \frac{N_{Ga}}{2} \left( 1 + \frac{g_{Ga0}}{g_{Ga2}} \left( \frac{p}{N_e} \right) \exp \left( \frac{E_{Ga0}}{kT} \right) \right) \]
\[ = \frac{N_{Ga}}{2} \left( 1 + \frac{g_{Ga0}}{g_{Ga2}} \left( \frac{p}{N_e} \right) \exp \left( \frac{E_{Ga0}}{kT} \right) \right) \]

The solid line in Fig. 3 is obtained by the least-square fit with the degeneracy factors \( g_{Ga0} \) under no splitting of the \( T_2 \) state. The degeneracy factors for CAs, Ga\(\text{As}\)/Ga\(\text{As}\), and Ga\(\text{As}\)/Ga\(\text{As}\) are, respectively, 4 and 1. The value used for \( N_e \) is \( 1.7 \times 10^{15} \) T-3/2. The activation energies are 23, 71, and 199 meV, which can be attributable to CAs, Ga\(\text{As}\)/Ga\(\text{As}\), and Ga\(\text{As}\)/Ga\(\text{As}\). For example B Hall data were analyzed with two acceptor levels due to CAs and Ga\(\text{As}\)/Ga\(\text{As}\).

Table I shows the results of our experiment. First, CAs is a major shallow acceptor. The concentration of C determined by SSMS agrees within a factor of 2 with that determined by Hall measurements. Second, the values determined for the second acceptor level are consistent with other well-known examples of double acceptors. First, let us consider Ga\(\text{As}\)/Ge. We note that these elements are isoelectronic with Ga and As. Therefore, ionization energies of Ga\(\text{As}\) can be obtained by adjusting the acceptor parameters involved in the acceptor model of Balderis and Lipari. We obtain 86 and 225 meV for Ga\(\text{As}\)/Ga\(\text{As}\), and Ga\(\text{As}\)/Ga\(\text{As}\) by using 32.6 and 85.8 meV for \( Zn^{2+}/Zn^+ \) and \( Zn^+/Zn^2+ \) in Ge, respectively. Similarly, we also obtain 82 and 245 meV for Ga\(\text{As}\)/Ga\(\text{As}\) and Ga\(\text{As}\)/Ga\(\text{As}\), using 34 and 102 meV for GaSb intrinsic acceptor levels. Also it is mentioned that other examples of double acceptor can be found in the metal vacancy system in II-VI compounds.

In conclusion, the present work shows that p-type conduction in materials grown under nonstoichiometry condition is well explained by CAs and an intrinsic acceptor. The intrinsic acceptor is due to Ga\(\text{As}\). Therefore, the intrinsic acceptor Ga\(\text{As}\) play important roles in compensation mechanism in Ga\(\text{As}\) as predicted by van Vechten. In practical Ga\(\text{As}\) technology, this work presents the importance of stoichiometry control during crystal growth.

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