Anti-Phase-Boundary Defects in GaAs-on-Si Films: 
1. characterization by SHG
2. suppression by ART

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The microelectronics industry is trying to marry III-V and Column IV semiconductors via hetero-epitaxy to combine the favorable properties of each
GaAs/Si interfaces are susceptible to formation of defects

**Threading Dislocations (TDs)**
- Where: any hetero-interface
- Cause: lattice mismatch
- Characterization: selective etching + TEM

<table>
<thead>
<tr>
<th>Substrate</th>
<th>Lattice Mismatch w. GaAs</th>
<th>Typical TDD [cm$^{-2}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si (001)</td>
<td>4%</td>
<td>$&gt;10^9$</td>
</tr>
<tr>
<td>Ge (001)</td>
<td>&lt;1%</td>
<td>$&lt;10^8$</td>
</tr>
</tbody>
</table>


**Anti-Phase Domains (APDs)**
- Where: polar-on-nonpolar hetero-interfaces
- Cause: single-atom steps, nonpolar substrate (↑)


Ga-Ga bonds along Anti-Phase Boundaries (APBs) degrade carrier mobility

TDs and APBs are challenging to distinguish in TEM micrographs


To evaluate strategies for suppressing these defects, a fast, noninvasive diagnostic that clearly distinguishes APBs from TDs is needed
Neighboring APDs generate SH fields of opposite sign

SHG characterizes APBs sensitively and non-invasively

\[ I_s(2\omega) \propto |\sin 2\phi|^2 \]

\[ I_s(2\omega) \propto |\cos \alpha (f_c t_p \cos 2\phi_0 \cos \alpha + t_s \sin 2\phi_0 \sin \alpha)|^2 \]
To test SHG sensitivity to TD Density (TDD), we prepared $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ samples.

Integrated SHG Intensity [$10^4$ cts/s]

Conclusion: SHG is uncorrelated with TDD
Substrate off-cut angle $\alpha$ strongly affects APD density & SHG suppression

$\alpha < 1^\circ$: single-atom steps dominate; SHG suppression correlates with APD density

$\alpha \geq 4^\circ$: double-atom steps dominate; APDs suppressed, SHG recovers

<table>
<thead>
<tr>
<th></th>
<th>GaAs</th>
<th>GaAs/Si(001)</th>
<th>GaAs/Ge(001)</th>
<th>GaAs/Si: 4$^\circ$</th>
<th>GaAs/Ge: 6$^\circ$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\langle$SHG intensity$\rangle$</td>
<td>1</td>
<td>$2.4 \times 10^{-3}$</td>
<td>$7.7 \times 10^{-3}$</td>
<td>0.74</td>
<td>0.24</td>
</tr>
<tr>
<td>Roughness nm</td>
<td>0.9</td>
<td>1.0</td>
<td>5.8</td>
<td>1.8</td>
<td>16</td>
</tr>
<tr>
<td>TDD /cm$^2$</td>
<td>N/A</td>
<td>$8 \times 10^9$</td>
<td>$2.5 \times 10^8$</td>
<td>$5.5 \times 10^8$</td>
<td>$2.4 \times 10^7$</td>
</tr>
</tbody>
</table>
Scanning SHG microscope yields mottled SHG response from APD-laden surfaces

Lei et al., APL 102, 152103 (2013)

St. Dev. → of SHG intensity

GaAs/GaAs

0.027

10 µm

GaAs/Si(001)

0.35

10 µm

GaAs/Ge(001): 6°

0.037

GaAs/Ge(001)

0.26

10 µm

• The SHG images are NOT direct maps, but rather higher-order moments, of the APD distribution.

• Bright areas indicate dominance of one type of domain within the laser spot.

• Dark areas indicate equal areas of $+\chi^{(2)}$ and $-\chi^{(2)}$ domains within the laser spot.

• **SHG NSOM** may be able to image individual APDs directly.

Growth of GaAs on exactly oriented Si(001) is preferred for high-volume manufacturing.

Aspect-Ratio Trapping (ART) is an established technique for suppressing TDs on Si(001)

We found (serendipitously) that ART patterning of oriented Si(001) substrates also dramatically suppresses APDs in GaAs epi-films.

Nearly complete recovery of GaAs reference SHG signal!
GaAs pillars evidently coalesce commensurately into a single domain epi-layer.

ART appears to solve 2 problems simultaneously!
SUMMARY

- SHG characterizes APDs in polar-on-nonpolar semiconductor epi-films sensitively, quickly, non-invasively and selectively.

- Scanning SHG microscopy indirectly probes APD size distribution; SHG-NSOM promises direct APD imaging.

- SHG APD probe helps develop methods to suppress APDs: 
  - e.g. 1. vicinal substrates; 2. ART

- Compared to RAS, SHG is equally useful as an ex-situ & in-situ APB probe, requires only a single-\(\lambda\) source for any material system, and enables microscopic (possibly single APD) imaging.

Lei et al., Appl. Phys. Lett. 102, 152103 (2013)

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