Short-range In-segregation in InGaN and InAlN. Band structure and light emission related effects .

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theory: *'Unipress'*

Department of Physics and Astronomy, University of Aarhus, Denmark

Experiment:

Outline

Info about UNIPRESS (and TopGaN) concerning nitride activity

Lasers and importance of bulk GaN crystals for laser substrates

Band gap in InGaAlN ternary alloys. Absorption vs. Luminescence

Modelling within the short-range In-fluctuation approach

- Band gaps and their pressure coefficients

Alternative results on InGaN layers and InGaN/GaN QWs

Summary

UNIPRESS, Institute of High Pressure Physics of the Polish Academy of Sciences

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Director: Izabella Grzegory

Head of Semicondutors Lab: T. Suski

Polish Academy of Sciences is a corporation of famous professors and an „owner" of research institutions covering all fields. From humanistics to engineering and natural sciences.

UNIPRESS is one of 80 institutes of PAS

UNIPRESS is located in Warsaw (Warszawa) and consists of 7 Labs Largest - Semiconductor Laboratory

Institute of High Pressure Physics, UNIPRESS
Polish Academy of Sciences
One of about 80 research Institutes of PAS

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Research areas:

* physics, optoelectronics: mainly in green-blue-violet spectral region
* electronics: mainly nitride epi-strucures for HEMTs and THz
* nanomaterials: ceramics, metals, superconductors
* biological materials

Untypical (for PAS) structure of research activity

* basic research	- 40%
* applied research	- 40%
* high pressure methods and instrumentation	- 20%

Semiconductor Laser Diodes
Semiconductor families used

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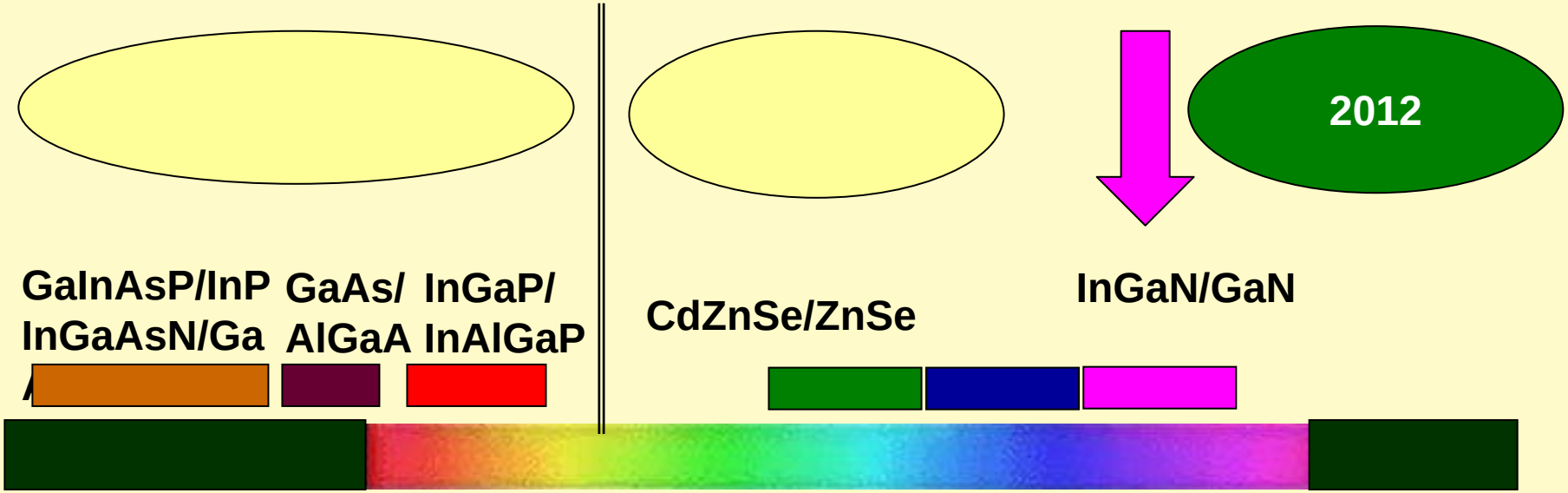

Choice of GaN, InN, AlN and their alloys for construction of green, blue and ulraviolet Light Emitting Diodes and Laser Diodes

Second semiconductor system after Silicon

GaN-AlN-InN properties
Important aplications

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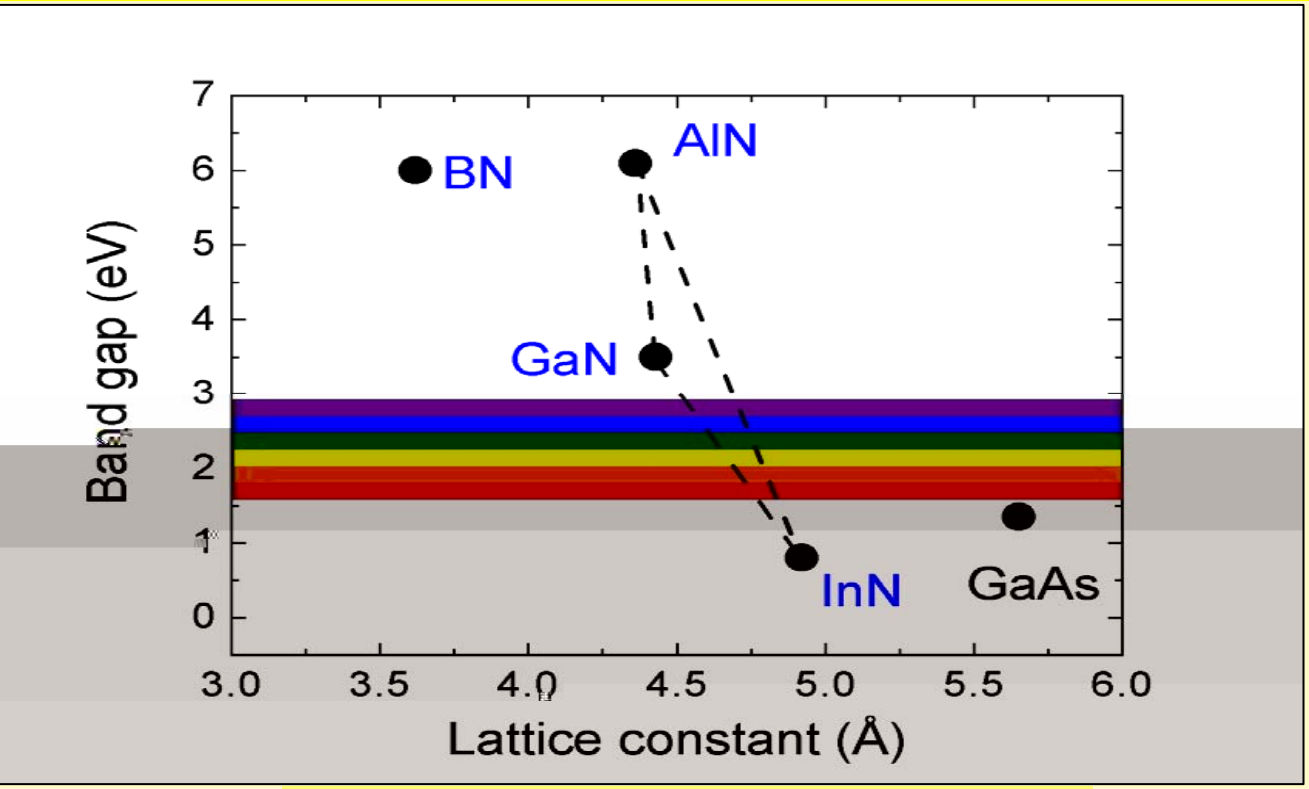

A BEST MOCVD GaN
on sapphire **Large lattice mismatch leads to misfit dislocations**

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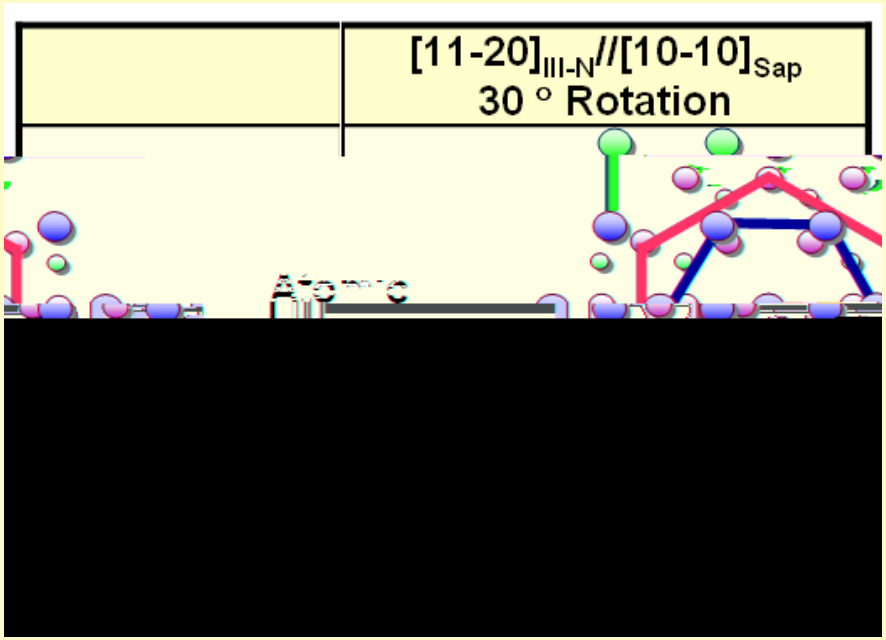

