Lattice-mismatched GaAsP Solar Cells Grown on Silicon by OMVPE


National Renewable Energy Laboratory

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Motivation

- Monolithic, two (or more) junction single crystal solar cell on Si
- Old idea (SERI 1980’s)

Advantages of silicon substrates:

- Excellent solar cell material
- Lower cost than III-V or Ge
- Mature Si technology
- Mechanically robust
- Two-junction cell using Si bottom junction is nearly optimal theoretical efficiency
  - 34% efficiency at 1 sun AM0
  - 44% efficiency at 500 sun AM1.5G
Challenges for III-V on Si growth

- Silicon oxides
- Surface contamination
- Antiphase domains
- Etching by sources
- Interdiffusion
- Lattice-mismatch
- Thermal expansion mismatch

New developments
- Improved characterization techniques
- Better understand for III-V nucleation
- Lattice-matched GaNPAs materials
P-on-N GaAsP Cell Structure

- III-V grown by OMVPE
- Smooth GaP nucleation on Si
- Step graded GaAsP buffer to reduce dislocations
- Constant lattice GaAsP junction with GaInP passivation

![Diagram of GaAsP cell structure with bandgap vs. lattice constant graph.](image-url)
GaP Nucleation on Si

- Antiphase domains during GaP nucleation revealed by AFM
- Growth of LM GaNP smoothes surface and reduces APD

5.7 nm GaP
RMS = 1.2 nm

17 nm GaP
33 nm GaNP
RMS = 1.9 nm

18 nm GaP
403 nm GaNP
RMS = 0.4 nm
Step graded buffer layer

- 0.25 or 0.5 μm \( \text{GaAs}_x \text{P}_{1-x} \) steps
- Composition change \( \Delta x = 0.07 \) per step
- 3.75 or 6.5 μm total buffer thickness
- Many dislocations in grade, but few in active layers

Cross-sectional TEM
Composition and Strain

- Grown under compression because growing epilayers have larger lattice constant
- Relaxes at $T_g$ above critical thickness
- Cools toward tension
- Residual compressive strain at $T_g$ results in less tension at RT (no cracks)

X-ray diffraction
224GI reflection RSM
Threading Dislocations

- Electron-Beam-Induced Current (EBIC)
- $9 \times 10^7 - 1 \times 10^8 \text{ cm}^{-2}$ threading dislocations

Plan-view EBIC
GaAsP/Si Device Performance

- Single-junction 8.7% efficiency AM1.5G w/o AR coat
- Increase $J_{sc}$ with lower $E_g$ (need about 20 mA/cm$^2$ for 2-junction current matching)
- Improve QE with better passivation, thinner window
Literature Comparison

GaAsP/GaAs $\sim 10^6$ cm$^{-2}$
Vernon, 19th PVSC, (1987), 108
Wanlass, 19th PVSC, (1987), 530

GaAs/SiGe/Si $\sim 10^6$ cm$^{-2}$
Ringel, Prog. PV 10, (2002), 417

GaAsP/Si (TCA)

AlGaAs/Si $\sim 10^7$ cm$^{-2}$

$V_{oc}$ is excellent measure of quality for mismatched solar cells

LM GaNP(As)/Si or GaP
Geisz, 31st PVSC, (2005), 695

GaNP(As)/Si or GaP

GaInP/GaAs

$V_{oc} = E_g/q - 0.4$

This work

GaAsP/Si (TCA)
Hayashi, 1st WCPEC, (1994), 1890

$V_{oc}$ is excellent measure of quality for mismatched solar cells.
Conclusions

- Lattice-mismatched GaAsP solar cells grown on Si
- Compositional step grade reduced dislocations to \( \sim 10^8 \text{ cm}^{-2} \)
- \( V_{oc} \) not ideal, but comparable to best III-V grown on Si with transparent buffer
- Diffusion lengths better than LM GaNP
- Want to reduce dislocations to \( 10^6 \text{ cm}^{-2} \)
Thermal Expansion

- Can measure strain at RT with XRD
- Would like to measure strain during growth
- Can calculate strain state at T_g assuming
  - change in in-plane lattice constant of epilayers constrained by thick Si
  - no relaxation upon cool-down
- Linear coefficients of thermal expansion (K^{-1})
  - Si: 3.7 \times 10^{-6}
  - GaP: 5.3 \times 10^{-6}
  - GaAs: 6.8 \times 10^{-6}
  - GaN: 6 \times 10^{-6} ?
  - InAs: 5.2 \times 10^{-6}
- Scales with T_g
- Biaxial strain energy
  \[ U = Y \varepsilon_x^2 t \]
Cracking from Tensile Strain on Si

