Lawrence Berkeley National Laboratory
Recent Work

Title
CHARACTERIZATION OF GaAs FILM GROWN ON Si SUBSTRATE BY PHOTOLUMINESCENCE AT 77 K

Permalink
https://escholarship.org/uc/item/1mp3c1rd

Author
Huang, Y.

Publication Date
1987-12-01
Characterization of GaAs Film Grown on Si Substrate by Photoluminescence at 77 K

Y. Huang, P.Y. Yu, H. Lee, and S. Wang

December 1987
DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.
Characterization of GaAs Film Grown on Si Substrate
by Photoluminescence at 77 K

Yihe Huang and Peter Y. Yu

Department of Physics, University of California, Berkeley
and
Materials and Chemical Sciences Division,
Lawrence Berkeley Laboratory, University of California,
Berkeley, California 94720

Henry Lee and Shyh Wang

Department of Electrical Engineering and Computer Science
and
Electronics Research Laboratory,
University of California, Berkeley,
Berkeley, California 94720

December 1987
Characterization of GaAs Film Grown on Si Substrate by Photoluminescence at 77 K

Yihe Huang and Peter Y.Yu.
Department of Physics, University of California

and

Materials and Chemical Sciences Division,
Lawrence Berkeley Laboratory, Berkeley, California 94720

Henry Lee and Shyh Wang
Department of Electrical Engineering and Computer Science,

and

Electronics Research Laboratory, University of California
Berkeley, CA 94720

Abstract

Photoluminescence of GaAs films grown on Si substrate has been investigated quantitatively at 77 K. The peak shift and splitting of the exciton luminescence are shown to result from tensile stress in the film. Information on carrier lifetime has been deduced from the lineshape of the photoluminescence.

PACS numbers: 78.55.
GaAs film grown on Si substrate by molecular beam epitaxy has been of much interest recently.\textsuperscript{1-4} Many different type of devices have been fabricated successfully on these thin films. But there are still serious problems remaining to be solved. One such problems is the high density of dislocations resulting from the lattice mismatch between GaAs and Si. This high dislocation density results in short minority carrier lifetime making it difficult to fabricate high quality laser diodes. The second problem is thermal stress which results from difference in thermal expansion coefficients between GaAs and Si. Several techniques have been used to measure this thermal stress in GaAs films grown on Si. Measurement of the stress-induced curvature is possible for large wafers such as those grown by metalorganic chemical vapor deposition.\textsuperscript{5} The lattice constant of the strained GaAs films can also be measured by X-ray diffraction.\textsuperscript{6} But both techniques measure the magnitude of the stress averaged over large areas. The lineshape and frequency shift of phonon Raman scattering have been shown to yield information on both the crystal quality and stress.\textsuperscript{7} This technique suffers from low sensitivity. Determination of stress in GaAs film on Si using photoluminescence technique has been reported previously.\textsuperscript{8} Zemon et al. found that the band edge luminescence peak was shifted and split. They suggested that this shift and splitting were caused by strain and could be used to determine the thermal stress in the GaAs film.\textsuperscript{9} In this Letter we report a quantitative analysis of the photoluminescence (PL) of several GaAs on Si samples with different film thicknesses and
widths. We show that from an analysis of the splitting of the PL peaks, their lineshapes and relative intensities, one can deduce besides the thermal stress other useful information on sample quality such as minority carrier lifetime.

Our GaAs films were grown by molecular beam epitaxy on either Si or GaAs substrates. The film thicknesses are listed in Table 1. Sample D is only 10 μ wide while other samples were more than 2 mm wide. The samples were unintentionally n-type doped to less than $10^{16}$ cm$^{-3}$. The 5145 Å line of an Ar$^+$ laser was used to excite the PL. Since the lineshape of the PL spectra changed at high excitation power densities, the laser power density was kept at a low level of 29 W/cm$^2$ which we will show to cause minimal heating of the samples. A Spex 1403 double monochromator and a photon counting system was used to measure the PL spectra. The experiment was performed at liquid nitrogen temperature with all the samples mounted side by side on the same cold finger. The penetration depth of the laser light in GaAs is about 2000 Å, so the information we deduced from the PL is representative of the top 2000 Å of the film.