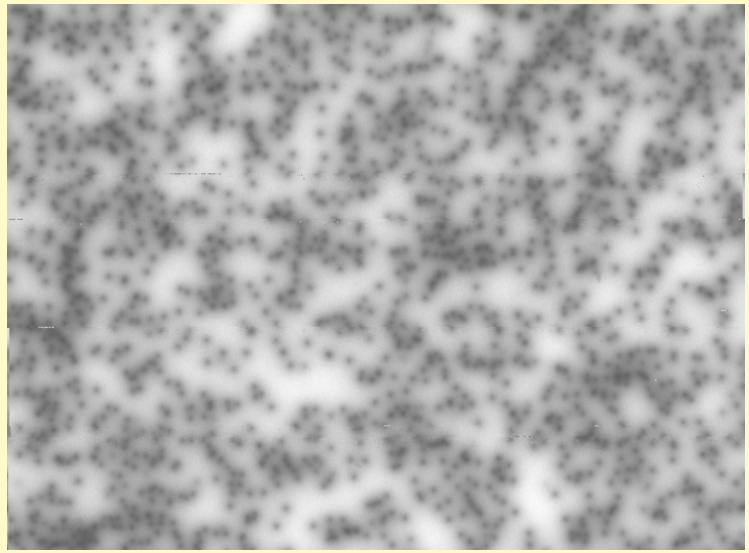

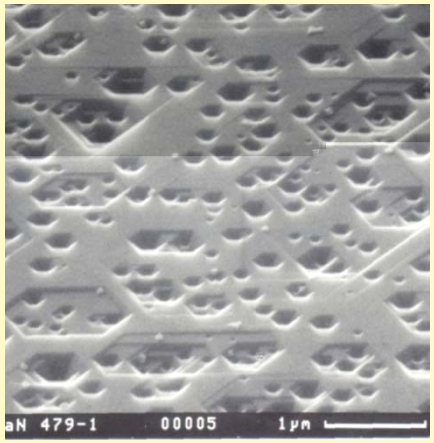

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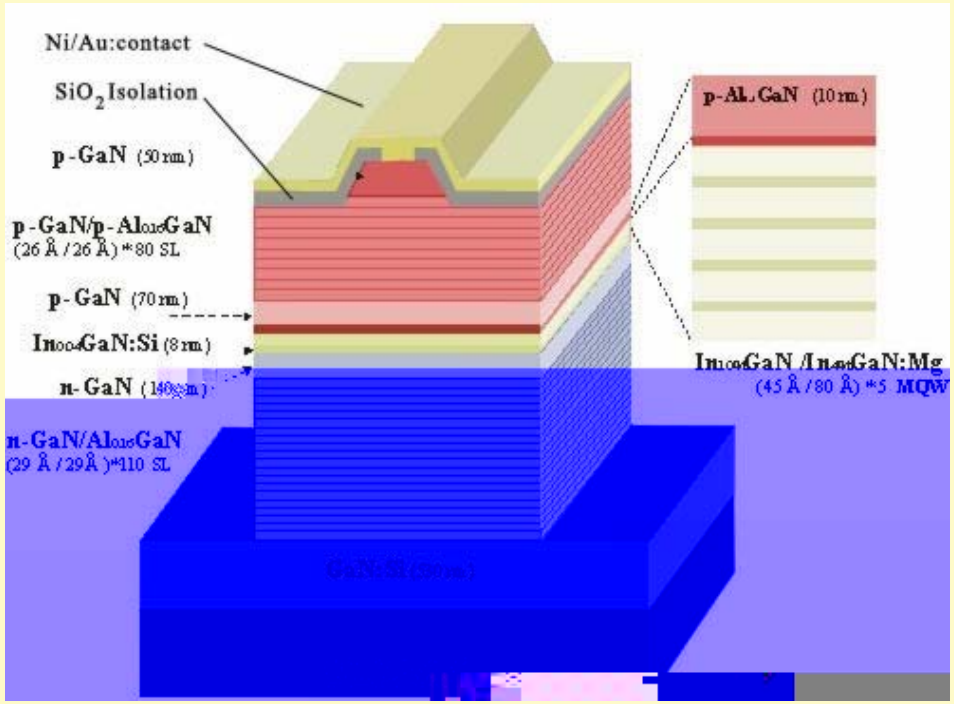
Ni/Au:contact
SiO2 Isolation
p-GaN (50nm)
p-GaN/p-Al0.15GaN
(26 Å / 26 Å) *80 SL
p-GaN (70nm)
In0.04GaN:Si (8nm)
n-GaN (1400nm)
n-GaN/Al0.15GaN
(29 Å / 29 Å) *110 SL
p-Al0.2GaN (10nm)
In0.08GaN /In0.16GaN:Mg
(45 Å / 80 Å) *5 MQW

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GaN	2500	45 000
AlN	2800	>100
InN	2200	>60 000

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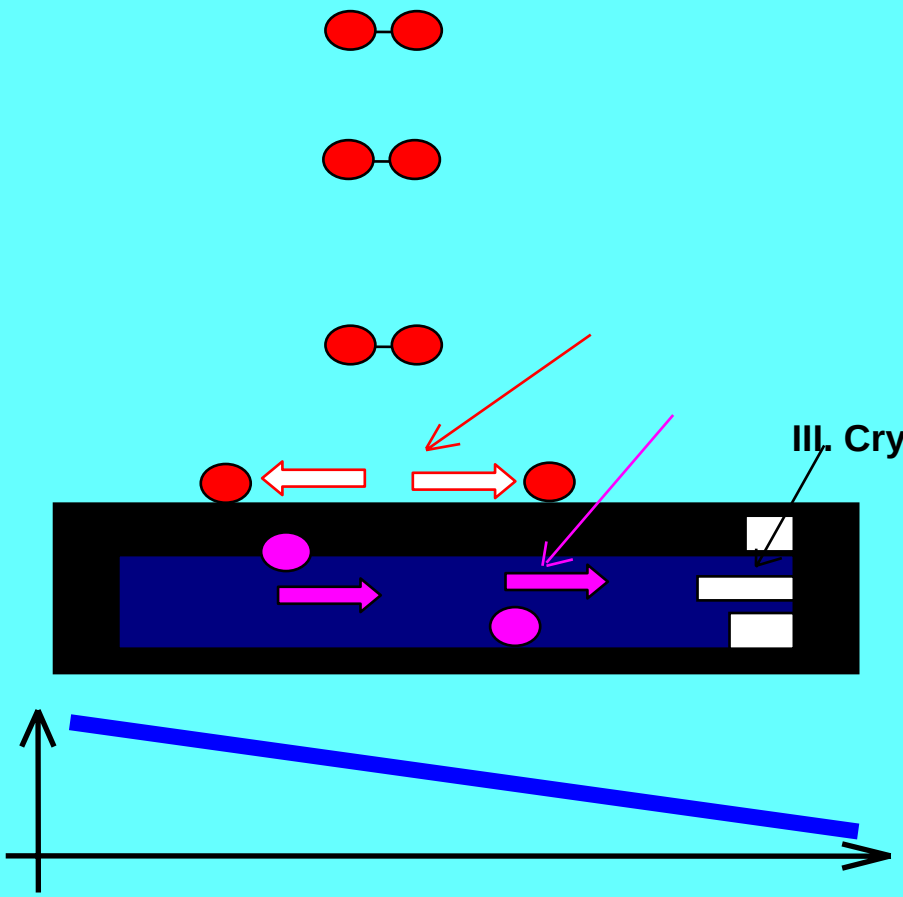
Three stages of HPSG growth of GaN



T=1500° C

P_{Nitrog}=15 000-20 000 atm

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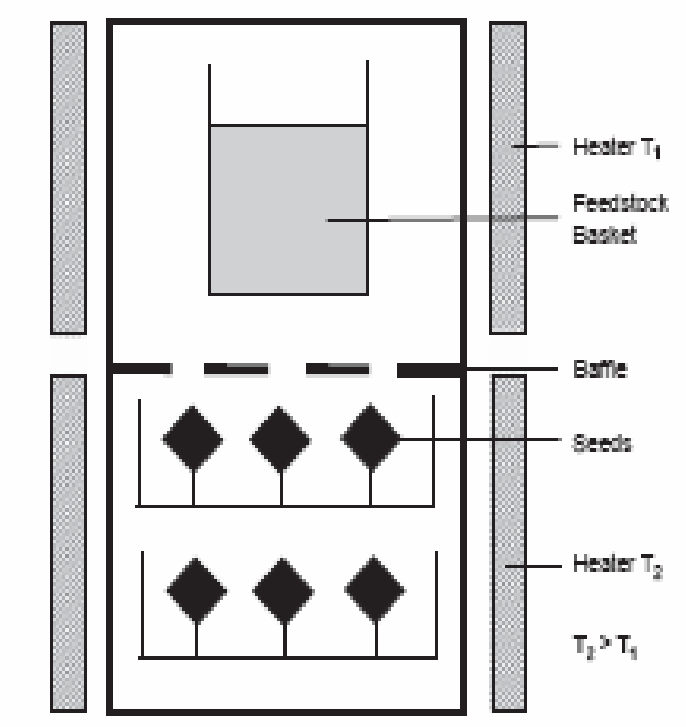
Working volume **4500 cm^3**

Max pressure
15 000 atm

Temperature
1550°C

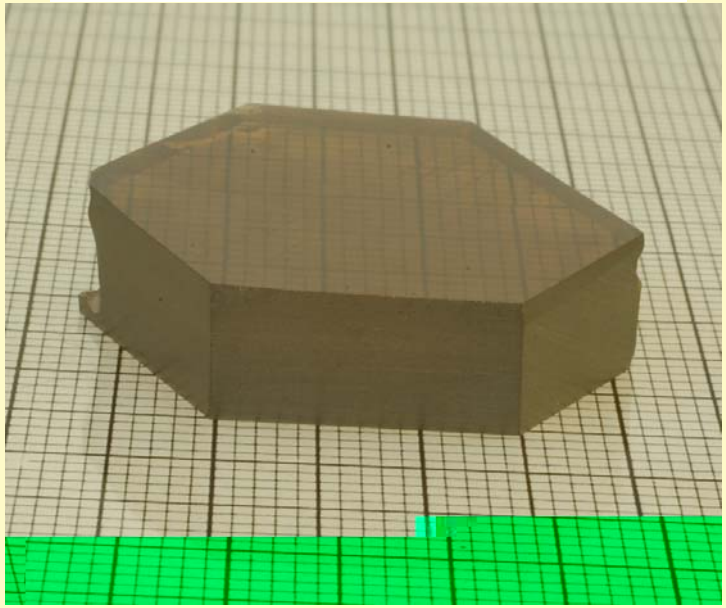
Pressure stabilization
10 atm

Temp. stabilization 0.1°C


Heater T_1
Feedstock
Basket
Baffle
Seeds
Heater T_2
$T_2 > T_1$

High Quality GaN Substrates for Laser Diodes

ammono



High Pressure
Multi-feed -seed method

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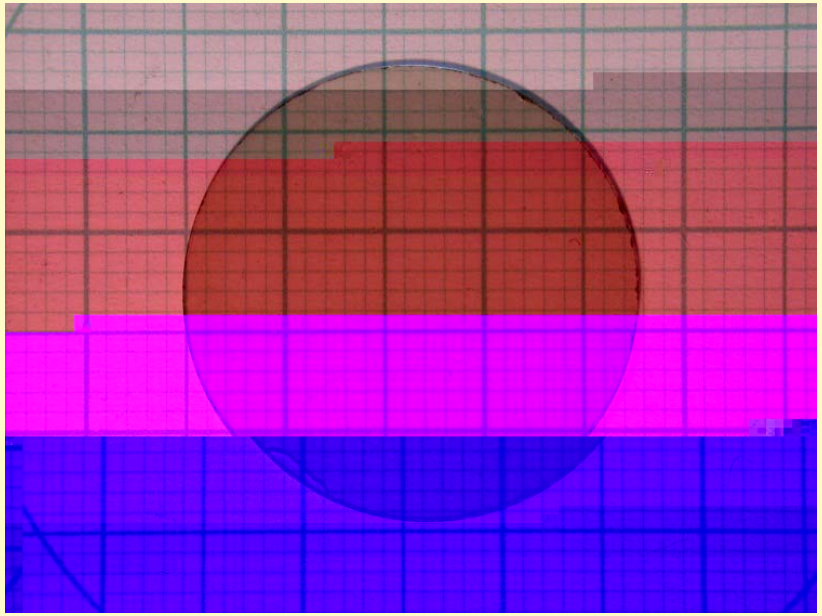

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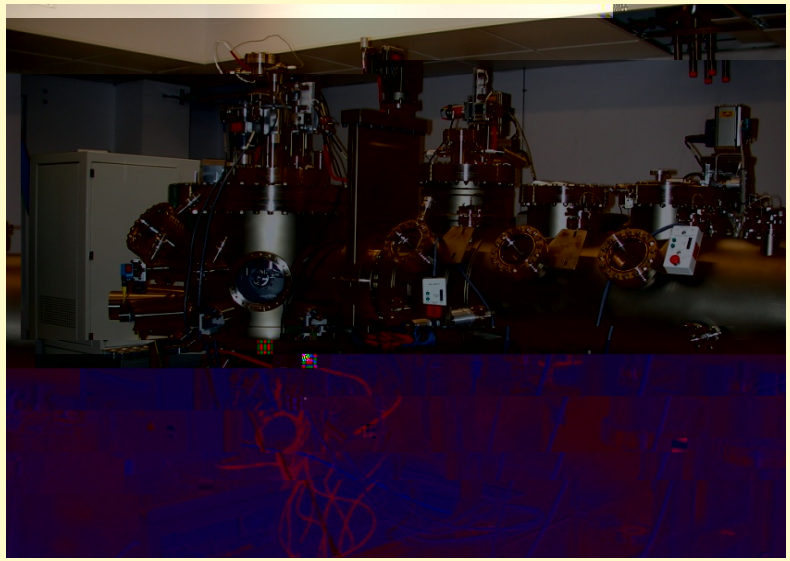
Surface preparation difficult.
Mechano-chemical polishing

