Determination of interface state densities in CdTe heterostructures using photoluminescence intensity measurements

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MBE Growth and Characterization complex at Texas State University

- II-VI MBE
- Oxide I MBE
- Oxide II MBE
- As-based MBE
- Sb-based MBE
- H₂ Cleaning Chamber
- IV-VI MBE
- XPS Chamber
- SPM Chamber
- Oxide III

7 growth chambers, an atomic hydrogen cleaning station, and XPS and SPM chambers
The Challenge: Measured Characteristics Did Not Seem To Correlate With Materials Properties

TRPL data from bulk \( \tau \) in single-crystal, large-grain, and poly CSS CdTe.
Comparison with confocal PL

In general, single photon TRPL and overall PL efficiency independent of dislocations & twins

CdTe /GaAs (211)  
Dislocation density  
2x10⁷ cm⁻²

CdTe/CdTe (211)  
Dislocation density  
5x10⁵ cm⁻²

CdTe/InSb (100)  
Twin Density  
5x10⁴ cm⁻²

Conclusion: PL efficiency is mainly a function of surface/interface passivation.
Photoluminescence Intensity (PLI) measurement

- Nondestructive
- No fabricated structures, temperature dependence, or conducting substrates needed.
- Characterizes recombination centers.
- Lower detection limit for near-interface effects than Capacitance-Voltage/DLTS.


Numerical modelling

\[
\frac{dn}{dt} = -D \frac{d^2n}{dx^2} - \frac{d}{dx} (\mu nE) - R + G = 0
\]

\[
\epsilon \frac{d^2V}{dx^2} = -n + p + N_D - N_A + Q_T
\]

- Includes recombination center charging effects
- Surface/interface recombination is a result of recombination behavior – it does not remain fixed as the intensity changes!
- Recombination center concentration \((N_T)\) and Energy \((E_T)\) can be found.

\[
G = I_\alpha \exp(-\alpha x)
\]

\[
R_{rad} = B_{rad} np
\]

\[
R_{SRH} = \frac{N_T}{n + n_1 + p + p_1} np
\]

\[
N_1 = N_C e^{(E_T - E_G)/k_B T}, \quad p_1 = N_V e^{-E_T/k_B T}
\]
Basic Concepts

Input Intensity approaches 100% internal quantum efficiency (Radiative).

Well-defined lifetime and surface recombination velocity.

Slope is a function of trap energy.

High injection with input intensity.

Input intensity is well known: not adjustable.

Log (Normalized PLI efficiency)

100%
Measured PLI fits well to a single trap 70 meV above the valence band.

\[ E_{CNL} = 1.12 \text{ eV} \]

\[ E_T \approx 70 \text{ meV} \]

\[ N_s(E) = N_{so} \times \exp\left(\frac{\left| E - E_{CNL} \right|}{E_0}\right)^2 \]

\[ E_0 \approx 400 \text{ meV} \]

This single trap model falls in line with Disorder-Induced Gap State (DIGS) model.
DH structure and band edge diagram

**CdTe DH**

- **CdTe cap**
- **X CdTe barrier**
- **CdTe**
- **X CdTe barrier**
- **CdTe**

10 nm
30 nm
1000 nm
30 nm

**CdTe/Mg0.18Cd0.82Te**

- Type-I heterojunction
- $\Delta E_v = 80$ meV*
- $\Delta E_c = 188$ meV*
- Mismatch < 0.2%
- Stable in air ($x < 0.5$)

Excitation Intensity (W/cm²)

Normalized PL Efficiency

Bare
CdZnTe
CdZnSe
CdMgTe
CdMgTe DH

ET = 70 - 100 meV

Most Likely: Recombination at Homoepitaxial interface

Comparison of CdMgTe Single and Double Heterostructures (DH)
CdMgTe DH Results

Normalized PL Efficiency versus Excitation Intensity (W/cm²)

- InSb substrate
  - 1 micron film
  - 0.5 micron buffer
- Bare
- CdZnTe
- CdZnSe
- CdMgTe
- InSb substrate
  - 1 micron film
  - 1 micron buffer
- InSb substrate
  - 0.5 micron film
  - 1.5 micron buffer
- CdMgTe DH
- Fit
- AlGaAs/GaAs

Normalized PL Efficiency values:
- 6-8 × 10^{10}
- 2.6 × 10^{10}
- 1.3 × 10^{10}
- 1.6 × 10^{11}
- 6.7 × 10^{10}
- 2.1 × 10^{10}
Correspondence with TRPL

For DH: \( \frac{1}{\tau_e} \sim \frac{2S}{d} \)

- Excitation Intensity (W/cm²)
  - 0.1 1 10 100 1000

- Normalized PL Efficiency
  - \(10^{-5}\)  \(10^{-4}\)  \(10^{-3}\)  \(10^{-2}\)  \(10^{-1}\)  100

- InSb substrate
- 1 micron film
- 0.5 micron buffer
- Bare
- CdZnTe
- CdZnSe
- CdMgTe
- DH

ET = 70 - 100 meV

- 240 nS
- 40-50 nS

- Correspondence with TRPL
The combination of PLI and TRPL measurements and analysis provides a reliable method for estimation of the recombination parameter $B_{rad}$.

- The trap parameters resulting from the fit to the PL-I data ($N_T = 2.5 \times 10^{10}$ cm$^{-2}$) were used to simulate the time dependent distribution of carriers after a pulse of photo-generated electron-hole pairs — without the use of any additional parameters.
- The low injection lifetime is one of the longest ever measured for CdTe.
- Analysis assumes $B_{rad} \sim 1.1 \times 10^{-10}$ cm$^3$s$^{-1}$.
c-PL dark spot Simulation

Pixels (80 nm)

Intensity (Arb.)

\[ \tau = 220 \text{ ns} \ (N_T = 2 \times 10^{10} \text{ cm}^{-2}) \]

\[ \tau = 20 \text{ ns} \ (N_T = 1.2 \times 10^{11} \text{ cm}^{-2}) \]

\[ \tau = 2 \text{ ns} \]

Z275 SH

Z278 DH

Z323 DH
Correspondence with TRPL

For DH: \[ \frac{1}{\tau} \sim \frac{2S}{d} \]

- Does NOT track with DH thickness
- More closely related to buffer thickness
- Need to get away from interface (?)
The final word is not yet in regarding lifetime and defects….

<table>
<thead>
<tr>
<th>Sample</th>
<th>Peak (nm)</th>
<th>Band Gap Energy (eV)</th>
<th>x</th>
<th>Thickness (nm)</th>
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<tr>
<td>z328</td>
<td>587.9</td>
<td>2.11</td>
<td>0.38</td>
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<tr>
<td>z335</td>
<td>649.7</td>
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<td>0.25</td>
<td>35</td>
</tr>
</tbody>
</table>

3x10^5 cm^-2 twins
1x10^7 cm^-2 dislocations
Conclusions

• Currently achievable interface state density between the CdTe and CdMgTe of $\sim1.6 \times 10^{10}$ cm$^{-2}$

• CdMgTe/CdTe DH now rivals high quality AlGaAs/GaAs DH in radiative efficiency