Sample A was assumed to be free of thermal stress since its substrate was also GaAs. Indeed its PL spectra showed one sharp peak (see Fig. 1) with no detectable sign of splitting. The frequency of this peak was used as the reference for determining the stress induced shift in the PL of other GaAs/Si samples. In contrast the PL spectra of all the GaAs/Si films showed two peaks similar to those reported by Zemon et al. Although these spectra were qualitatively similar to each other, the widths of
the PL peaks were quite different between spectra B, C and D.

To interpret these PL spectra quantitatively, we have used the following model. First we assume that each peak in the PL spectrum contains two contributions: transitions due to the lowest (1s) exciton level and the corresponding band-to-band transition. These two contributions were not fully resolved in our experiment because of the smallness of the exciton binding energy \( E_{\text{ex}} \) in GaAs and the high temperature \( ( \geq 77 \, \text{K} ) \) of the experiment. In the absence of strain the heavy hole (hh) and light hole (lh) bands are degenerate at the Brillouin zone center so these bands contribute only one luminescence peak. The split-off band is 0.34 eV higher in energy so at 77 K its population is negligible. To simplify the calculation, we have neglected the discrete excited states of the excitons and the excitonic enhancement of the continuum band-to-band transition.\(^\text{10}\) The error introduced by this simplification was not serious for GaAs because of its very small exciton binding energy. The exciton luminescence is represented by a Lorentzian \( L_i(E) \) centered at the exciton energy \( ( E_{\text{gi}} - E_{\text{exi}} ) \) while the band-to-band transition is described by the function \( F_i(E) \):

\[
L_i(E) = |M_i|^2 \mu_i^2 \frac{3}{2} \frac{\Delta_i^2 e^{- \frac{E_{\text{gi}}-E_{\text{exi}}}{kT}}}{(E-E_{\text{gi}}+E_{\text{exi}})^2 + \Delta_i^2} \tag{1}
\]

and \( F_i(E) = |M_i|^2 \mu_i^2 \left\{ \begin{array}{ll} \sqrt{\frac{E}{E_{\text{gi}}} - 1} e^{- \frac{E}{kT}} & \text{if } E \geq E_{\text{gi}} \\ 0 & \text{if } E < E_{\text{gi}} \end{array} \right. \tag{2} \)

In Eqns. (1) and (2), \( i \) refer to either hh or lh bands, \( |M_i|^2 \) are
their optical transition matrix elements, $E_{gi}$ and $\mu_i$ are their bandgaps and joint-density-of-states masses, $E_{exi}$ and $\Delta_i$ are the exciton binding energies and linewidths, $T$ is the carrier temperature, and $k$ is the Boltzmann constant. The function $F(E)$ describes an asymmetric peak whose high energy side is determined by the temperature $T$ of the carriers. The total PL intensity is obtained by summing the contributions from both the heavy hole and light hole bands:

$$I_{PL} \propto \sum_{i=hh}^{lh} (A L_i(E) + F_i(E))$$

(3)

$A$ is an adjustable parameter, which represents the relative intensity of the lowest exciton level to the band-to-band transition.

An external hydrostatic stress change the lattice constant and shift the energy bands, while an uniaxial stress can lift some of band degeneracies. The stress induced bandgap shifts and splittings in GaAs have been studied extensively by PL and many other experiments.\textsuperscript{11,12} We assume that the stress distribution inside the GaAs/Si films is biaxial with the stress perpendicular to the film equal to zero, while the stress in the plane of the GaAs films is isotropic. One can show easily that for a GaAs film grown on (100) Si substrate this stress is equivalent to the sum of a hydrostatic pressure and an uniaxial stress perpendicular to the film. The effect of such uniaxial stress on the optical transitions of GaAs can be described by the strain Hamiltonian proposed by Bir et al.\textsuperscript{13} For GaAs subjected to a tensile stress in the [100] direction this
Hamiltonian gives the following stress-induced bandgap shifts to the lowest order in stress:

\[
\frac{\Delta E_h}{X} = \left[-\frac{2}{3} \left( \frac{\partial E_g}{\partial P} \right) + b(S_{11} - S_{12})\right] = -10.4 \text{ meV/kbar}
\]

\[
\frac{\Delta E_l}{X} = \left[-\frac{2}{3} \left( \frac{\partial E_g}{\partial P} \right) - b(S_{11} - S_{12})\right] = -4.9 \text{ meV/kbar}
\]

where \(\Delta E_l\) and \(\Delta E_h\) are respectively the lh and hh band gap shifts, \(S_{11}\) and \(S_{12}\) are components of the compliance tensor of GaAs, \(X\) is the magnitude of the isotropic stress in the plane of the films and \(\frac{\partial E_g}{\partial P}\) is the hydrostatic pressure coefficient of the bandgap and \(b\) is the deformation potential for uniaxial stress along the \([100]\) direction. To fit the PL spectra for GaAs films grown on Si substrate, we use Eq.(4) to calculate the bandgaps \(E_{gi}\) under stress and substitute these values into Eq.(3). Figure 1 shows the experimental PL spectra (solid lines) and the corresponding theoretical fits (broken curves). In fitting curve A (GaAs/GaAs sample) the adjustable parameters are \(A, E_{ex}',\) and \(T\) and their values are listed in Table 1. Within our experimental accuracy we found that \(E_{ex} = 0\) meV gave the best overall fit to the experimental spectrum. If we have used \(E_{ex} = 5\) meV, which is the generally accepted exciton binding energy in GaAs, the theoretical curves show a dip between the exciton peak and the continuum band-to-band contribution. The dip would not be present if the higher discrete exciton states plus the exciton enhancement to the continuum density of states were included in our model. Thus the use of the adjustable parameter \(A\) and the assumption that \(E_{ex} = 0\) compensate for these omissions. We also...
noted that in sample A the carrier temperature $T$ was very close to the lattice temperature suggesting that laser heating of the samples was negligible. In fitting the spectra for the GaAs/Si samples we again assumed $E_{\text{exi}} = 0$ for both hh and lh transitions. The adjustable parameters in these cases are $X, \Delta_1, \Delta_h, T$ and $A$. The results are shown in Table 1 also. From Eq. (4) the stress $X$ causes a shift in the 'center of gravity' of the hh and lh transitions in addition to splitting them. The fact that a single value of $X$ can fit both the shift and splitting of the hh and lh transitions is a strong indication that the biaxial stress we have assumed is basically correct. Furthermore the fact that $X$ deduced from the different GaAs/Si samples are more or less the same is consistent with its thermal origin.

Besides the splitting of the PL peaks, there are also differences in lineshapes and relative peak intensities between all the samples. For example the linewidths of the exciton peaks in the GaAs/GaAs sample was considerably narrower than those of the GaAs/Si samples. The broadening of the exciton peaks in the GaAs/Si samples can result from either shorter exciton lifetimes in the GaAs/Si samples due to dislocations or from inhomogeneous broadening due to variation of stress in the sample. We will show later that the exciton lifetime in our GaAs/Si samples are longer than tens of picoseconds (ps) so homogeneous lifetime broadening in these samples are negligible. Thus to reconcile this inhomogeneous stress broadening with the biaxial stress distribution, we have to assume that the stress is locally homogeneous and isotropic but there are variations over an area of the size of our focal spots which were typically larger.
than three hundred microns across. Presumably this stress variation is largest near the edge of the film. This will explain the larger exciton linewidth in the narrower sample D. The stress variation over the film can be mapped out by a tighter focusing of the laser spot and this will be the subject of future investigations.