Metalorganic vapor phase epitaxy (3 MOVPE reactors) and molecular beam epitaxy (2 PA MBE reactors) growth of nitrides layers and structures in Unipress



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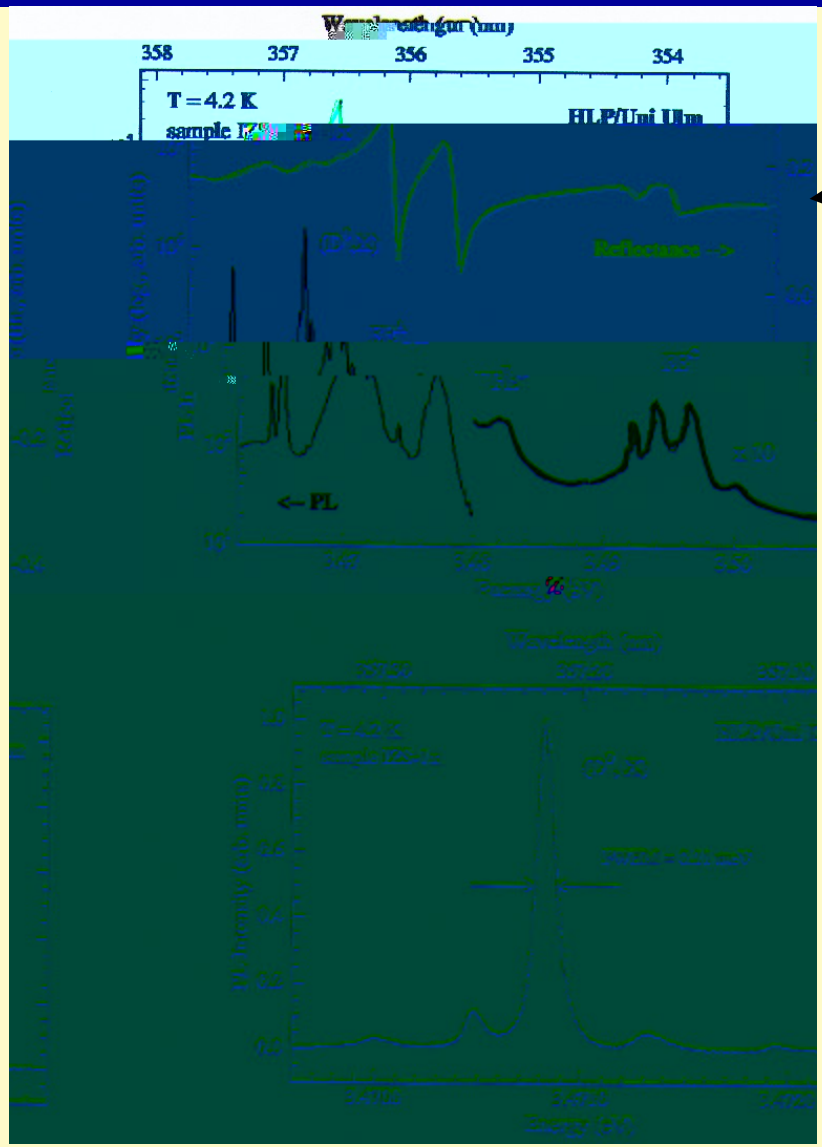

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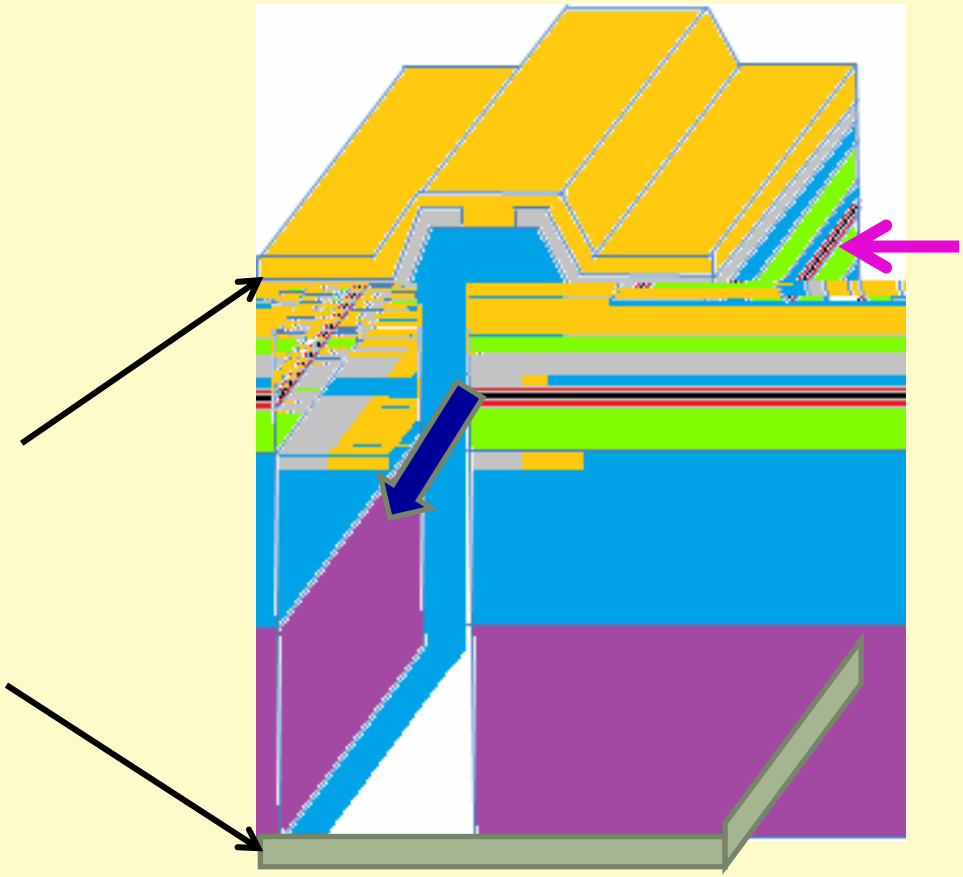
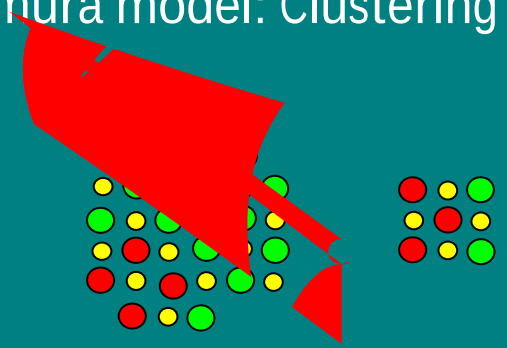


$In_xGa_{1-x}N/GaN$ $GaN/In_yGa_{1-y}N$

Compositional inhomogeneities and carrier localization in InGaN & AlInN. Almost commonly accepted concept

Chichibu/Nakamura model: Clustering of indium.



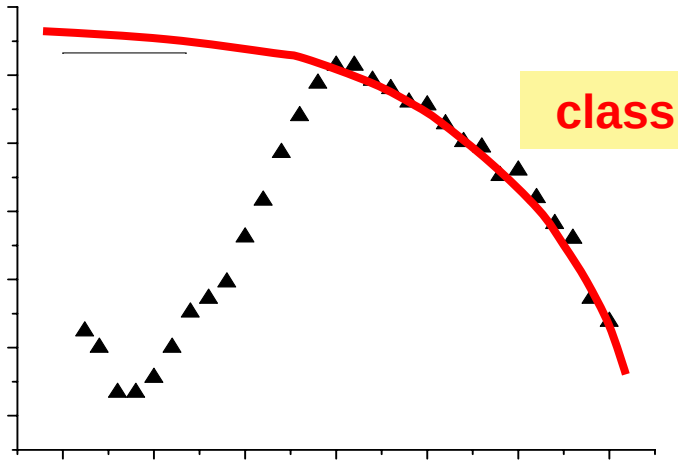
In- fluctuations

- clustering, spinodal decom tion, phase separation
  -Chichibu et al. Appl. Phys. , 4188 (1996))
- short range order/statisti fluctuations
  - Gorczyca et al.. Phys. Re 9, 2010), Bellaiche et al. 74, 1842 (1999);

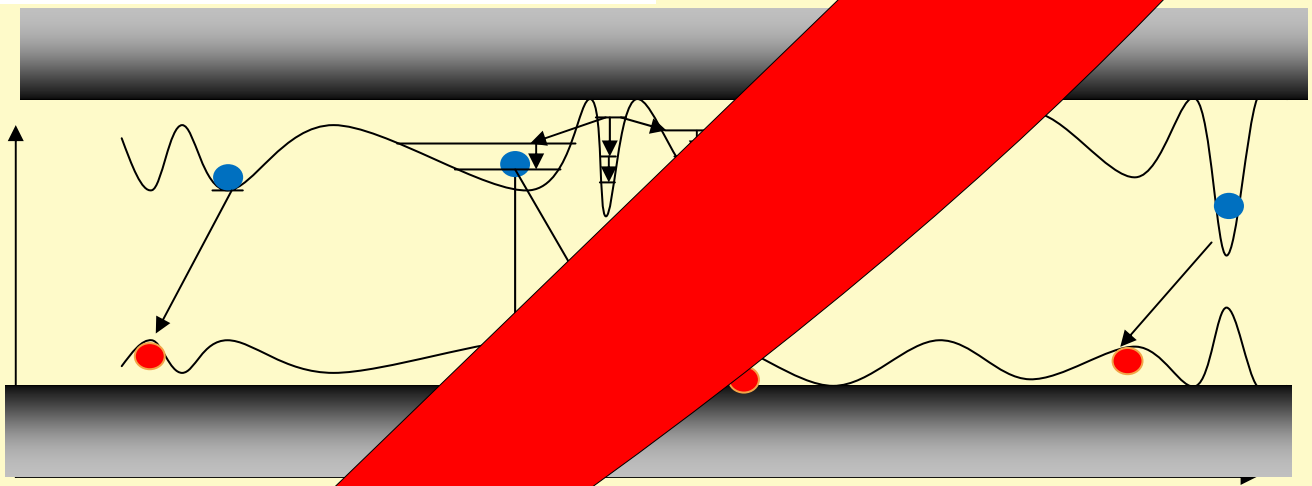
There are results of optical s emonstrating that potential fluctuations within spatial scale of below 50-10 portant for luminescence data (SNOM, CL)

What is a common understanding of the potential fluctuations contribution to the light emission in In-containing alloys.

Electron-hole pair or exciton transport before radiative recombination



classical" behavior of semiconductor band gap



In-fluctuations are particularly enhanced when structural defects appear

Strained and relaxed layers with different In concentration were observed when InGaN layers increased in thickness. Above the critical layer thickness stacking faults start to appear with increased density toward the surface. Stacking faults cause an appearence of multipeak PL and CL.

