Pyroelectric and Piezoelectric Properties of GaN-based Materials and Devices
Outline

Pyroelectric effect and pyroelectric sensors
Piezoelectric properties and piezoelectric sensors
Polarization doping in GaN-based heterostructures
Strain energy band engineering
Conclusions
It is complex!

“The Universe is full of magical things patiently waiting for our wits to grow sharper”

Eden Phillpotts
Zinc blende structure
No PE or SP effect in <100> direction
PE coefficient <111> ~0.15 C/m²
No PE/SP ‘doping’ reported

• Wurtzite structure
• c-axis growth direction
• PE coefficient in c-direction ~1 C/m²
• PE/SP ‘doping’ demonstrated
Ga and N faces

Polarization sign


SDM-2, ©Michael Shur 1999-2009
Spontaneous polarization

<table>
<thead>
<tr>
<th>Material</th>
<th>AlN</th>
<th>GaN</th>
<th>InN</th>
<th>ZnO</th>
<th>BeO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spontaneous polarization (C/m²)</td>
<td>-0.081</td>
<td>-0.029</td>
<td>-0.032</td>
<td>-0.057</td>
<td>-0.045</td>
</tr>
</tbody>
</table>

For comparison, in BaTiO₃, $P_s = 0.25$ C/m²
Equivalent circuit of pyroelectric sensor

Pyroelectric material $I_p$
Primary and secondary pyroelectric effects


Fast heat transfer

Slow heat transfer
Pyroelectric voltage for primary pyroelectric effect (changing flux magnitude)

From A. D. Bykhovski, V. V. Kaminski, M. S. Shur, Q. C. Chen, and M. A. Khan
Pyroelectric voltage for primary pyroelectric effect (changing flux magnitude and direction)


Heat Flux Counter!
Two time constants for primary pyroelectric effect

\( \tau_T \) reflects the rate of the sample cooling due to free convection

\( \tau_s \) reflects the pyroelectric charge relaxation.

Primary pyroelectric effect at 300 °C
(High Temperature Operation!)

Constant temperature of “cold” contact (94 °C) is shown by dotted line.
Pyroelectric coefficients

From M. S. Shur, A. D. Bykhovski, R. Gaska, and M. A. Khan, GaN-based Pyroelectronics and Piezoelectronics, to be published.
Curie temperature

Piezoelectric Properties of GaN

![Graph showing ionicity vs. $e_{14}$ (C/m$^2$)]

- GaN
- ZnSe
- ZnTe
- CdTe
- InP
- InSb
- AlSb
- InAs
- GaSb
- GaAs
- AlAs

$e_{14}$ (C/m$^2$)

Ionicity
# Piezoelectric constants

<table>
<thead>
<tr>
<th>Material</th>
<th>$\varepsilon_{33}$</th>
<th>$\varepsilon_{31}$</th>
<th>$\varepsilon_{15}$</th>
<th>$\varepsilon_{14}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN (electromechanical coefficients)</td>
<td>1</td>
<td>-0.36</td>
<td>-0.3</td>
<td></td>
</tr>
<tr>
<td>GaN (mobility)</td>
<td>0.44</td>
<td>-0.22</td>
<td>-0.22</td>
<td>0.375</td>
</tr>
<tr>
<td>GaN (from optical phonons)</td>
<td>0.65</td>
<td>-0.33</td>
<td>-0.33</td>
<td>0.56</td>
</tr>
<tr>
<td>GaN (ab initio)</td>
<td>0.73</td>
<td>-0.49</td>
<td></td>
<td></td>
</tr>
<tr>
<td>InN (from optical phonons)</td>
<td>0.43</td>
<td>-0.22</td>
<td>-0.22</td>
<td>0.37</td>
</tr>
<tr>
<td>InN (ab initio)</td>
<td>0.97</td>
<td>-0.57</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AlN (surface acoustic waves)</td>
<td>1.55</td>
<td>-0.58</td>
<td>-0.48</td>
<td></td>
</tr>
<tr>
<td>AlN (ab initio)</td>
<td>1.46</td>
<td>-0.60</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SiC</td>
<td>0.2</td>
<td></td>
<td>0.08</td>
<td></td>
</tr>
<tr>
<td>ZnO</td>
<td>1.32</td>
<td>-0.57</td>
<td>-0.48</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>-0.185</td>
<td>0.093</td>
<td>0.093</td>
<td>-0.16</td>
</tr>
</tbody>
</table>

