DOE/ER/10939--1

DE82 011083

MASTER

INVESTIGATION OF THE ELECTRICAL AND OPTICAL
PROPERTIES OF ORGANOMETALLIC VAPOR-PHASE
EPITAXIAL $\text{Ga}_{1-x}\text{Al}_x\text{As}$ AND $\text{Ga}_{1-x}\text{Al}_x\text{As}/\text{GaAs}$ IN
SOLAR CELLS

DEPARTMENT OF ENERGY CONTRACT

DE AM06 76RL02227

TA DE AT06 81ER10939

PROGRESS REPORT

16 June 1981 - 15 December 1981

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INTRODUCTION

The results presented in this report cover work carried out under contract T 81ER10939 DE-AM06-76RL02227. Transport measurements have been carried out on $\text{Al}_x\text{Ga}_{1-x}\text{As}$ with $x \leq 0.3$ and the results compared with theory. In addition, measurements of transient capacitance have been used to investigate GaAs p-n homojunctions and GaAs/ $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ heterojunctions. Activation energies of dominant electron traps and their cross section have been calculated and the variations in emission rate for electron traps in the heterostructure has been obtained.

The results of this study together with measurements on photoluminescence, which allows determination of the excitonic spectra and binding energies of impurity and defect levels as a function of x , are the subject of a scientific paper soon to be submitted for technical publication. The final version of this paper will be forwarded to the Department of Energy at a later stage.

EXPERIMENTAL RESULTS AND DISCUSSION

Hall Effect Measurements on $\text{Al}_x\text{Ga}_{1-x}\text{As}$

The $\text{Al}_x\text{Ga}_{1-x}\text{As}$ layers were grown on the (100) surface of Cr doped, semi-insulating GaAs by organo-metallic chemical vapor deposition (OMCVD). The layers were prepared by Varian Associates, at a growth temperature of 750°C and with a V/III ratio of 10. This ratio is defined by

$$\text{V/III} = P_{\text{AsH}_3} / (P_{\text{TMA}} + P_{\text{TMG}})$$

where P_{AsH_3} , P_{TMA} and P_{TMG} are the respective partial pressures of arsine, trimethyl aluminum and trimethyl gallium within the growth reactor. The growth rate was $0.08 \mu\text{m}/\text{min}$ and the thickness of the epitaxial layers was about $10 \mu\text{m}$. All the grown layers were unintentionally doped n-type and had room temperature carrier concentrations of 10^{16} - $10^{17}/\text{cm}^3$.

The temperature dependence of the carrier concentrations of layers with $x = 0.1$, 0.2 and 0.3 are shown in Figure 1. At these alloy compositions the majority of the conduction band electrons occupy the Γ minimum of the conduction band at temperatures below 300 K . However, at higher temperatures some electrons will transfer to the higher energy X and L minima. This effect is reflected in the high temperature range in Figure 1 in which the observed carrier concentrations reach a maximum and then decrease with further increase in temperature. The carrier concentration for $x = 0.3$ decreases rapidly as the temperature is lowered below room temperature. This behavior may suggest the presence of a deep level.

The temperature dependence of the electron mobility for layers with $x = 0.1$, 0.2 and 0.3 is shown in Figures 2, 3 and 4 respectively. Measured values of mobility are shown by closed circles and the theoretical value is

plotted as the solid line μ_{total} . Various scattering mechanisms used to calculate the total mobility included polar optical phonon scattering (μ_{PO}), deformation potential scattering (μ_{DP}), piezoelectric scattering (μ_{PE}), alloy scattering (μ_{A}), space charge scattering (μ_{SC}) and ionized impurity scattering (μ_{II}). The total mobility μ_{total} is given by:

$$\frac{1}{\mu_{\text{total}}} = \sum_i \frac{1}{\mu_i}$$

The equations used in the calculations of electron mobility are¹, in $\text{cm}^2/\text{V.S.}$,

$$\mu_{\text{PO}} = 25.4 \frac{1}{(1/\epsilon_{\infty} - 1/\epsilon_s)} \frac{T^{1/2}}{(m^*/m_0)^{3/2}} \frac{\exp(\frac{\theta}{T}) - 1}{\theta} G(\frac{\theta}{T})$$

$$\mu_{\text{DP}} = \frac{3.17 \times 10^{-5} \rho \mu_{\ell}^2 T^{-3/2}}{E_1^2 (m^*/m_0)^{5/2}}$$