From the relative intensities of the hh and lh exciton peaks and the lineshapes of the higher energy tail of the band-to-band contribution, we found that the carrier temperatures in the GaAs/Si samples are considerably higher than the lattice temperature. (See Table 1 for the carrier temperatures). We propose to explain this 'hot carrier' effect in the GaAs/Si samples by the shorter lifetime of photoexcited carriers in these samples due to the higher density of dislocations. To correlate the carrier lifetime with their temperature we assume that the photoexcited electron-hole (e-h) pairs lifetime is $\tau$. The rate at which energy is transferred to each e-h pair from the laser beam is given by: $H = \frac{\hbar \omega - E_g}{\tau}$ where $\hbar \omega$ is the laser photon energy. The rate at which each e-h pair will lose energy due to emission of longitudinal optical (LO) phonon is:

$$L = \frac{\hbar \omega_{LO}}{\tau_0} \left[ \exp\left(- \frac{\hbar \omega_{LO}}{k T}\right) - \exp\left(- \frac{\hbar \omega_{LO}}{k T_L}\right) \right] \quad (5)$$

where $\hbar \omega_{LO}$ is the LO phonon energy, $\tau_0$ is the time for an e-h pair to emit a LO phonon and is $\sim 0.1$ ps $^{15}$ and $T_L$ is the lattice temperature assumed to be 77.4 K. At steady state we expect $H = L$ and from this equation we can calculate $\tau$ from the experimentally deduced carrier temperature. The resultant $\tau$'s are
shown in Table 1 for samples A to D. The shorter carrier lifetimes in Samples C and D as compared with sample B are presumably caused by their smaller thickness so there are more dislocations at the surface of these films. The carrier lifetimes estimated in this way from these films are somewhat shorter than the lifetime of photoexcited free carriers in GaAs containing nonradiative recombination centers such as Cr. They are consistent with the relative quantum efficiencies of these films determined with the same optical setup. The results of these quantum efficiency measurements will be published elsewhere.

In conclusion we have shown that from the photoluminescence spectra of GaAs films grown on Si, one can determine the thermal stress, carrier lifetime and stress inhomogeneity in these films.

This work is supported by the director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098 and by the Joint Services Electronic Program AFOSR F49620-84-C-0057.
References:


Figure Captions:

Fig. 1: The experimental photoluminescence spectra of GaAs films at 77 K (solid curves).

A: GaAs on GaAs substrate.
B: GaAs on Si substrate (3μ thick).
C: GaAs on Si substrate (1.5μ thick).
D: GaAs on Si substrate (1.5μ thick and 10μ wide).

The broken curves are theoretical fits to the experimental curves as discussed in the text.
Table I

Summary of characterization of GaAs films and sample parameters deduced by fitting the experimental photoluminescence spectra.

<table>
<thead>
<tr>
<th>Sample</th>
<th>A GaAs/GaAs</th>
<th>B GaAs/Si</th>
<th>C GaAs/Si</th>
<th>D GaAs/Si</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thickness (μ)</td>
<td>1.5</td>
<td>3</td>
<td>1.5</td>
<td>1.5 (10μ wide)</td>
</tr>
<tr>
<td>Exciton Linewidth (cm⁻¹)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Δ_h (heavy hole)</td>
<td>13</td>
<td>44</td>
<td>53</td>
<td>85</td>
</tr>
<tr>
<td>Δ_l (light hole)</td>
<td>52</td>
<td>70</td>
<td>110</td>
<td></td>
</tr>
<tr>
<td>Carrier Temperature (K)</td>
<td>81</td>
<td>127</td>
<td>187</td>
<td>216</td>
</tr>
<tr>
<td>Stress (kbar)</td>
<td>0</td>
<td>3.7±0.5</td>
<td>3.2±0.4</td>
<td>3.6±0.5</td>
</tr>
<tr>
<td>A</td>
<td>1.8</td>
<td>1.9</td>
<td>3.5</td>
<td>4.8</td>
</tr>
<tr>
<td>Carrier lifetime (ps)</td>
<td>2000</td>
<td>79</td>
<td>28</td>
<td>18</td>
</tr>
</tbody>
</table>
Fig. 1