How Piezoelectric constants are determined?

Electromechanical coefficients (difficult)
Optical experiments (indirect)
Estimate from transport measurements (very indirect)
Strain from the lattice mismatch

\[ u_{xx} = \frac{a_{\text{GaN}} - a_{\text{AlGaN}}}{a_{\text{GaN}}} \]

Strain with metal - to be analyzed?

Thermal expansion - important for sapphire substrate, relatively unimportant for AlGaN/GaN interfaces

\[ P_{pe} = 2 \, u_{xx} \, (e_{31} - e_{33} \, \frac{C_{13}}{C_{33}}) \]
Effect of Strain on Dislocation-Free Growth

Critical thickness as a function of Al mole fraction in $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$: superlattice (solid line), SIS structure (dashed line).

From A. D. Bykhovski, B. L. Gelmont, and M. S. Shur, J. Appl. Phys. 81 (9), 6332-6338 (1997)

Can it be exceeded?
Effect of Critical Thickness on Electron Mobility

- High Al- Heterostructures
- Origin of Doping?

<table>
<thead>
<tr>
<th>AlGaN Thickness (A)</th>
<th>Hall Mobility (cm²/Vs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al₀.₂₅Ga₀.₇₅N</td>
<td></td>
</tr>
<tr>
<td>i-GaN</td>
<td></td>
</tr>
<tr>
<td>AlN</td>
<td></td>
</tr>
<tr>
<td>SiC</td>
<td></td>
</tr>
</tbody>
</table>

Critical Thickness $d_{cr} \sim 30$ nm
Model Assumptions

Isotropic approximation
Averaged (over the layers) elastic constants
Ideal crystal (except, of course, for misfit dislocations)
The critical thickness is found by minimizing the deformation energy with respect to the misfit dislocation density
Piezoelectric sensors
Pyroelectric sensors

After R. Gaska, J. Yang, A. D. Bykhovski, M. S. Shur, V. V. Kaminski, S. M. Soloviev,
SIS structure and Band Diagram

<table>
<thead>
<tr>
<th>Top Contact</th>
<th>Bottom Contact</th>
</tr>
</thead>
<tbody>
<tr>
<td>n - GaN 0.4 μm</td>
<td>Sapphire</td>
</tr>
<tr>
<td>AlN 30 Å - 100 Å</td>
<td></td>
</tr>
<tr>
<td>n - GaN 1.0 μm</td>
<td></td>
</tr>
<tr>
<td>i - GaN 1.0 μm</td>
<td></td>
</tr>
<tr>
<td>AlN Buffer</td>
<td></td>
</tr>
</tbody>
</table>

SIS capacitance

Resistance of SIS structure with 50 nm top GaN layer versus compressive strain.

Twice as large as in SiC

Short range superlattice is four times larger than in SiC


SDM-2, ©Michael Shur 1999-2009
Possible domain structure

Fig. 1 Epilayer design of \([\text{AlN}_m-\text{GaN}_n]_p\) SRSLS structure. The constant current was maintained by ohmic contacts 1, 4, and sample resistance was estimated by measuring voltage drop between contacts 2 and 3. Arrows show the directions of the strain component, \(u_{xx}\).
Superlattice Band Diagram

Fig. 2 Relative change in resistance under applied strain. (o) - correspond to $[(\text{AlN})_6-(\text{GaN})_3]_{150}$ SRSL; ($\Delta$) - $[(\text{AlN})_3-(\text{GaN})_8]_{150}$ SRSL; solid line 1 shows dependence measured for GaN-AlN-GaN SIS $^1$; dashed line 2 - SiC $p$-$n$ junction $^1$; 3 - GaAs $^2$. The GF for the measured samples was in the 30 to 90 range. The larger GF (higher sensitivity to strain) was measured in SRSLs with higher Al content.