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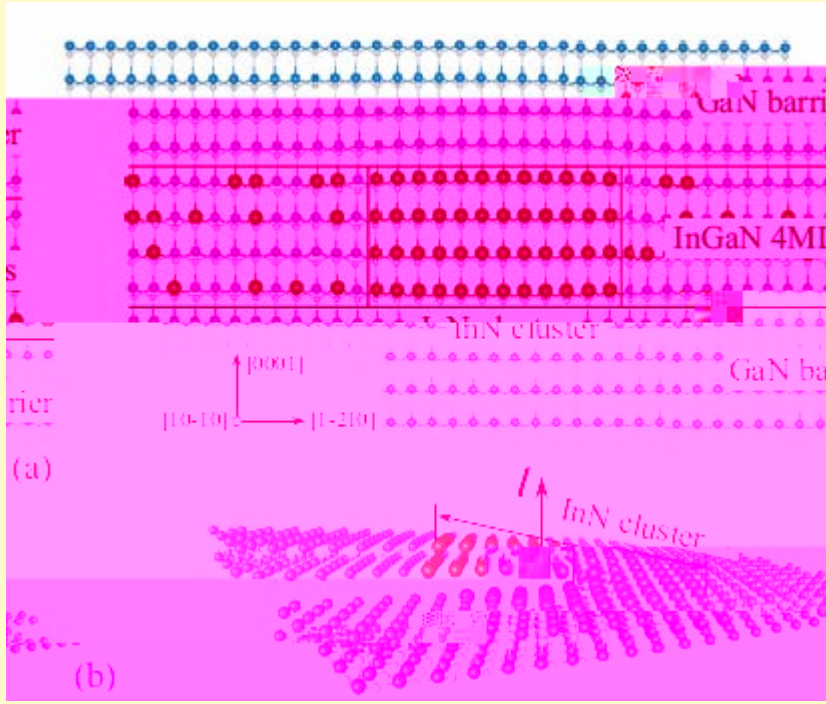
Influences of the biaxial strain and *c*-screw dislocation on the clustering in InGaN alloys

Huaping Lei,[1,a] Jun Chen,[2] and Pierre Ruterana[1]



$In_xGa_{1-x}N$ alloy „real” band gap determination

Differences between absorption-type and luminescence type of measurements

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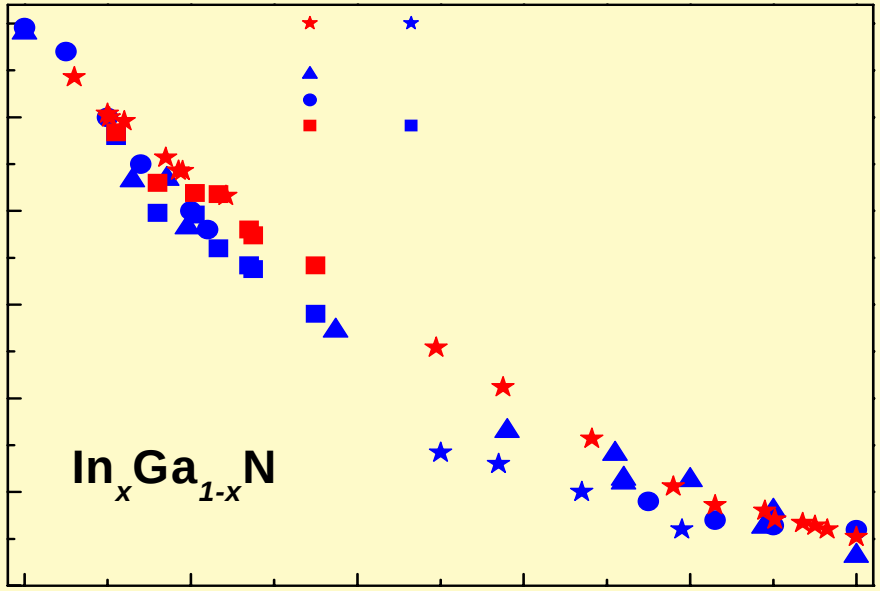

$Al_xGa_{1-x}N$ alloy band gap determination

Differences between absorption-type and luminescence type of measurements

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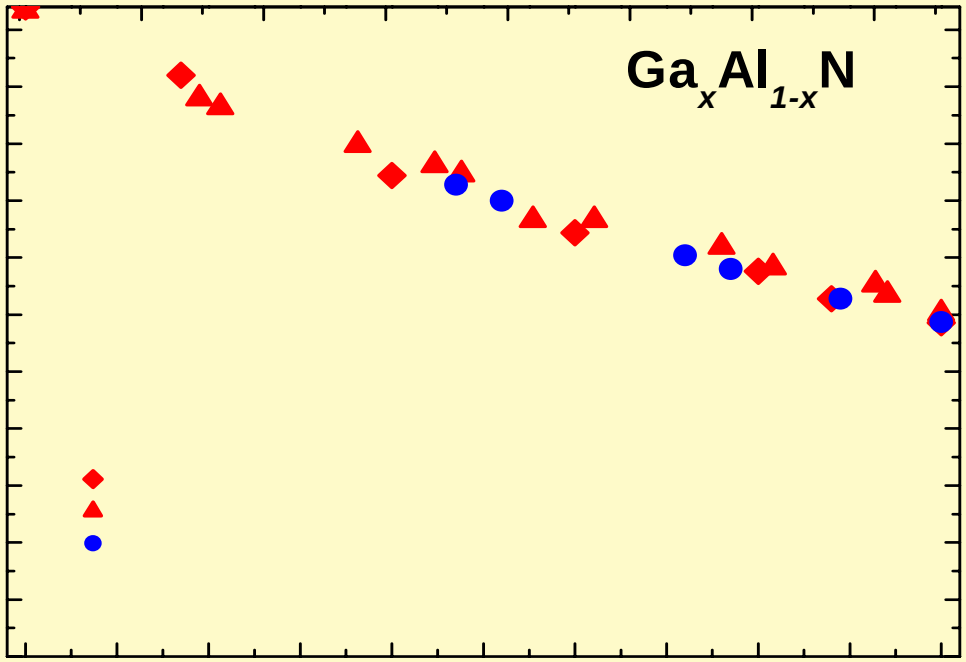

$In_xAl_{1-x}N$ alloy band gap determination

Differences between absorption-type and luminescence type of measurements

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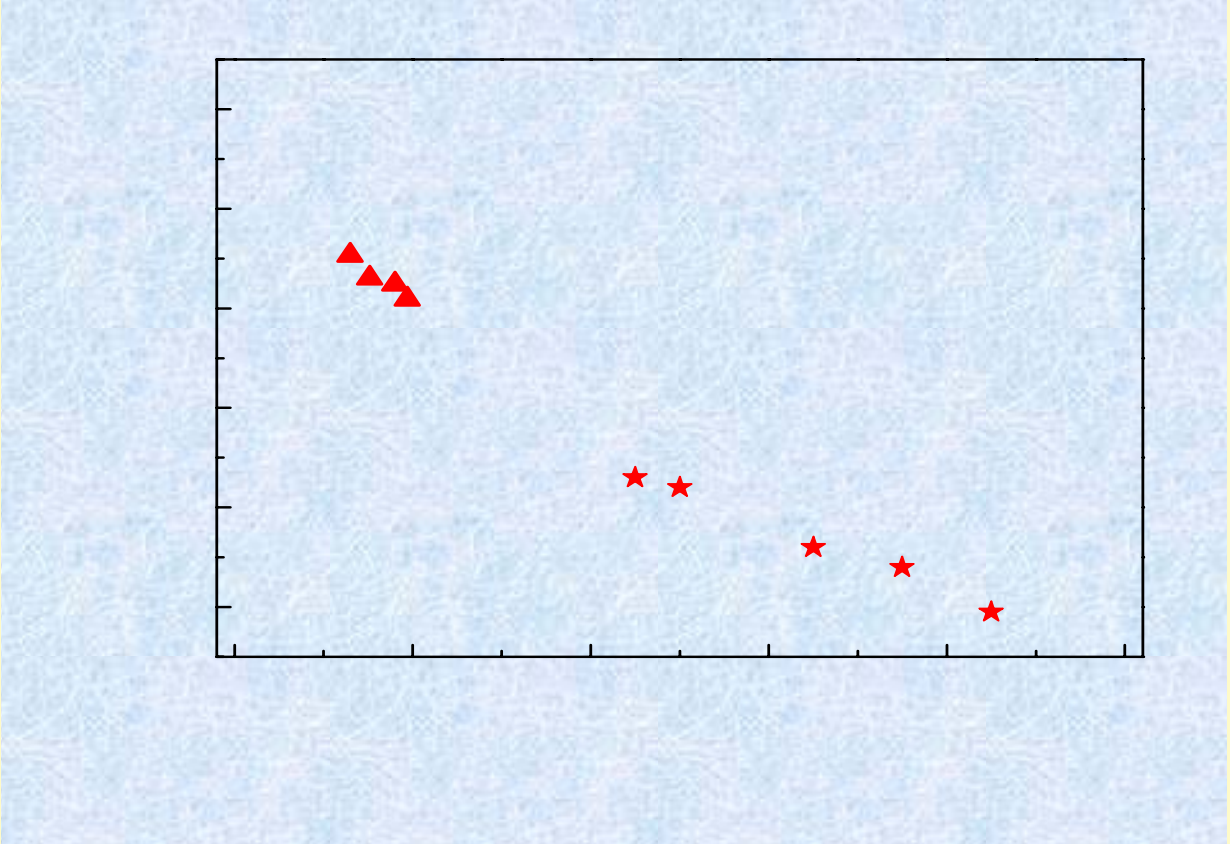
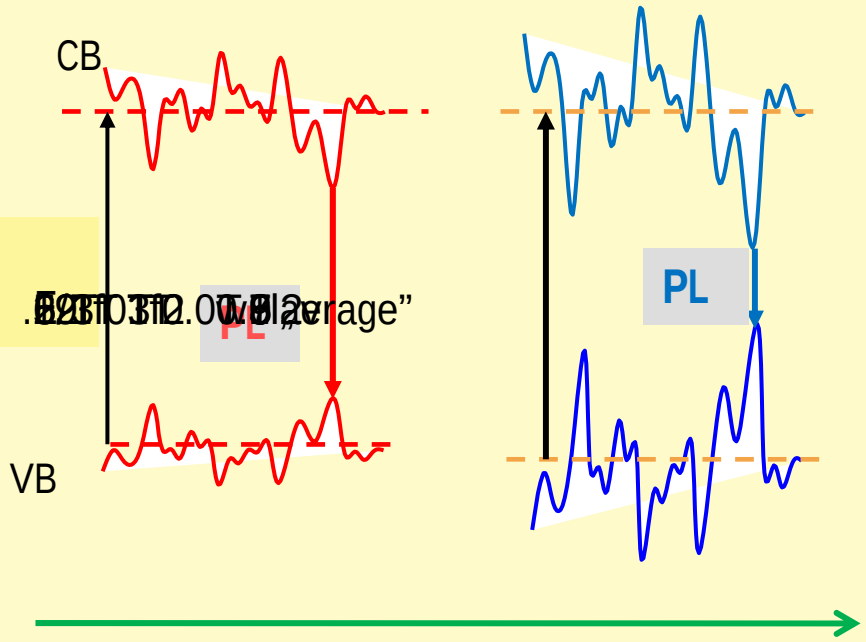


