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Electrical and Computer Engineering

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**Wide Band Gap III-Nitride**

**Compound Semiconductor Devices:**

**The Universal Solution for Energy Applications**

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**ECE and**

**Energy Production Infrastructure Center**



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# EPIC and CRI





# Typical EPIC floor plan



# Solar Decathlon House UNCC



<http://www.youtube.com/watch?v=j1H6ojXcitY>



# Solar Decathlon House GaTech



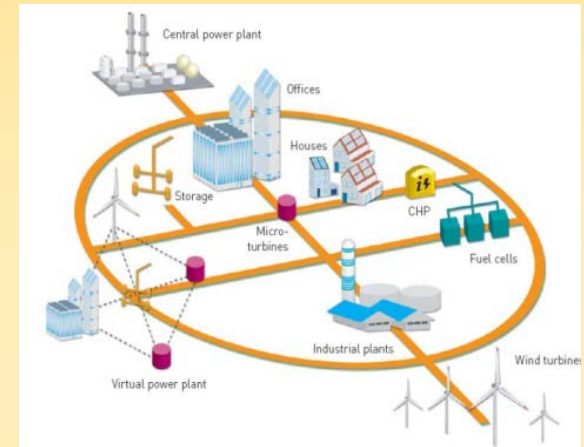
# EPIC Education Focus

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- Undergraduate Education
  - Energy Concentrations within ME, ECE, CE and ET
  - “Introduction to Energy” for all Engineering students
  - Expand Co-op and Internship program
  - Undergraduate Research Assistance
  - Student participation in Leadership Academy
  - Senior Design Project – Energy related
- Graduate Education in Development
  - MBA with Energy concentration
  - Energy certifications in all disciplines – retraining
  - Certifications – Energy Efficiency, Nuclear, Smart Grid, etc.
  - Energy Certification for Non-engineers
  - Graduate Research Assistance
  - Accredited short courses – PE through MS
- Coordination with Regional Universities
  - Concentrations and MS programs

# EPIC Applied Research Clusters (1)

- *Power Systems Modernization*
  - Duke Energy Smart Grid Laboratory with RTDS and system analysis – NSF MRI
  - Distribution Automation and Micro-grids
  - Electric Vehicle and Energy Storage Integration
- *Large Energy Component Design and Manufacturing*
  - Siemens Large-scale Manufacturing Laboratory
  - Materials Characterization Laboratory (MCL)
  - Robotics and Welding Technologies
- *Power Infrastructure & Environmental Development*
  - Large-structures laboratory and T&D designs
  - Utilization and recycling of spent fuels and emission controls
- *Renewables and Energy Efficiency*
  - Clean-room with PV cell and LED research
  - Off-shore wind, biomass and small-scale hydro technologies
  - Integration of renewables and energy efficiency measures
- *Energy Markets and Systems Engineering*
  - Quality Assurance, Nuclear Safety, Regulatory and Standards
  - Distributed energy markets
  - Improved supply chain utilization

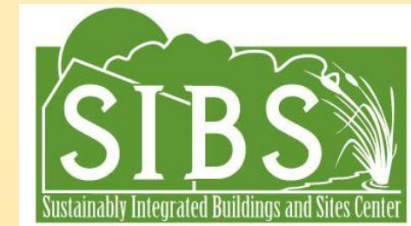




# EPIC Applied Research Clusters (2)

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- The Infrastructure, Design, Environment and Sustainability Center (*IDEAS*)  
[ideas.uncc.edu](http://ideas.uncc.edu)
  - Development and utilization of biofuels
  - Natural and Built Site Design and Analysis (Green Buildings)
  - Materials Characterization Laboratory (MCL)
  - Environmental impact analysis
  - Environmental Assistance Office for Small Business (EAO)
- *Sustainable Integrated Buildings and Sites* ([SIBS](#))
  - I/UCRC NSF Center with industry related research
  - PV integration in dense urban settings with limited roof space poor orientation, insurance issues, etc.
  - Optical collectors to guide light into PV building
  - Energy modeling for DSM, energy storage, and renewables
  - Thermal-energy storage for peak-shaving
  - Thermal storage technologies



# Founding Industrial Partners in EPIC

## Board Members from Representative Organizations:

- Duke Energy
- Siemens
- Westinghouse
- AREVA
- URS Corp
- Shaw Group
- Electric Power Research Institute (EPRI)
- Tessera
- Steag Energy Services

The Siemens logo, featuring the word "SIEMENS" in a bold, blue, sans-serif font.The Duke Energy logo, consisting of a red stylized flame icon to the left of the words "Duke Energy" in a bold, black, sans-serif font.The Westinghouse logo, featuring a circular icon with a crown-like symbol inside, followed by the word "Westinghouse" in a black, sans-serif font.The Areva logo, featuring a large, red, stylized letter "A" above the word "AREVA" in a red, sans-serif font.The Shaw logo, featuring a white triangle with a smaller triangle inside, set against an orange square background, with the word "Shaw" in white below it.The URS logo, featuring the letters "URS" in a bold, blue, sans-serif font.The EPRI logo, featuring the letters "EPRI" in a blue, sans-serif font.The Tessera logo, featuring the word "TESSERA" in a blue, sans-serif font, followed by a small graphic of a cluster of blue and white dots.The Steag logo, featuring the word "steag" in a blue, sans-serif font, with a horizontal line underneath.

# Aba Ebong - EPIC Professor

## Photovoltaic Research Laboratory (PVRL)



### Vision Statement

Establish a world class research and education program at UNC Charlotte to attract young and talented minds in Science and Engineering to give USA a competitive advantage in the field of Photovoltaic Science, Engineering and Technology

#### Milestones:

- Conduct high quality research in Renewable Energy to foster fundamental understanding of the science and technology of photovoltaic cells, modules, systems, integration and distribution.
  - Train undergraduate and graduate students
- Establish collaborative research with the industry to develop new materials for photovoltaic devices and serve as an R&D arm of the Photovoltaic industry
- Establish collaborative research with other universities within NC, USA and internationally.
- Establish certificate courses in Renewable Energy to position UNC Charlotte at the fore front in the field.
- Serve as a training center to provide experience for engineers and scientists.

#### Area of expertise:

- Silicon solar cell – Design, modeling, analysis, fabrication and characterization.
- III-V Light Emitting Diodes – Design, modeling, fabrication and characterization

#### Research Highlight:

- Cost effective and high efficiency solar cells through advanced structures, processes, understanding and reducing the parasitic losses.
- Understanding and improving every layer of a solar cell through optical, electrical, thermal and mechanical characterization of a solar cell
- Development of new and low-cost dielectrics for effective passivation of solar cells
- Development of novel contacting schemes including ink jet printing and light induced plating of Ni/Cu and Ag dip for crystalline silicon solar cell
  - Development and optimization of inline process for <50 μm thick silicon application
- Investigate the microstructures of Ag and Al metal pastes and the liquid phase sintering thereof
  - New module concepts and materials thereof
    - Systems integration and connectors

### Previous industry collaboration and funding:

| Company name             | Period    | Amount    |
|--------------------------|-----------|-----------|
| Heraeus Inc.             | 2006-2009 | \$609,000 |
| Dupont Electronics       | 2010-2011 | \$200,000 |
| Dow Advanced Electronics | 2008-2009 | \$125,000 |
| Konca Solar              | 2010-2011 | \$100,000 |
| Despatch Solar           | 2009-2011 | \$200,000 |
| TP Solar                 | 2009-2011 | \$60,000  |
| Wuxi Calex               | 2010-2011 | \$180,000 |
| BASF                     | 2006-2011 | \$510,000 |
| Air Product              | 2009-2011 | \$180,000 |
| Five Star Technologies   | 2008-2010 | \$260,000 |
| Varian Semiconductors    | 2009-2010 | \$100,000 |

**Number of graduate students envisaged: 10**

**Number of postdocs: 4**

**Expected Funds:** Industry to start and then DOE and NSF

#### Associated Publications

- A. Ebong et. al “On the ink jetting of full front Ag gridlines for cost effective metallization of Si Solar Cells,” IEEE Electron Device Letters, vol. 33, no. 5, 637-639, 2012.
- A. Ebong et al “Capitalizing on the glass etching effect of silver plating chemistry to contact silicon solar cells with homogeneous 100-110 ohm/sq emitters” IEEE Electron Device Letters, vol. 32, no. 6, 779-781, 2011.
- A. Ebong et al “Overcoming the technological challenges of contacting homogeneous high sheet resistance emitters (HHSE)” Proceedings 26th European PVSEC, Hamburg-Germany, September 5th-9th 2011.
- A. Ebong et al ““Impact of surface cleaning on random texturing of crystalline silicon wafers” Proceedings 26th European PVSEC, Hamburg-Germany, September 5th-9th 2011.
- A. Ebong et al ““Implementing narrow front silver gridlines through ink jet machine for high quality contacts to silicon solar cells” Proceedings 37th IEEE PVSC, Seattle, June 2011.



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# Aba Ebong - EPIC Professor

## Photovoltaic Research Laboratory (PVRL)

### Laboratory space required

**4100 ft<sup>2</sup>**

### Equipment needed



Wet bench for wafer clean & texturing



Inline Diffusion furnace for B & P diffusion



Tube Diffusion & PECVD furnace for p-n junction formation & AR coating



Inline Oxidation furnace for passivating oxide growth



Inkjet printer for Ag front contacts



Screen-printer for Ag front contacts



Belt line contact firing for contacts sintering



Plating station for Ni/Cu & Ag LIP



Solar cell simulator for measuring solar cell efficiency

Expected funding per year: \$200K (Estimate)

Funding source: Industry, DOE and NSF

### Equipment in storage awaiting installation



TP Solar donated Contact firing furnace

Tube Diffusion & PECVD furnace for p-n junction formation & AR coating

TP Solar donated Dryer

TP Solar donated inline diffusion furnace for p-n junction formation

Start up funds: \$400K from EPIC  
 Donation through equipment: \$1,050K for equipment received in storage.

Equipment donation pending: \$600K

Installation cost: \$400K (Estimate)

Annual running cost: \$50K (funds from sponsored projects)



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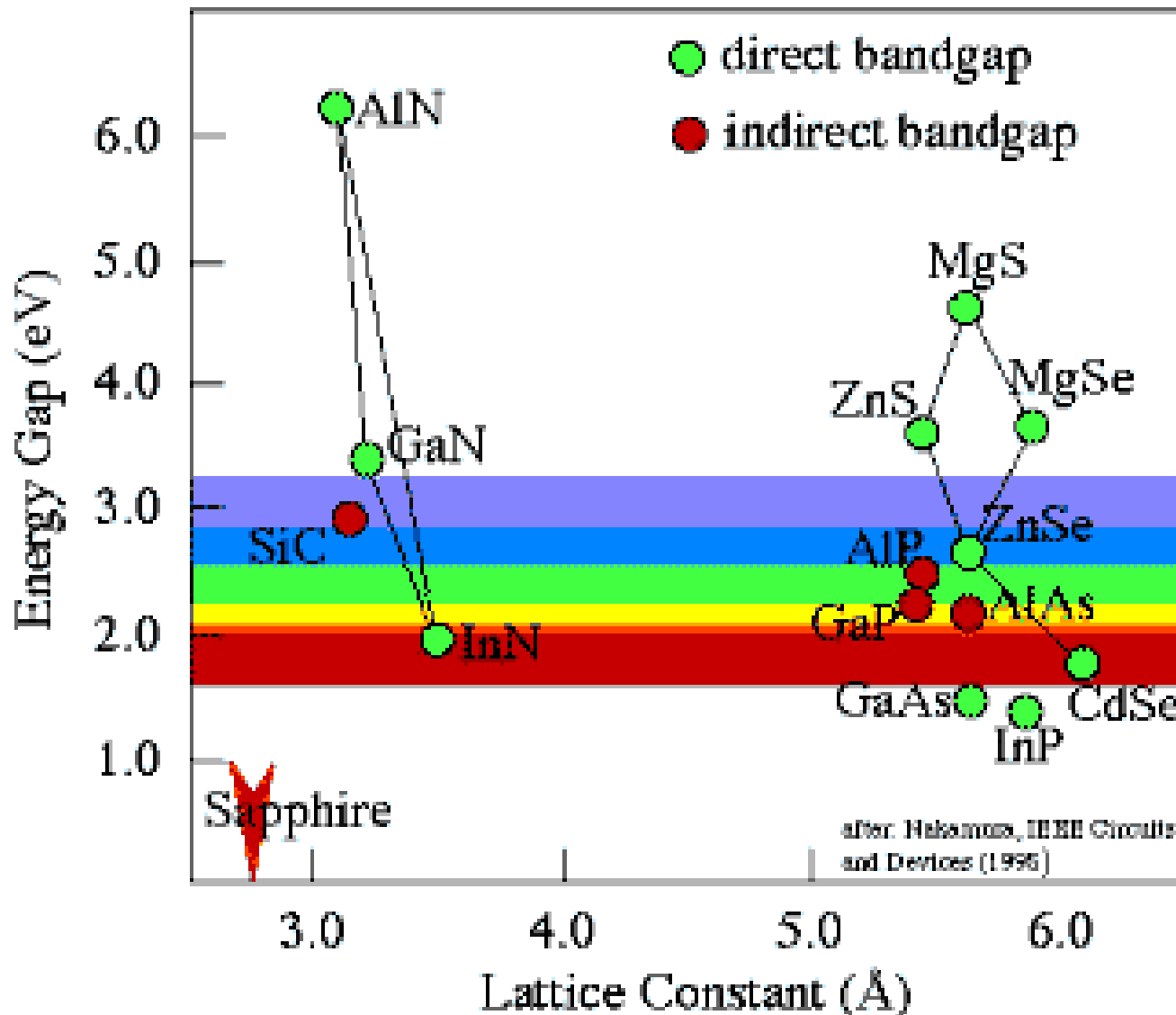
**Anything you can do GaN can do better...**



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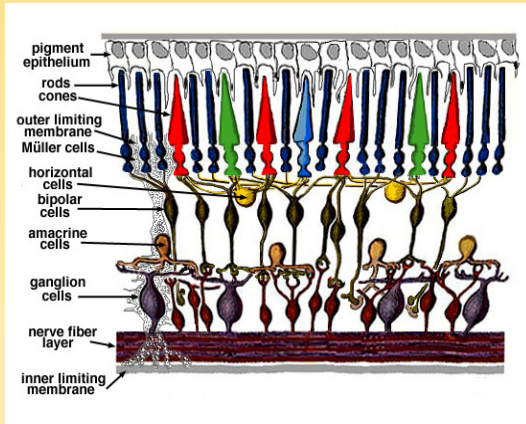
Electrical and Computer Engineering

# Lattice Constant vs Bandgap

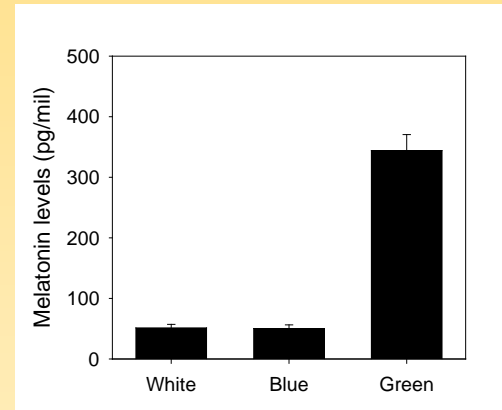




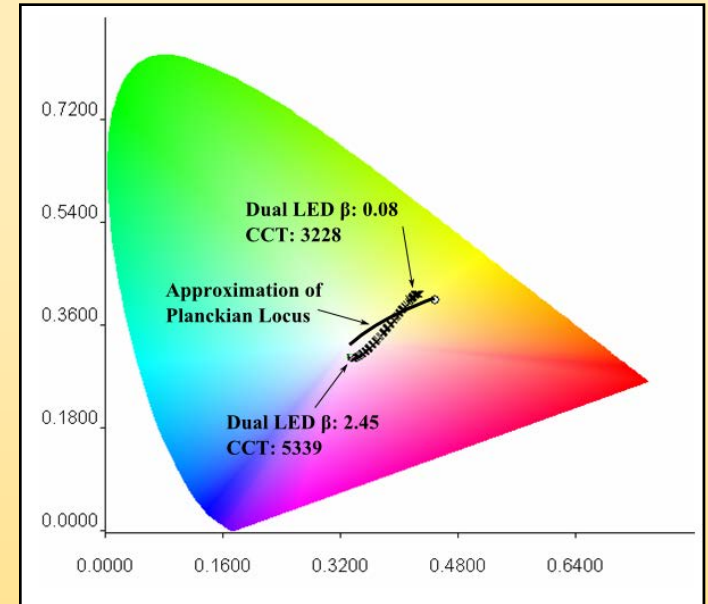
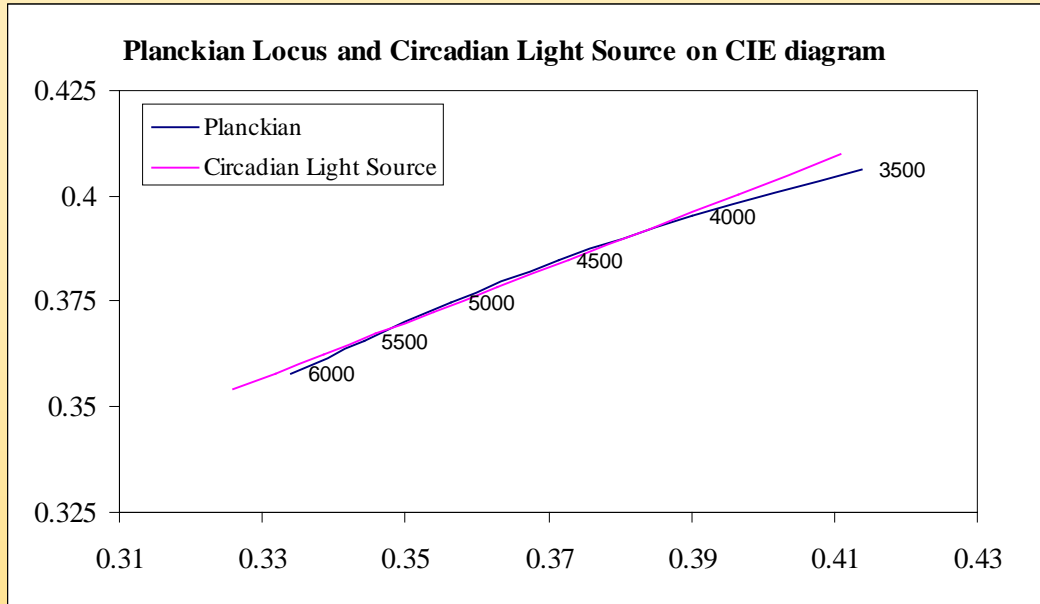
# New Approaches to Solid State Lighting: A Diurnal Light Source



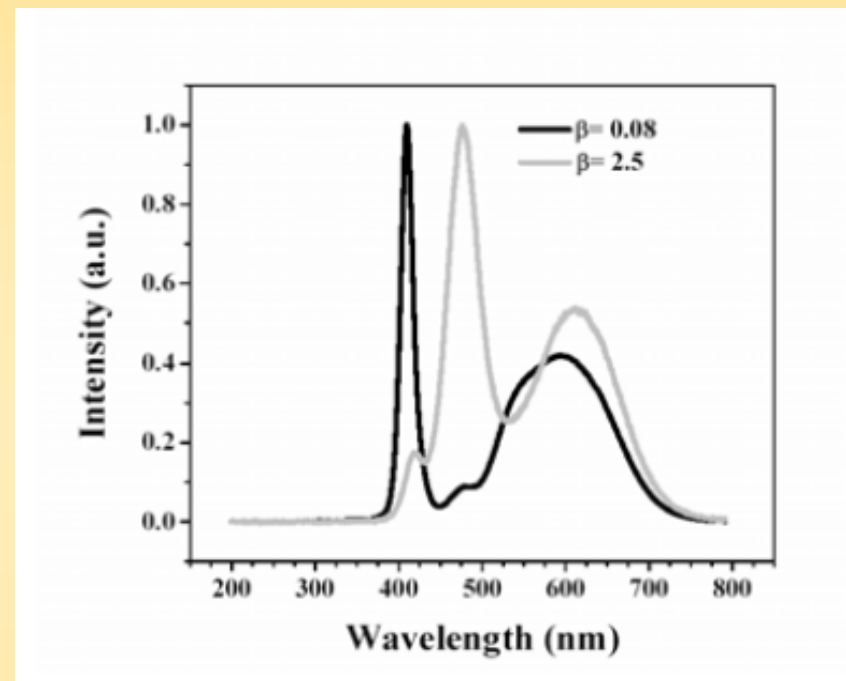
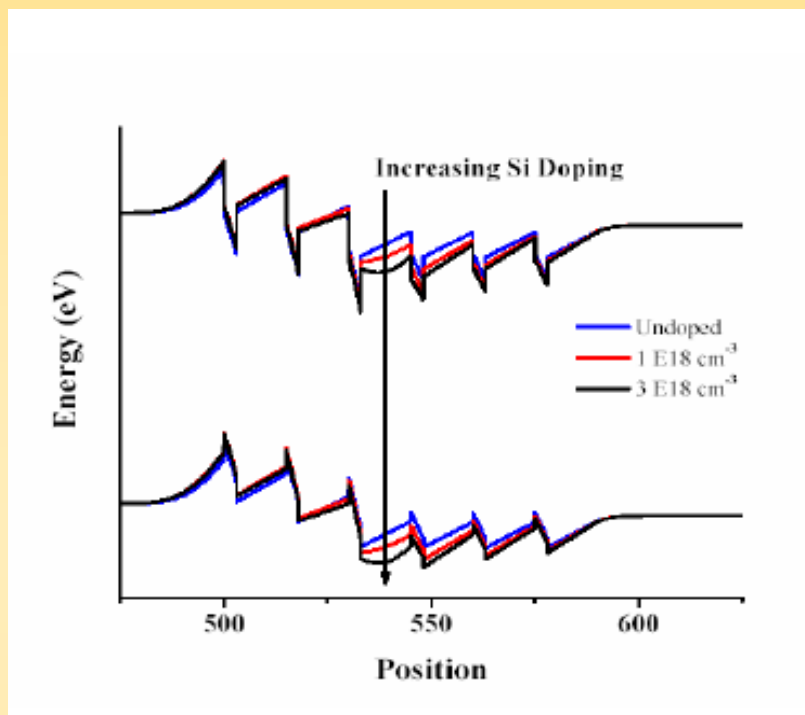
Melatonin response peaks around 464 nm



Visual Acuity → Psychological → Physiological



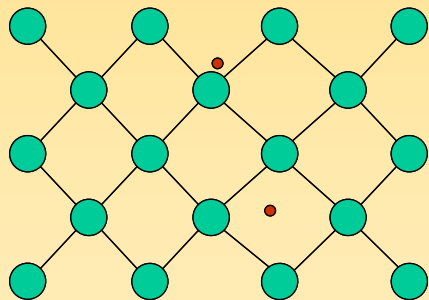
# Optimizing the dual emitter



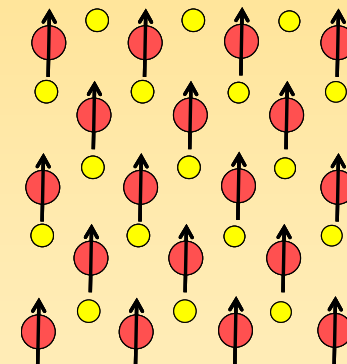
| Sample) | Doping ( $cm^{-3}$ ) | Min $\beta$ | Max $\beta$ | $\beta=1$            |
|---------|----------------------|-------------|-------------|----------------------|
| A       | None                 | 0.89        | 1.47        | $4 \frac{A}{cm^2}$   |
| B       | $1.5 \times 10^{18}$ | 0.08        | 2.5         | $220 \frac{A}{cm^2}$ |
| C       | $3 \times 10^{18}$   | 0.08        | 1.1         | $305 \frac{A}{cm^2}$ |

# New materials for semiconductor spintronics

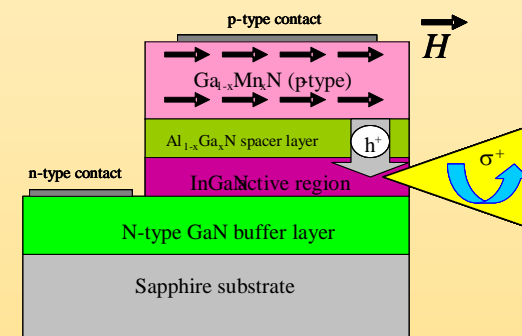
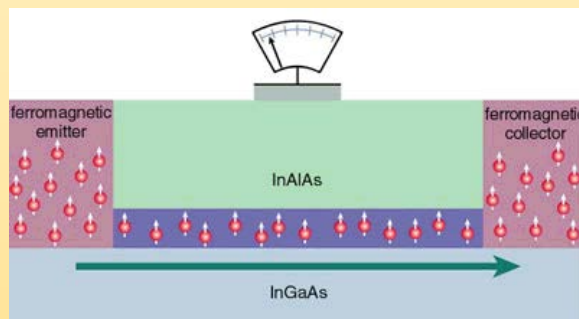
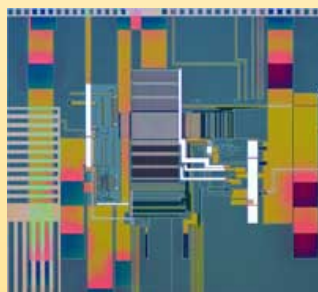
Semiconductor



Ferromagnet



Dilute Magnetic Semiconductors



Nonvolatile memory

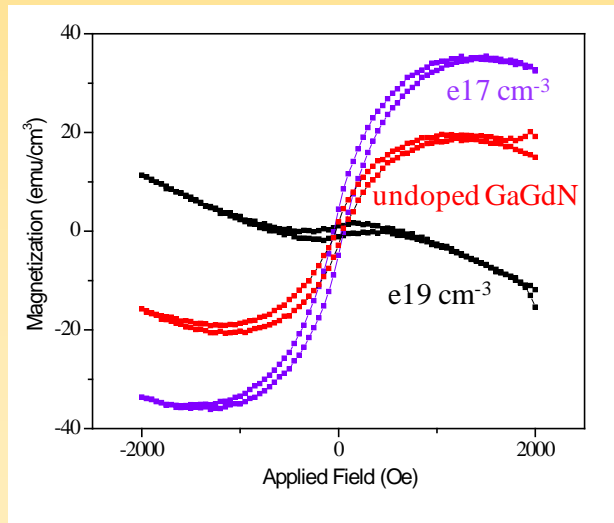
Spin-based logic and computation

Spin emitters

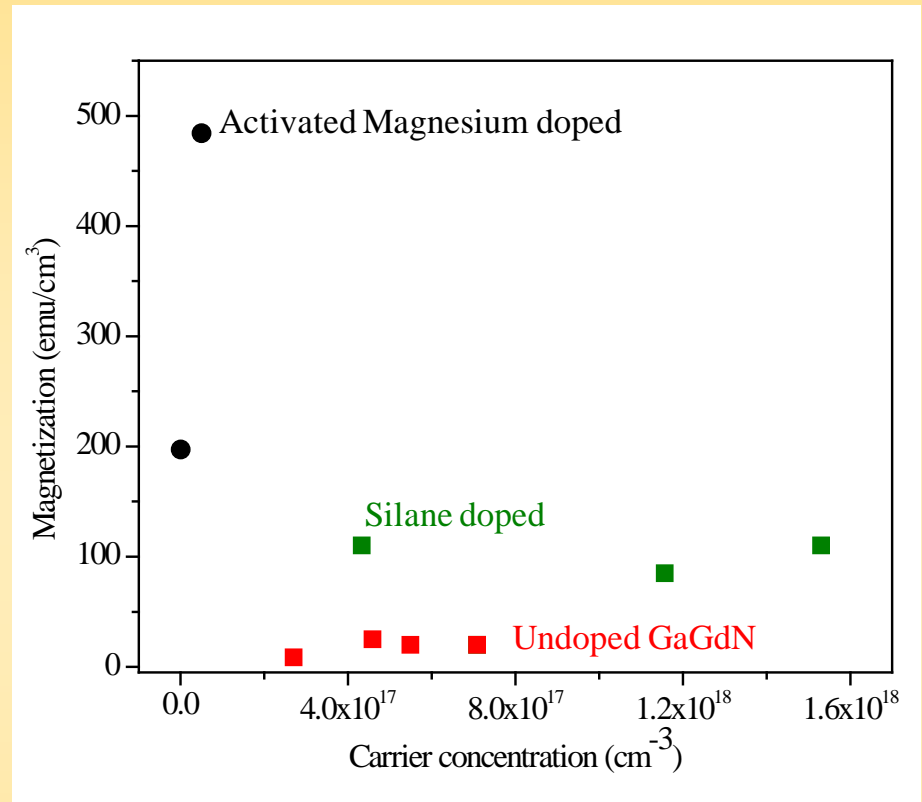
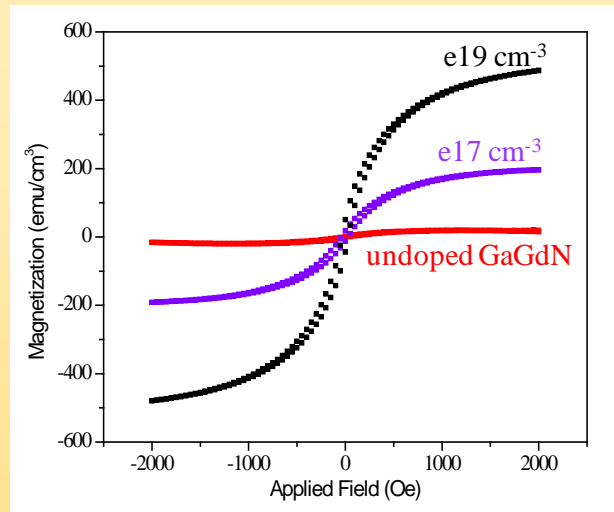


# Effect of doping on $\text{Ga}_{1-x}\text{Gd}_x\text{N}$

*p-Unactivated*



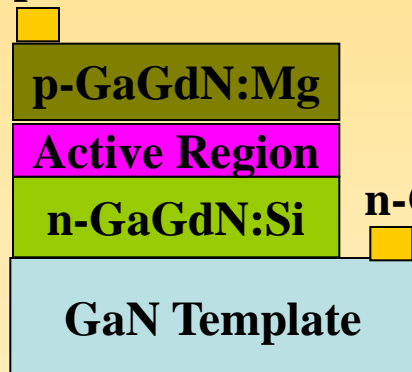
*p-activated*



Activated p-doped  $\text{Ga}_{1-x}\text{Gd}_x\text{N}$   
results in a large magnetic moment