$$\mu_{\text{PE}} = \frac{2.52 \times 10^{12} T^{-1/2}}{(m^*/m_0)^{3/2} (e_{14}/\epsilon_s \epsilon_0)^2 (4/C_t + 3/C_{\ell})}$$

$$\mu_{\text{A}} = \frac{52.83 T^{-1/2}}{(m^*/m_0)^{5/2} x (1 - x) (\Delta U)^2}$$

$$\mu_{\text{SC}} = \frac{3.2 \times 10^9 T^{-1/2}}{(m^*/m_0)^{1/2} (N_s A)}$$

$$\mu_{\text{II}} = \frac{3.28 \times 10^{15} (m_0/m^*)^{1/2} \epsilon_s^2 T^{3/2}}{(N_D + N_A) [\ln(b + 1) - b/(b + 1)]}$$

$$\text{with } b = \frac{1.29 \times 10^{14} (m^*/m_0) \epsilon_s T^2}{n^*}$$

and n^* is equal to the carrier concentration if the temperature is low enough

for intrinsic conduction to be neglected and is assumed to be equal to a constant value, $10^{16}/\text{cm}^3$ for these calculations. The other symbols in the previous equations have their usual meaning and the values are given in Table 1. The value of ΔU , the alloy scattering potential, is given by²

$$\Delta U = 0.3 + 0.0011 x \text{ eV.}$$

The values of $N_s A$, where N_s is the density of the space charge region and A the effective electron scattering cross section, and $N_D + N_A$ were adjusted to give the best fit between measured and calculated values. These are

x	$N_s A \text{ cm}^{-1}$	$(N_D + N_A) \text{ cm}^{-3}$
0.1	9.2×10^4	7.2×10^{16}
0.2	1.8×10^5	1.8×10^{17}
0.3	2.4×10^5	1.0×10^{17}

The layer with $x = 0.2$ has the highest value of $N_D + N_A$ which is consistent with the results plotted in Figure 1, in which this sample has the highest carrier concentration. For the alloy composition $0 \leq x \leq 0.32$ intervalley scattering may be neglected^{3,4}. The dominant scattering mechanisms in the OMCVD $\text{Al}_x\text{Ga}_{1-x}\text{As}$ layers used in this investigation appear to be ionized impurity scattering at low temperatures, and space charge scattering or polar optical phonon scattering at high temperatures.

Detailed analysis of the temperature-dependent Hall-concentration data using a Multi-Vally conduction model is in progress. In addition to the bandstructure, the analysis will give information regarding deep levels in the ternary alloys.

Measurements on GaAs p-n junctions

A multi-layer structure grown by OMCVD on a n^+ - GaAs substrate was used in this study. A conventional buffer layer was first grown on the substrate followed by a n-type GaAs layer. This layer was undoped with a carrier concentration of $3 \times 10^{15}/\text{cm}^3$ and a thickness of 4 to 5 μm . The subsequent layers are p-type GaAs with a carrier concentration of $10^{17}/\text{cm}^3$ and a layer thickness of 1.5 μm , and p-type $\text{Al}_x\text{Ga}_{1-x}\text{As}$ with a carrier concentration of $10^{17}/\text{cm}^3$ and a thickness of 0.5 to 1.0 μm . The third layer has an energy gap greater than 2 eV and can act as a window layer of a solar cell. A p-type GaAs cap layer with a thickness of 0.5 to 1 μm was grown on the p- $\text{Al}_x\text{Ga}_{1-x}\text{As}$ layer to facilitate ohmic contact. This structure is described on pages 2 and 3 of our original proposal.

Measurements on this multilayered structure have concentrated upon the GaAs n-p junction, which, because of the differences in carrier concentration, may be treated as an abrupt, one-sided, asymmetric step junction. Under reverse bias the depletion region lies almost entirely within the lighter doped n-type region. Capacitance measurements may therefore be used to yield information about the n-type region.

Transient capacitance measurements are used to obtain information about electron traps within the material. The activation energy and the thermal cross-section of electron traps were determined from the following equation⁵,

$$\frac{1}{\tau T^2} = 3.26 \times 10^{21} g_n \sigma_{\infty} \frac{m^*}{m_0} \exp(\alpha/k) \exp[-(\Delta E_T^0 + \Delta E_B)/kT]$$

Here τ is the time constant for thermal emission of carriers from the trap level, $\Delta E_T = \Delta E_T^0 - \alpha T$ where α , the temperature coefficient of the trap level, is assumed to be zero, $\sigma = \sigma_{\infty} \exp(-\Delta E_B/kT)$ is the captive cross section with

an energy barrier ΔE_B , g_n the degeneracy factor is assumed to be 1/2 and m^* the effective mass of the electron.