≈ E_G



Larger E_{PL} smaller fluctuations

Smaller E_{PL} larger fluctuations

along the sample

Theoretical description

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Method

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Electronic band structures of wurtzite $In_xGa_{1-x}N$, $In_xAl_{1-x}N$, and $Ga_xAl_{1-x}N$

by DFT with corrected band gaps

2 steps :

1. relaxed atomic positions

Pseudopotential method

- **Vienna simulation package (VASP)**

2. energy band structure

Full-potential linear muffin-tin-orbital (FP-LMTO)

- **semicore cation-*d* states included as local orbitals**
- **band gaps correction**

Method – superlattice like structure

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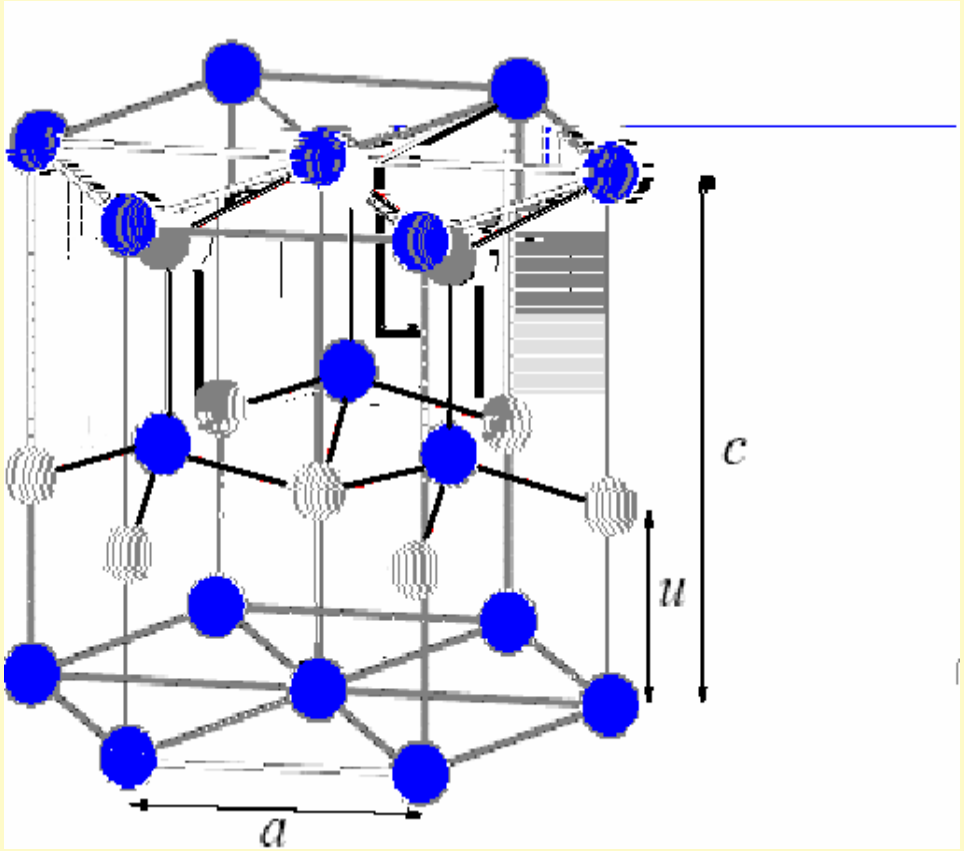
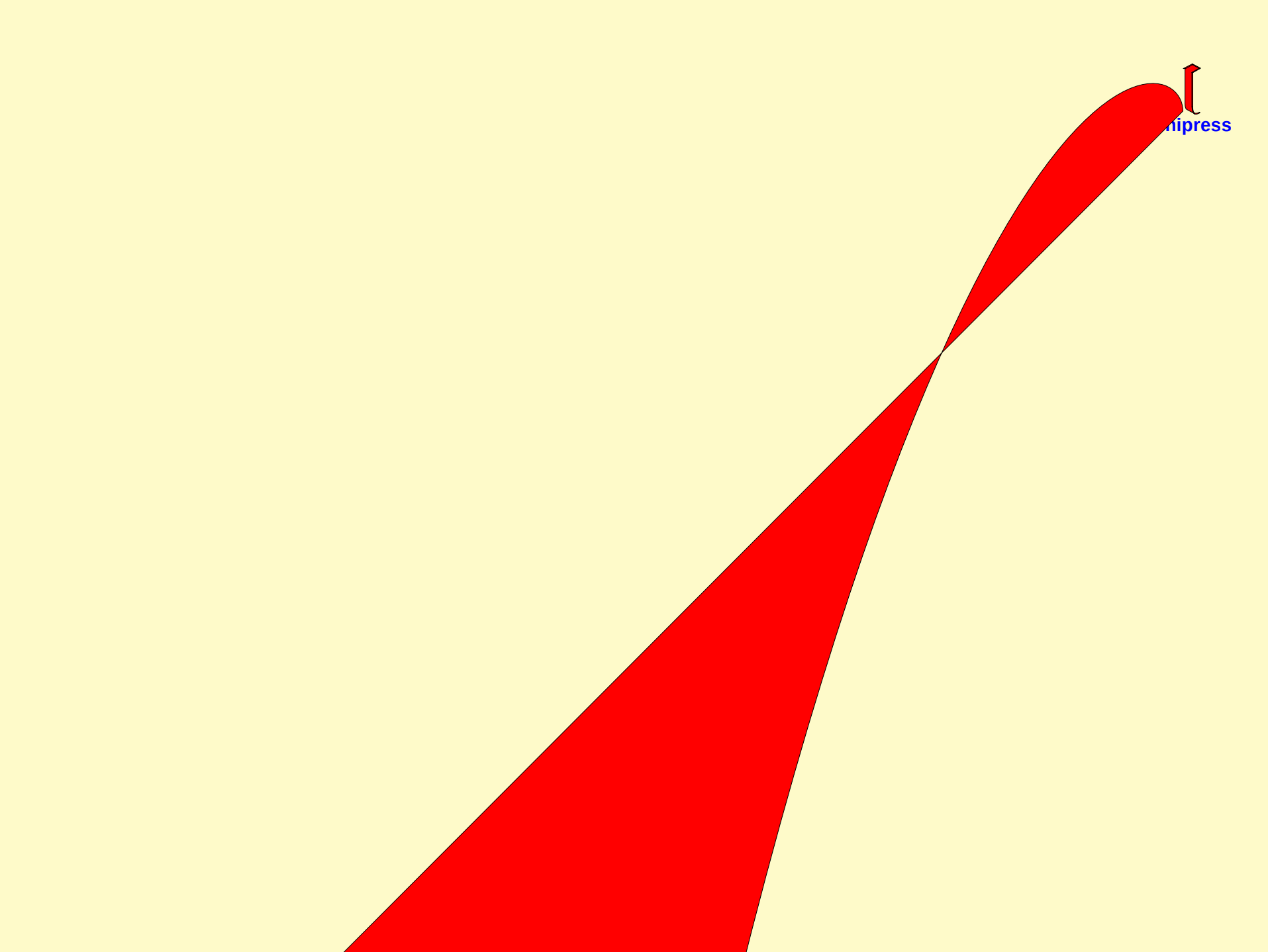
$In_xGa_{1-x}N$, $In_xAl_{1-x}N$

32 atoms supercell
wurtzite structure

No of In atoms	x
2	0.125
3	0.19
4	0.25
6	0.375
8	0.50
10	0.625
12	0.75
14	0.875





X

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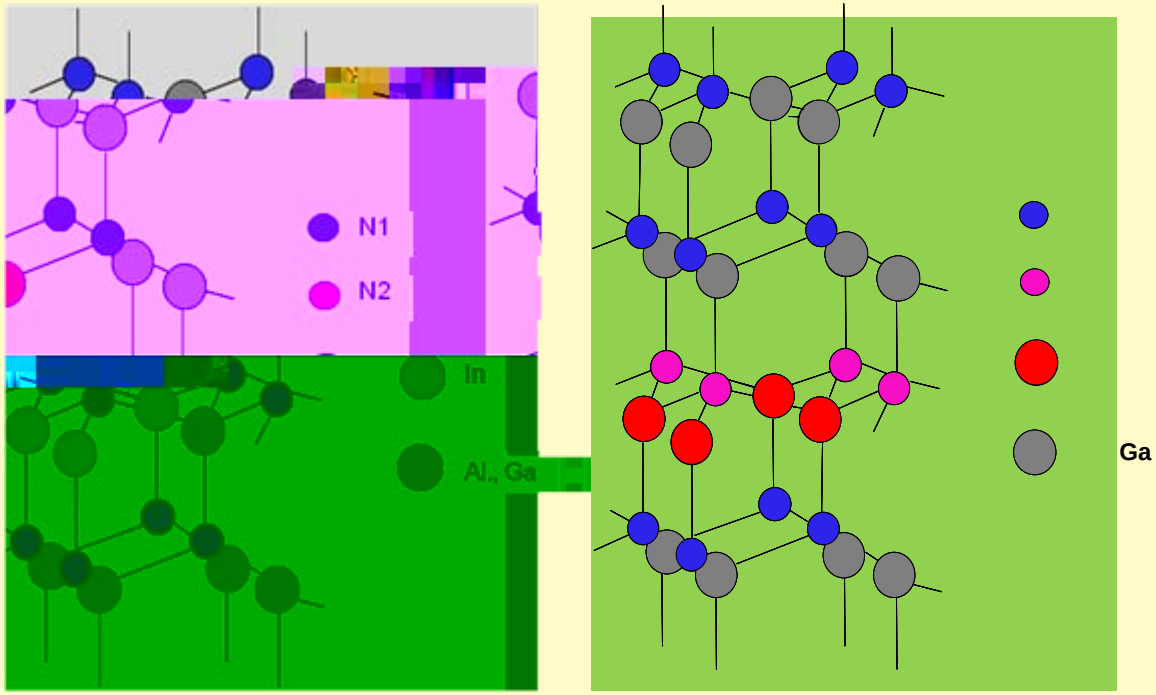
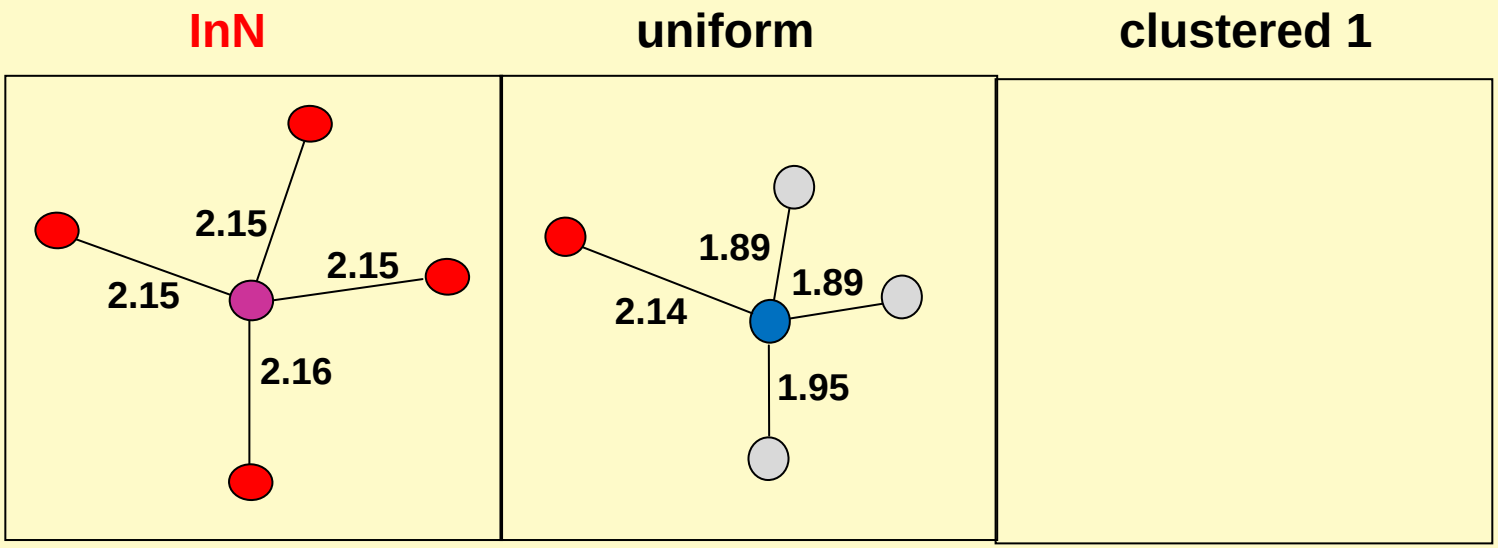


What is the effect of different arrangements of indium atoms on the band structure?