# Spin-polarized LED emission

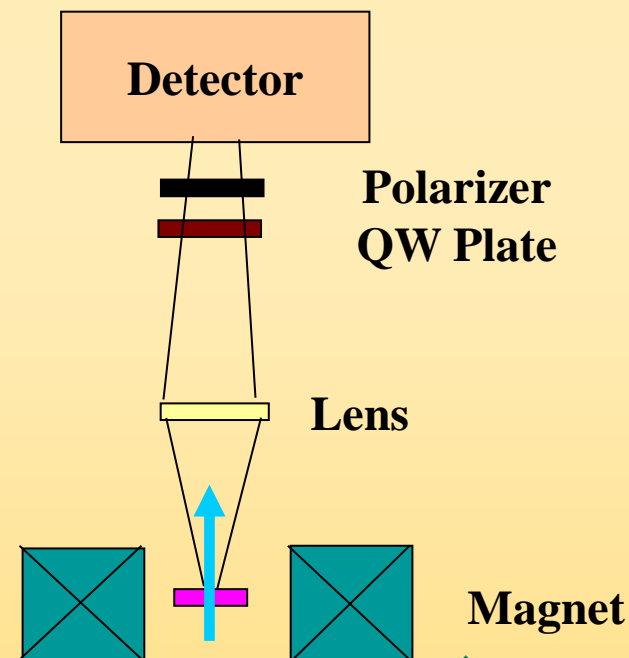
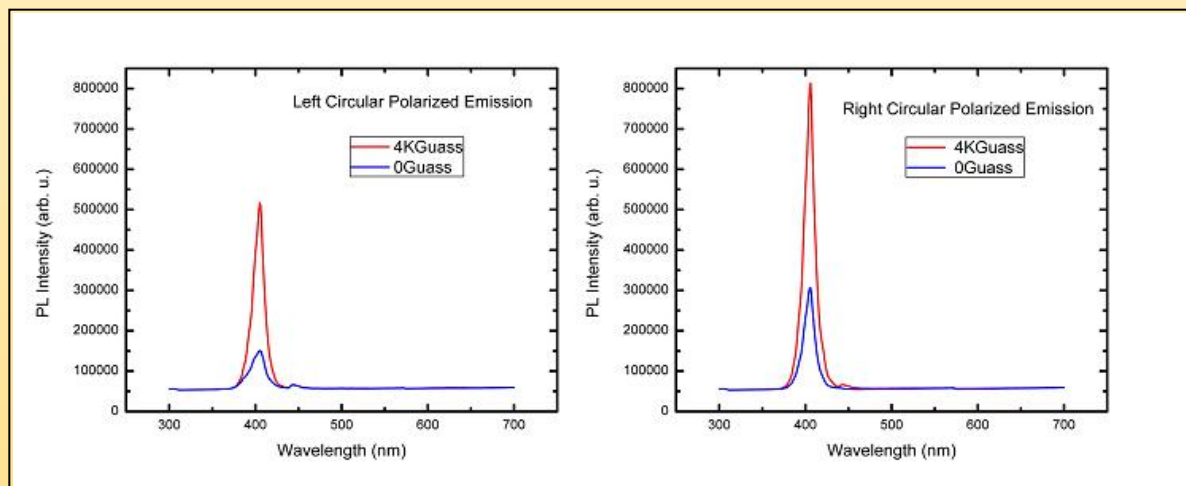
p-Contact



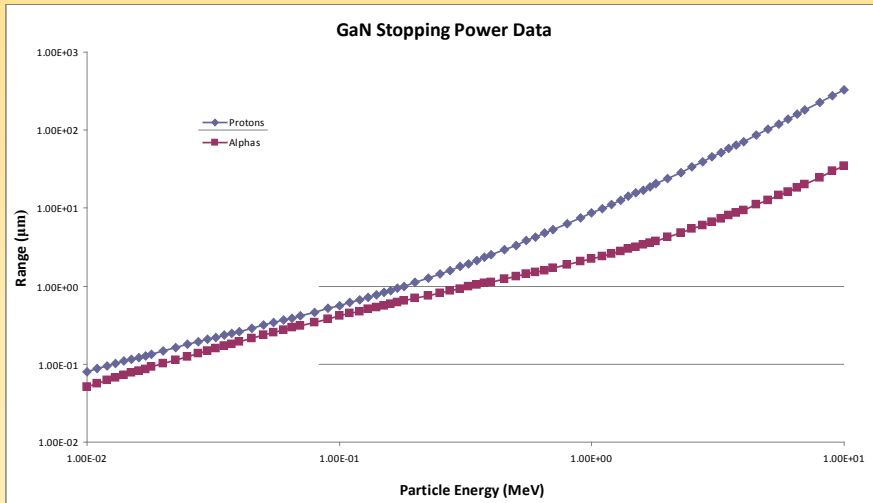
Spin LED Structure

- First MOCVD Gd doped GaN thin film report
  - Increase conductivity with Gd doping
- Both n- and p-type films grown on GaN template
- p-n diode and LED structures with Gd doped GaN
  - Spin-polarized LED fabricated – Under test

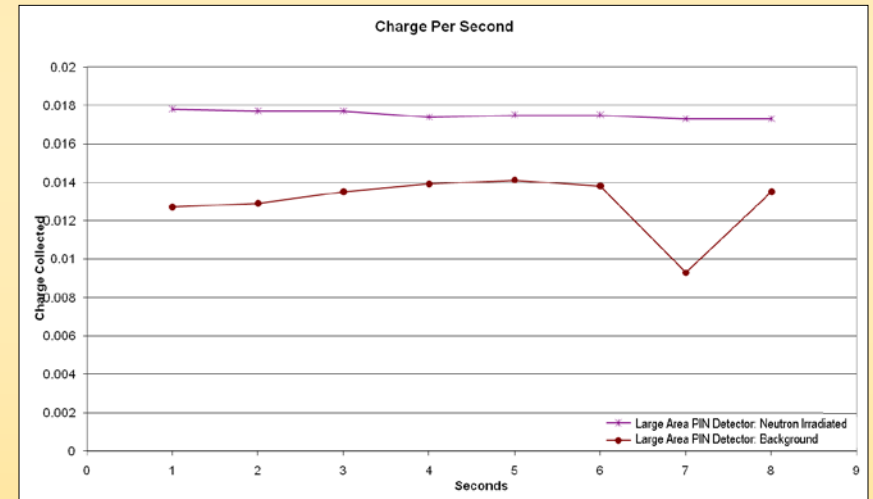
$$P = (\sigma^- - \sigma^+) / (\sigma^- + \sigma^+) = 0.34 (0G) \\ = 0.22(4kG)$$



# III-Nitrides for Neutron Detection

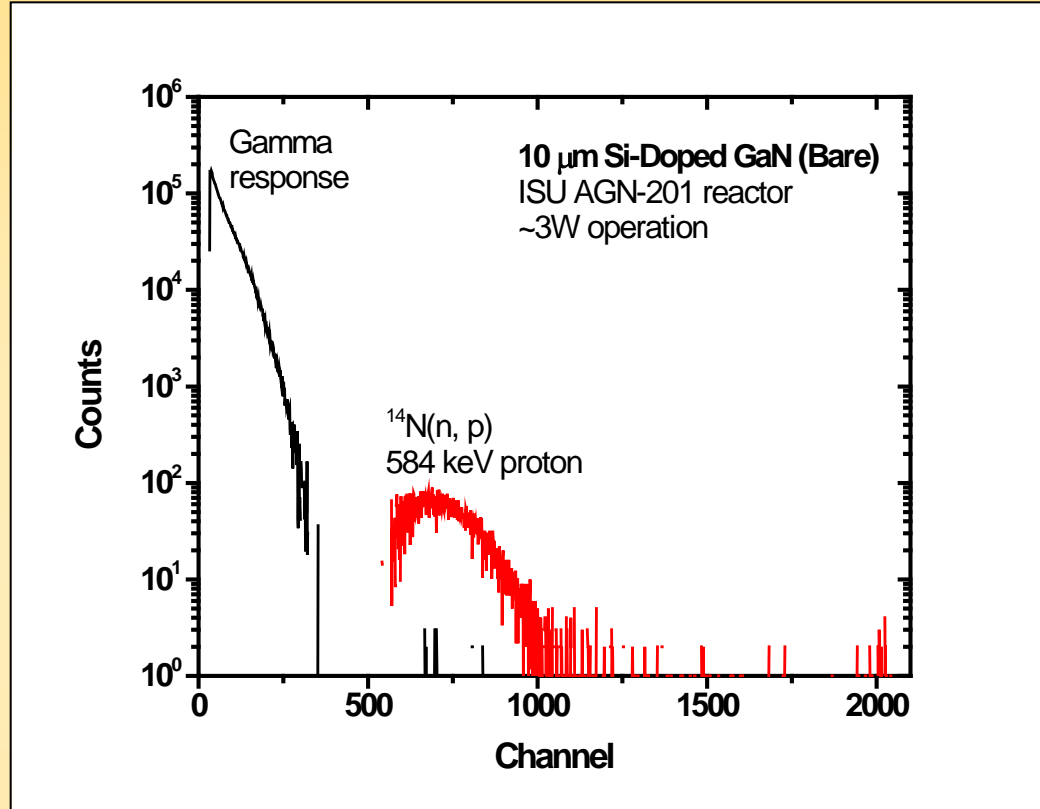


| Reaction  | Deposited Energy (MeV) | Range of Proton (µm) | Range of Alpha (µm) |
|-----------|------------------------|----------------------|---------------------|
| 10B@ 5MeV | 2.8                    | -                    | 13.6                |
| 14N@ 2.65 | 2.626                  | 36.1                 | -                   |



**Clear trend in increased collected charge is indicator of (n,p) events**

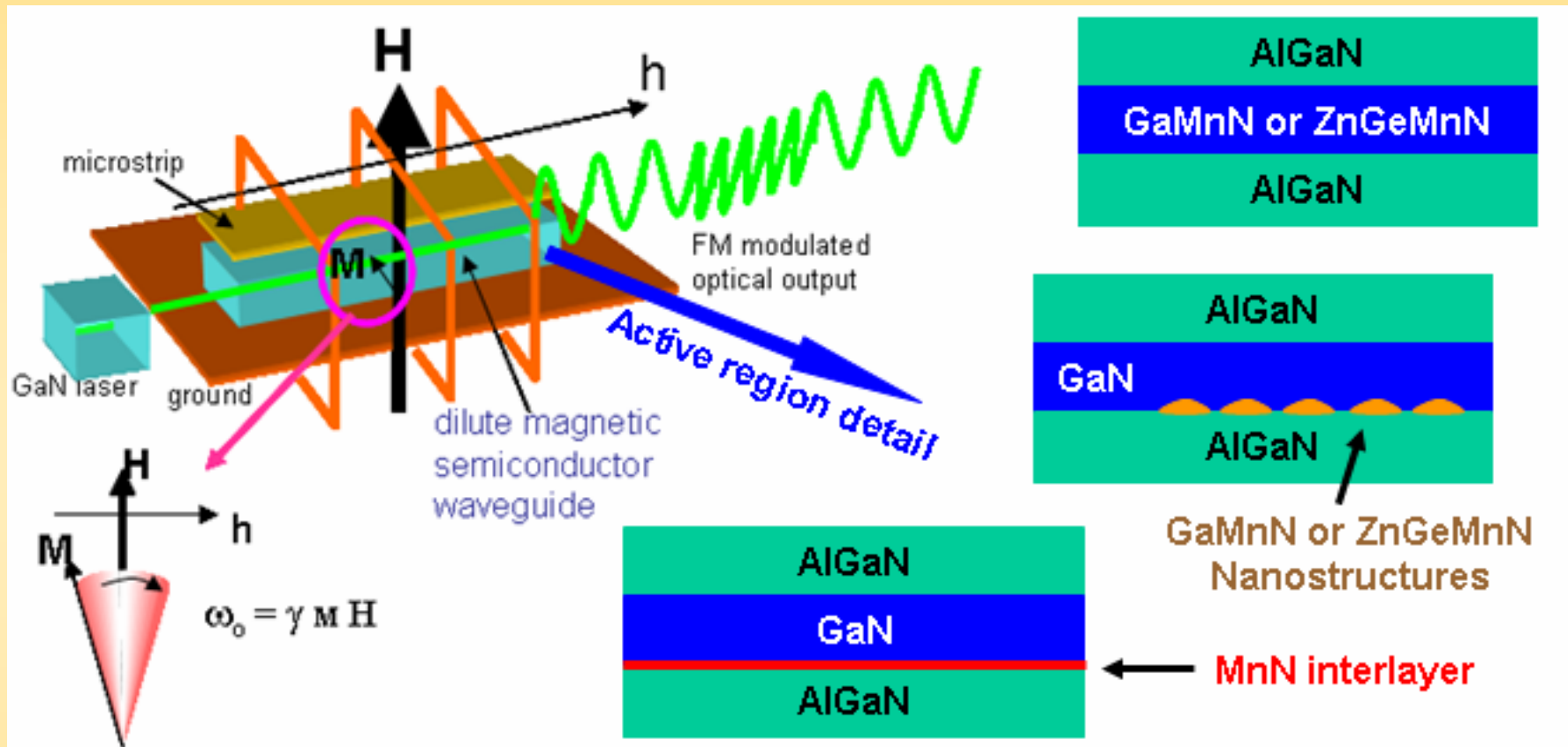
# Neutron-Induced Scintillation



Excellent gamma discrimination observed



# Future Direction: Multifunctional EMO devices



Devices where the Electrical, Magnetic and Optical (EMO) can interact.



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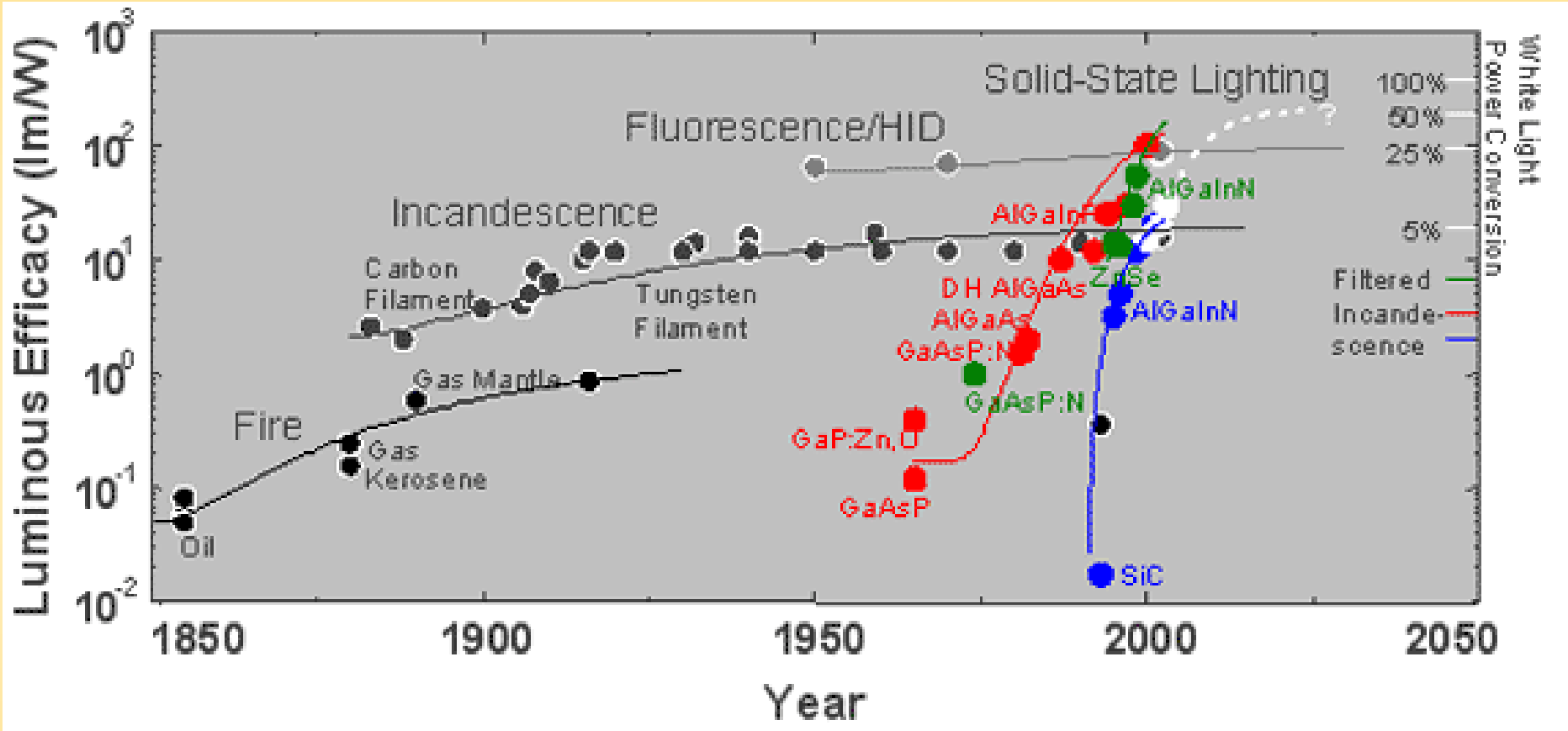
**III-Nitrides for Solid State Lighting**  
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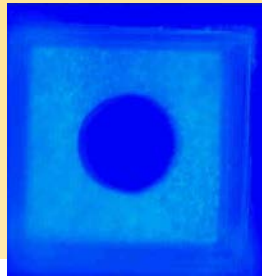
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Electrical and Computer Engineering

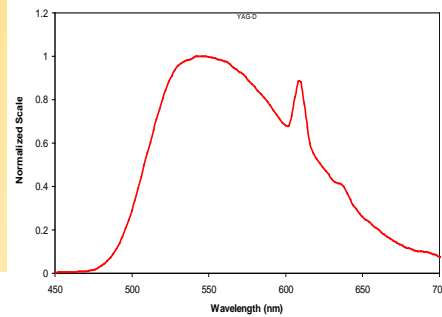
# Historical Development of Lighting and LEDs



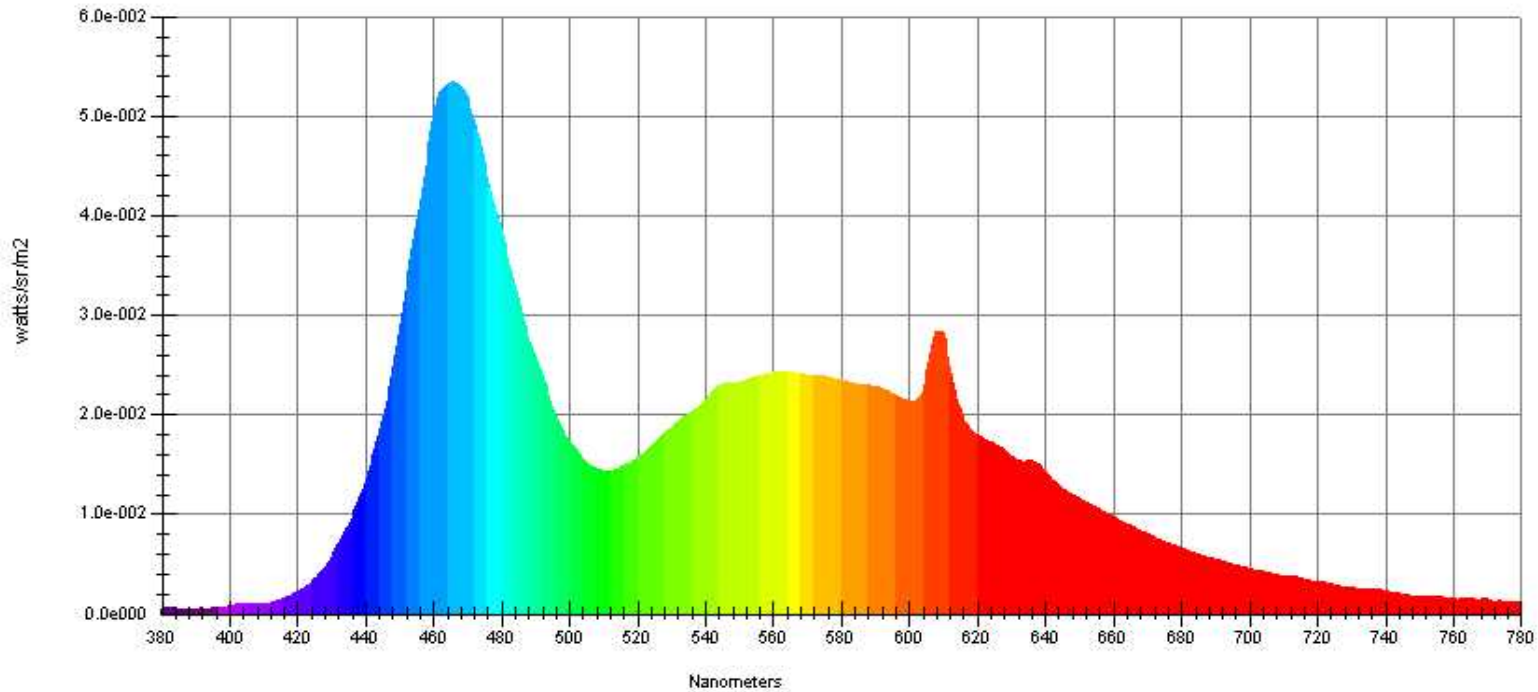
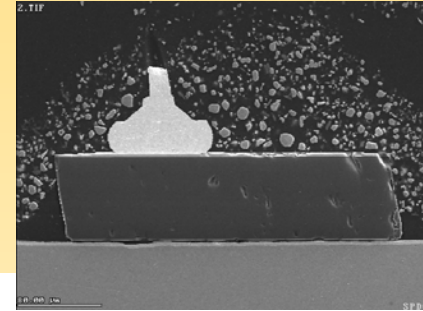
# Combined Blue LED and YAG:Ce,Pr Spectra=White



+



+



(Mueller et al., IDW 2000, Lumileds)



# Solid State Lighting

## Clyde Bridge, Glasgow

- 100 years after the discovery of electroluminescence in a semiconductor, solid state illumination is enabled by advances in high power LED technology during the past 10 years
- Early history of the visible LED
- Development of high-power LEDs at Philips Lumileds
  - Light extraction
  - Packaging
  - Materials technology
- Emerging applications and new figures of merit



## Palace in Nancy, France

# Street Lighting

- Ann Arbor
  - Replacing 1,500 streetlights
  - Payback 4 years
  - Using \$100K less energy/yr
- Welland, Ontario
  - Retrofitted streetlights
- Tianjin, China
  - 1,500 streetlights
  - Energy savings and economic driver





# Lighting in Egypt...



# $\text{Al}_2\text{O}_3$ Transition layer-Schematic illustration

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Atomic layer deposition (ALD) is used to provide a transition layer of  $\text{Al}_2\text{O}_3$  on Si/ZnO substrates before nitride growth by MOCVD.

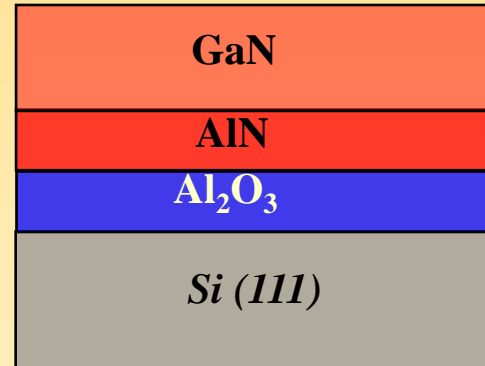
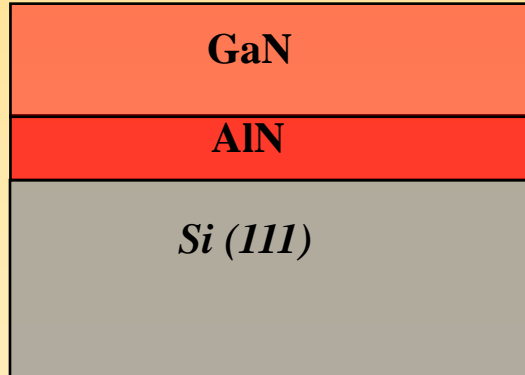
$\text{Al}_2\text{O}_3$  was grown at  $100^\circ\text{C}$  for 5nm and 20nm, then annealed in a furnace at  $1100^\circ\text{C}$  followed by AlN/GaN in MOCVD





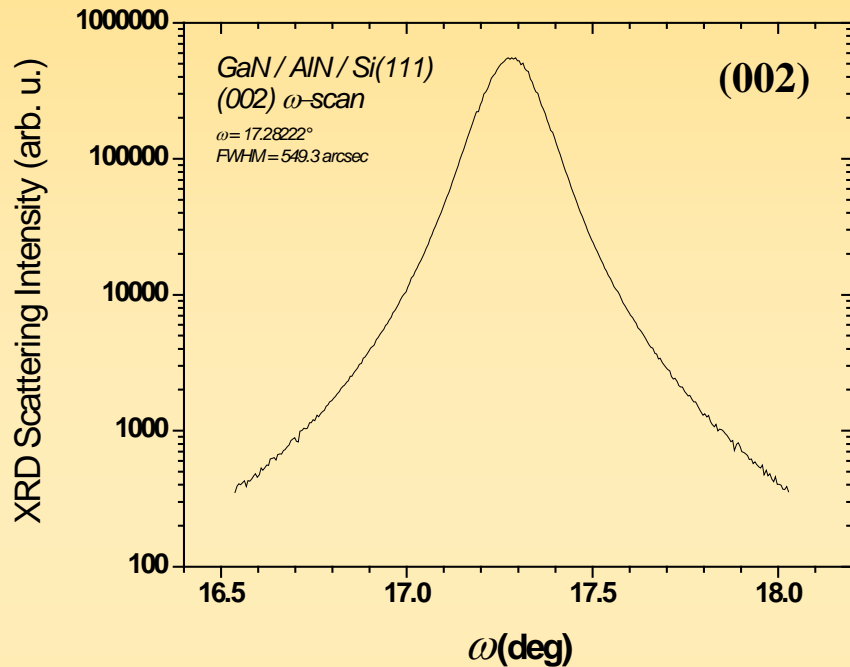
# MOCVD Growth of GaN on Si-Approaches

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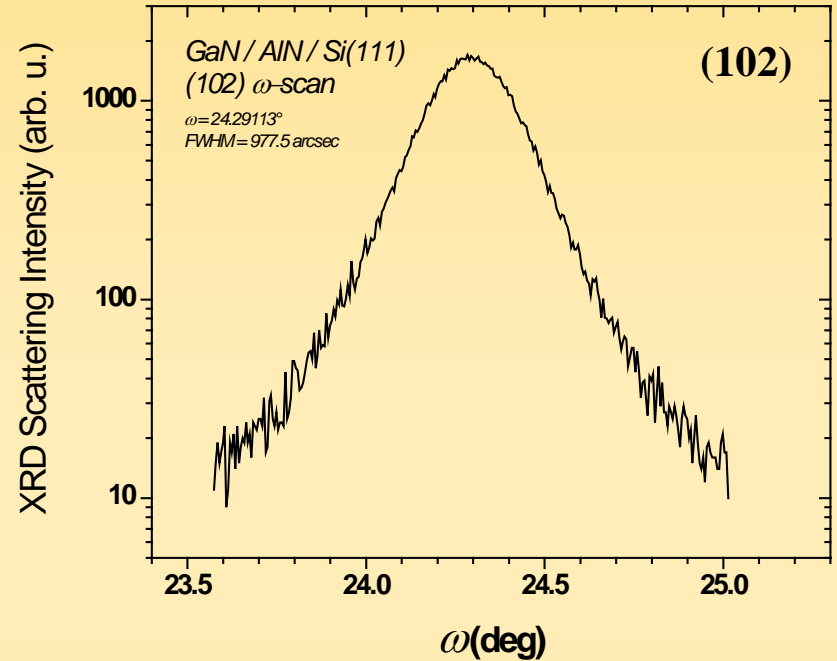


- Develop MOCVD process for GaN on Si
- Transfer the process to Al<sub>2</sub>O<sub>3</sub>/Si
- Determine and compare the characteristics
- Grow LED device structures and remove substrate

# Structural Properties of GaN on Bare Si



FWHM = 549.3 arcsec



FWHM = 977.5 arcsec

- XRD shows good quality GaN (1.5  $\mu\text{m}$ ) material on Si

# GaN on Bare Si - Summary

|                       | XRD                    |                        | PL            |       | AFM                  |
|-----------------------|------------------------|------------------------|---------------|-------|----------------------|
|                       | (002) FWHM<br>(arcsec) | (102) FWHM<br>(arcsec) | FWHM<br>(meV) | BL/YL | RMS roughness<br>(Å) |
| HT-AIN<br>buffer      | 549.3                  | 977.5                  | 49.3          | 5.396 | 5.67                 |
| LT-AIN<br>interlayers | 436.8                  | 1041.9                 | 46.9          | 5.521 | 3.99                 |

MOCVD process developed for growth of high quality GaN on Si(111)