The temperature dependence of the emission time constant for the 0.8 eV electron trap in the n-type GaAs, is shown as a function of distance d from the junction, in Figure 5. The emission time constant for the electron trap is observed to decrease with distance from the p-n junction. However, the activation energy $\Delta E_T + \Delta E_B$ does not change appreciably with corresponding distance.

Spatial profiles of electron concentration and the 0.8 eV electron trap is shown in Figure 6. The electron concentration, calculated from measurements of the capacitance/voltage characteristic, is almost constant, $3.6 \times 10^{15}/\text{cm}^3$ over the distance 0.6 μm . The trap density, $N_T(d)$ is given by⁶

$$N_T(d) = - \frac{\Delta C}{C} \frac{\bar{W}^2}{d} \frac{N^+(\bar{W})}{\Delta d}$$

where $\Delta C/C$ is the relative capacitance change due to the $N_T(d)$ trapped electrons in the interval Δd at d , $\bar{W}$ is the width of the space charge layer at a quiescent reverse bias, and $N^+(\bar{W})$ is the positive space-charge concentration at the edge of the depletion region. This equation is valid for $\Delta C \ll C$. In the region $d \geq 0.8 \mu\text{m}$ the 0.8 eV trap is nearly uniformly distributed but the trap density was observed to decrease rapidly near the p-n junction. Similar decreases in trap concentrations have been reported for two hole traps in p-type GaAs grown by liquid phase epitaxy⁷.

The effect of changes in electric field on the emission time constant has also been examined. For electric fields of strength 2.7×10^4 to 7.6×10^4 V/cm no significant change in the emission time constant was observed.

Measurements on GaAs-Al_{0.2}Ga_{0.8}As Heterojunctions

The active layers used in this study were grown by OMCVD on a n⁺ - GaAs substrate similar to that described in the previous section. For this sample the first active layer is undoped n-type Al_{0.2}Ga_{0.8}As with a carrier concentration of $\sim 10^{16}/\text{cm}^3$ and a thickness of $\sim 2.5 \mu\text{m}$. This is followed by a layer of undoped n-type GaAs with a carrier concentration of $\sim 10^{16}/\text{cm}^3$ and a thickness of $\sim 1.1 \mu\text{m}$. The third active layer is p-type Al_{0.2}Ga_{0.8}As with a carrier concentration of $\sim 10^{17}/\text{cm}^3$ and a thickness of $\sim 1.5 \mu\text{m}$. A p-type cap layer of GaAs is again used to facilitate ohmic contact.

The temperature dependence of emission time constants for electron traps in the n-type GaAs and the n-type Al_{0.2}Ga_{0.8}As layers are shown in Figures 7 and 8 respectively. The activation energy ($\Delta E_T + \Delta E_B$) and the capture cross section of the electron trap in the GaAs were calculated to be $0.84 \pm 0.02 \text{ eV}$ and $\sim 6 \times 10^{-13} \text{ cm}^2$. Measurements on the electron trap in the Al_{0.2}Ga_{0.8}As yield values of $0.67 \pm 0.02 \text{ eV}$ and $\sim 1 \times 10^{-15} \text{ cm}^2$ for the activation energy and capture cross section, respectively.

A study of the spatial distribution of the electron concentration and the electron trap in both the n-type GaAs and n-type Al_{0.2}Ga_{0.8}As is shown in Figure 9.

A noticeable drop in electron concentration occurs near the interface between the n-type GaAs and n-type Al_{0.2}Ga_{0.8}As. This reduction in electron concentration suggests the presence of compensating acceptor levels, possibly due to lattice defects near the interface. The compensatory levels are distributed in the region from $0.9 \mu\text{m}$ to $1.7 \mu\text{m}$. In addition the trap density was observed to decrease near the interface. The transient capacitance measurements, carried out ^{near} room temperature, have concentrated solely on traps with activation energies in the range ~ 0.7 to 0.8 eV . At room temperature

the thermal emission rate of the trapped electrons are strongly dependent upon position within the layer. At a distance of $d = 1.0 \text{ } \mu\text{m}$ (in the interface region) the emission rate for electron traps is some 25 times faster than that for the traps situated at $d = 0.5 \text{ } \mu\text{m}$, within the GaAs, and 5 times faster than at $d = 1.7 \text{ } \mu\text{m}$, which is within the $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$. Furthermore, the capacitance transient due to traps within the interface region is highly non-exponential, this is in comparison to the fairly exponential capacitance transients observed for traps outside the interface region. One outcome of this is that traps with various different activation energies appear to be located in the interface region. These results suggest that a highly detailed study of the interface region needs to be carried out.