Clustered $In_xAl_{1-x}N$ x=0.25
very short bond-length of In-N(2)



Å Å

$In_xGa_{1-x}N$ alloy band gap determination

Theory vs. experiment

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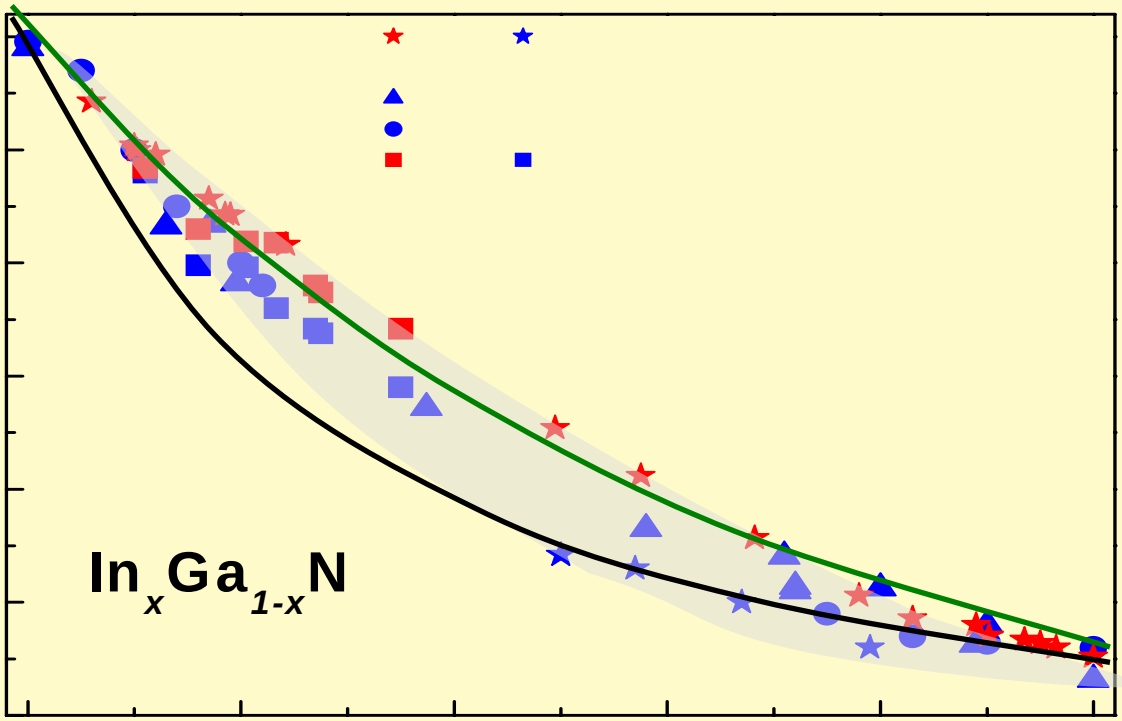

$Al_xGa_{1-x}N$ alloy band gap determination

Theory vs. Experiment, comparison with InGaN

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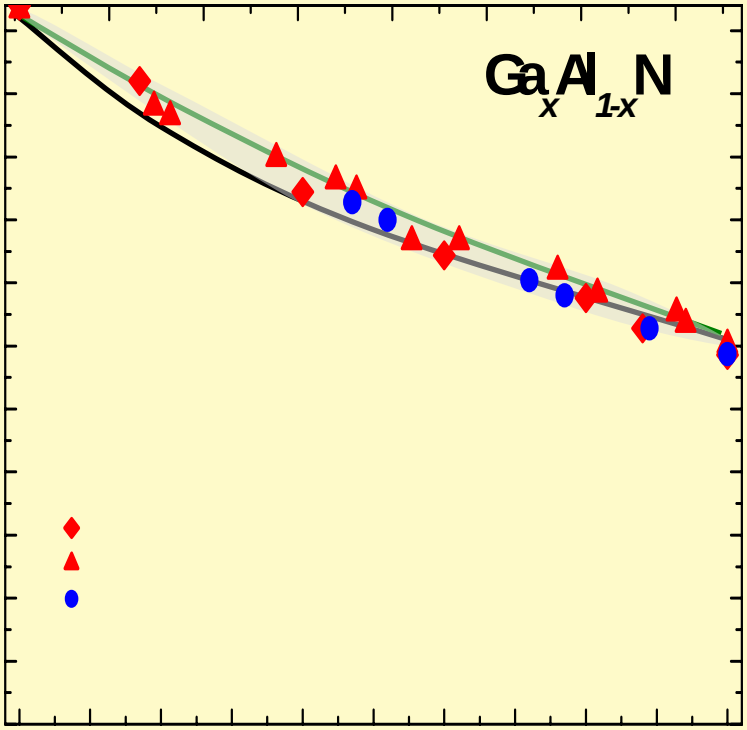

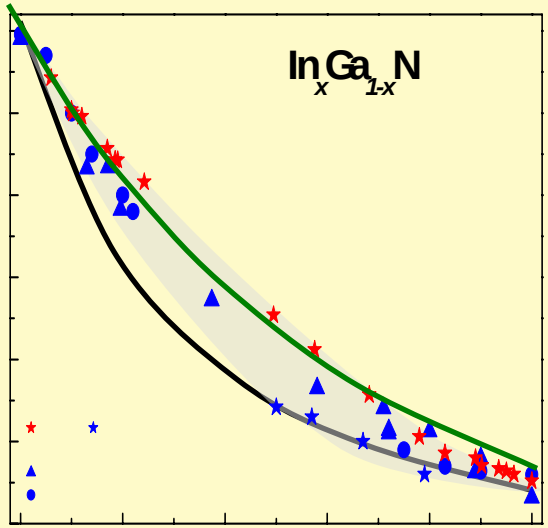

$Al_xGa_{1-x}N$

$In_xAl_{1-x}N$ alloy band gap determination

Theory vs. Experiment,

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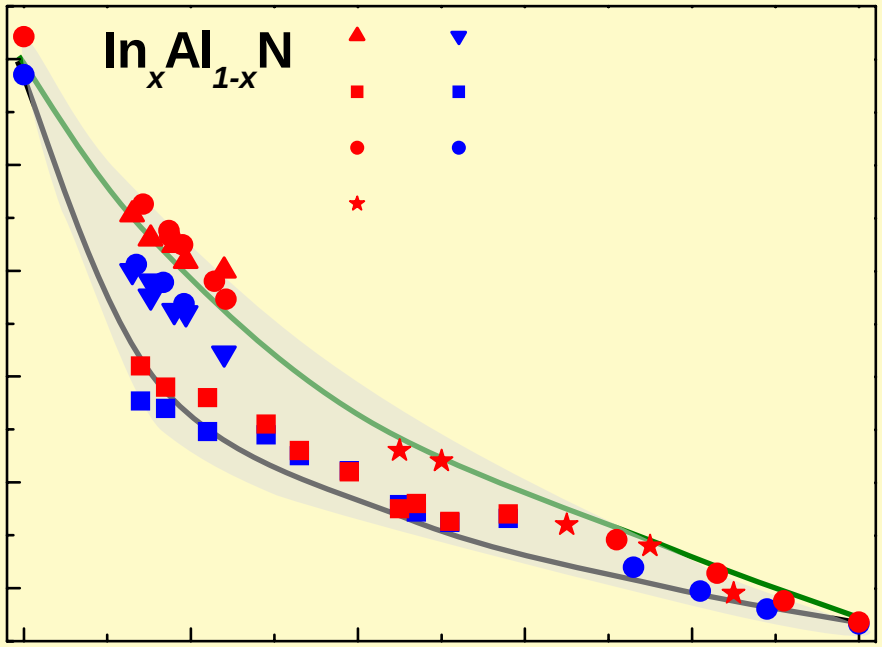

$In_xAl_{1-x}N$

Valence-band density of states (VB DOS)