# GaN on ALD/Si Substrate

Bare Si



1.5um GaN on bare Si

10nm ALD- $\text{Al}_2\text{O}_3/\text{Si}$

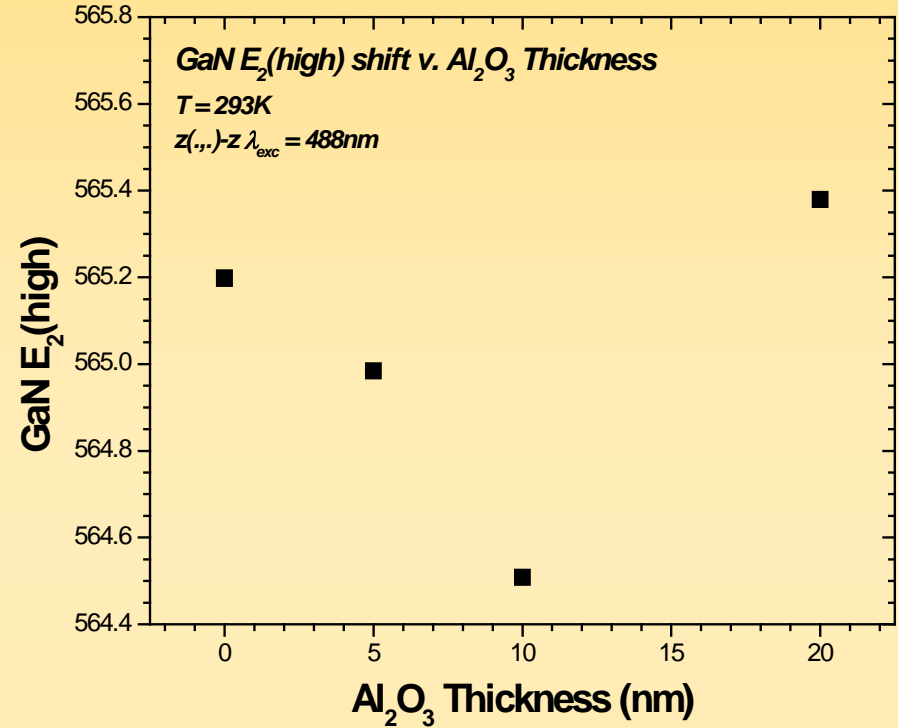
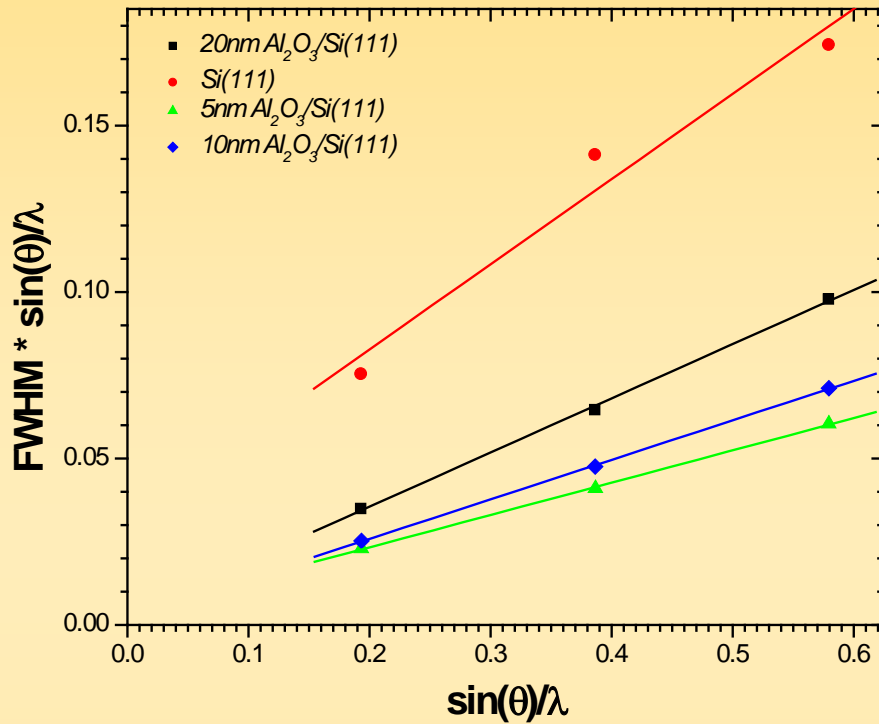


1.5um GaN on 10nm ALD- $\text{Al}_2\text{O}_3/\text{Si}$

**The cracking issue has been resolved**



# Strain and Defect Density



- Al<sub>2</sub>O<sub>3</sub> layer reduces strain in GaN layer
- Decrease in tilt angle ( $\alpha_{\text{tilt}}$ )
- Decrease in dislocation density using ALD-Al<sub>2</sub>O<sub>3</sub> layer

# Process Summary - Comparison

|   | XRD                    |                        | PL            |        | AFM                  |
|---|------------------------|------------------------|---------------|--------|----------------------|
|   | (002) FWHM<br>(arcsec) | (102) FWHM<br>(arcsec) | FWHM<br>(meV) | BL/YL  | RMS roughness<br>(Å) |
| HT-AlN buffer                           | 549.3                  | 977.5                  | 49.3          | 5.396  | 5.67                 |
| LT-AlN<br>interlayers                   | 436.8                  | 1041.9                 | 46.9          | 5.521  | 3.99                 |
| 5nm Al <sub>2</sub> O <sub>3</sub> /Si  | 378.6                  | 849.5                  | 46.5          | 7.395  | 3.93                 |
| 10nm Al <sub>2</sub> O <sub>3</sub> /Si | 433.9                  | 1344.6                 | 47.7          | 4.497  | 5.65                 |
| 20nm Al <sub>2</sub> O <sub>3</sub> /Si | 416.6                  | 740.1                  | 43.4          | 28.223 | 3.70                 |

Increased structural, optical, and surface quality compared to layers on bare Si

XRD linewidth approaching typical values for GaN on sapphire

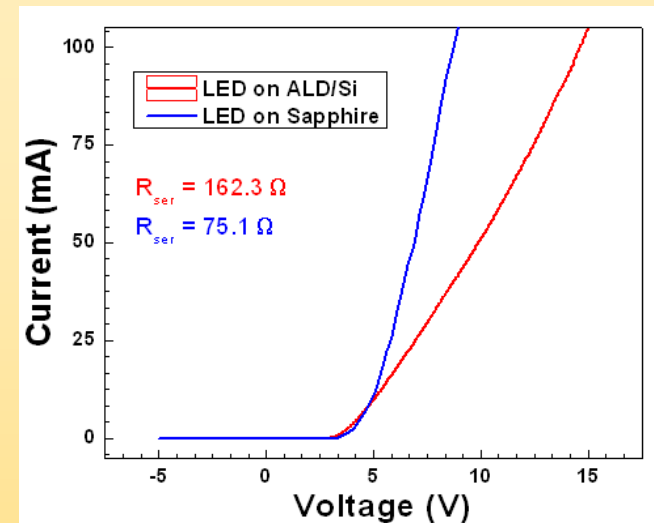
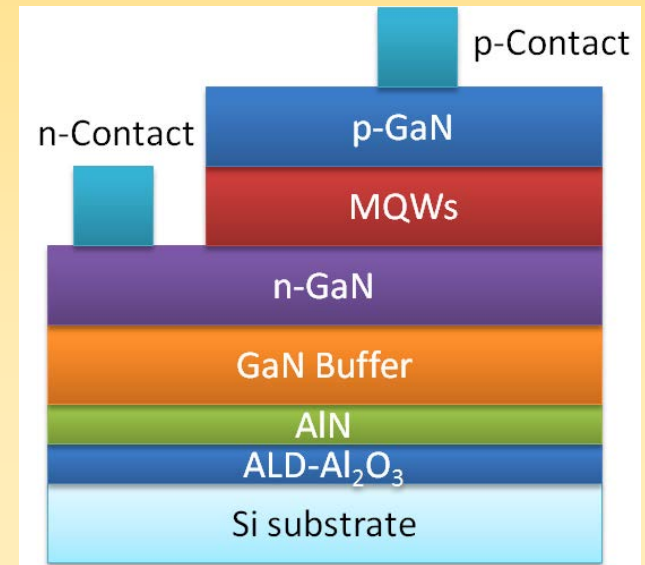
# Electrical Properties of GaN LEDs on Si and Sapphire

GaN-based LEDs were grown on ALD-  $\text{Al}_2\text{O}_3$ /Si and sapphire

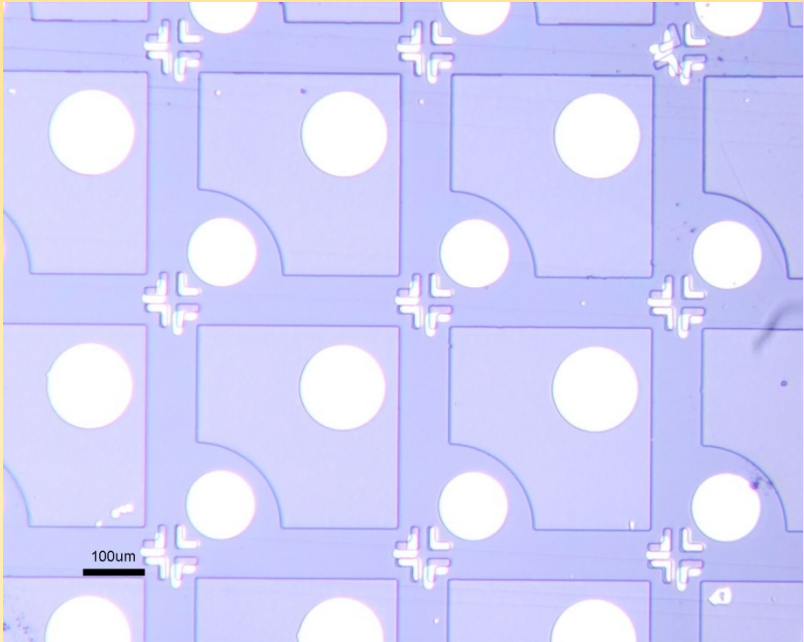
Device structures consisted 1.0  $\mu\text{m}$  n-GaN, 3-periods InGaN/GaN (3 nm/12 nm) MQWs and 150 nm p-GaN

Fabrication was performed to the device sizes of  $350 \times 350 \mu\text{m}^2$

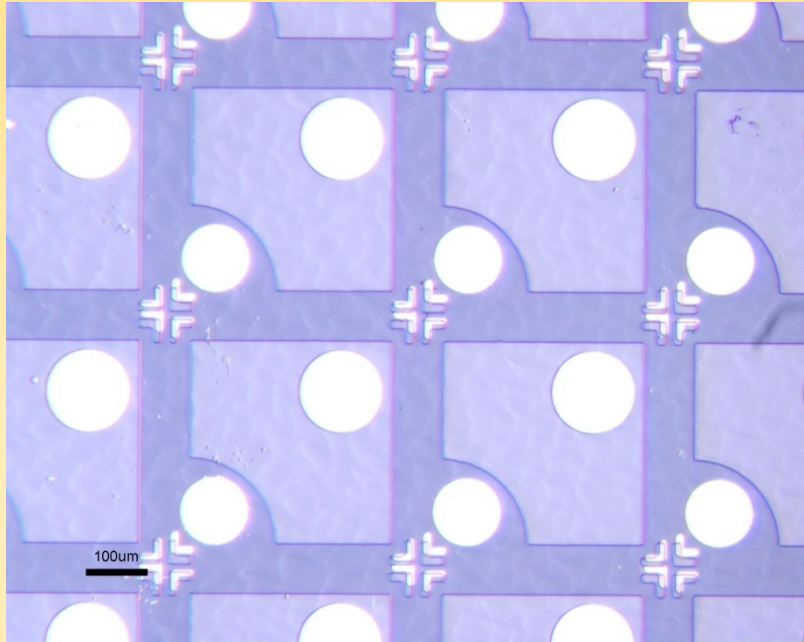
Similar turn-on voltage but higher series resistance for LED on ALD/Si than on sapphire.



# Crack-free LEDs on Si



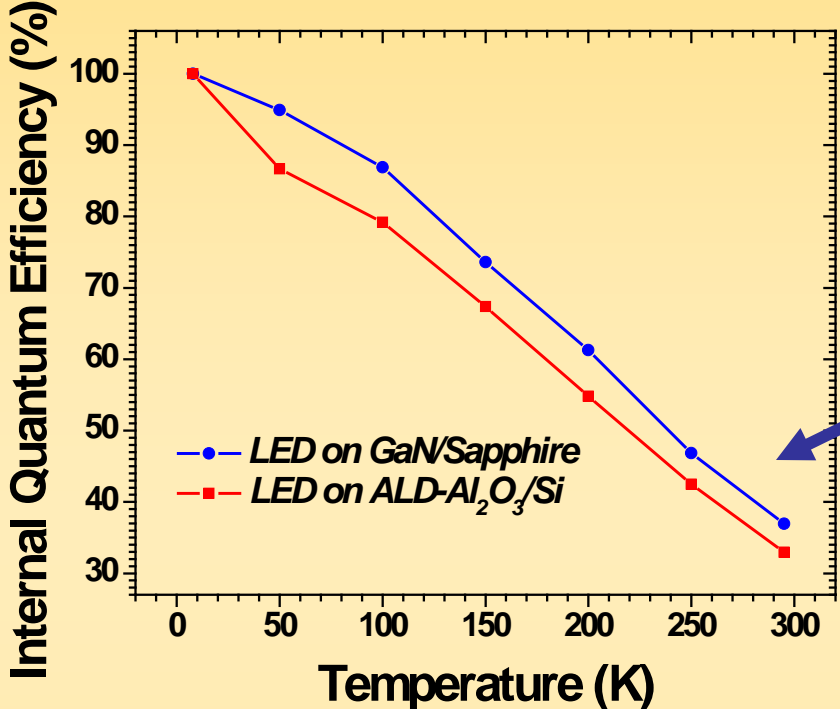
LEDs on ALD- $\text{Al}_2\text{O}_3/\text{Si}$



LEDs on GaN/sapphire

Crack-free GaN LEDs on ALD- $\text{Al}_2\text{O}_3/\text{Si}$  substrates

# Internal Quantum Efficiency (IQE)



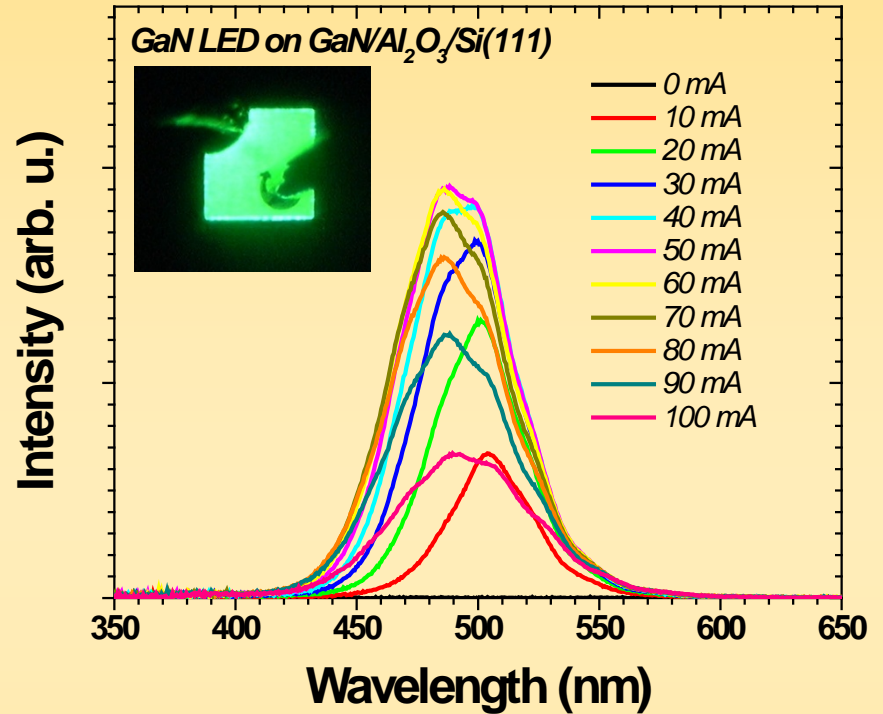
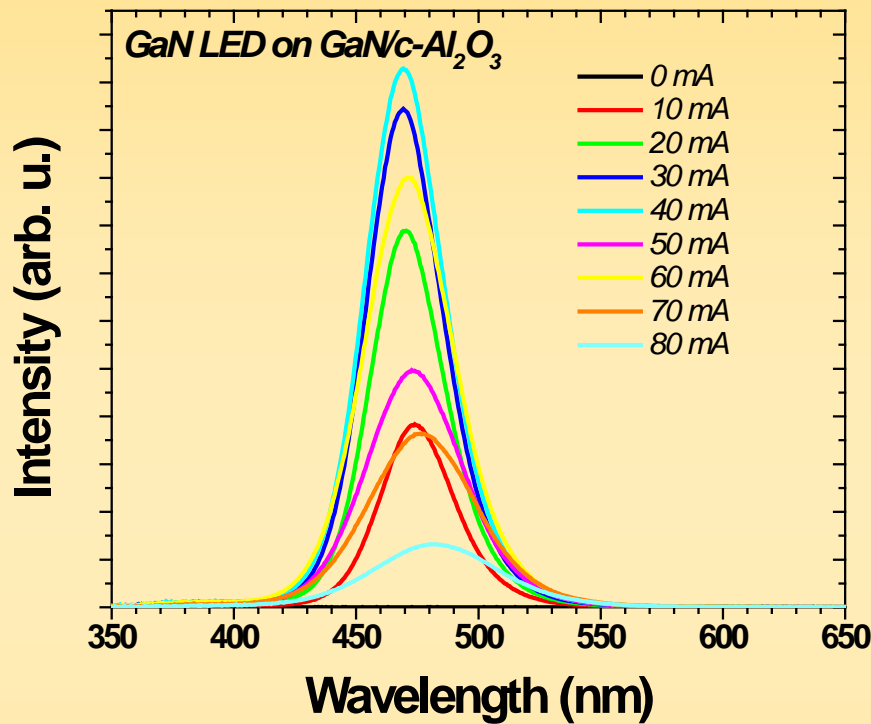
LEDs on sapphire and Al<sub>2</sub>O<sub>3</sub>/Si shows similar IQE values

Al<sub>2</sub>O<sub>3</sub> /Si shows significant improvement in IQE over bare Si

| Substrate                          | IQE |
|------------------------------------|-----|
| Sapphire                           | 37% |
| Al <sub>2</sub> O <sub>3</sub> /Si | 32% |
| Bare Si                            | ~4% |

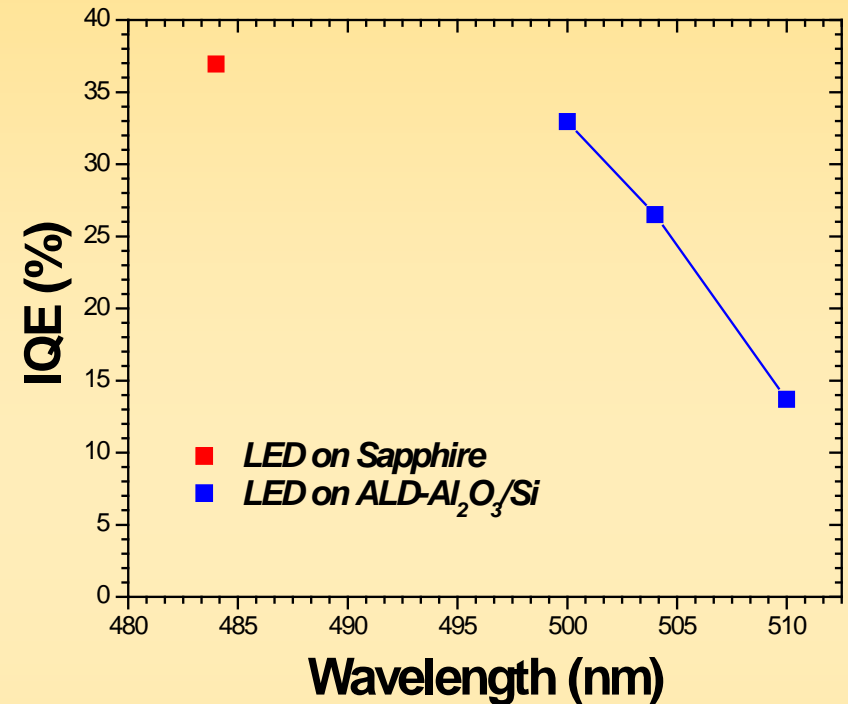
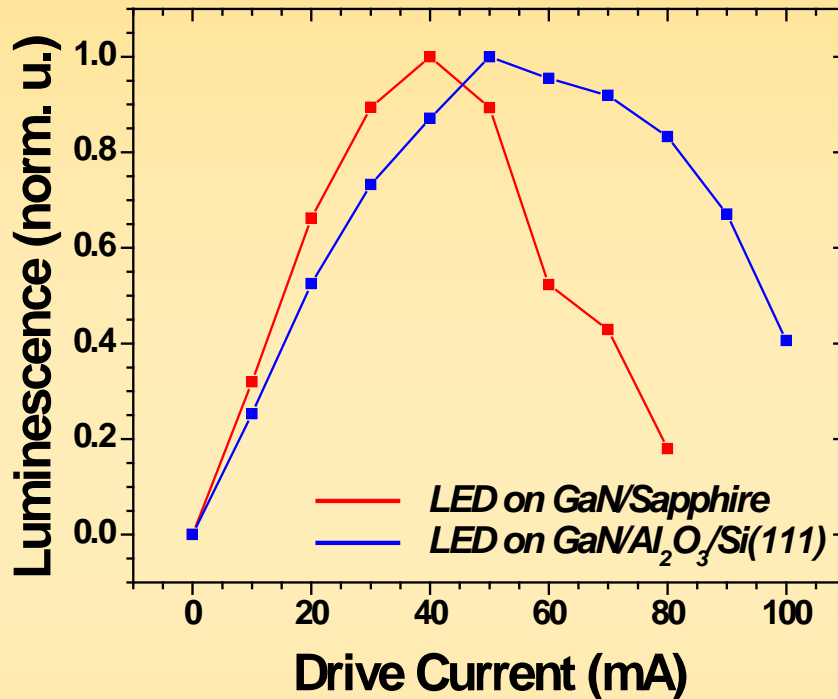


# Electroluminescence



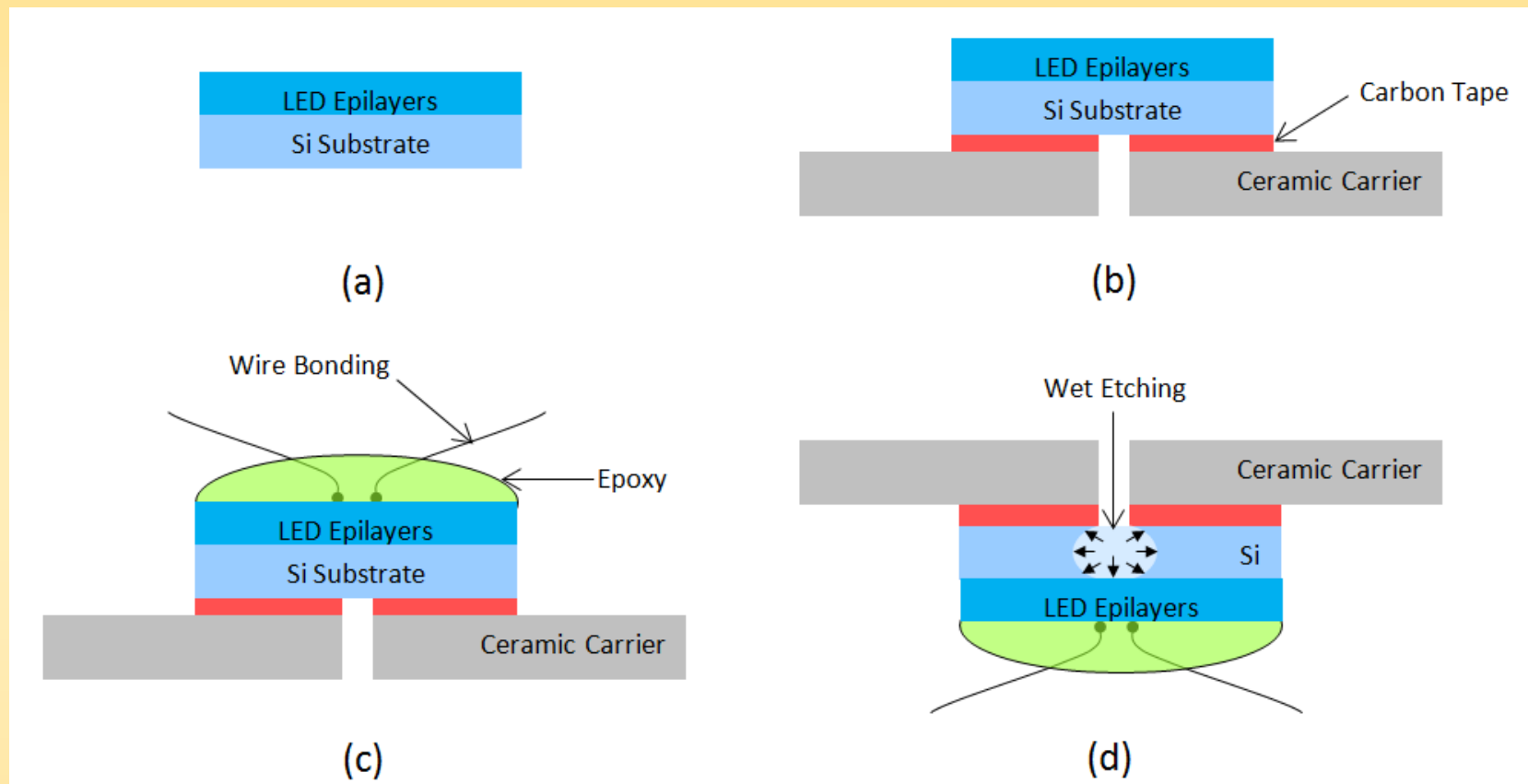
LEDs on ALD-Al<sub>2</sub>O<sub>3</sub>/Si substrates shifted to longer wavelengths

# L-I curves



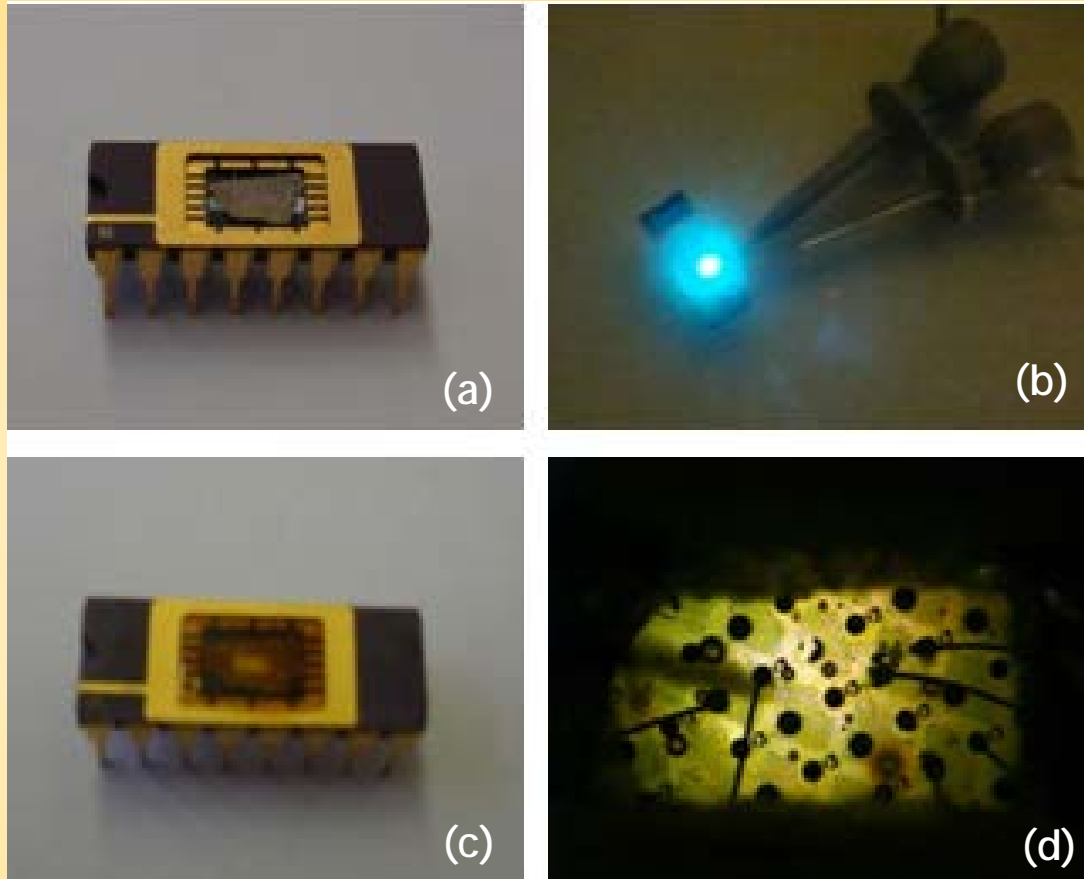
Higher efficiency at high drive currents for LEDs on ALD-Al<sub>2</sub>O<sub>3</sub>/Si  
Drop in IQE with the shift toward longer wavelengths

# Si Substrate Removal Process



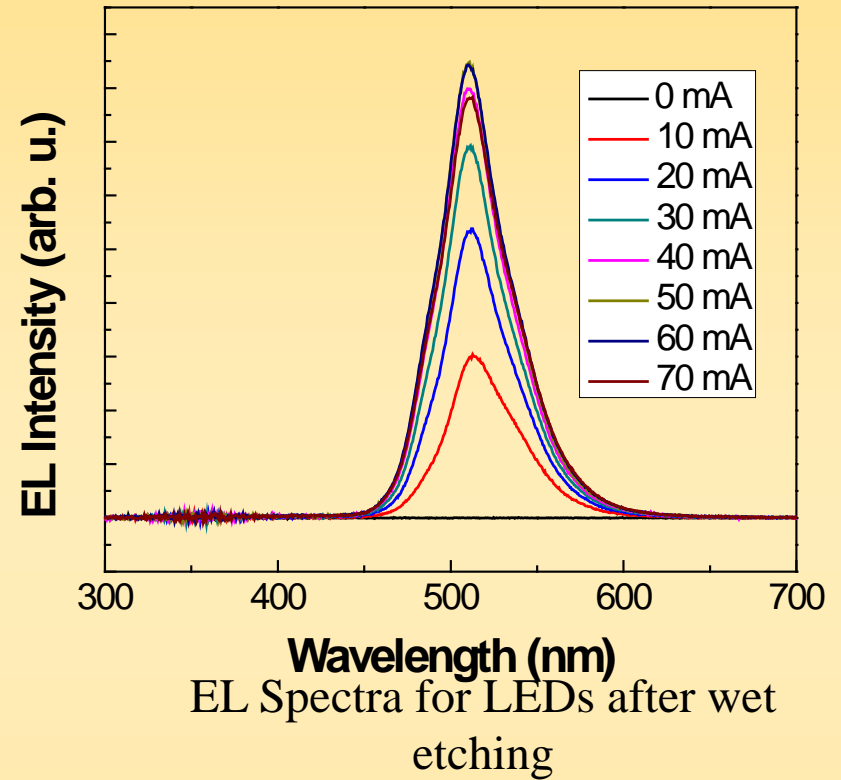
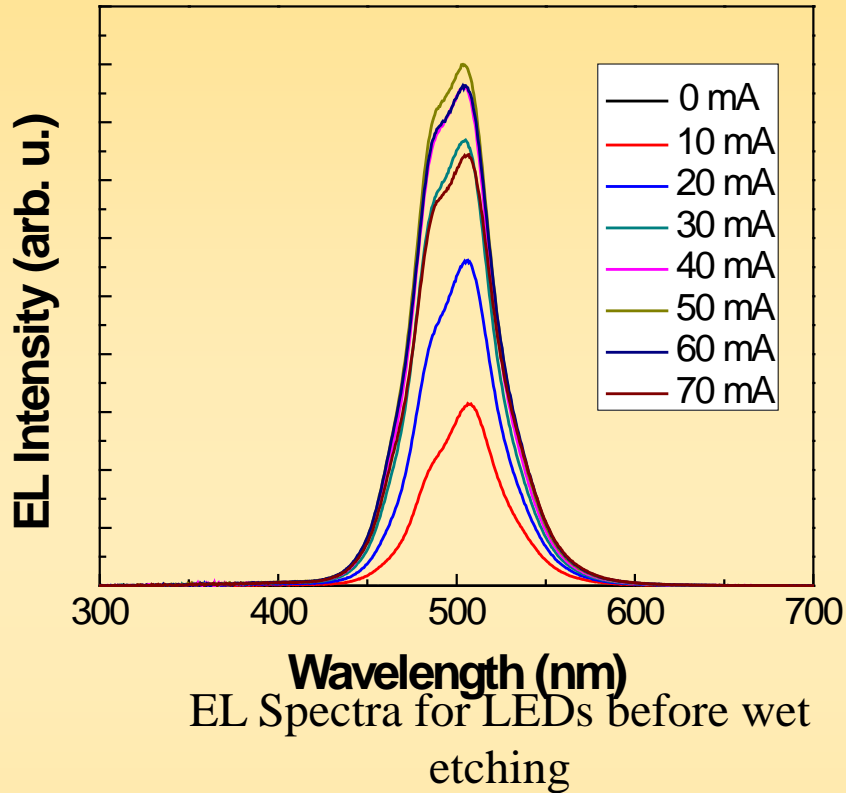
Selective wet etching process flow  
( $\text{HNO}_3:\text{HF}:\text{CH}_3\text{COOH} = 3:1:1$ )

# Images of Substrate Removal Process Flow



- (a) GaN LEDs mounted on ceramic DIP holder by wire bonding
- (b) LED lit up under forward driving current
- (c) Si substrate selectively removed by wet etching
- (d) Free-standing transparent GaN LED devices seen from back side.