Other non-exponential behavior of the capacitance transient is observed for traps near the anisotype p- $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}/\text{n-GaAs}$ heterojunction. The behavior of the traps near the GaAs p-n junction is, however, exponential. It appears therefore, that the non-exponential nature of the transient decay is a definite feature of GaAs/ AlGaAs heterojunction. The heterojunctions used in this investigation have been those in which the doping concentrations lead to voltage division between the two sides of heterojunction. For detailed examination of the nonexponential behavior it may be preferable to examine semiconductor heterojunctions in which deliberate asymmetric doping has been introduced. This would serve to restrict the band bending to the more lightly doped material and hence to reduce the effects of voltage division. Both isotype and anisotype heterojunctions should be studied. In addition it is essential to study materials with a higher Al content which would be appropriate for solar cell applications.

In addition to the traps discussed above, we have detected electron and hole traps with ΔE_T ranging from 0.18 to 0.37 eV in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ with $x = 0.1$ and 0.2 . The characteristics of these traps are being further investigated and will be described in a report to follow in the near future. We expect to complete a detailed investigation of deep levels in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ layers and heterojunctions by the end of the first year, as proposed.

Photoluminescence Measurements

Photoluminescence measurements at 1.8K and with a resolution $\sim 2\text{\AA}$ were carried out on the ternary alloys with $0.1 \leq x \leq 0.8$ and on one of the heterojunctions mentioned above. The measurements were also performed as a function of excitation intensity. The alloys in the direct bandgap range (up to $x = 0.36$ eV) exhibit excellent edge luminescence. On the contrary, the samples with $x > 0.4$ supplied to us do not show any luminescence. More material is being grown for our studies. A report on the photoluminescence measurements will follow in the near future.

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Table 1. Parameters for calculating electron mobilities in $\text{Al}_x\text{Ga}_{1-x}\text{As}$.

	GaAs (x=0)	AlAs (x=1)
m^*/m_0	0.067	0.128
ϵ_s	12.9	10.06
ϵ_∞	10.9	8.16
θ (K)	420	580
ρ (g/cm ³)	5.37	3.6
U_ℓ (km/s)	5.24	5.5
E_1 (eV)	8.6	13
e_{14} (C/m ²)	0.16	0.16
C_t (dyne/cm ²)	0.487×10^{12}	0.493×10^{12}
C_ℓ (dyne/cm ²)	1.404×10^{12}	1.422×10^{12}

Figure 1. Temperature dependences of electron concentrations in
 $\text{Al}_x\text{Ga}_{1-x}\text{As}$ layers grown by OMCD.

Figure 2. Experimental (closed circles) and calculated (solid curves) mobilities as a function of temperature for $\text{Al}_{0.1}\text{Ga}_{0.9}\text{As}$.

Figure 3. Experimental (closed circles) and calculated (solid curves) mobilities as a function of temperature for $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$.

Figure 4. Experimental (closed circles) and calculated (solid curves) mobilities as a function of temperature for $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$.

Figure 5. Temperature dependences of thermal emission time constants for electron traps in n-GaAs at various positions from a p^+ -n junction. The distance d from the p^+ -n junction and the spatial resolution Δd are shown in the figure.

Figure 6. Carrier concentration n and 0.8-eV electron trap concentration N_T versus distance into n-GaAs from a p^+ -n junction.

Figure 7. Temperature dependence of thermal emission time constant for an electron trap in n-GaAs in the interval Δd at distance d from a p^+ -n junction.

Figure 8. Temperature dependence of thermal emission time constant for an electron trap in $n\text{-Al}_{0.2}\text{Ga}_{0.8}\text{As}$ in the interval Δd at distance d from a $p^+\text{-}n$ junction.

Figure 9. Carrier concentration n and electron trap concentration N_T versus distance into n-type material from a $p^+-Al_{0.2}Ga_{0.8}As/n-GaAs$ heterojunction. The metallurgical interface position between n-GaAs and n- $Al_{0.2}Ga_{0.8}As$ is shown in the figure.