Comparison for various nitrides

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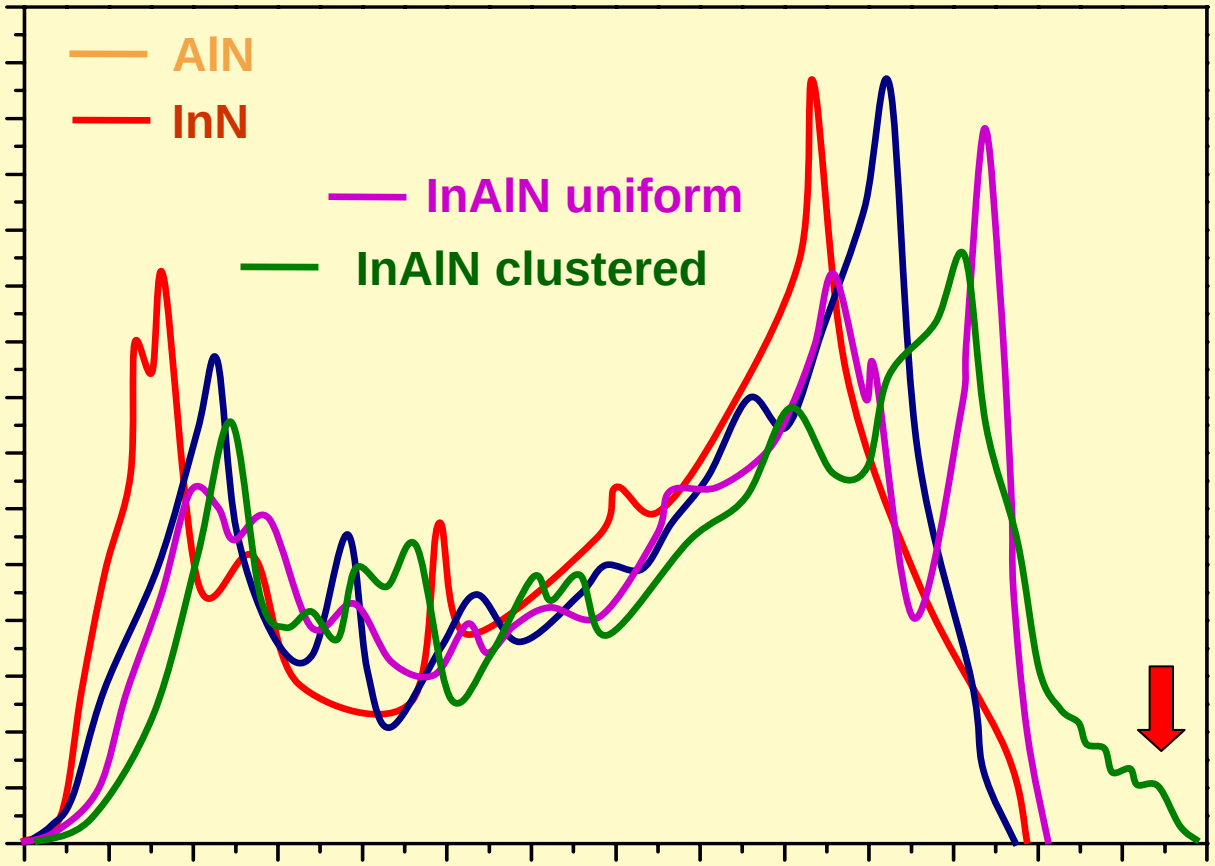
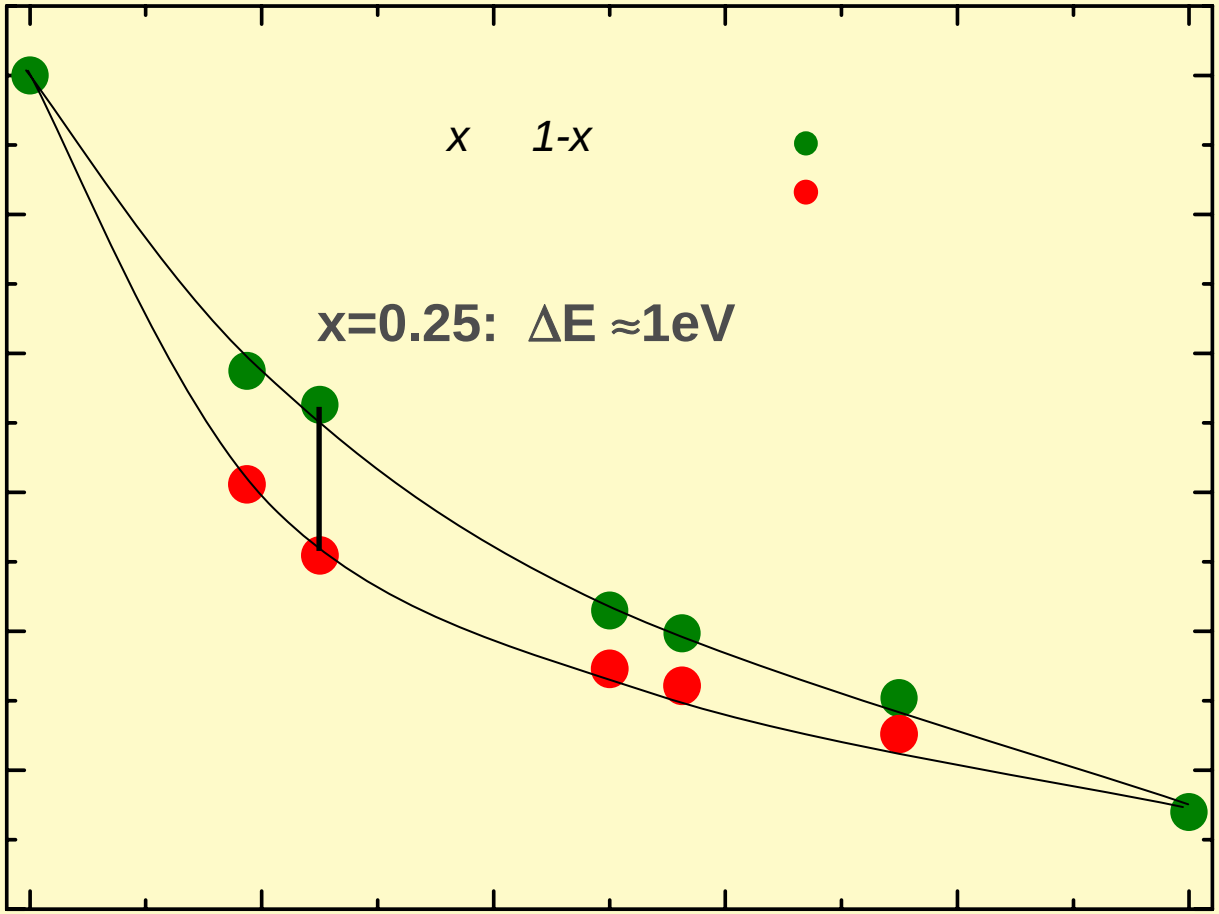


ΔE
about 1eV

Bandgap bowings – results od calculations



Decrease of the band gap comes from the valence band width reduction

Pressure coefficients of bandgap – calculations
Sensitive tool to detect In-segregation?

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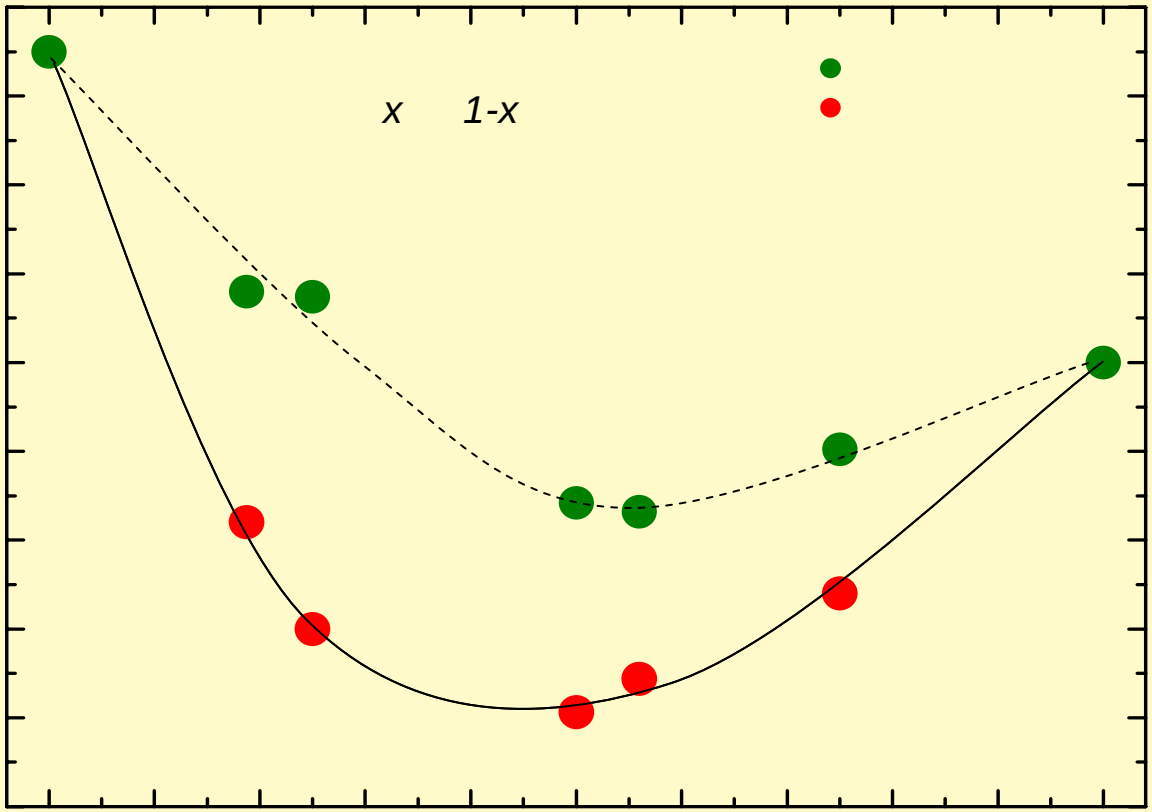

Experimental techniques in high-pressure studies
of the optical properties of semiconductors.

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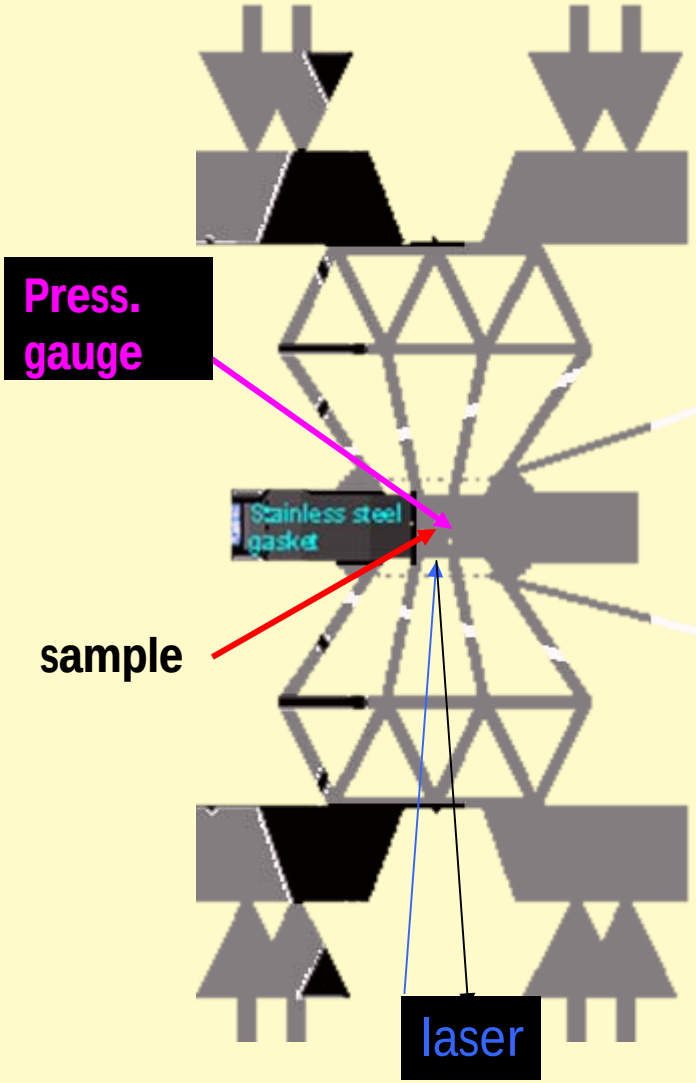
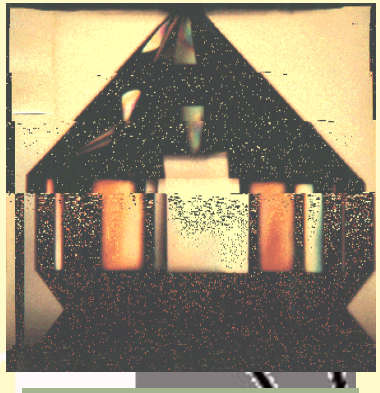
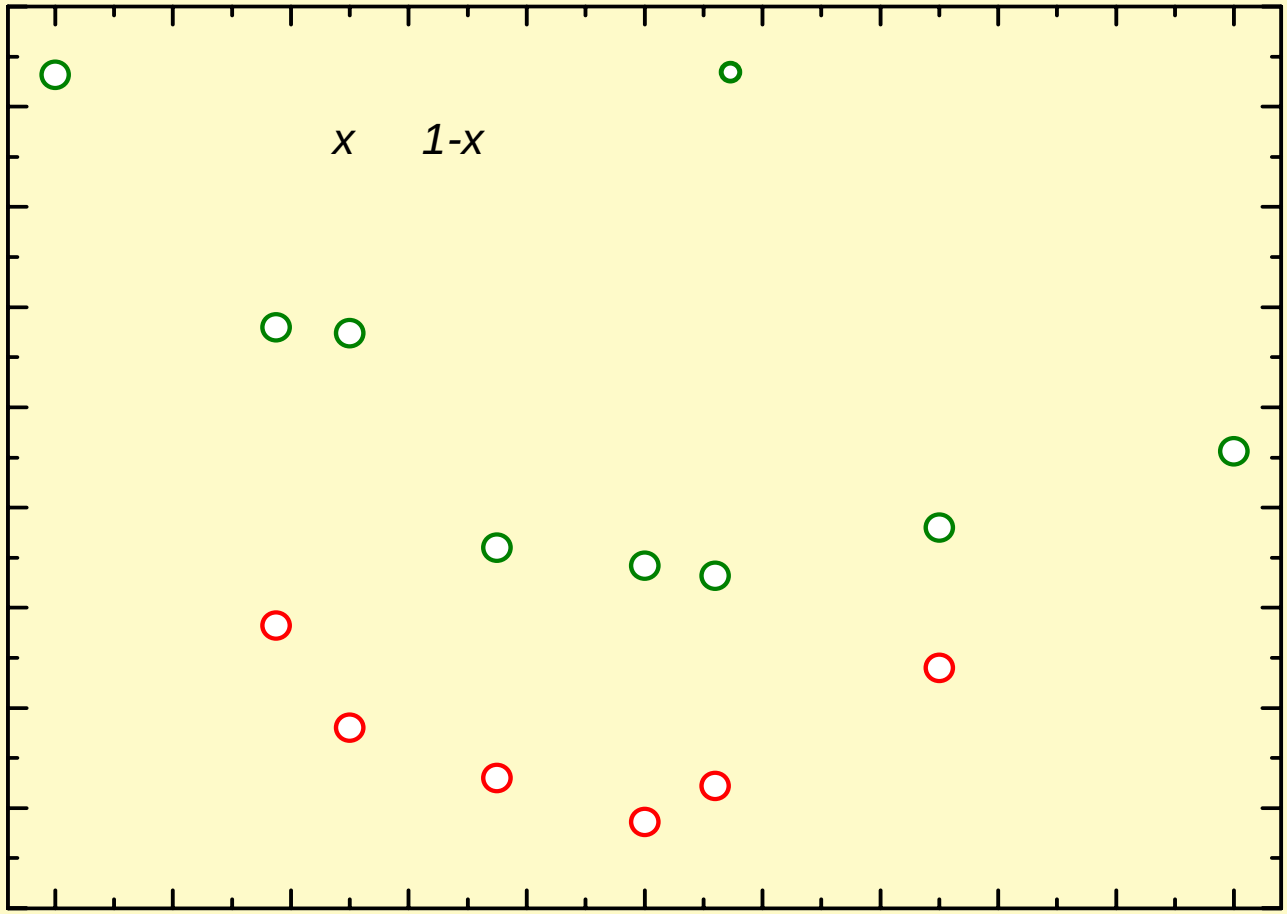
Diamond Anvil Cell