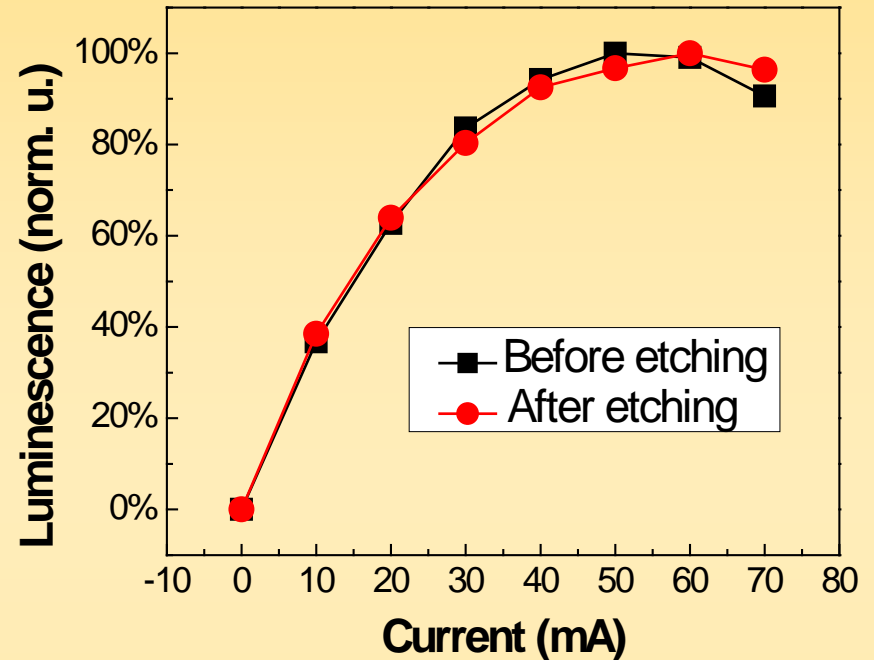
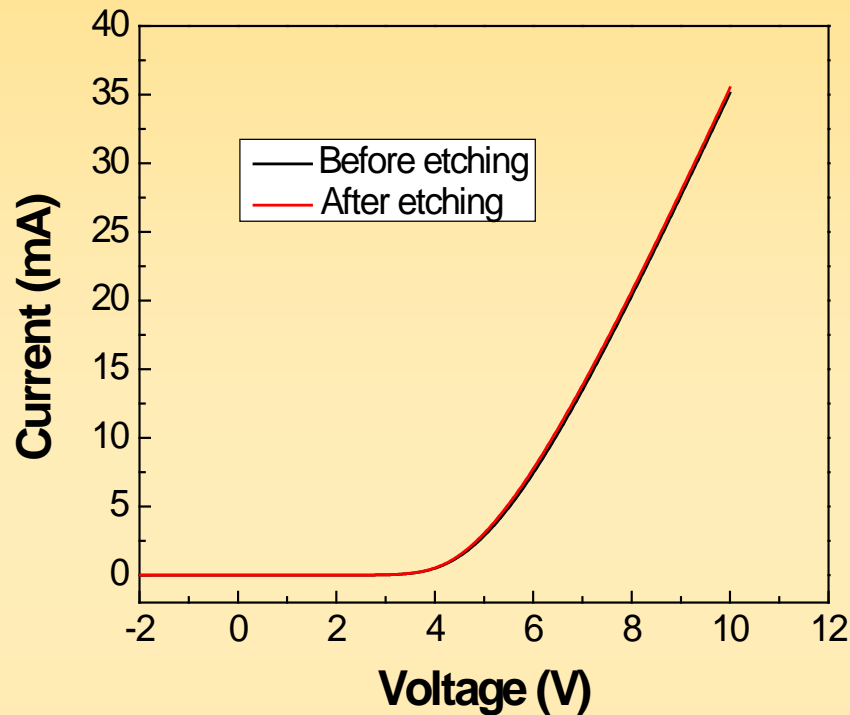
# Optical Properties Before and After Wet Etching



**No significant change in peak emission wavelength and EL intensity Vs drive current.**

**Wet etching process was effective to protect the devices from being damaged by acid etchant.**

# Electrical and Optical Properties



No degradation observed for electrical properties after the substrate removal process.

Efficiency of devices drop at higher drive current due to inefficient heat dissipation





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**III-Nitrides for Solar Cells**

Electrical and Computer Engineering

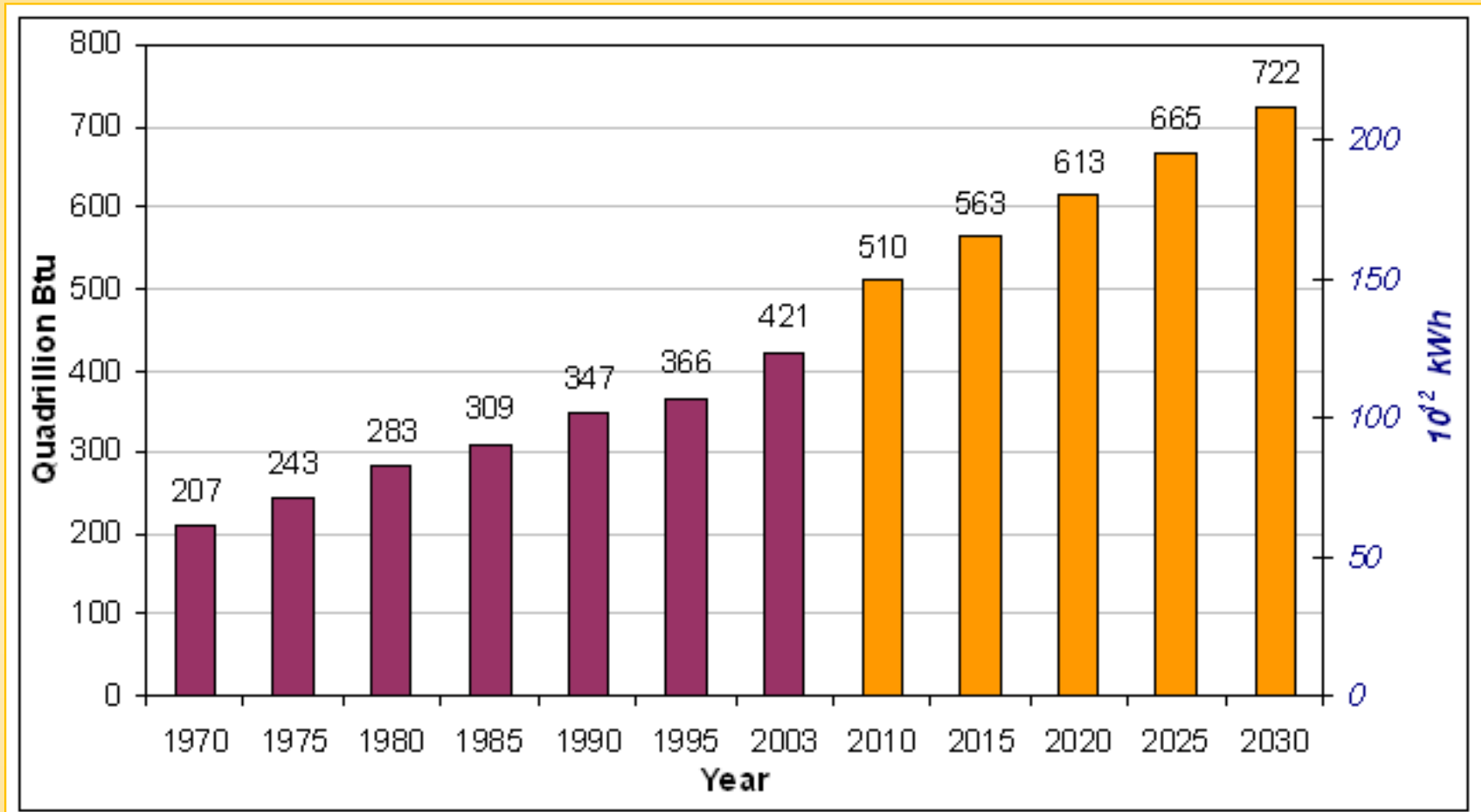


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Electrical and Computer Engineering

# Motivation for PV: Energy demand

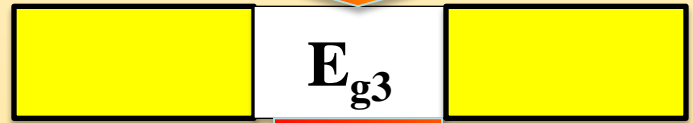
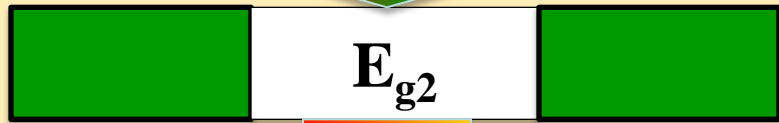
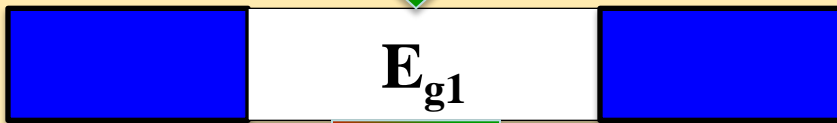
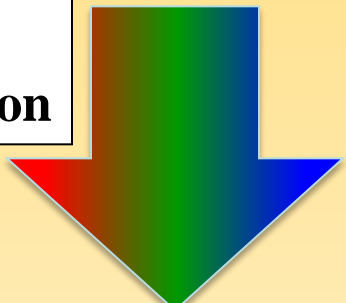


**World marketed energy consumption, 1970 - 2030.**

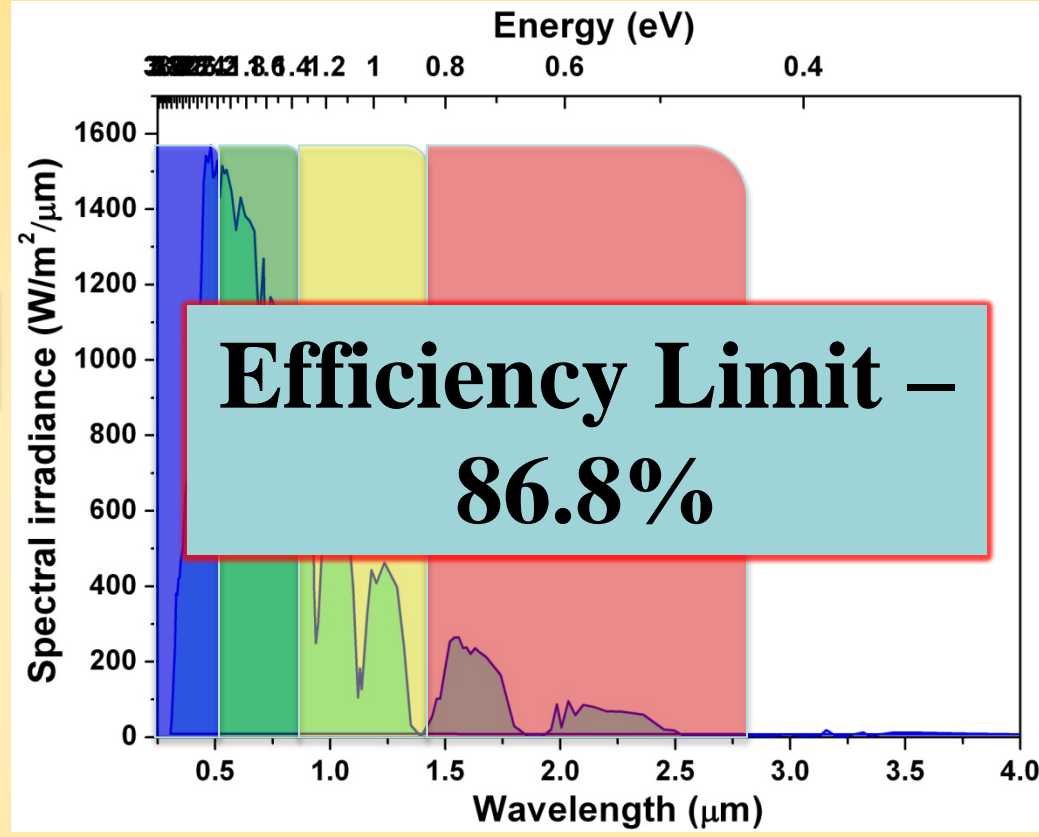
Source: DOE/EIA, Annual Energy Review, 2004.

# High efficiency approach

Solar Radiation



Band Gap  $E_{g1} > E_{g2} > E_{g3} > E_{g4}$



Optical absorption edge → **Sharp**  
(No absorption below band gap)

# Towards achieving efficiency > 50%

## Detailed Balance Calculations for 6000K Black Body Radiation, 500X.

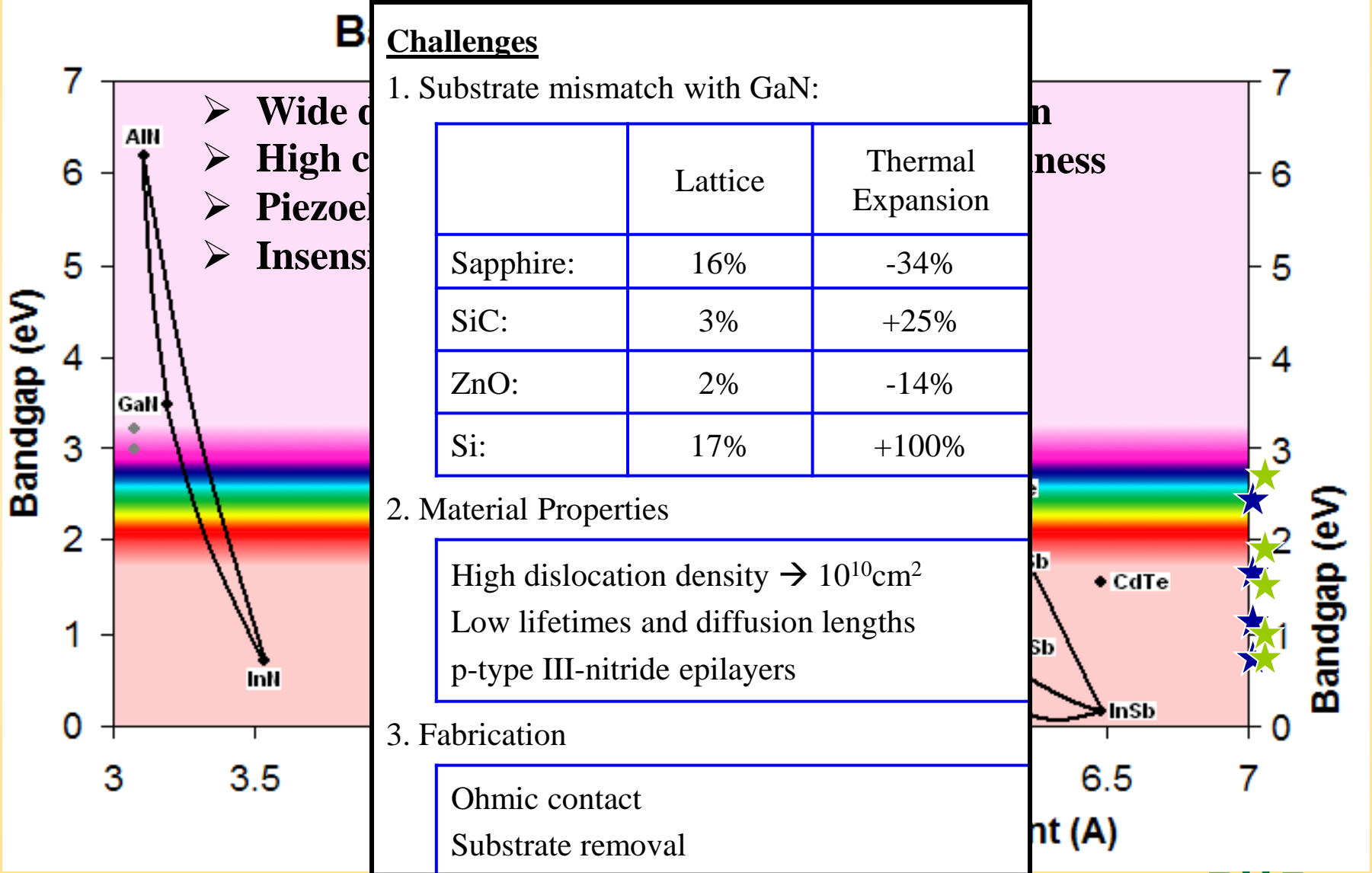
| n | Values of Band Gap |      |       |      |      |      |      |      | $\eta$ (%) | $0.8 \cdot \eta$ (%) |       |
|---|--------------------|------|-------|------|------|------|------|------|------------|----------------------|-------|
| 3 | 0.7                | 1.37 | 2     |      |      |      |      |      | 56         | 44.8                 |       |
| 4 | 0.6                | 1.11 | 1.69  | 2.48 |      |      |      |      | 62         | 49.6                 |       |
| 5 | 0.53               | 0.95 | 1.4   | 1.93 | 2.68 |      |      |      | 65         | 52                   |       |
| 6 | 0.47               | 0.84 | 1.24  | 1.66 | 2.18 | 2.93 |      |      | 67.3       | 53.84                |       |
| 7 | 0.47               | 0.82 | 1.191 | 1.56 | 2    | 2.5  | 3.21 |      |            | 68.9                 | 55.12 |
| 8 | 0.44               | 0.78 | 1.09  | 1.4  | 1.74 | 2.14 | 2.65 | 3.35 | 70.2       | 56.16                |       |

Source: A. De Vos, "Detailed balance limit of the efficiency of tandem solar cells", Journal of Physics D (Applied Physics) 1980, 839-46

**5 or more effective band gaps  $\rightarrow$  50%  $\eta$**

**50%  $\eta$   $\rightarrow$  Band gap > 2.4 eV**

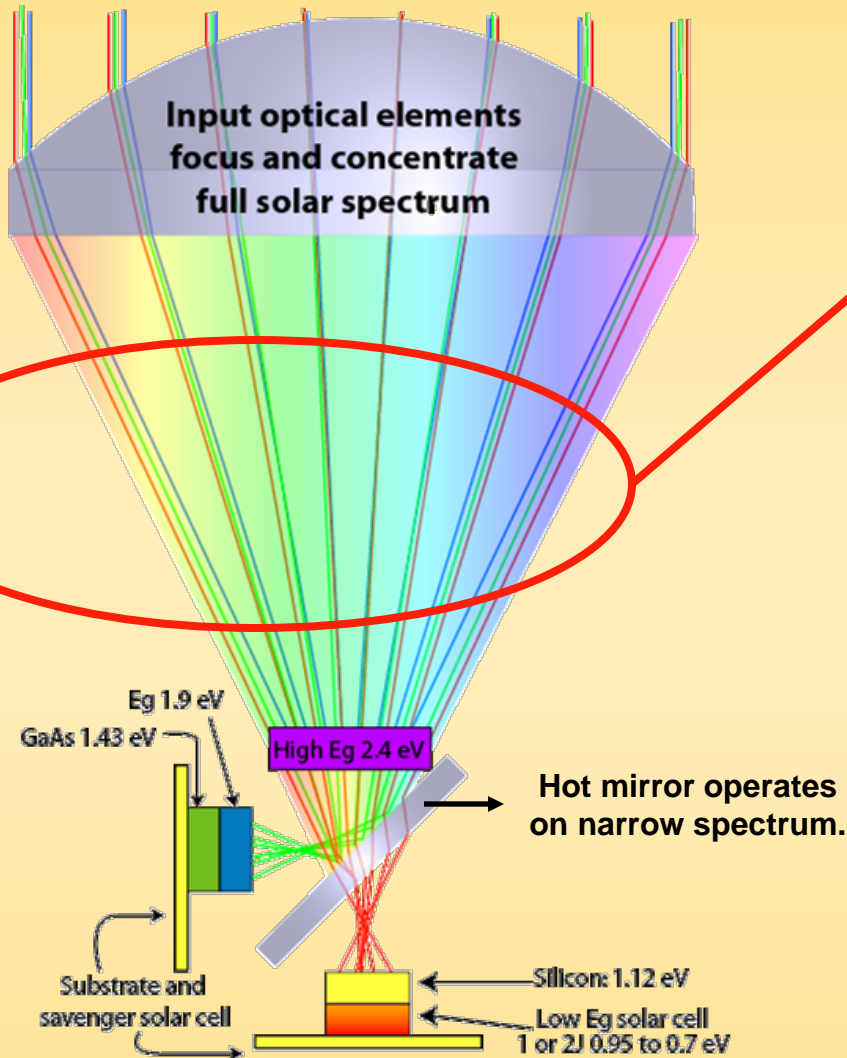
# III-Nitride material system





# Very High Efficiency Solar Cells

## InGaN solar cells



Operation of VHESC.

| 6J Solar Cell Band Gaps | Thermodynamic efficiency          | De-rating factor | Ideal target efficiency                           |
|-------------------------|-----------------------------------|------------------|---|
| High Eg 2.4 eV          | 14.9%                             | 0.89             | 13.3%   |
| GaN 1.84 eV             | 16.6%                             | 0.86             | 14.3%   |
| GaAs 1.43 eV            | 13.9%                             | 0.84             | 11.7%   |
| Si 1.12 eV              | 9.7%                              | 0.80             | 7.8%  |
| 0.95 eV                 | 5.0%                              | 0.74             | 3.7%  |
| 0.70 eV                 | 4.1%                              | 0.70             | 2.9%  |
| <b>Total</b>            | <b><math>\eta = 64.2\%</math></b> |                  | <b>Total</b><br><b><math>\eta = 53.5\%</math></b> |

Predicted efficiency contribution of each junction .

# Research approach

**Modeling**  
PC1D, SiLENSe, etc.

**Growth**  
MOCVD, MBE  
(*Characterization:*  
*PL, XRD, Transmission*)

**Analysis &  
Optimization**  
Decrease band gap

**2.4 – 2.9 eV  
InGaN solar cell**

**Fabrication**  
Current spreading layer,  
Interdigitated contacts

**Characterization**  
I-V, QE

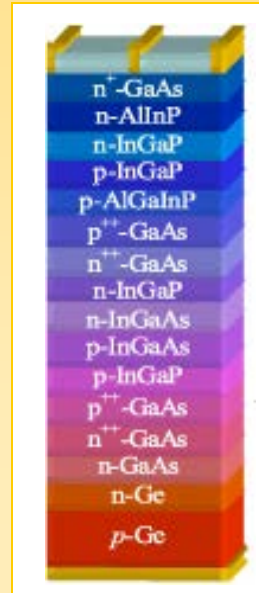
# Design principles

## FIRST ATTEMPT @ InGaN solar cells

- III-V solar cell technology
- III-nitride LED, photodetector, laser technology

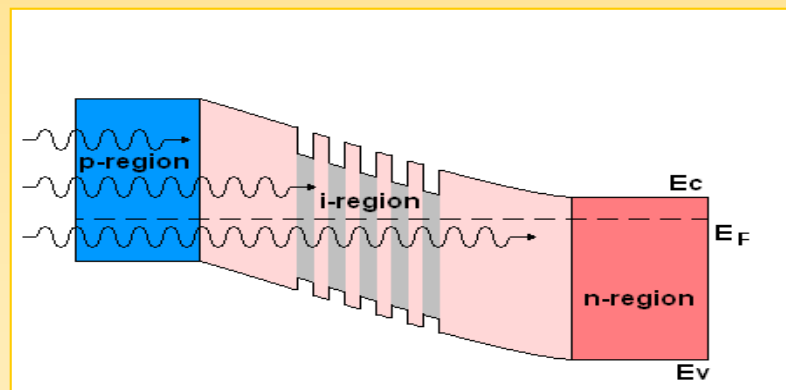
## DESIGN PRINCIPLES

- Maximize light absorption
  - Thickness, light trapping, ARC, surface texturing, shadowing.
- Maximize collection
  - Surface passivation, electric fields, band engineering, gettering.
- Minimize dark current
  - Recombination, passivation, doping.
- Minimize resistive losses
  - Ohmic contacts, doping, spreading resistance, tunneling.

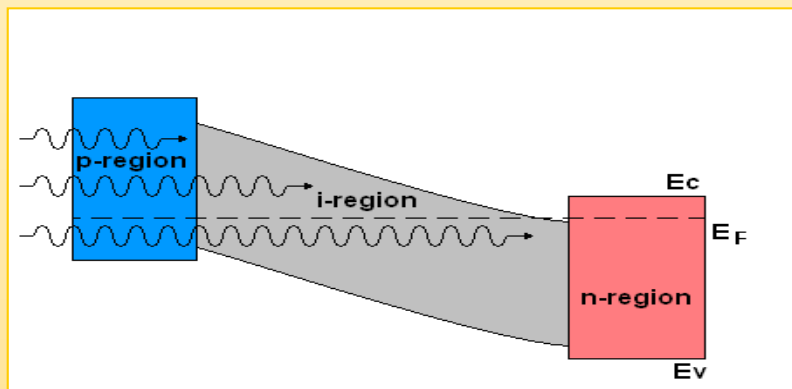


# Preliminary design: p-i-n solar cell

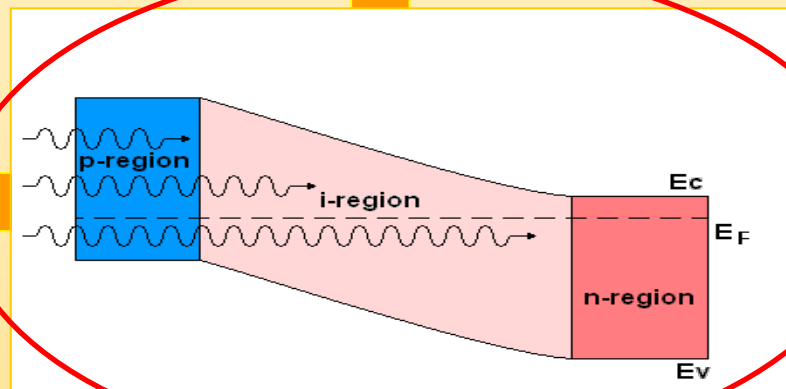
- p-region ~ 100 nm
  - Maximize absorption in i-region.
  - Provide charge to junction.
- n-region ~ 200 nm (effective)
  - Hole diffusion length ~ 200 nm.
- Test material → i-region.



GaN/InGaN QW solar cell.



GaN/InGaN p-i-n solar cell.



GaN p-i-n solar cell.

# Modeling of solar cells: PC1D

## Device parameter files

Device design, structure,  
lifetime and recombination,  
doping profiles, etc.

## Material files

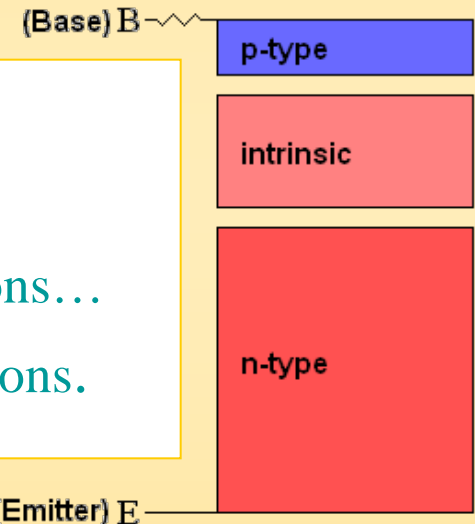
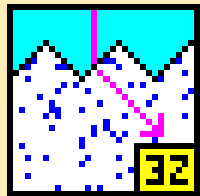
Band structure, recombination  
Optical:  
Absorption, refractive index



## PC1D core

### Solar cell simulation program

Solves fully coupled 1-D nonlinear equations...  
for quasi-1-D transport of holes and electrons.



## Result

- Graphical/numerical
- I-V, QE, band diagram, electric fields, generation/recombination



# Modification of PC1D for III-nitrides

Step 1: Preliminary modification

Step 2: Advance modification

- Polarization, convergence, etc.

## Material files

Band structure, recombination

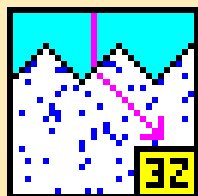
Optical:

Absorption, refractive index

## PC1D core

### Solar cell simulation program

Solves fully coupled 1-D nonlinear equations...  
for quasi-1-D transport of holes and electrons.