Cross-sectional TEM

Optical Nomarski

Plan-view SEM

220DF

GaAs$_{0.63}$P$_{0.37}$

GaAs$_{0.7}$P$_{0.3}$

GaAsP step grade

GaN-P

Si

Charging effect reveals cracks
Si junction

- Under current growth conditions, more P than Ga diffusion into Si from GaP
- Creates n-type emitter in silicon
- Emitter passivation from GaP if no interface defects

- $V_{oc}$ of silicon junction $\sim 535$ mV
- Currently using CZ Si, but float-zone may be better
- BSF from annealed Al contact
GaNPAs/Si Tandem Solar Cell Results

- Working tandem
- Good current in Si junction, but Voc could be a little better
- GaNPAs delivers half the current necessary to current match tandem

Geisz et al., PVSC 31 (2005) 695
Step Grading for Mismatch on GaP

- Top layer strained to match next in-plane lattice constant (residual strain)
- Mostly relaxes while next layer growing

XRD Reciprocal Space Maps
Lattice-matched GaNP
### GaNPAs/Si Tandem Solar Cell Structure

<table>
<thead>
<tr>
<th>Layer Description</th>
<th>Thickness</th>
<th>Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5 μm n-type GaAs:Se</td>
<td>70 nm</td>
<td>Au grid</td>
</tr>
<tr>
<td>0.1 μm n-type GaN$<em>{0.02}$P$</em>{0.98}$:Se</td>
<td>0.1 μm</td>
<td>n-type GaNP$<em>{0.02}$As$</em>{0.98}$:Se</td>
</tr>
<tr>
<td>1.0 μm intrinsic undoped GaNPAs</td>
<td>1.0 μm</td>
<td>p-type GaNP$<em>{0.02}$As$</em>{0.98}$:Zn</td>
</tr>
<tr>
<td>0.2 μm p-type GaN$<em>{0.02}$P$</em>{0.98}$:Zn</td>
<td>0.2 μm</td>
<td>n-type GaNP$<em>{0.02}$As$</em>{0.98}$:Se</td>
</tr>
<tr>
<td>0.5 μm GaN$<em>{0.02}$P$</em>{0.98}$:Se buffer layer</td>
<td>0.5 μm</td>
<td>GaNP$<em>{0.02}$As$</em>{0.98}$:Se</td>
</tr>
<tr>
<td>40 nm GaP nucleation layer</td>
<td>40 nm</td>
<td>GaNP$<em>{0.02}$As$</em>{0.98}$:Se</td>
</tr>
<tr>
<td>diffused n-type Si emitter</td>
<td></td>
<td>Si emitter</td>
</tr>
<tr>
<td>p-type Si:B substrate</td>
<td></td>
<td>Si:B substrate</td>
</tr>
<tr>
<td>diffused Si:Al back-surface-field</td>
<td></td>
<td>Si:Al back-surface-field</td>
</tr>
<tr>
<td>Al metal contact</td>
<td></td>
<td>Si substrate</td>
</tr>
</tbody>
</table>

**Diagram:**
- **Top Cell:**
  - n-i-p top cell
  - tunnel junction
  - silicon bottom cell
- **Bottom Cell:**
  - p-type Si:B substrate
  - diffused Si:Al back-surface-field

**Materials:**
- Au
- GaNP$_{0.02}$As$_{0.98}$:Se
- GaNP$_{0.02}$As$_{0.98}$:Zn
- GaNP$_{0.02}$As$_{0.98}$:Se
- GaNP$_{0.02}$As$_{0.98}$:Se buffer layer
- GaP
- Si substrate

**Notations:**
- 220DF
- 5 μm
GaAsP/Si Device Performance

- Single-junction 8.7% efficiency AM1.5G w/o AR coat
- Increase $J_{sc}$ by lower $E_g$ (need about 20 mA/cm$^2$ for 2-junction)
- Improved QE with wide depletion region, but decent with thinner depletion region
- GaAsP/Si better than GaNPAs/GaP
  - Longer diffusion length even with $10^8$ cm$^{-2}$ TD