Gauge factors for $[(\text{AlN})_m-(\text{GaN})_n]_p$ SRSL structures and different biases. (o) and line 1 correspond to $[(\text{AlN})_6-(\text{GaN})_3]_{150}$ SRSL; (Δ) and line 2 - $[(\text{AlN})_3-(\text{GaN})_8]_{150}$ SRSL. At each voltage, a number of measurements were taken for different strains in $0.5 \times 10^{-4} - 2.4 \times 10^{-4}$ range.
Static Gauge factors (GF)
(measured under longitudinal mechanical deformation)

<table>
<thead>
<tr>
<th>Material</th>
<th>GF</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN n-type</td>
<td>10</td>
</tr>
<tr>
<td>GaN p-type</td>
<td>&gt;200</td>
</tr>
<tr>
<td>GaN/AlN/GaN Sapphire</td>
<td>50</td>
</tr>
<tr>
<td>AlGaN/GaN Heterostructures</td>
<td>10-15</td>
</tr>
<tr>
<td>AlN/GaN Short Range Superlattices</td>
<td>30-80</td>
</tr>
</tbody>
</table>

**High Temperature p-GaN Pressure Sensor**
Piezoelectric effect in doped and undoped channel GaN/AlGaN HFETs

Up to $4 \times 10^{13}$ cm$^{-2}$ in GaN versus $2 \times 10^{12}$ cm$^{-2}$ in GaAs

Piezoelectric effect (opposite polarity)

C-V of AlGaN/GaN heterostructures show the presence of residual strain.

Piezoelectric and Pyroelectric Doping in AlGaN/GaN

State-of-the-art
Maximum Electron Sheet Density
Electronic island at the surface of semiconductor grain in pyroelectric matrix (MQDs - Moveable Quantum Dots)

Inversion electron and hole islands at the surface of pyroelectric grain in semiconductor matrix

Control by external field - Zero dimensional Field Effect (ZFE)

After V. Kachorovskiy and M. S. Shur, APL, March 29 (2004)
TERAHERTZ OSCILLATIONS

2D island might oscillate as a whole over grain surface. The oscillations can be exited by AC field perpendicular to \( P_0 \).

\[
\omega_0 = \sqrt{\frac{4\pi eP_0}{(\varepsilon + 2\varepsilon_p) mR}}
\]

**MOVABLE QUANTUM DOTS (MQD)**

Oscillation frequency is of the order of a terahertz:

\[
\omega_0 \pi/2 \sim 1 \text{ THz} \text{ to } 30 \text{ THz}
\]

**CAN SWITCH OR SHIFT FREQUENCY BY EXTERNAL FIELD OR BY LIGHT**

After V. Kachorovskiy and M. S. Shur, APL, March 29 (2004)
Key references


Piezoelectric constants and spontaneous polarization in III-N ab-initio—F. Bernardini and V. Fiorentini, Phys. Rev. B 56(16), 10024 (1997);


Conclusions

• Pyroelectric properties of GaN are comparable to those of the pyroelectric ceramics such as PZT or BaTiO$_3$.
• Both primary and secondary pyroelectric effects have been observed in GaN based structures.
• Piezoresistive effect in GaN/AlN multilayer structures up to 4 times larger than in SiC.
• Role of spontaneous polarization, the role of surface and interface states, and of the inversion domains must be ascertained.
• Polarization doping plays dominant role in AlGaInN/GaN HEMTs.