(Base) B

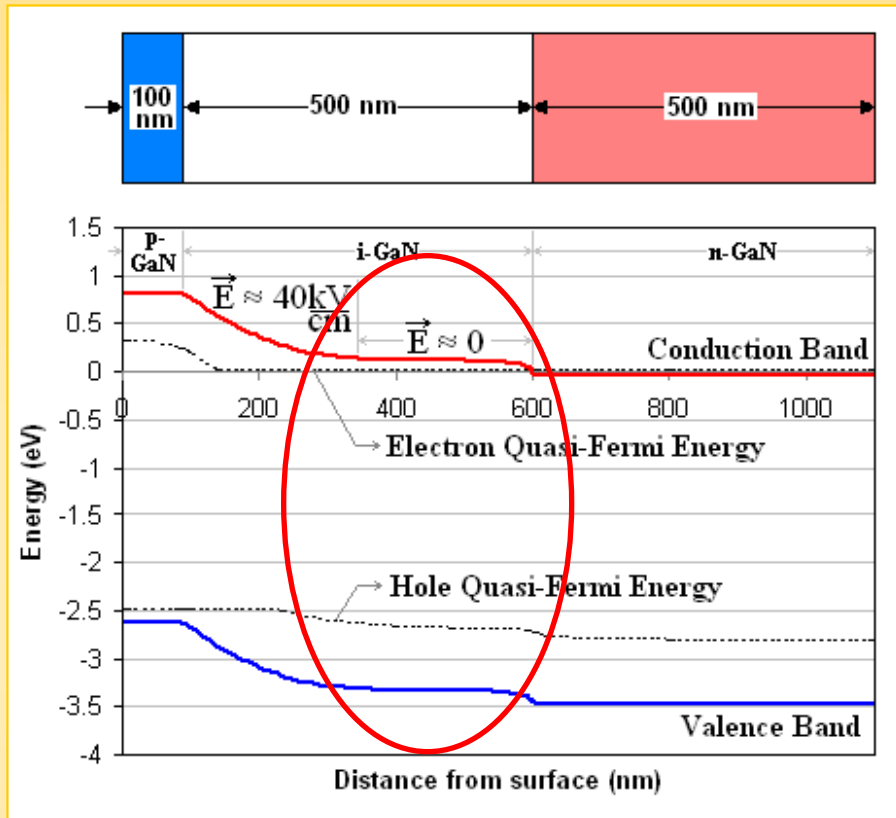
p-type

intrinsic

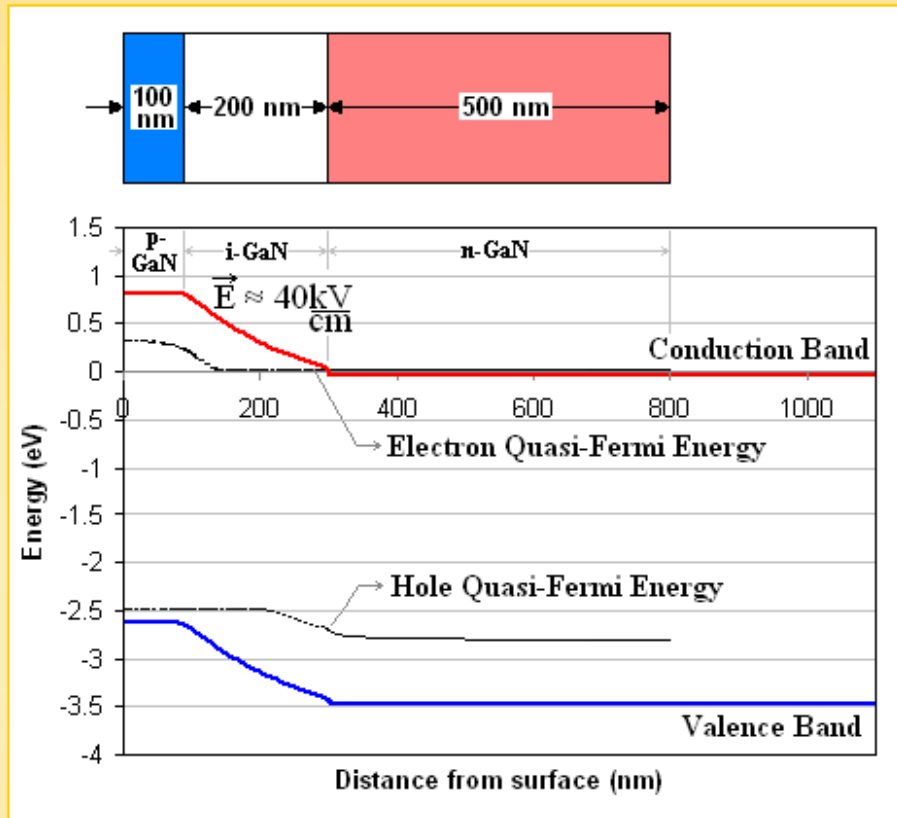
n-type

(Emitter) E

# Preliminary design: i-region thickness



Band diagram of GaN p-i-n solar cell with 500 nm thick i-region.



Band diagram of GaN p-i-n solar cell with 200 nm thick i-region.

- Background n-type concentration:  $10^{16} \text{ cm}^{-3}$ .
- **Result:** i-region thickness limited to 200 nm.

# Polarization parameter input in PC1D

**New Parameters - PC1D with Polarization for Windows**

File Device Excitation Compute Graph View Options Help

Select Region  
Insert Region  
Remove Region

Thickness...  
Material  
Doping  
Recombination  
**Polarization...** (2)  
Area...  
Texture...  
Surface charge...  
Contacts...  
Internal Elements...  
Reflectance...  
Substrate Polarization...

Thickness: 10  $\mu\text{m}$   
Material from program defaults  
Carrier mobilities from internal model  
Dielectric constant: 11.9  
Band gap: 1.124 eV  
Intrinsic conc. at 300 K:  $1 \times 10^{10} \text{ cm}^{-3}$   
Refractive index: 3.58  
Absorption coeff. from internal model  
Free carrier absorption enabled  
P-type background doping:  $1 \times 10^{16} \text{ cm}^{-3}$   
*No front diffusion*  
*No rear diffusion*  
Bulk recombination:  $\tau_n = \tau_p = 1000 \mu\text{s}$   
*No Front-surface recombination*  
*No Rear-surface recombination*  
**Polarization Model Disabled** (1)

Specify the polarization model

100 elements

**Polarization**

Enable Polarization Model

Polarity of region  
 In/Ga/Al Face  N-Face

Enable Spontaneous Polarization  Enable Piezoelectric Polarization

Use III-Nitride Model [ In(x) Ga(y) Al(100-x-y) ]

InN(%x) GaN(%y) AlN(%{100-x-y})  
70 30 0

External Polarization Model

Spontaneous Polarization (C/m<sup>2</sup>) -0.029  
Piezoelectric Constants (C/m<sup>2</sup>) e31 -0.33 e33 0.65  
Elastic Constants (GPa) c13 105 c33 395  
Lattice Constant of Current Region (Å) a 3.189 c 5.186

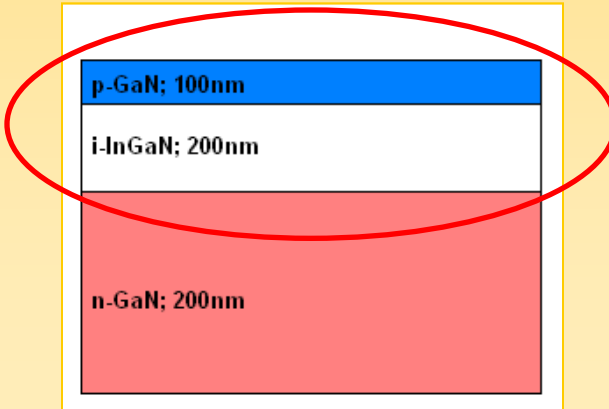
Strain Relaxation Constants (used for piezoelectric polarization)

Lattice Constant of underlying region a 3.112 (Å)  
Bulk Relaxation Constant 14.45  $\mu\text{m}$   
Interface Relaxation Factor 95 (%)

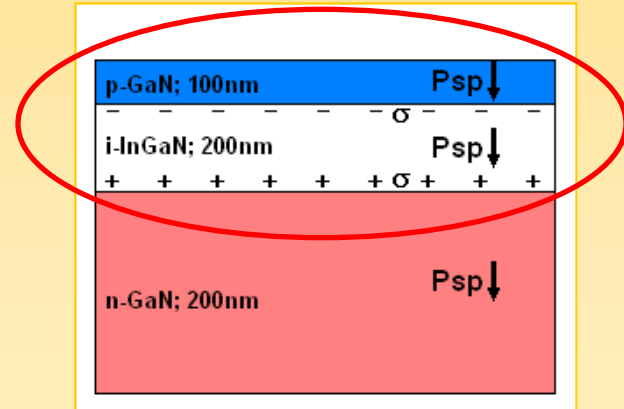
OK Cancel

# Test runs for polarization model

## 1. Spontaneous polarization in p-i-n GaN/InGaN structure

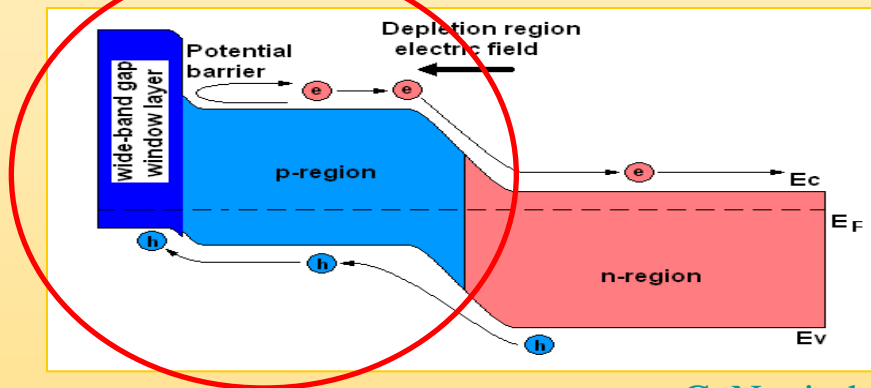


Without polarization.

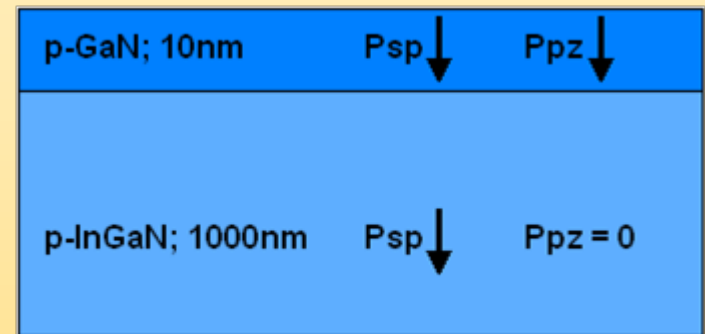


With spontaneous polarization.

## 2. Piezoelectric polarization in p-GaN window layer

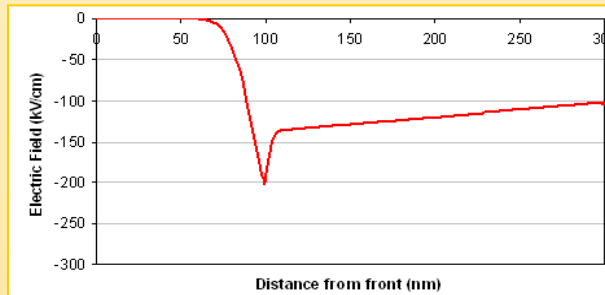
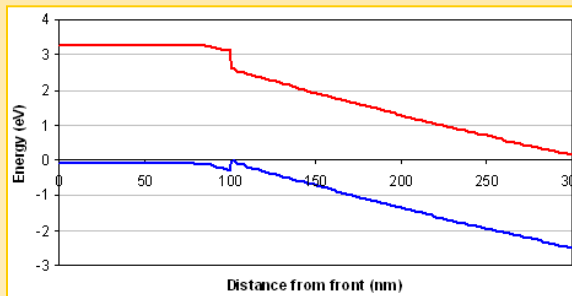
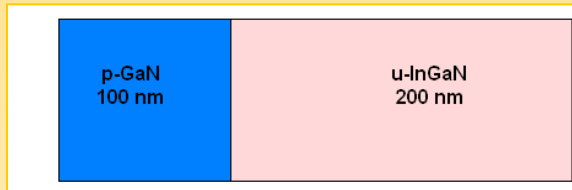


p-GaN window layer.

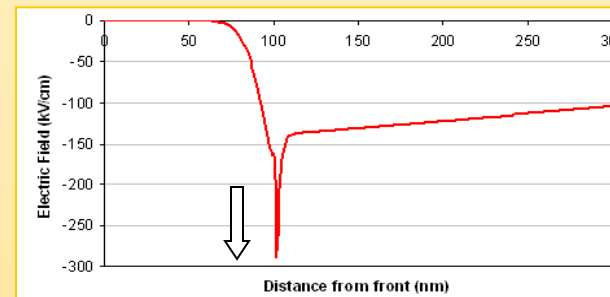
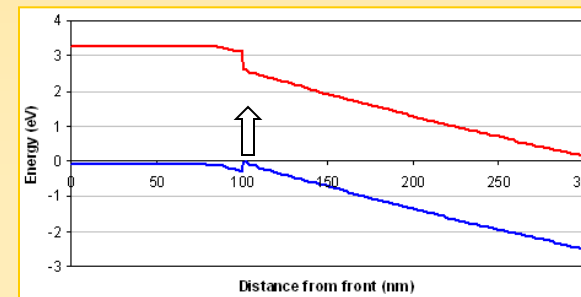
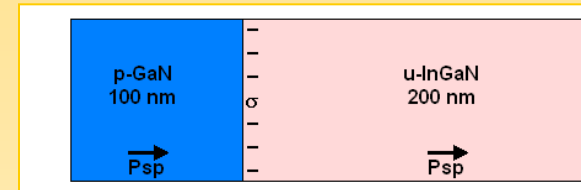


# Sample polarization results: Spontaneous polarization

Test 1: p-GaN/u-InGaN interface of a p-i-n GaN/InGaN solar cell.



Without spontaneous polarization.



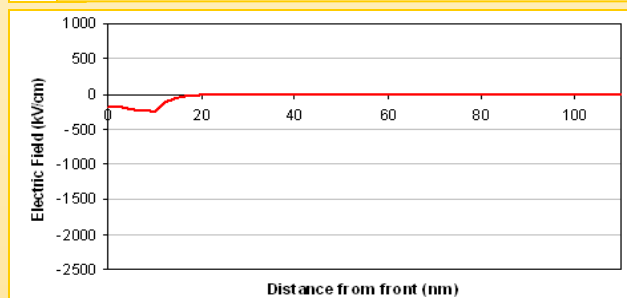
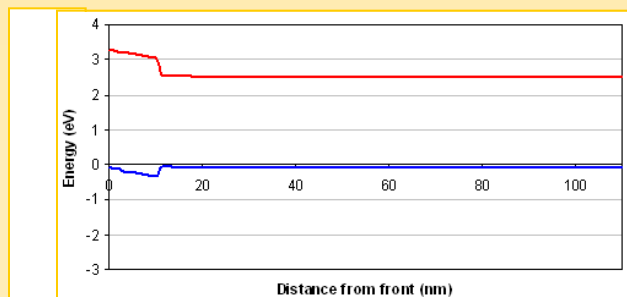
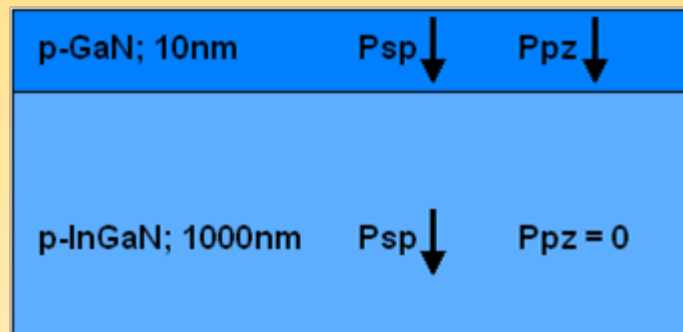
With spontaneous polarization.

- **Result:** Spontaneous polarization marginally enhances electric field.
- **Reason:** Marginal difference in  $P_{SP}$  between GaN and  $In_{0.2}Ga_{0.8}N$ .

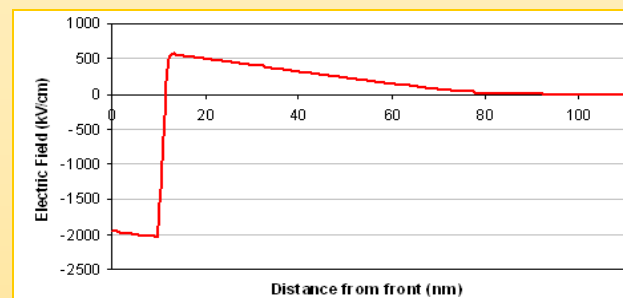
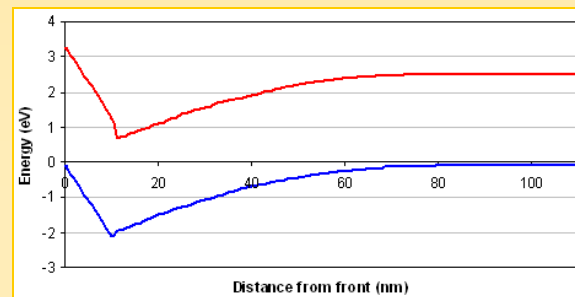
# Sample polarization results: Piezoelectric polarization

Test 2: Strained p-GaN window layer on p-InGaN junction.

- Conventional choice for window layer for InGaN.



**Completely relaxed window layer.  
(Without piezoelectric polarization.)**

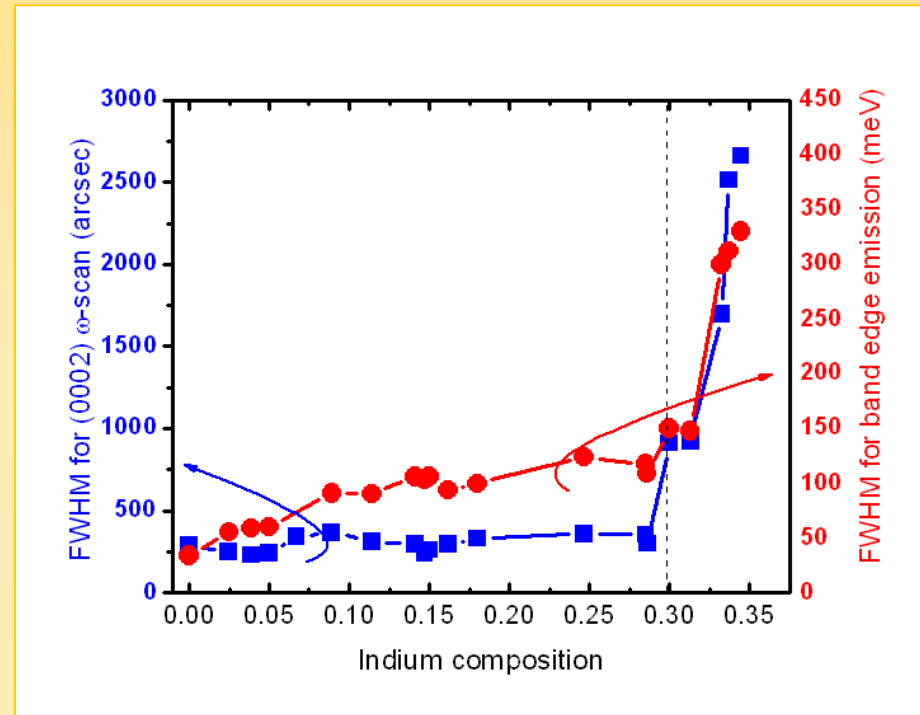
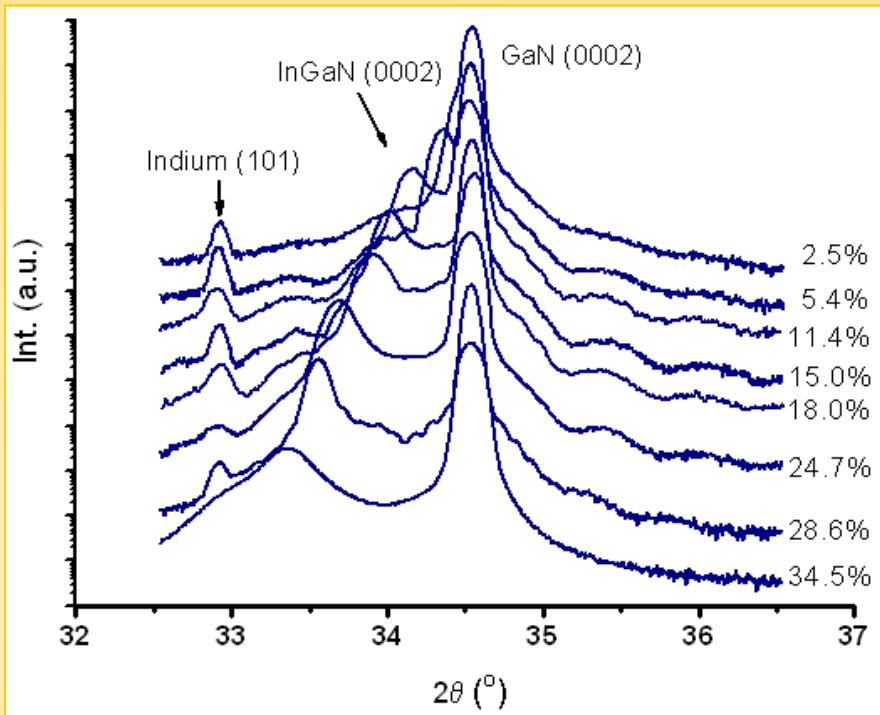


**Completely strained window layer.  
(With piezoelectric polarization.)**

- **Result:** Strong detrimental band bending at GaN/InGaN interface.



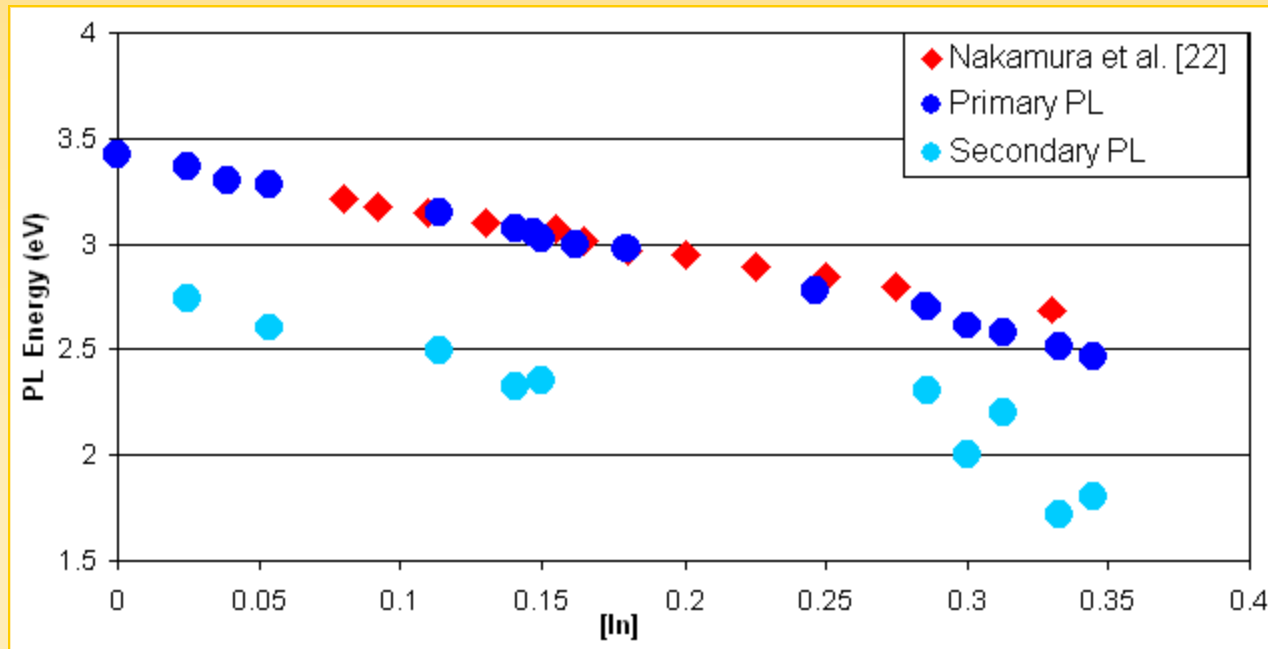
# InGaN material characterization



Summary of XRD & PL measurements of InGaN with variable [In] grown by MOCVD.

- Crystalline quality degrades for [In] > 30%
- In segregation observed

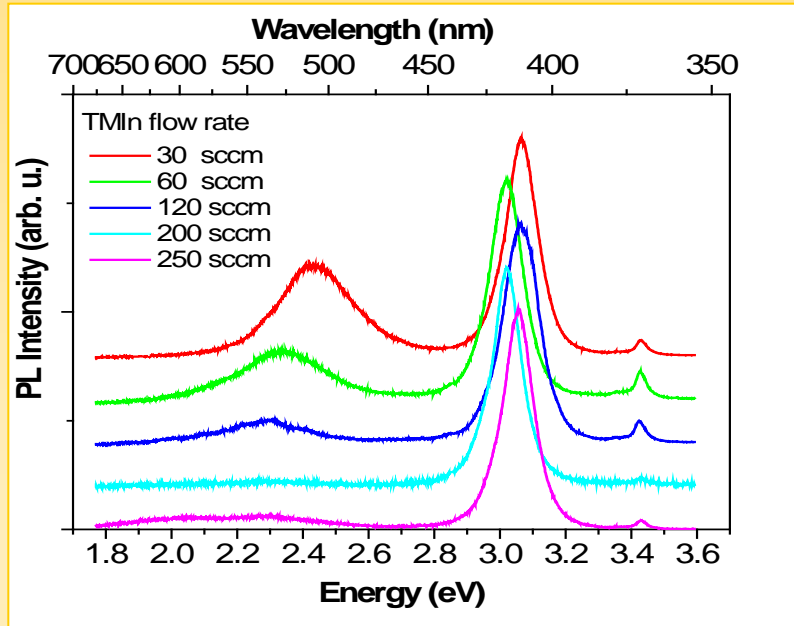
# InGaN material characterization - Photoluminescence



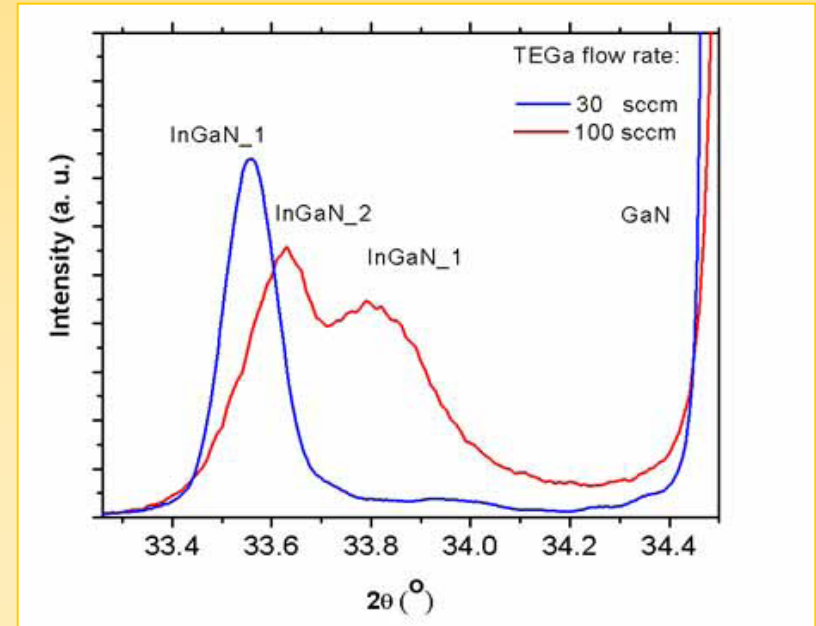
PL emission Vs. [In] from XRD

- InGaN growth consistent with literature
- Observation of secondary phase PL emission
  - → **Phase separation**
- Secondary phase emission intensity increases as [In] increases

# Control of phase separation in MOCVD samples



PL of InGaN grown at variable TMIn flow rate.

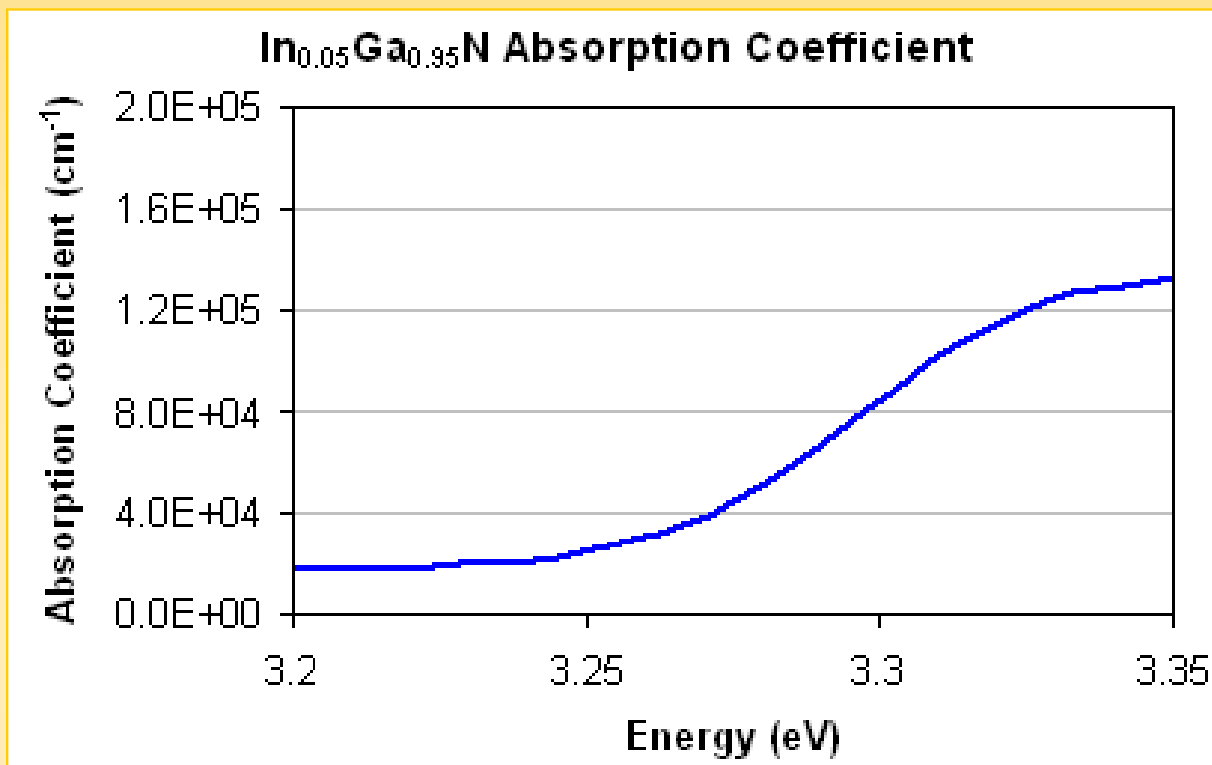


XRD of InGaN grown at variable TEGa flow rates.