Solid argon as pressure transmitting medium

Pressure units: 1 atm = 1 bar; 10 kbar=1 GPa


x
1-x

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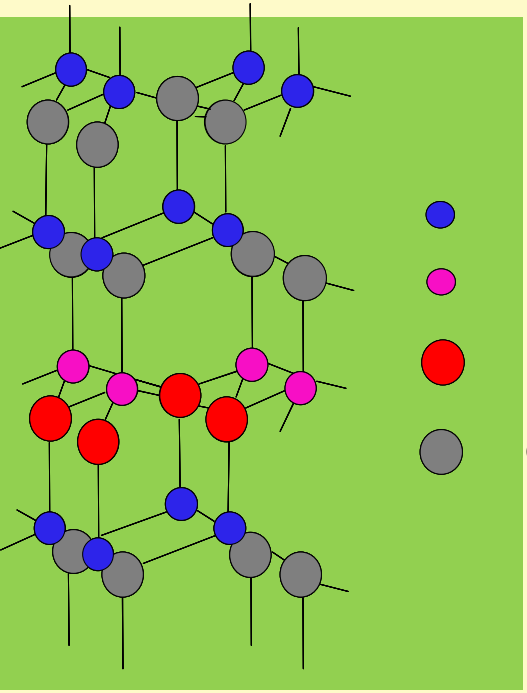
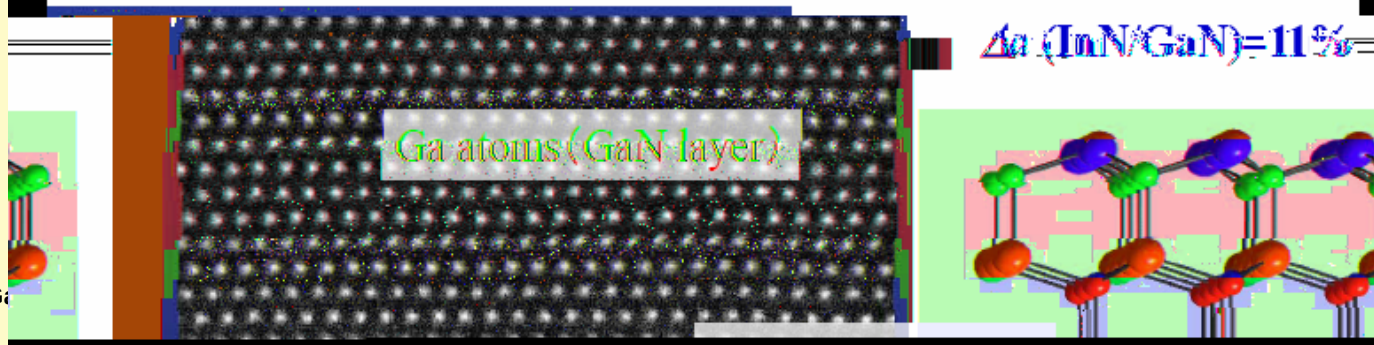


Ga

Fundamental structure of the proposed symmetrical structure 1ML-InN/GaN matrix quuntum well



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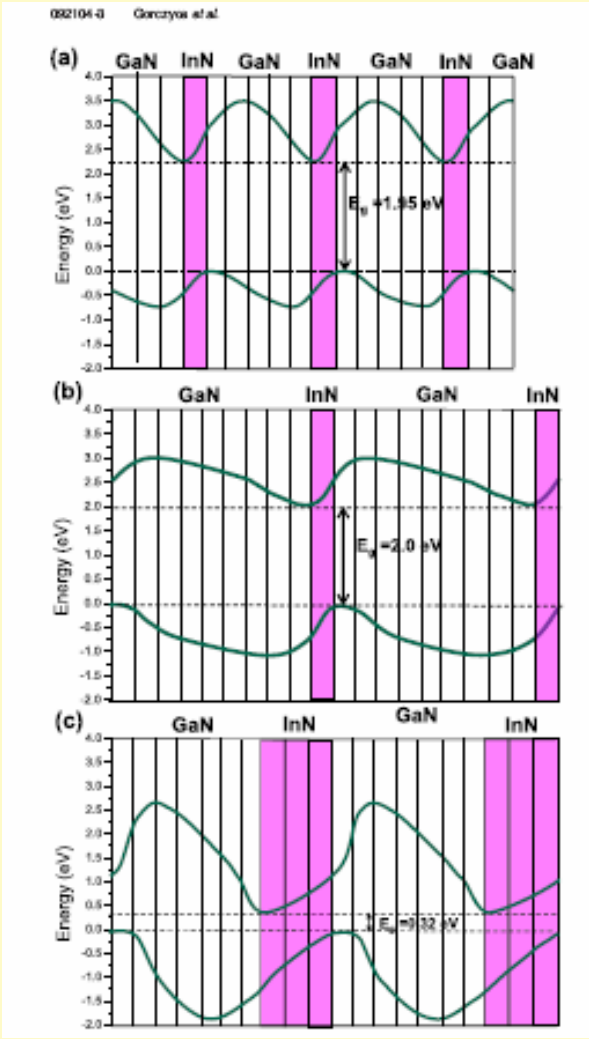

InN/GaN Superlattices: Band Structures and their Pressure Dependence


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Summary

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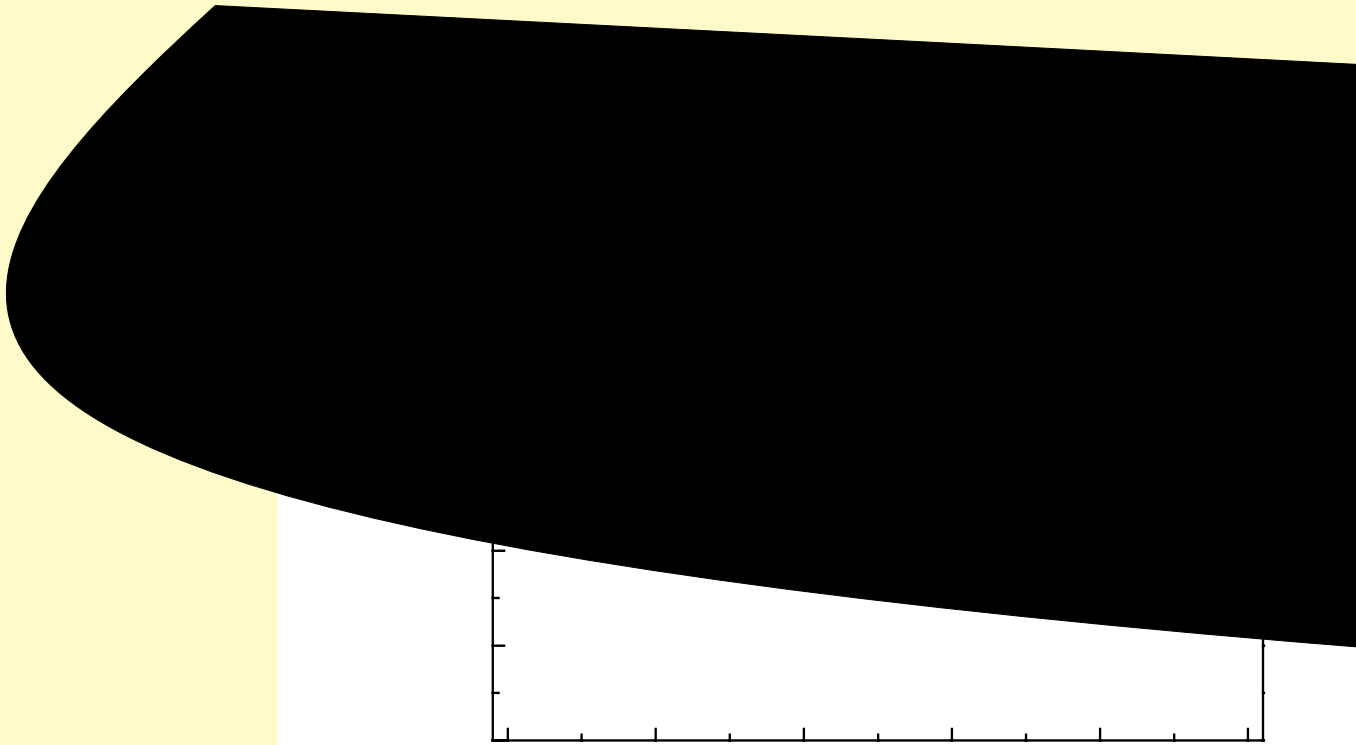
perfect

imperfect



Incoherent alloys (InGaN) demonstrate strong decrease of band gap - sophisticated calculations

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coherent alloys – precipitates having continuous crystal planes across the phase boundary between them and the crystal matrix

incoherent alloys – precipitates having the dislocations, grain boundaries Leading to disengaging them from the matrix