Epitaxy in the development of LEDs

Jean-Yves Duboz

CRHEA-CNRS

Valbonne Sophia Antipolis

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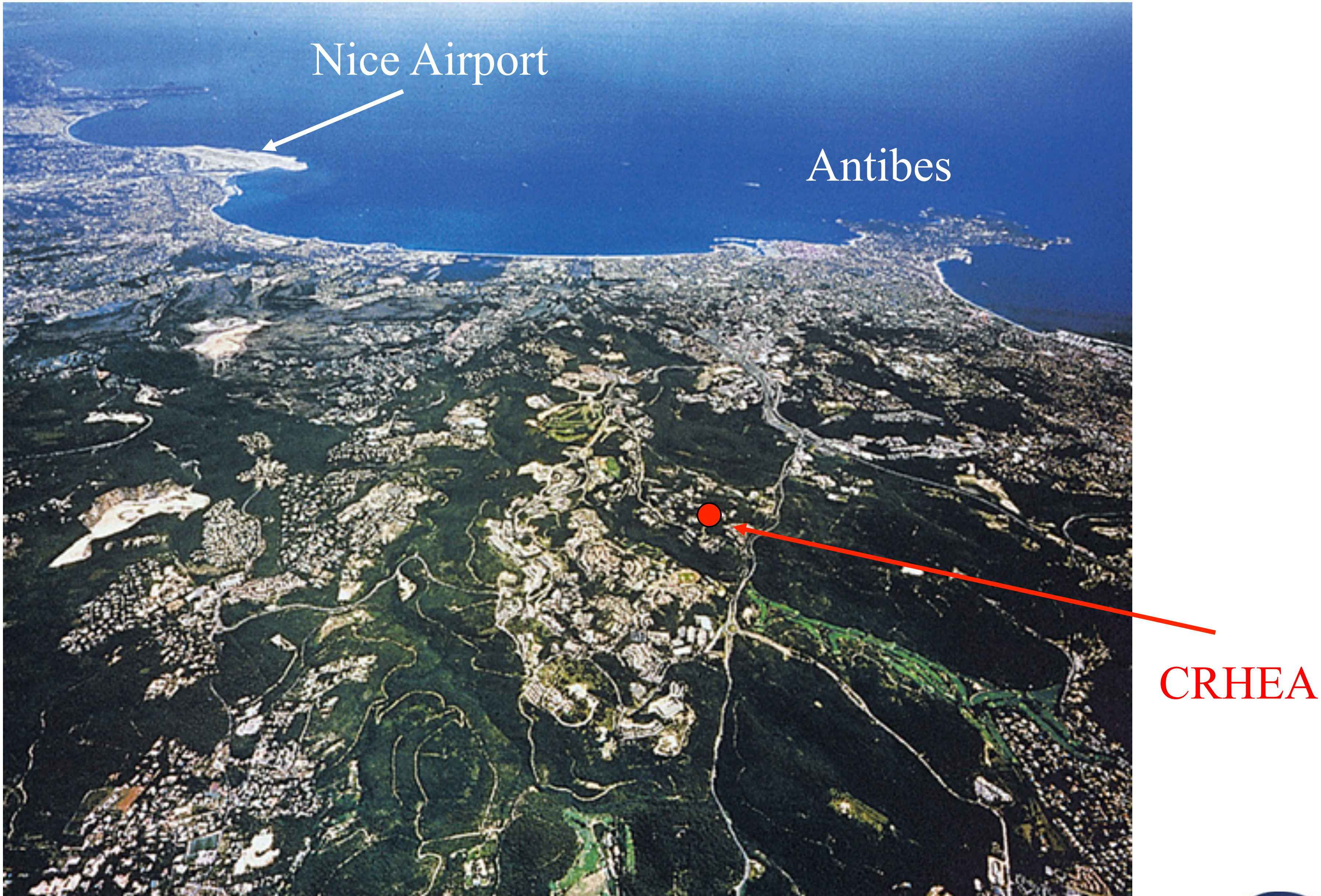
Nice Airport
Antibes
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Epitaxy (GaN, ZnO, SiC, graphene)

Characterization (structural, optical)

Device fabrication (LED, laser, transistors….)

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History of LEDs

- LED first discovery : the first known observation of electroluminescence was made in 1907 by H. J. Round using SiC Schottky diode.