➤ **Result:** Phase separation is controlled in MOCVD by:

- Increasing TMIn flow rate → Growth rate
- Moderating TEGa flow rate
- Limiting thickness of epitaxy.

# InGaN optical absorption: Implications



| Thickness    | Absorption |
|--------------|------------|
| 100nm        | 63%        |
| 200nm        | 86%        |
| 300nm        | 95%        |
| 400nm        | 98%        |
| <b>500nm</b> | <b>99%</b> |

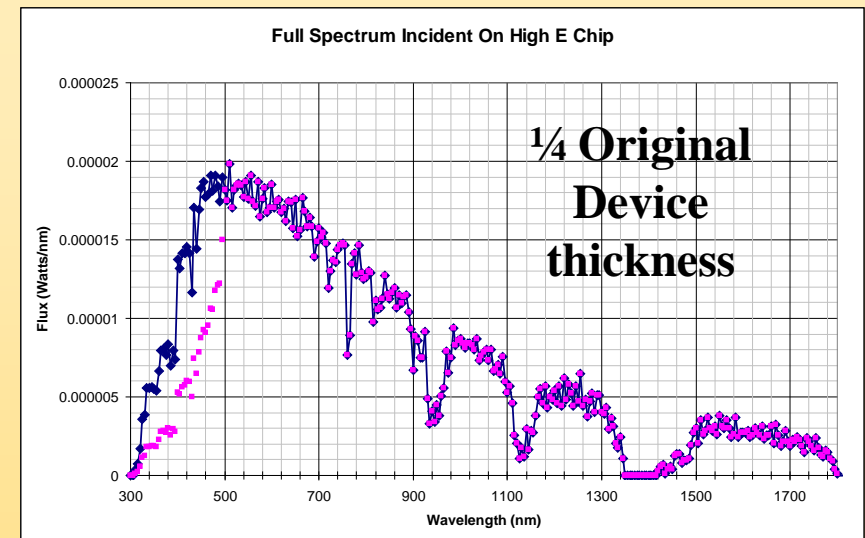
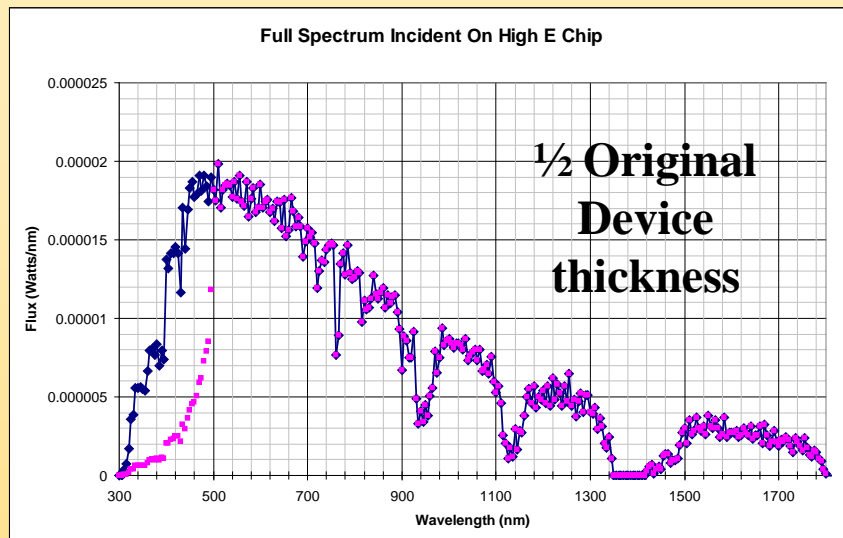
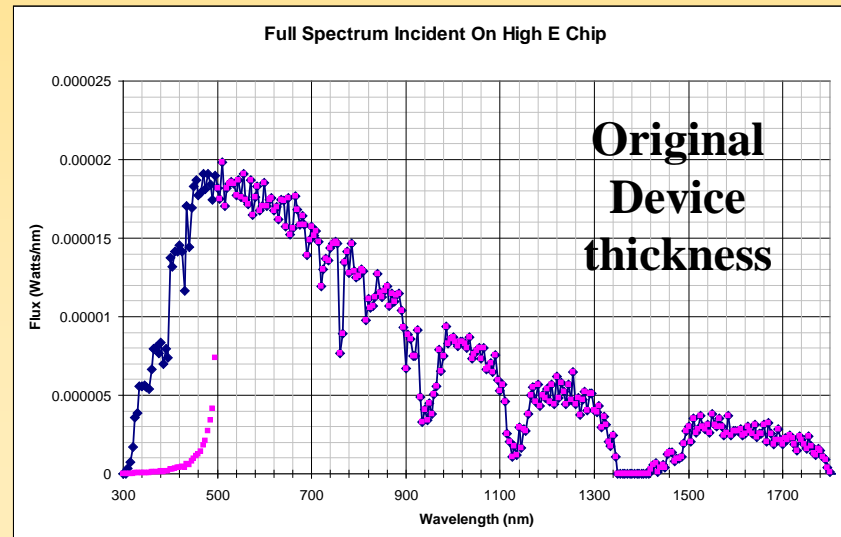
Measured absorption coefficient for In<sub>0.05</sub>Ga<sub>0.95</sub>N sample (EG = 3.3eV)

- High Absorption Coefficient:  $>10^5 \text{cm}^{-1}$  at band edge.
  - Absorption is ~ 10X greater than GaAs.
  - Device thickness ~ 500nm.
    - Complements low diffusion lengths.

# Lessons Learned – Flexibility in Optical Absorption

Device thickness can be tuned for optimal system performance

Blue is full spectrum on High E chip. Magenta is Spectrum expected to be passed by 25% InGaN (2.5 eV)



# P-type doping in InGaN

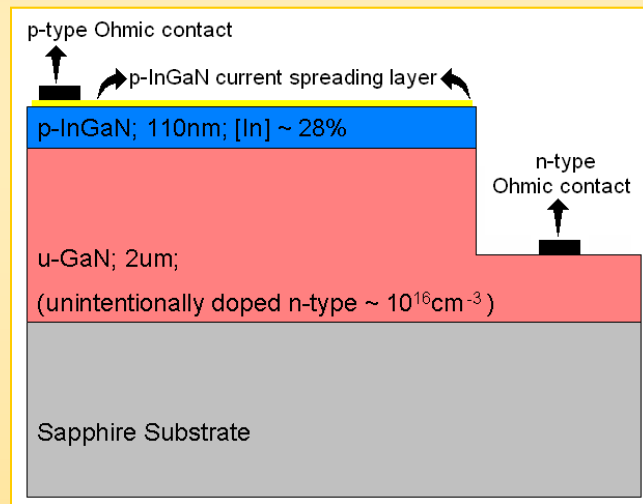
## ➤ Optimize:

1. Material quality,
2. Mg flow rate,
3. Anneal conditions.

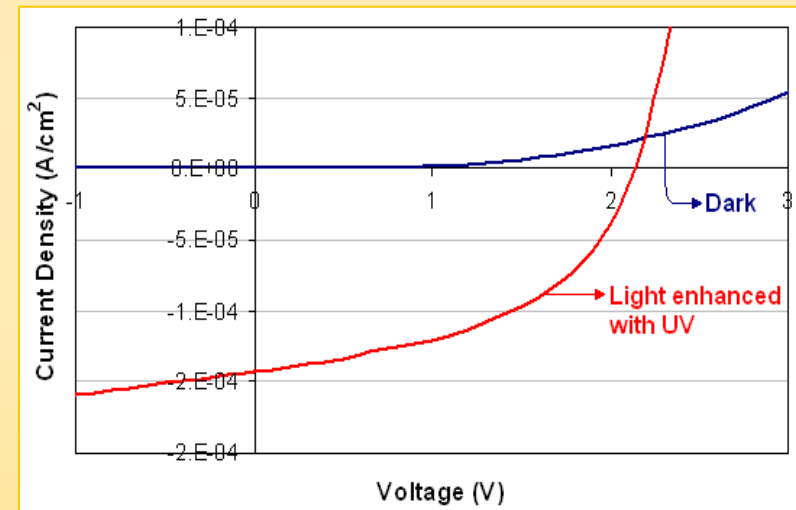
## ➤ Material result:

- [In] = 15% →  $10^{19} \text{ cm}^{-3}$
- [In] = 28% →  $10^{18} \text{ cm}^{-3}$

## ➤ High p-type doping also demonstrated in solar cell:



Test device for p-type  $\text{In}_{0.28}\text{Ga}_{0.72}\text{N}$ .

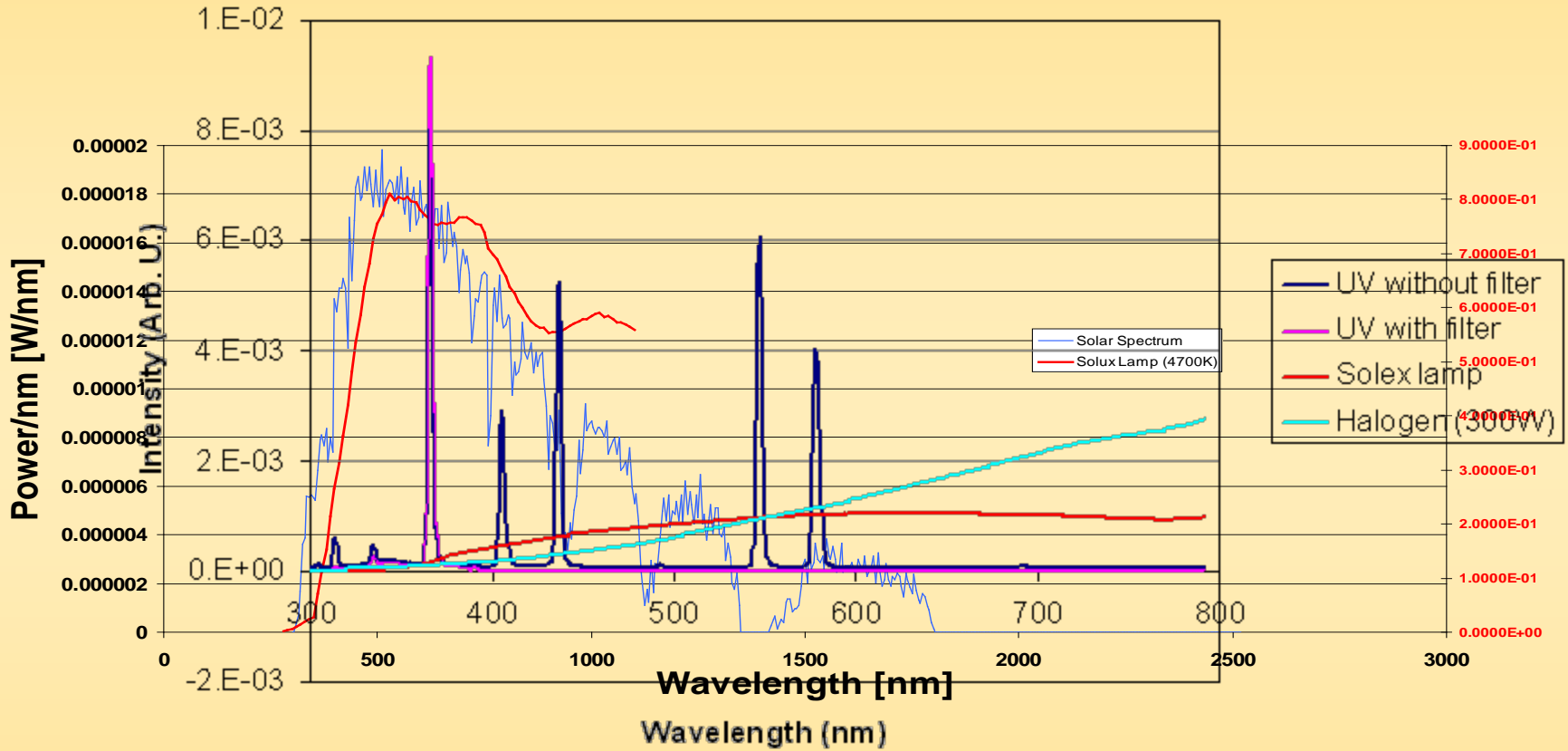


I-V curve for  $\text{In}_{0.28}\text{Ga}_{0.72}\text{N}$  test device.

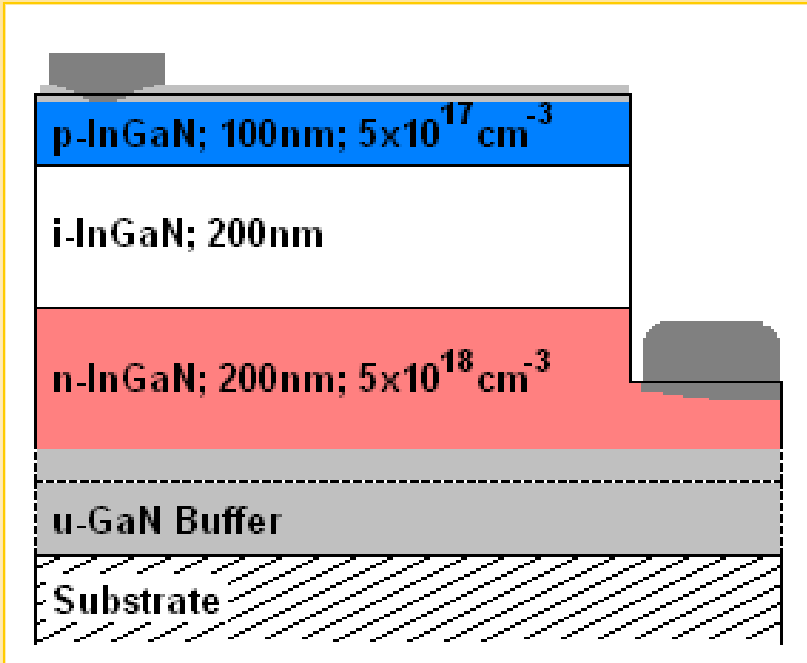
## ➤ Device result: Successful 2.1 $V_{\text{OC}}$ for 2.5 eV device.



# Test Validation Procedure



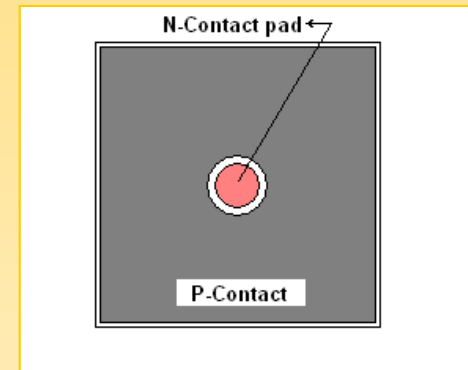
# Baseline solar cell fabrication



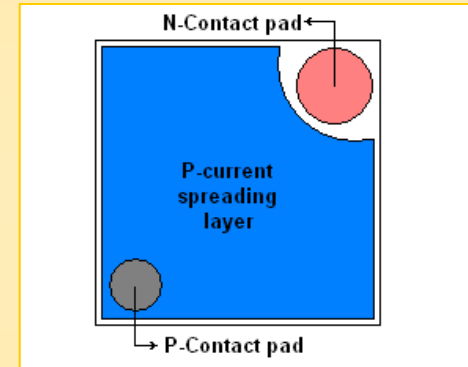
Current spreading layer position

## FINAL DEVICE

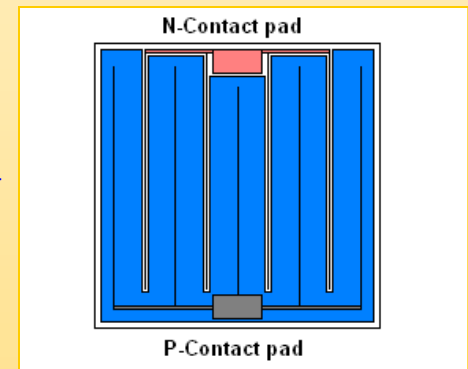
Solid contact device



Transparent contact device

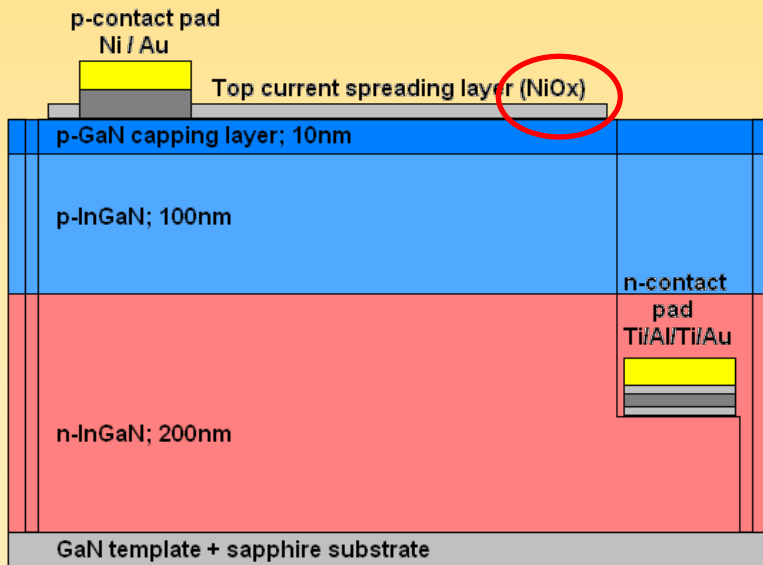


Interdigitated grid contact device

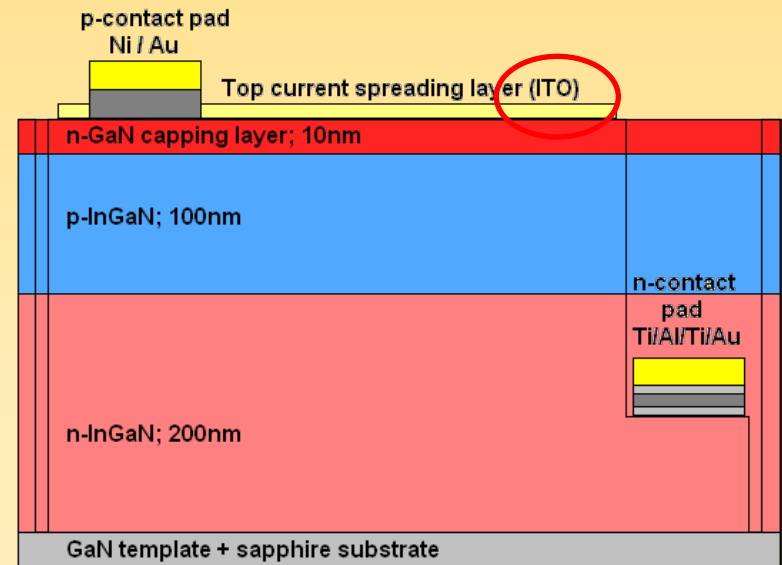


C  
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N  
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# InGaN test solar cell fabrication



**Fabricated solar cell with p-cap.**

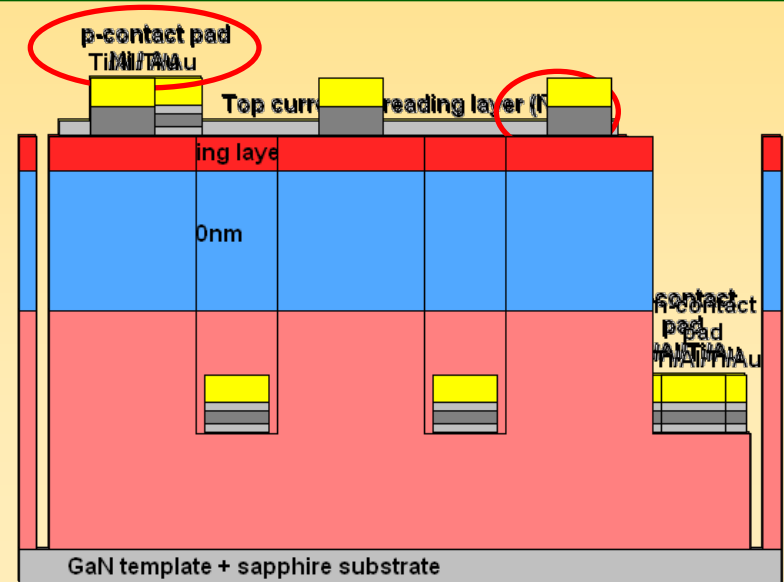
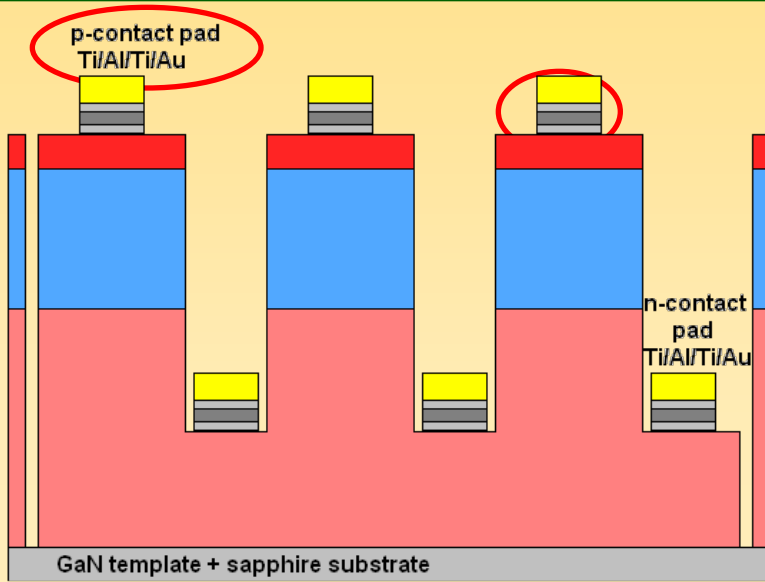


**Fabricated solar cell with n-cap.**

- $\text{NiO}_x$  is used for Ohmic contact to p-GaN cap layer.
- ITO is used for Ohmic contact to n-GaN cap layer.
- Additional contacting schemes for n-GaN cap layer are investigated...

# Contacting schemes for n-GaN cap layer

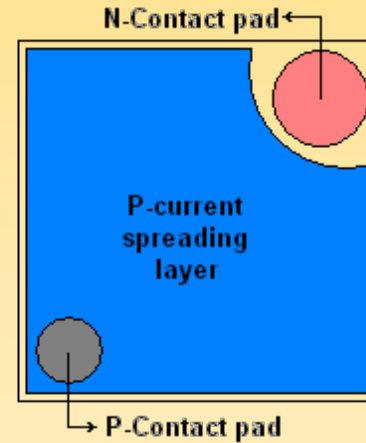
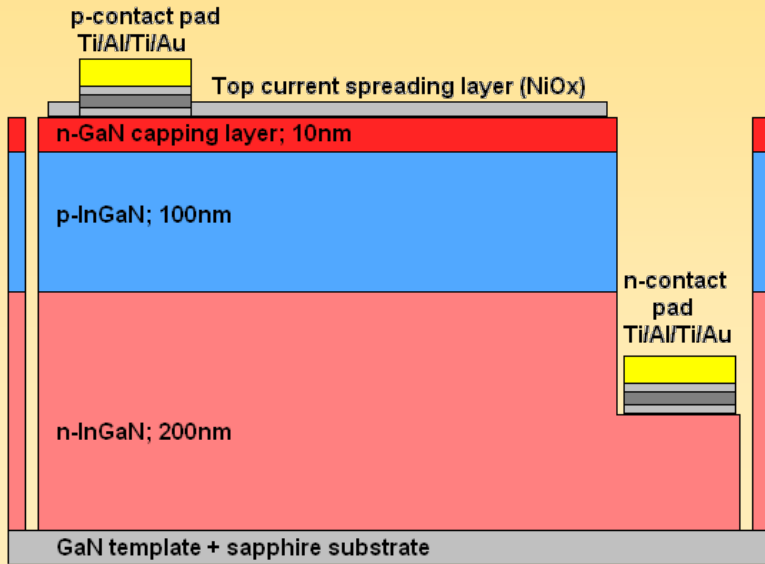
Current-spreading contact.



Grid contact.

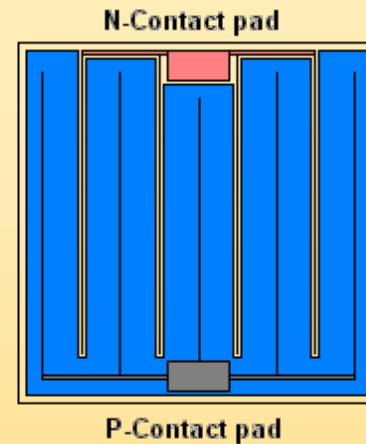
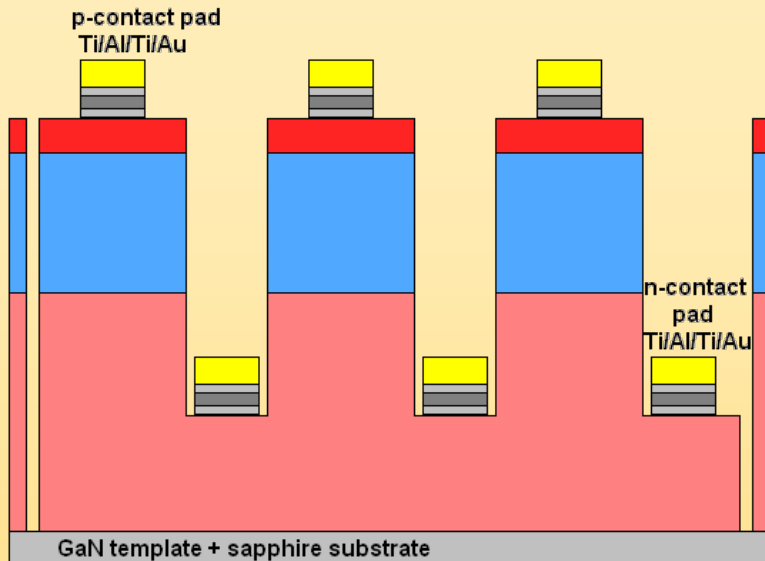
# Fabricated device structures

Current-spreading contact



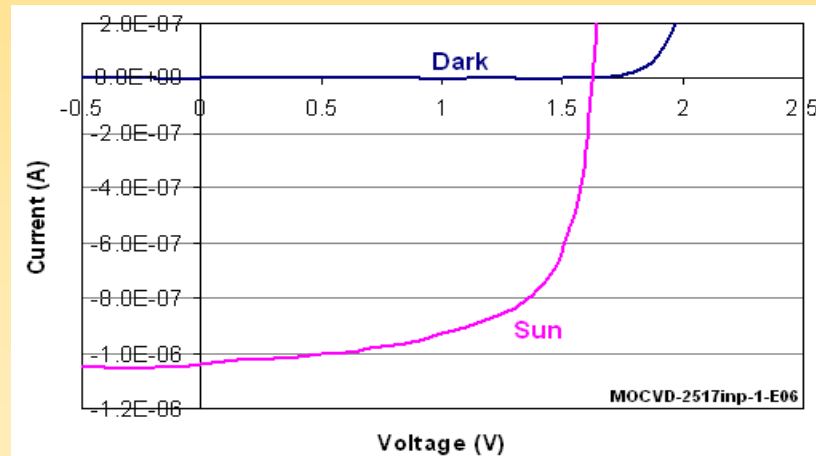
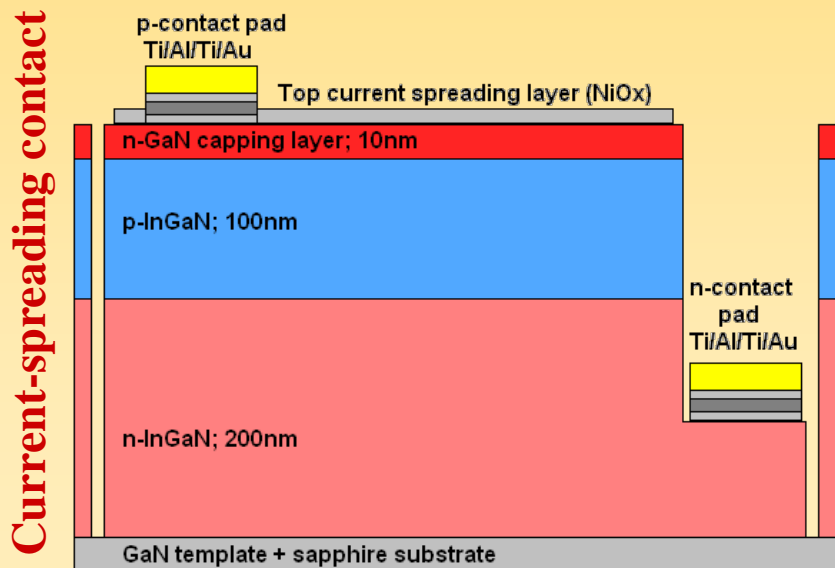
Device size: 1 mm<sup>2</sup>, 9 mm<sup>2</sup>, 25 mm<sup>2</sup>

Grid contact



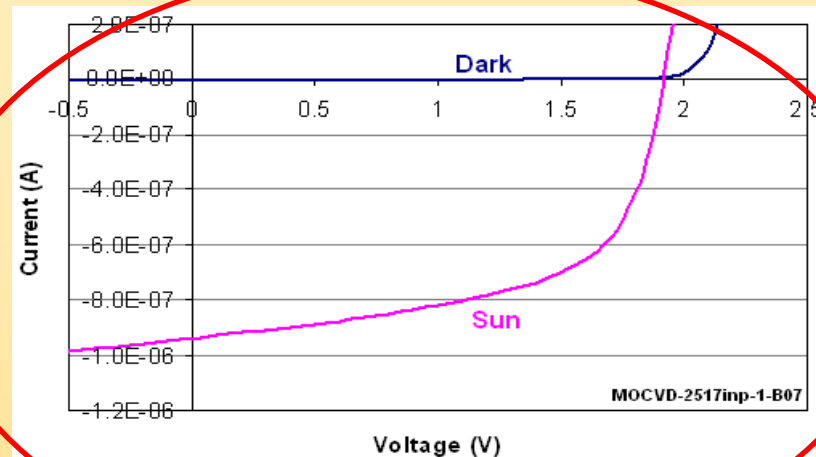
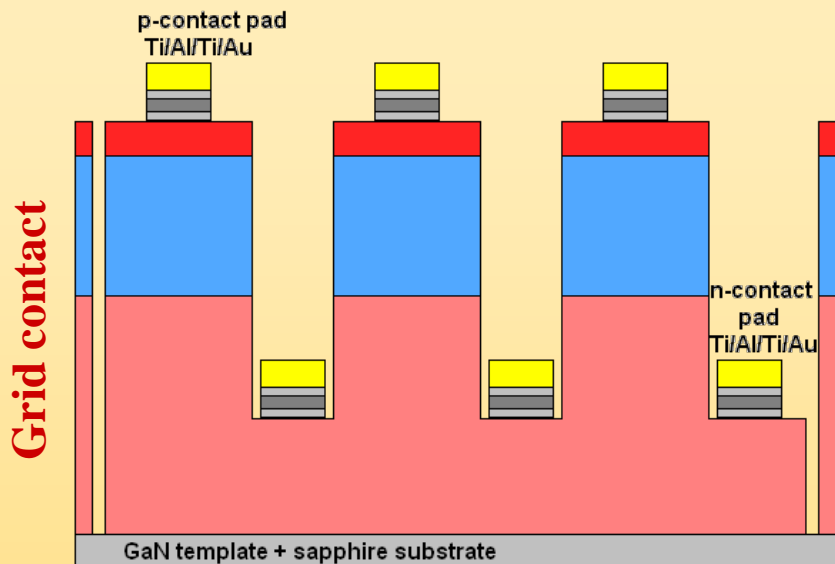
Device size: 1 mm<sup>2</sup>, 9 mm<sup>2</sup>, 25 mm<sup>2</sup>

# I-V characteristics: Best devices



**Voc = 1.7V;**

**FF = 61.3%**

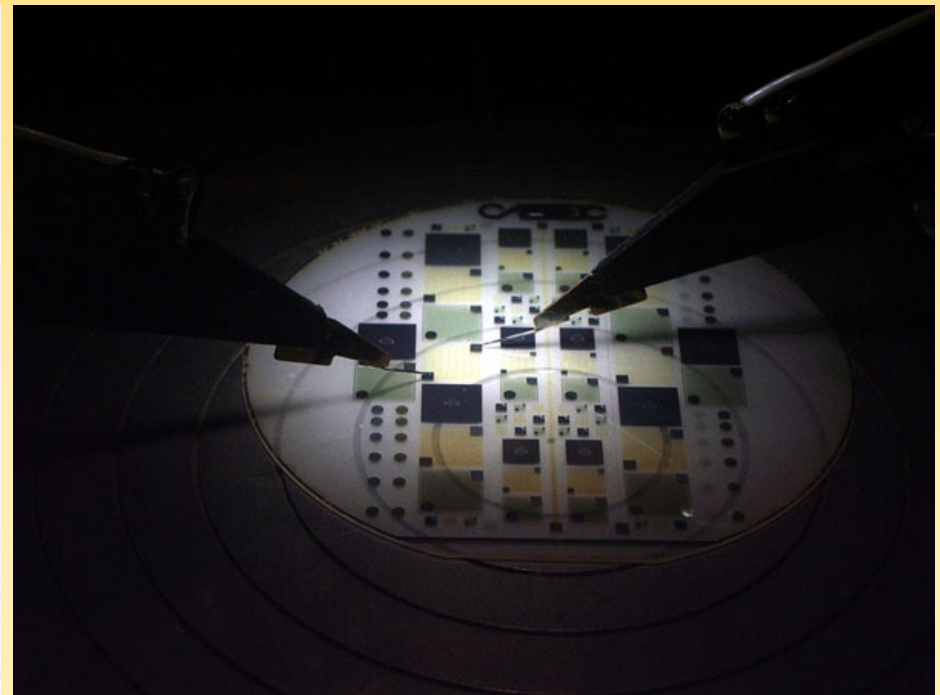


**Voc = 1.95V;**

**FF = 57.3%**



# Test I-V setup



**Fabricated InGaN solar cells under test.**

**I-V setup and test InGaN solar cell indicating a  $V_{OC}$  of 1.86V under 1 Sun.**



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# III-Nitrides for Thermoelectric Applications

Electrical and Computer Engineering

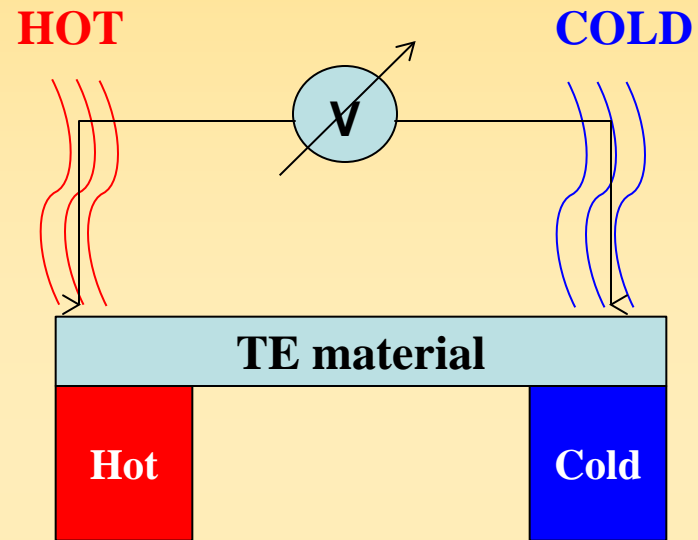


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Electrical and Computer Engineering

# Thermoelectric (TE) Effect

- Temperature difference induces a voltage difference, the Seebeck voltage
- $S = -\Delta V / \Delta T$
- Seebeck coefficient  $S < 0$  for n-type materials
- $S > 0$  for p-type materials



**$ZT = (S^2\sigma/\kappa)T = \text{“Thermoelectric Figure of Merit”}$**

$S =$  Seebeck coefficient

$\sigma =$  Electrical conductivity

$\kappa =$  Thermal conductivity  $= \kappa_e + \kappa_{ph}$

$T =$  Delta Temperature

# TE Equations: A Function of Carrier Concentration

## The Electrical Conductivity

$$1/\rho = \sigma = ne\mu$$

Electrical conductivity =  $\sigma$

Carrier concentration =  $n$

Electron charge =  $e$

Mobility =  $\mu$

## The Thermal Conductivity

$$\kappa = \kappa_e + \kappa_l$$

$$\kappa_e = L\sigma T = ne\mu LT$$

$\kappa$  = thermal conductivity

$\kappa_e$  = electronic thermal conductivity

$\kappa_l$  = lattice thermal conductivity

$L$  = Lorenz factor =  
 $2.4 \times 10^{-8} \text{ J}^2\text{K}^{-2}\text{C}^{-2}$

## The Seebeck Coefficient

$$\alpha = \frac{8\pi^2 k_B^2}{3eh^2} m^* T \left( \frac{\pi}{3n} \right)^{2/3}$$

$\alpha$  = Seebeck coefficient

$k_B$  = Boltzmann constant

$h$  = Planck's constant

$m^*$  = effective electron mass

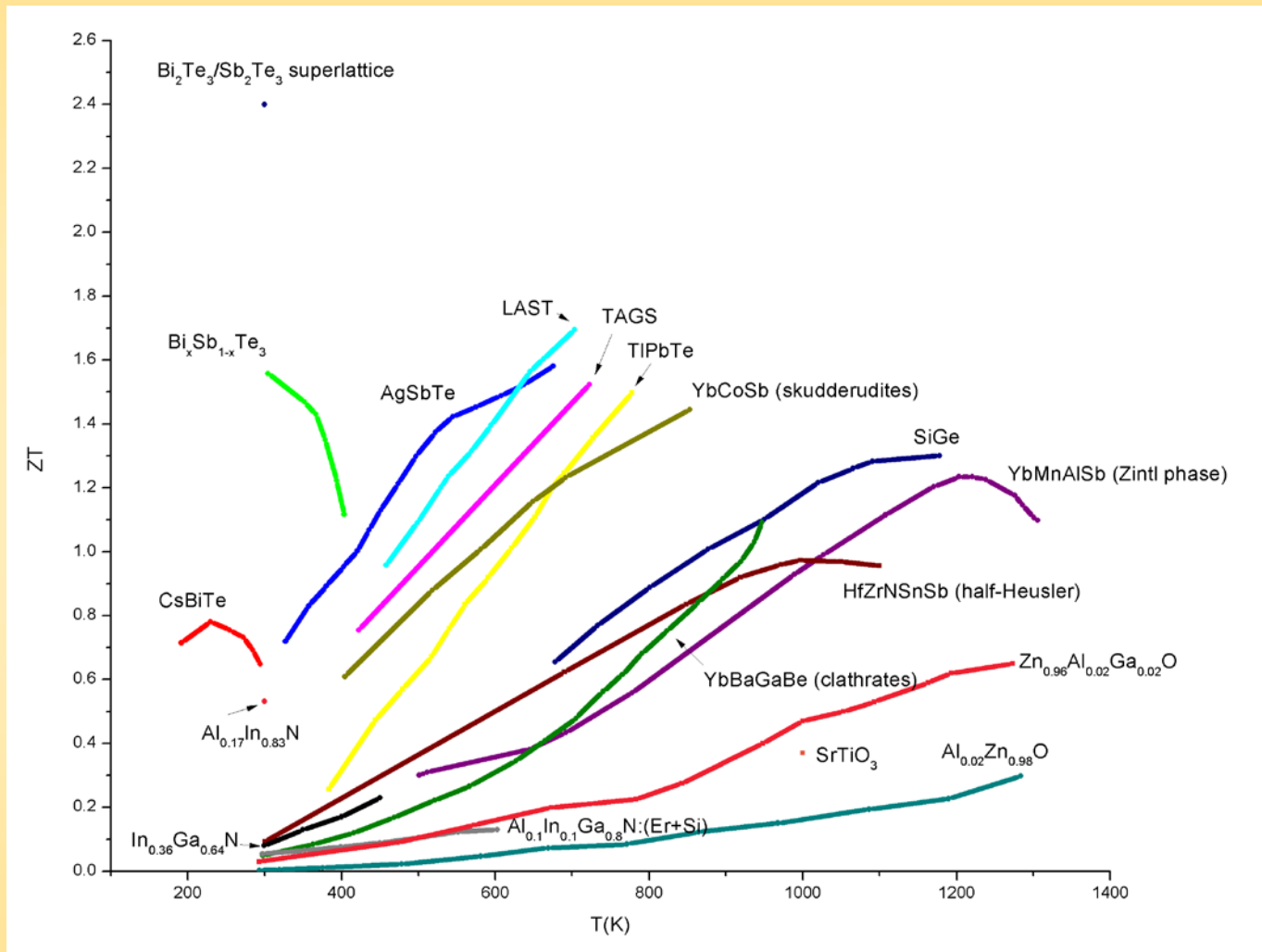
$T$  = operating temperature

**$ZT = (S^2\sigma/\kappa)T = \text{“Thermoelectric Figure of Merit”}$**

**$S^2\sigma = \text{“Power Factor”}$**

J.G. Snyder and E. Toberer Nat. Mat. 7, 105 (2008)

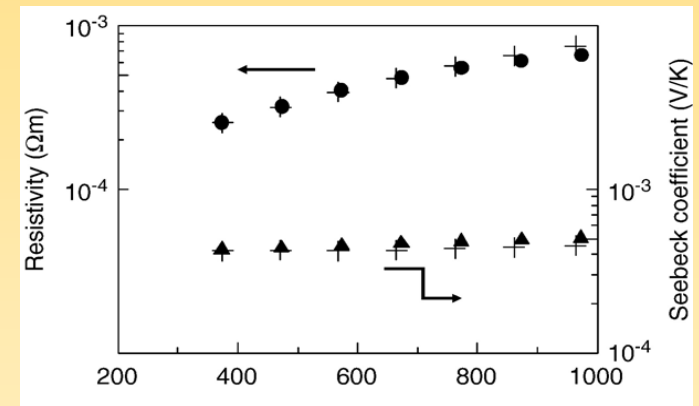
# State-of-the-Art Thermoelectric Materials



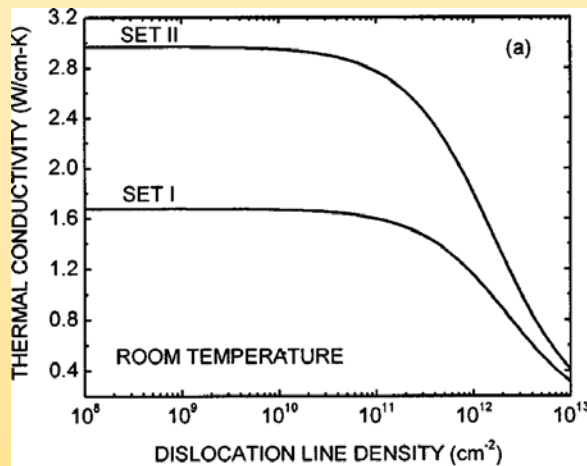
1. J.-F. Li et al. NPG Nature Mat. 2, 152 (2010)
2. M. Ohtaki et al. JAP 79, 1816 (1996)

# GaN: Thermal properties

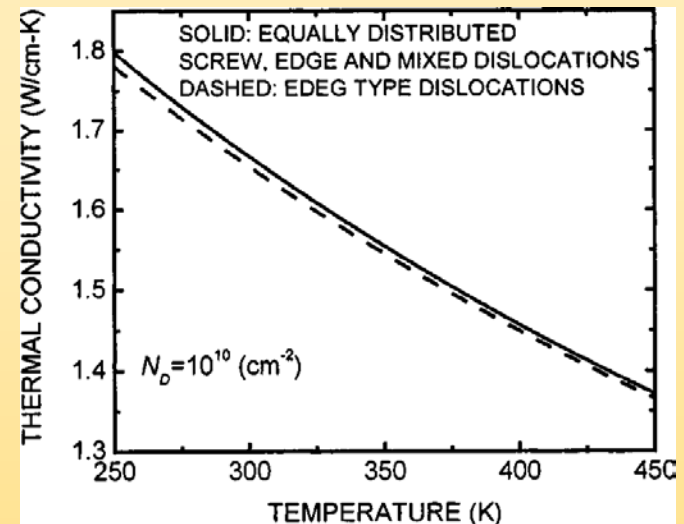
- Seebeck Coefficient is relatively constant up to 1000K
- Thermal Conductivity is decreased with T and doping concentration
- Piezoelectric acoustic phonons main contributor of thermal conductivity is at 3 orders of magnitude more than the electrical contribution in thermal conductivity



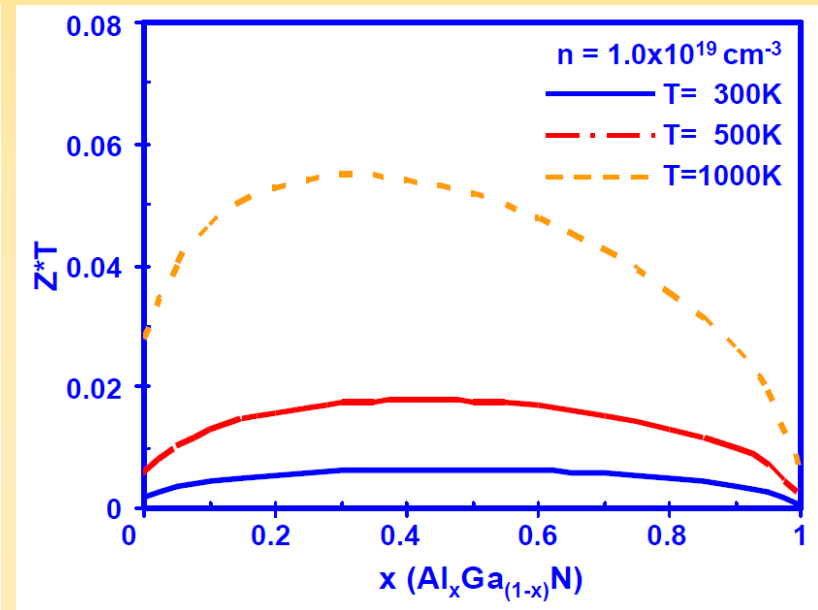
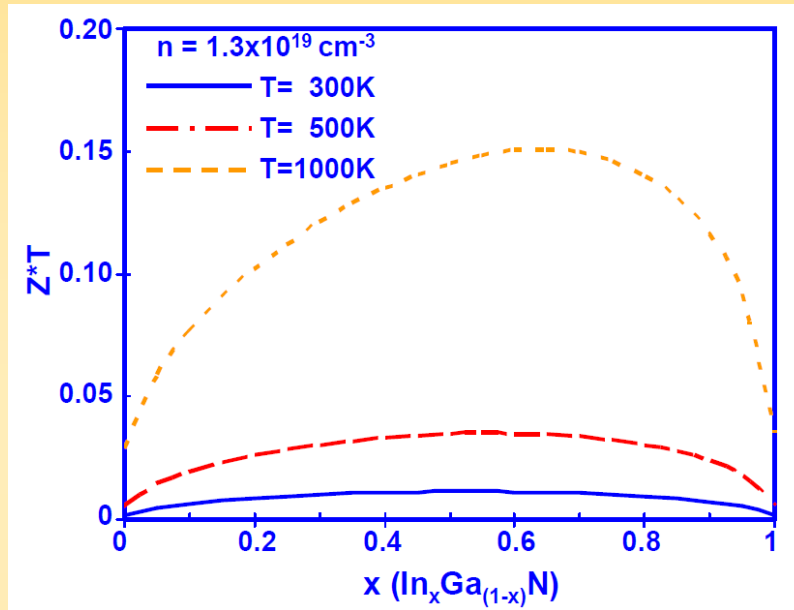
Temperature dependence of electrical resistivity (left ordinate) and Seebeck coefficient (right ordinate) of fr-GaN of experimental values (circles) and calculation values (crosses).



W. Liu & A. Balandin, JAP, 97, 123705 (2005)



# TE Properties of III-Nitrides

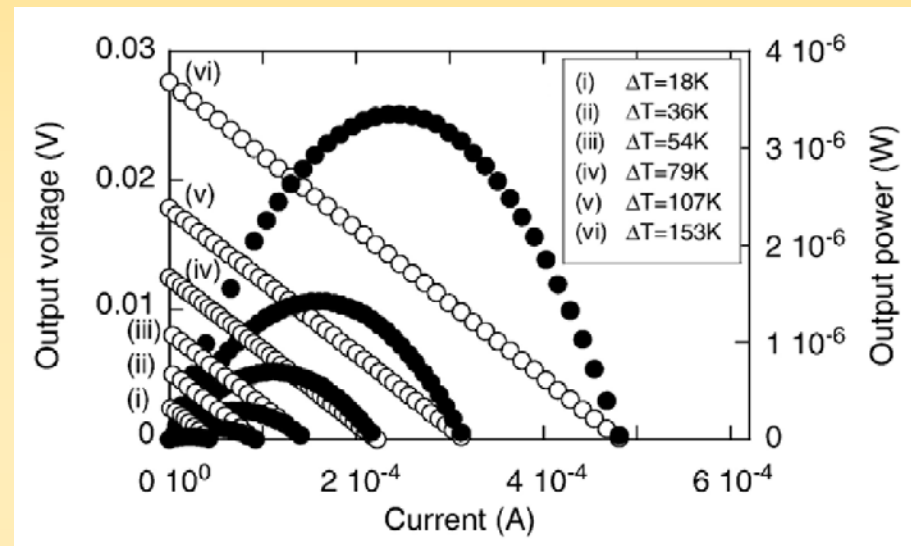
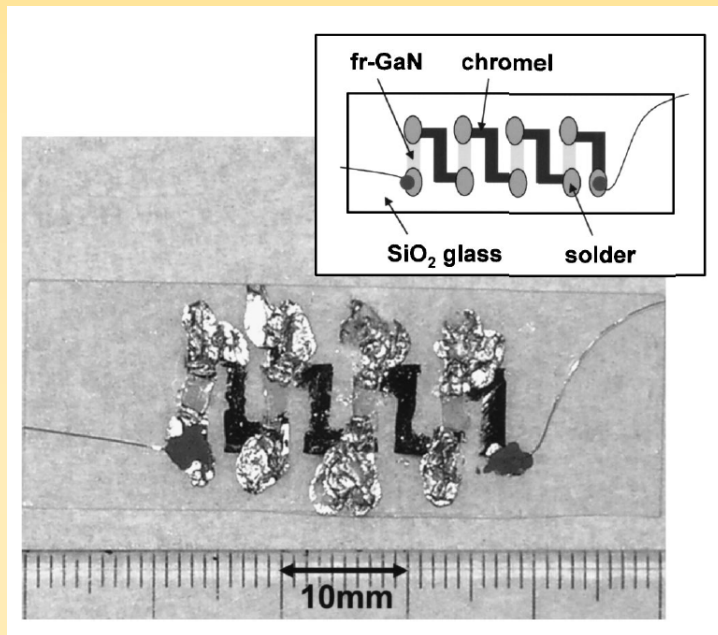


- $Z^*T$  of InGaN is at 3 times higher than AlGaN
- $Z^*T$  of InGaN could reach at 0.15 at 1000K with 60% Indium concentration

Tong et al., Proc. SPIE, vol. 7211, pg. 721103, 2009



# GaN TE Generator



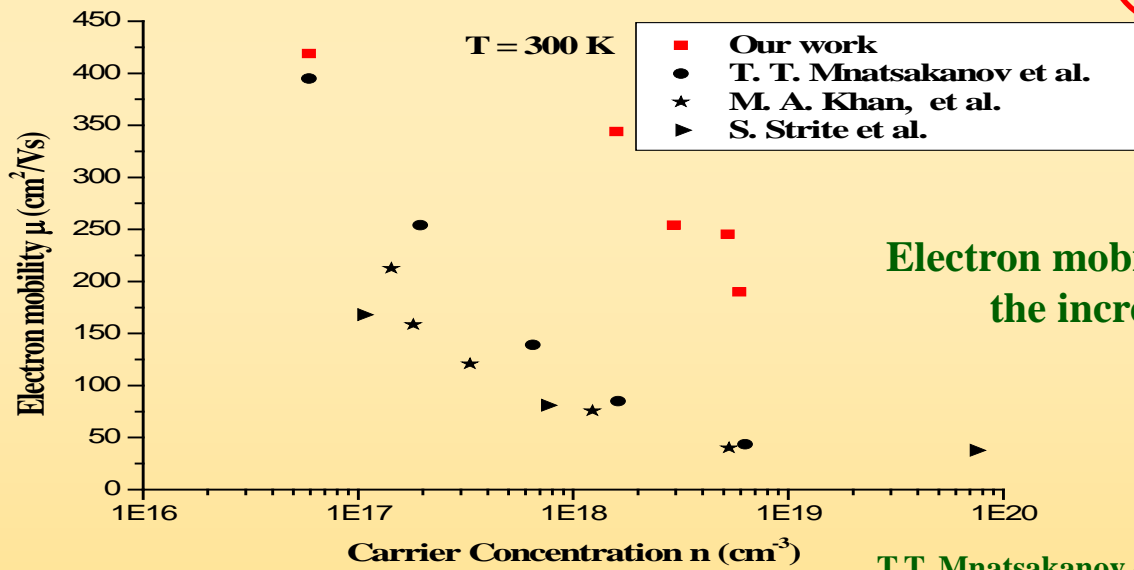
## Crude TE generators made from free-standing GaN (HVPE)

Yamaguchi et al., APL, vol. 86, pg. 252102, 2005

Kaiwa et al., TSF, vol. 515, pg. 4501, 2007

# Summary of GaN Data

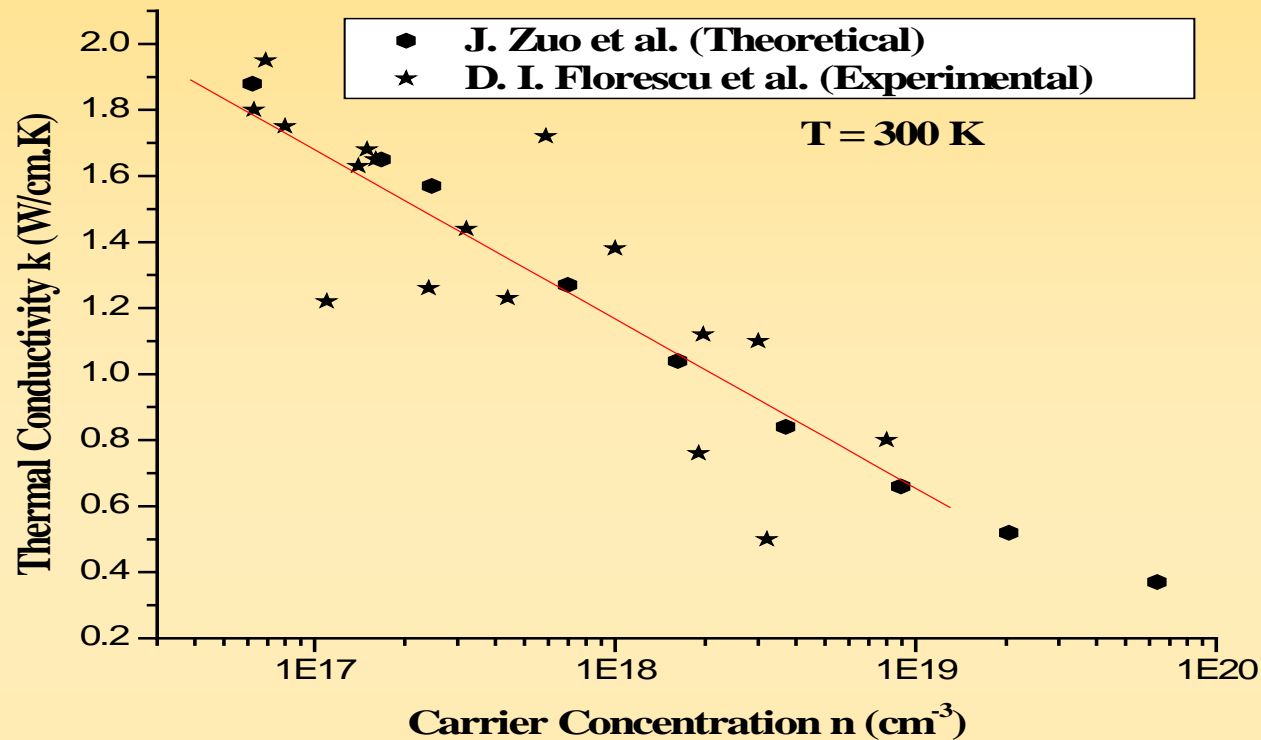
| Material | $\mu$ (cm <sup>2</sup> /(Vs)) | n or p (cm <sup>-3</sup> ) | $\sigma$ (1/( $\Omega$ cm)) | S ( $\mu$ V/K) | Power Factor (x10 <sup>-4</sup> W/m <sup>2</sup> ·K) |
|----------|-------------------------------|----------------------------|-----------------------------|----------------|--|
| GaN      | 419                           | -5.91E+16                  | 3.97                        | -304           | 0.37   |
| GaN:Mg   | 10.43                         | 1.55E+17                   | 0.26                        | 637            | 0.11   |
| GaN:Si   | 344                           | -1.59E+18                  | 87.87                       | -322           | 9.11   |
| GaN:Si   | 245.3                         | -5.24E+18                  | 205.90                      | -206           | 8.73   |
| GaN:Si   | 254                           | -2.94E+18                  | 119.50                      | -255           | 7.77   |
| GaN:Si   | 190                           | -5.91E+18                  | 180.00                      | -169           | 5.14   |



**Electron mobility in n type GaN decreases with the increase in carrier concentration**

T.T. Mnatsakanov *et al.* Solid. Stat. Elec., 47, 111 (2003)  
M. A. Khan *et al.* Appl. Phys. Lett., 58, 526 (1991)  
S. Strite *et al.* J. Vac. Sci. Tech. 10, 1237(1992)

# Thermal Conductivity vs. Carrier Concentration

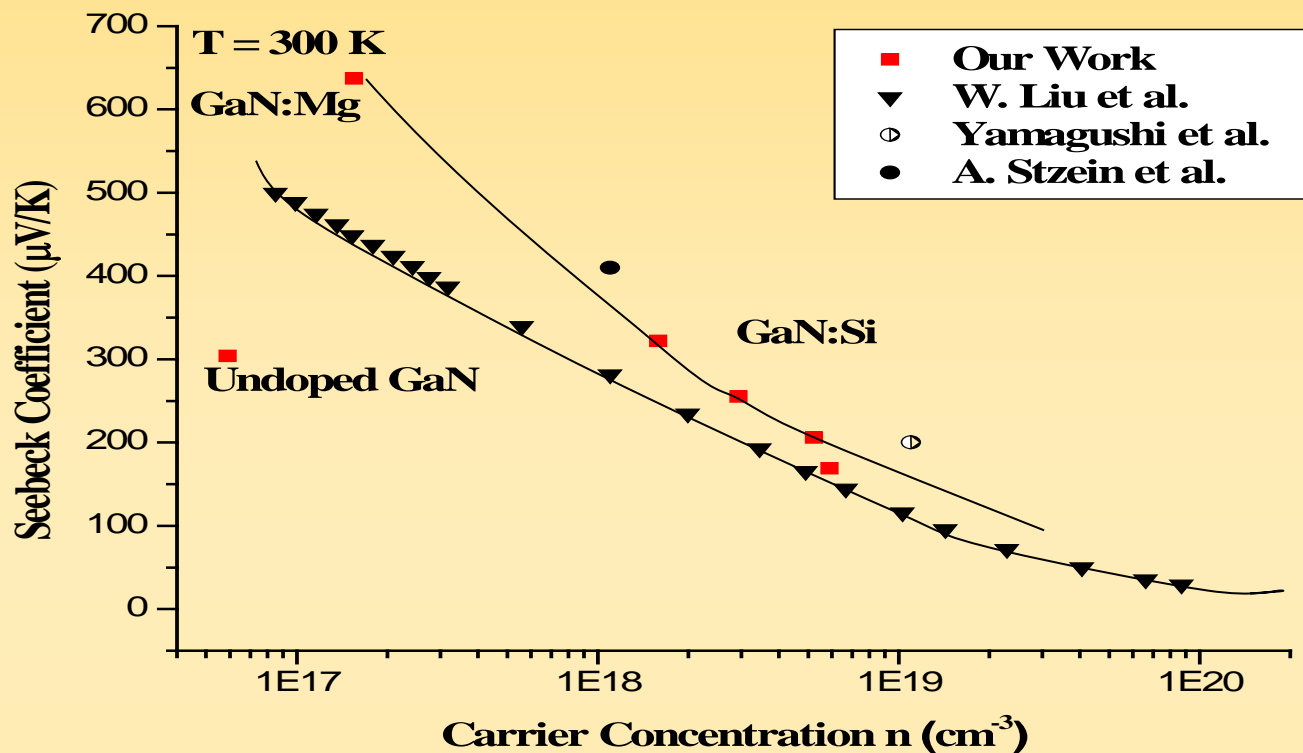


- Theoretical and experimental results follow the same trend
- Values of thermal conductivity were calculated by using first order exponential fit of experimental data. The equation used is  $k = 1.24 \cdot \exp(-n/1.87 \times 10^{18}) + .533$

D.I. Florescu *et al.* J. Appl. Phys. 88, 3295 (2000)

J. Zuo *et al.* J. Appl. Phys. 92, 2534 (2002)

# Seebeck Coefficient vs. Carrier Concentration



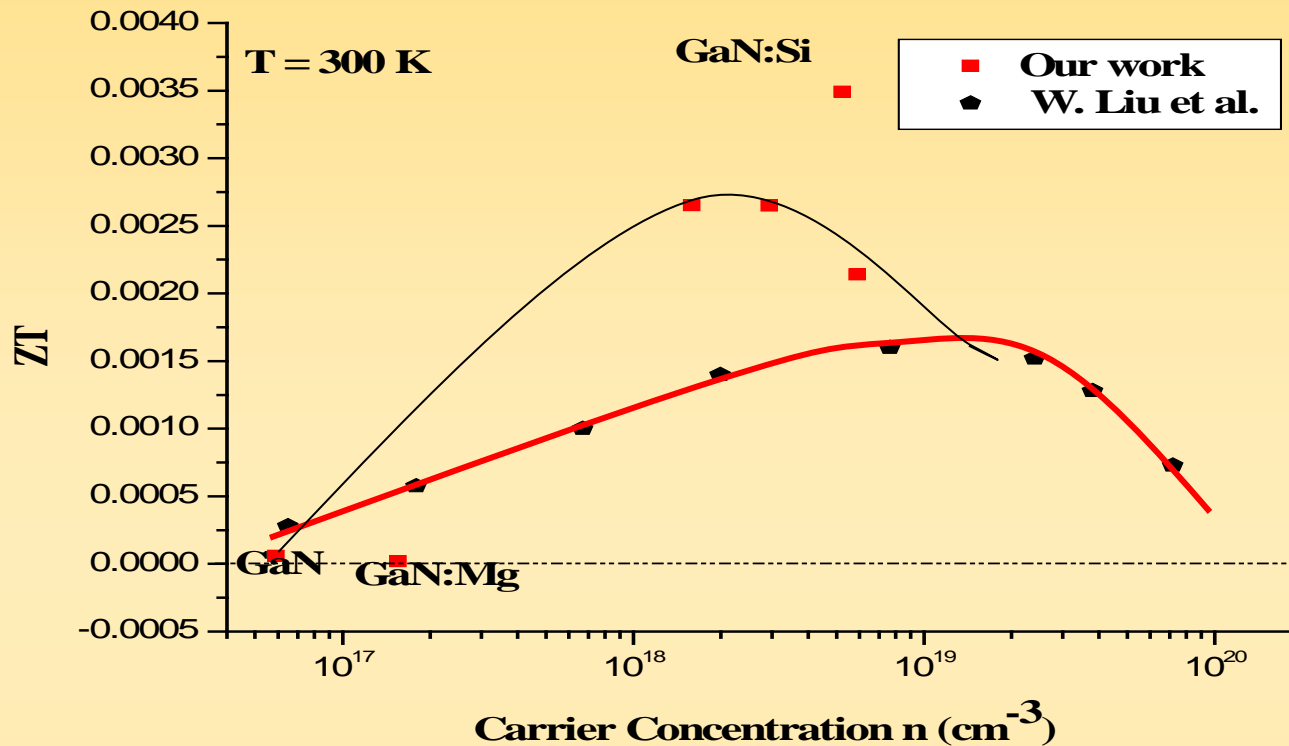
- Seebeck coefficient decreases with the increase of carrier concentration
- P-type doped GaN has higher Seebeck coefficient compared to N-type doped ones
- Seebeck coefficients for GaN:Si follow the trend reported in literature

A. Sztein *et al.* J. Appl. Phys., 110, 123709 (2011)

S. Yamagushi *et al.* Appl. Phys. Lett., 86, 252102 (2005)

W. Liu *et al.* J. Appl. Phys. 97, 123705 (2005)

# Figure of Merit ZT vs. Carrier Concentration

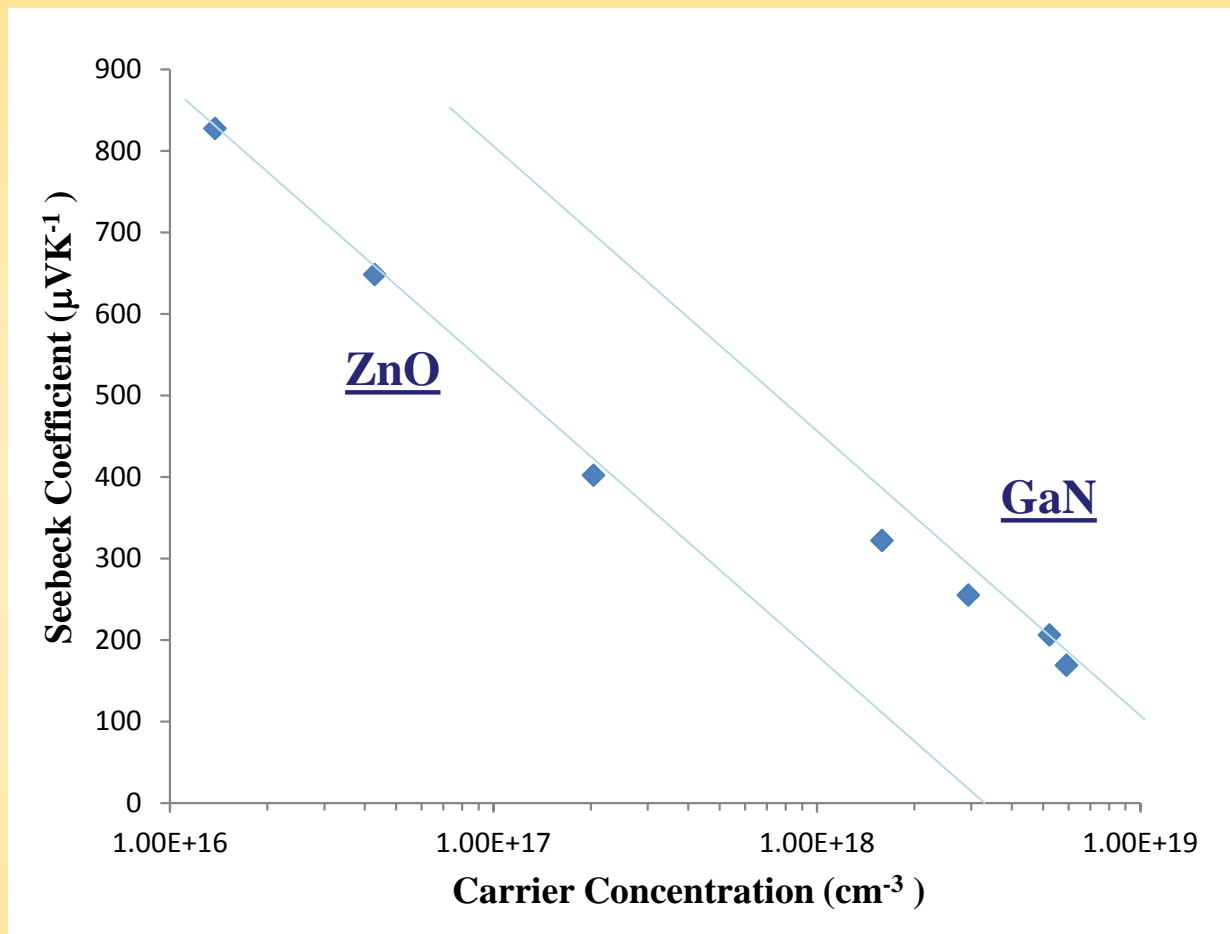


- **Our ZT values for GaN:Si are higher than reported in literature**
- **Higher Seebeck coefficient does not compensate for very low electrical conductivity of GaN:Mg**

D.I. Florescu *et al.* J. Appl. Phys. 88, 3295 (2000)

W. Liu *et al.* J. Appl. Phys. 97, 123705 (2005)

# Comparison of GaN and ZnO results



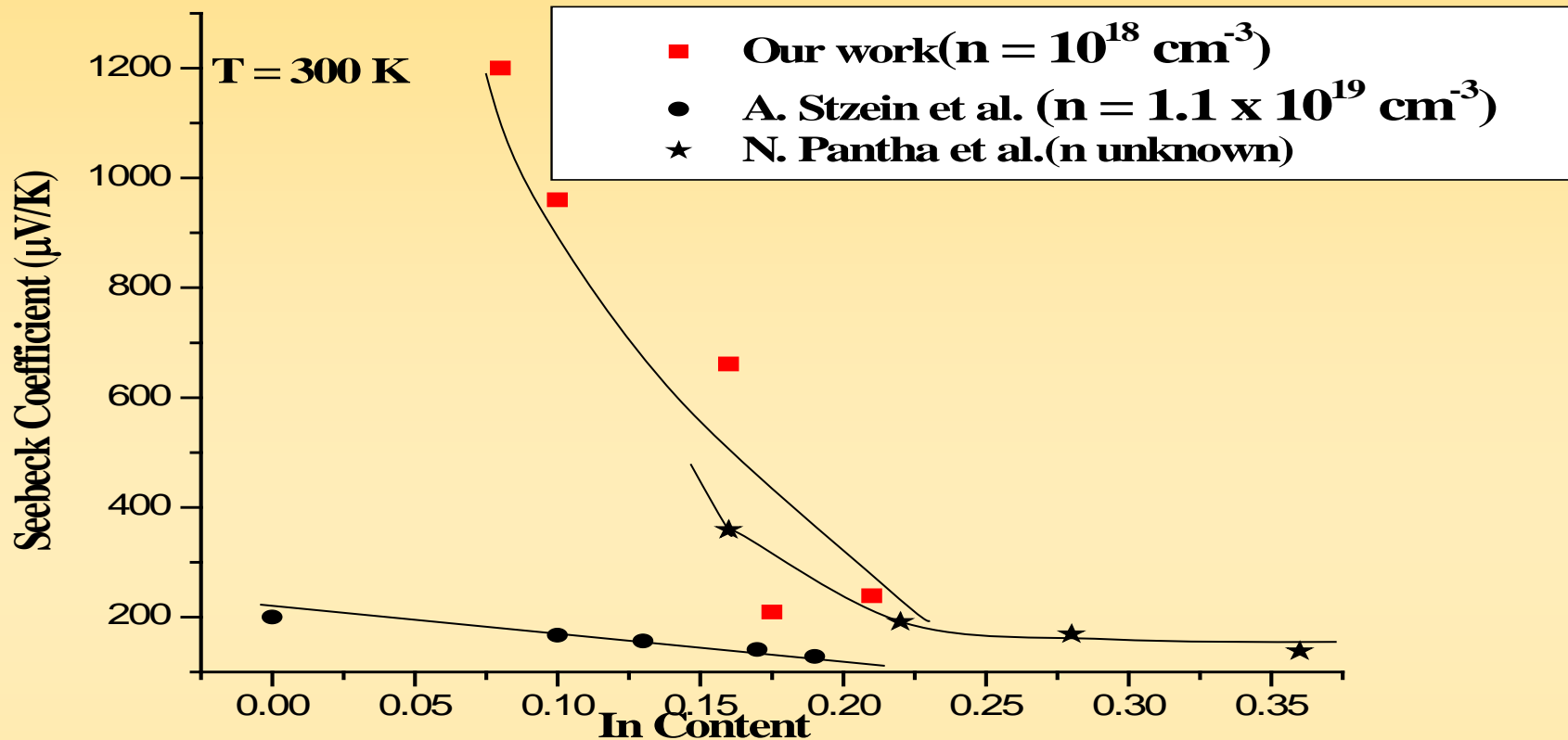
# Summary of InGaN Data

| Material                                   | $\mu$ (cm <sup>2</sup> /Vs) | n or p (cm <sup>-3</sup> ) | $\sigma$ (1/( $\Omega$ cm)) | XRD peak (°) | XRD FWHM (arcsec) | S ( $\mu$ V/K) | Power Factor ( $\times 10^{-4}$ W/m-K) |
|--|-----------------------------|----------------------------|-----------------------------|--------------|-------------------|----------------|--|
| In <sub>0.07</sub> Ga <sub>0.93</sub> N    | 15.55                       | 1.53E+18                   | 3.821                       | 17.0876      | 233.64            | 4050           | 62.67                                  |
| In <sub>0.08</sub> Ga <sub>0.92</sub> N:Mg | 1.22                        | 1.41E+18                   | 0.2747                      | 16.9697      | 240.84            | 1200           | 0.40                                   |
| In <sub>0.1</sub> Ga <sub>0.9</sub> N      | 597.20                      | 1.24E+18                   | 118.8                       | 16.8882      | 297.47            | -960           | 109.49                                 |
| In <sub>0.16</sub> Ga <sub>0.84</sub> N    | 110.40                      | 1.82E+18                   | 32.12                       | 16.7296      | 467.17            | -661           | 14.03                                  |
| In <sub>0.175</sub> Ga <sub>0.835</sub> N  | 48.82                       | 6.142E+17                  | 4.80                        | 16.7550      | 648.00            | -209           | 1.57                                   |
| In <sub>0.21</sub> Ga <sub>0.79</sub> N    | 200.90                      | 2.063E+18                  | 66.39                       | 16.5050      | 536.40            | -239           | 3.79                                   |

**Correlation between crystal quality and Seebeck coefficient**



# Seebeck Coefficient vs. Indium Content

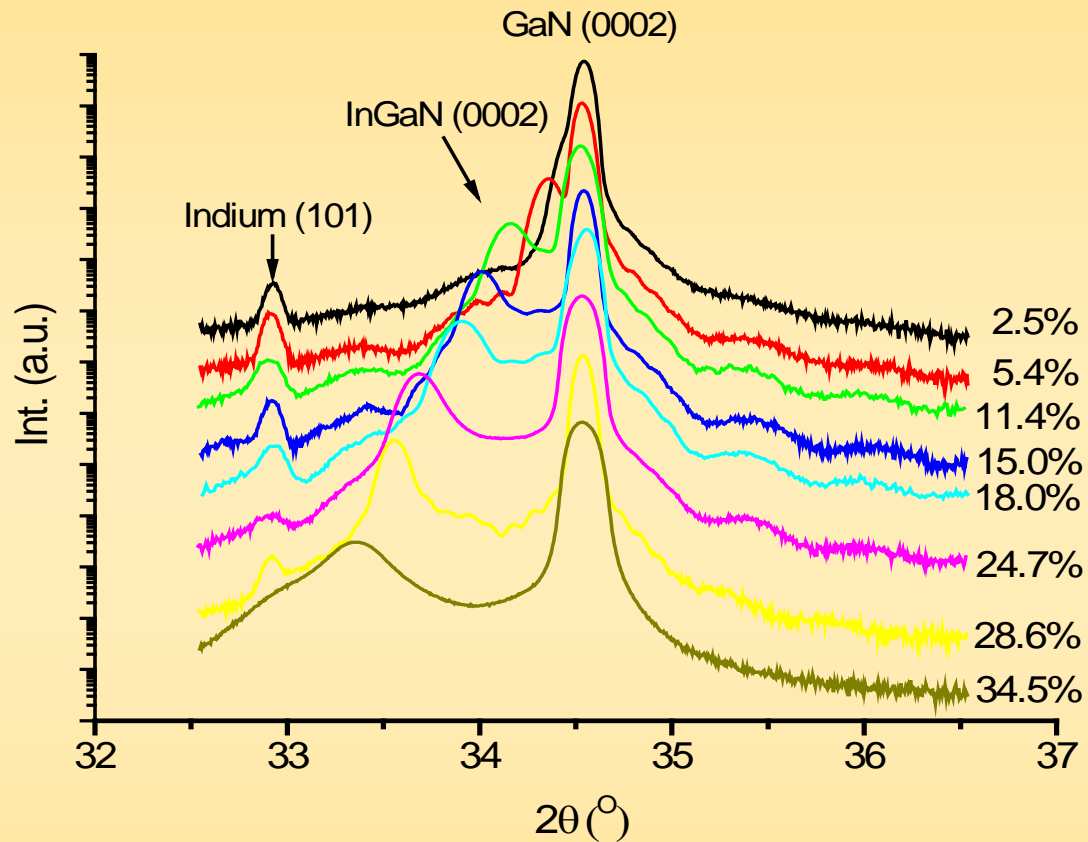


- Seebeck coefficient decreases with the increase in indium content
- Our Seebeck coefficients have higher values reported in literature

N. Pantha, *et al.* Appl. Phys. Lett. 92, 042112 (2008)

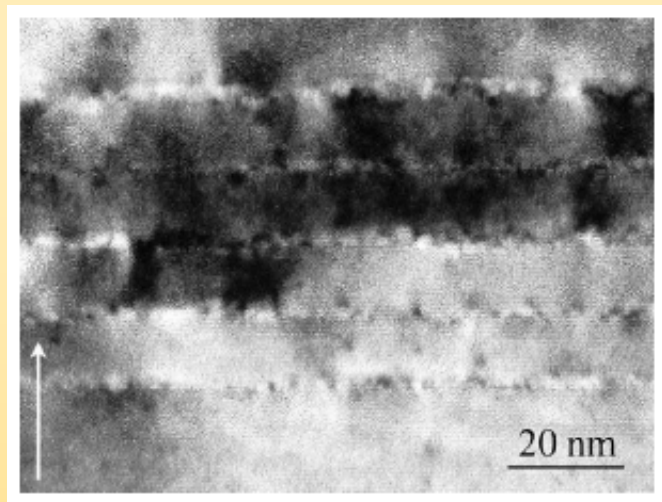
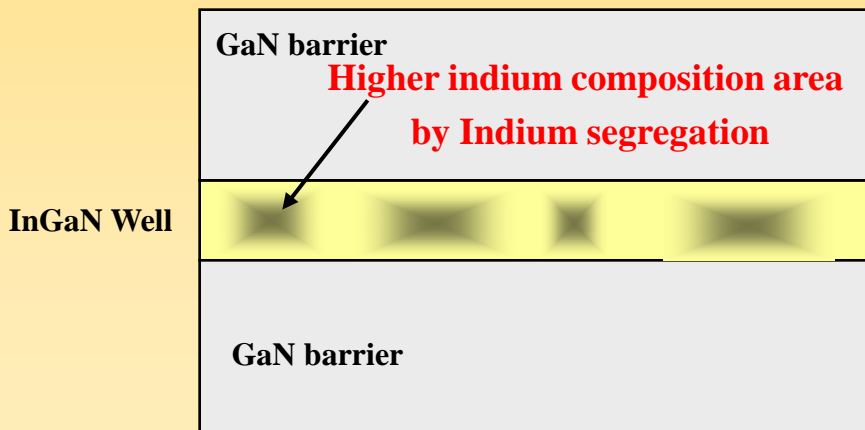
A. Szein, *et al.* J. Appl. Phys. 110, 123709 (2011)

# XRD patterns with different Indium concentration



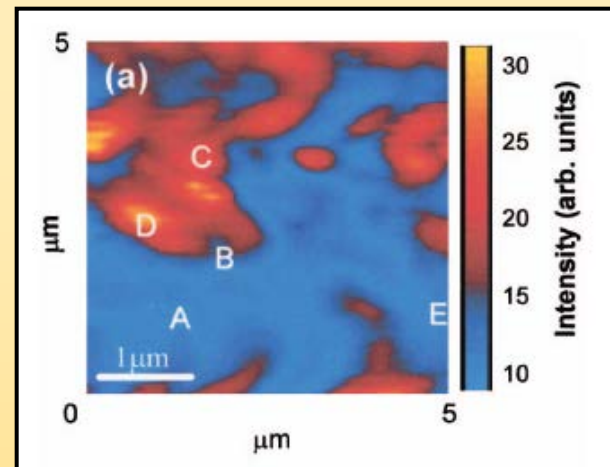
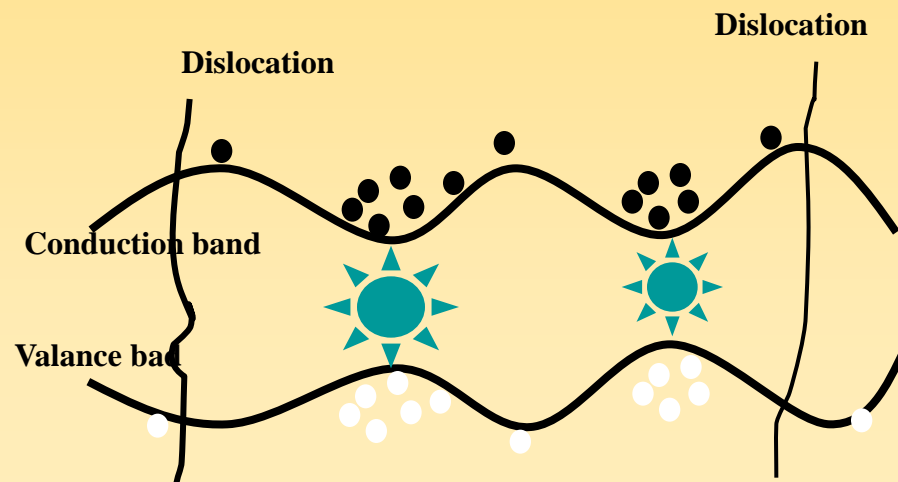
**InGaN shows phase separation with increasing indium content even when attempts are made to minimize it**

# Phase separation in InGaN



TEM image of indium segregated MQW

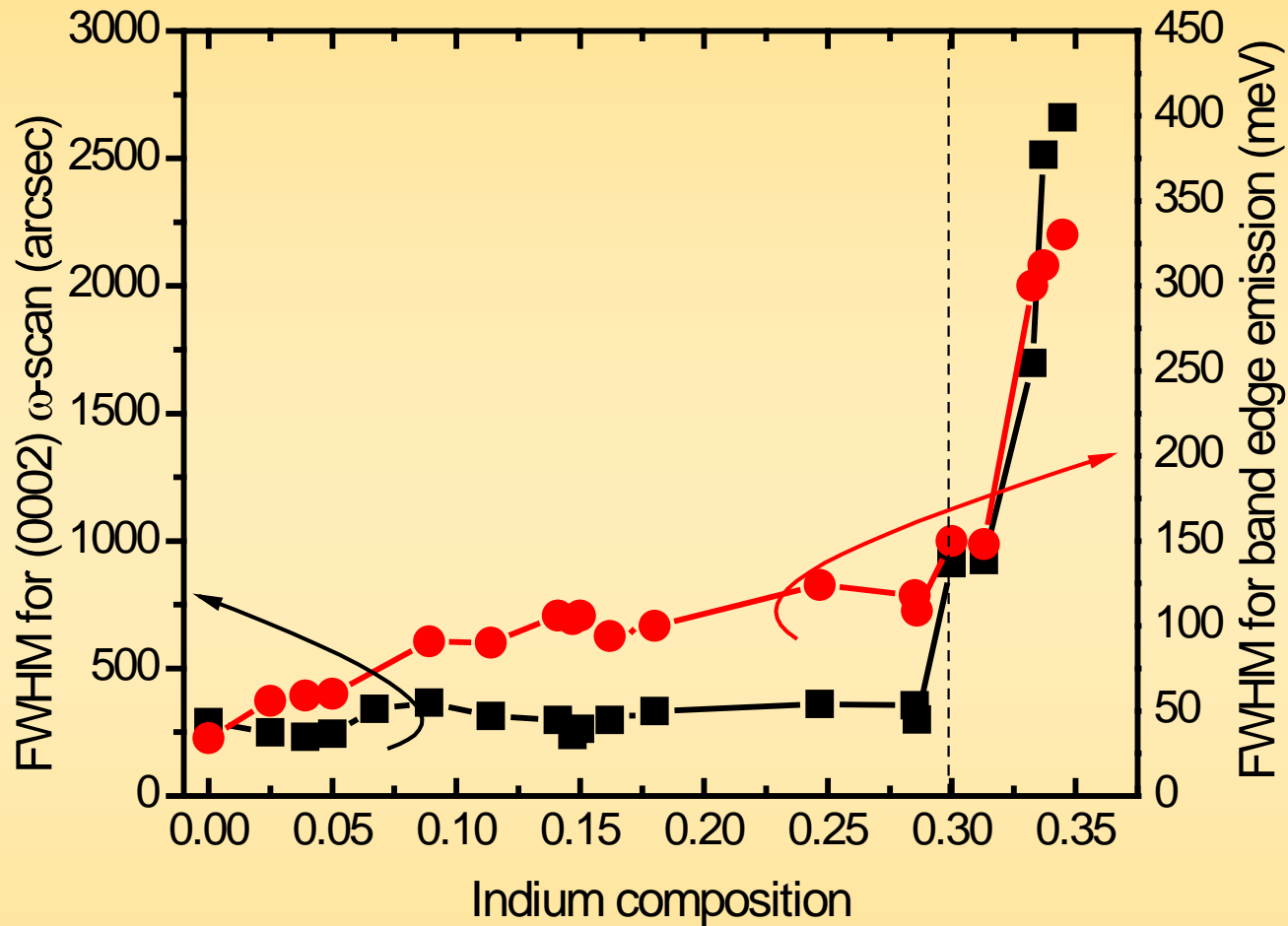
K.Jacobs et al, Journal of Crystal Growth 248(2003) 498



Micro-PL image of MQW

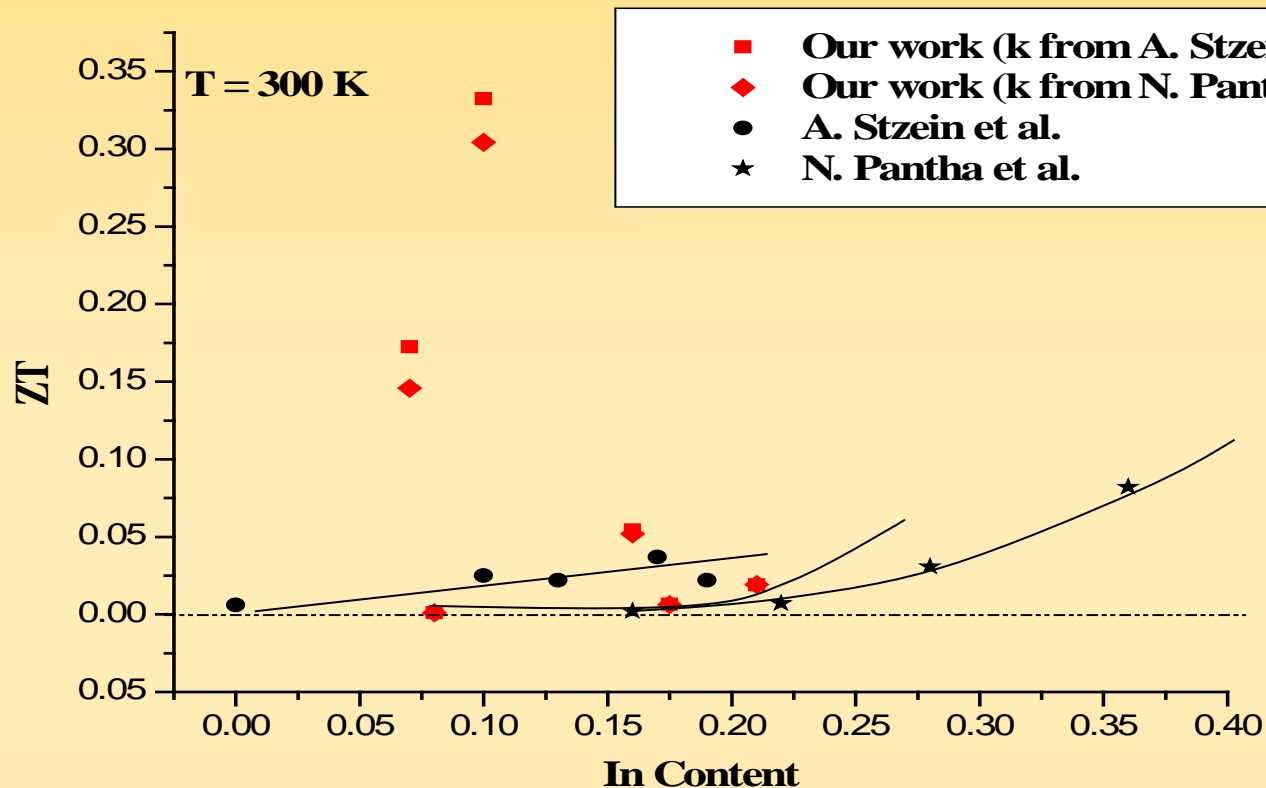
Koichi Okamoto et al. J. Appl.Phys. 98, 064503(2005)

# Crystal quality at different indium composition



**Sharp decrease of crystal quality when In% is > 25-30%**

# Figure of Merit ZT vs. Indium Content



- ZT values are decreasing with the increase in indium content

N. Pantha *et al.* Appl. Phys. Lett. 92, 042112 (2008)

A. Sztein *et al.* J. Appl. Phys. 110, 123709 (2011)



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Electrical and Computer Engineering

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**Wide Band Gap III-Nitride**

**Compound Semiconductor Devices:**

**The Universal Solution for Energy Applications**

**Ian Ferguson**

University of North Carolina at Charlotte

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Charlotte, NC 28223

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