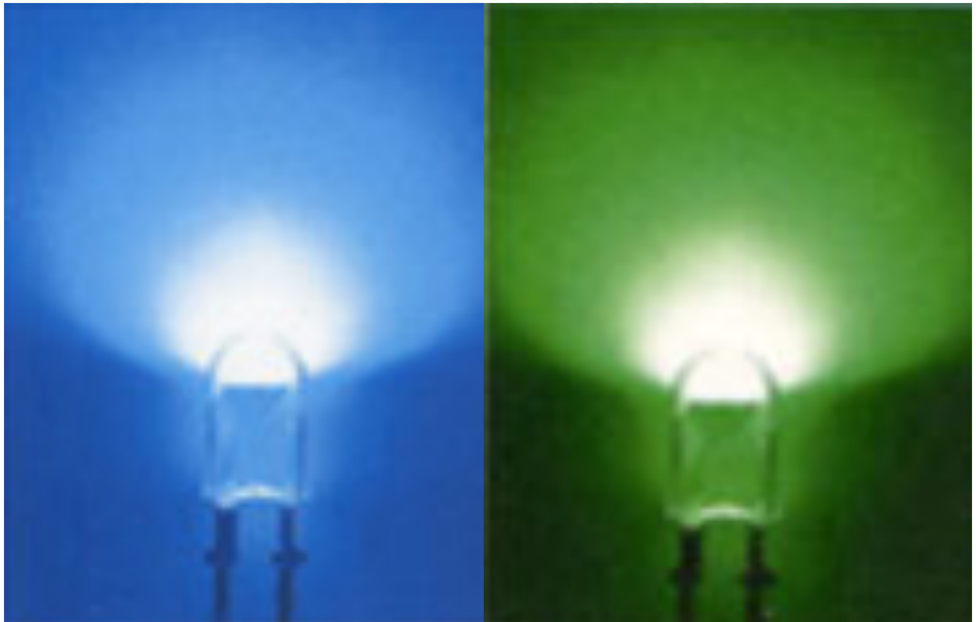
- In 1955, Rubin Braunstein of the Radio Corporation of America reported on infrared emission from gallium arsenide (GaAs) and other semiconductor alloys, patented in 1961

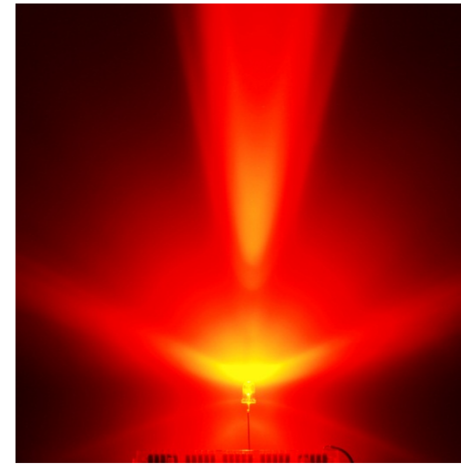
- In 1962, Nick Holonyak Jr., of the General Electric Company developed the first practical visible-spectrum LED. He is seen as the "father of the light-emitting diode".
- In 1972 first yellow LED and 10x brighter red and red-orange LEDs (by George Craford)

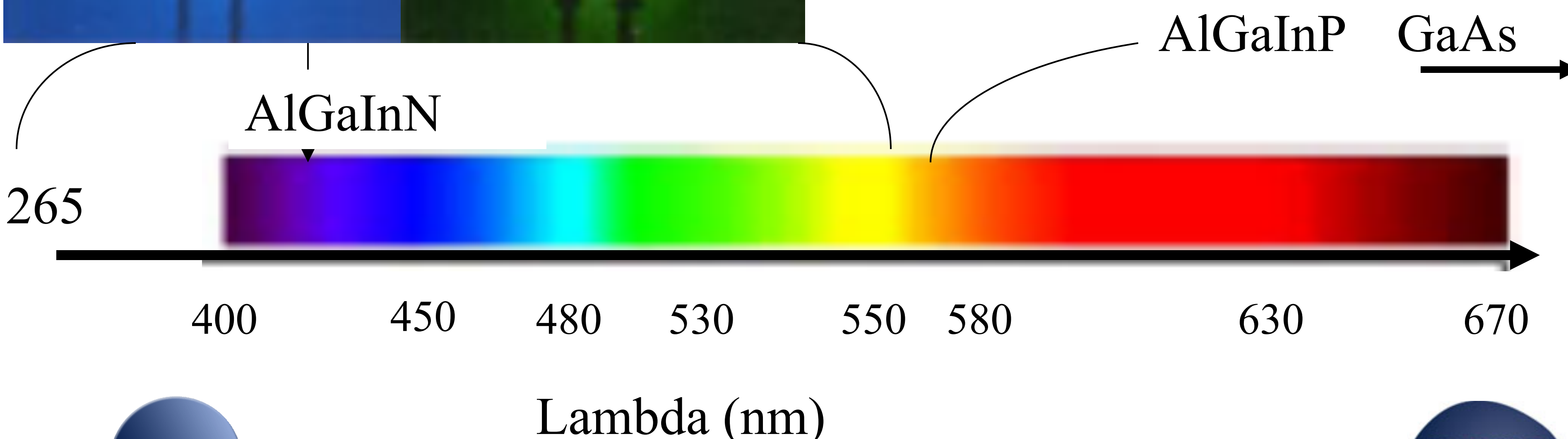
- 1993 Shuji Nakamura of Nichia Corporation of Japan demonstrated the first high-brightness blue LED based on InGaN. Beginning of the quest for white LEDs for solid state lightning. Nobel prize 2014.

http://www.myledpassion.com/History/History-of-leds.htm

LED






AlGaInP
GaAs
AlGaInN
265
400
450
480
530
550
580
630
670
Lambda (nm)

LED

Initial business

LED for signaling (traffic light), displays…

Monochromatic emission: low tolerance $\Delta\lambda <$ few nm

Low- medium power 10-50 mW

Current business

LED for lighting

Color rendering index, white temp.

High power: W

High efficiency !

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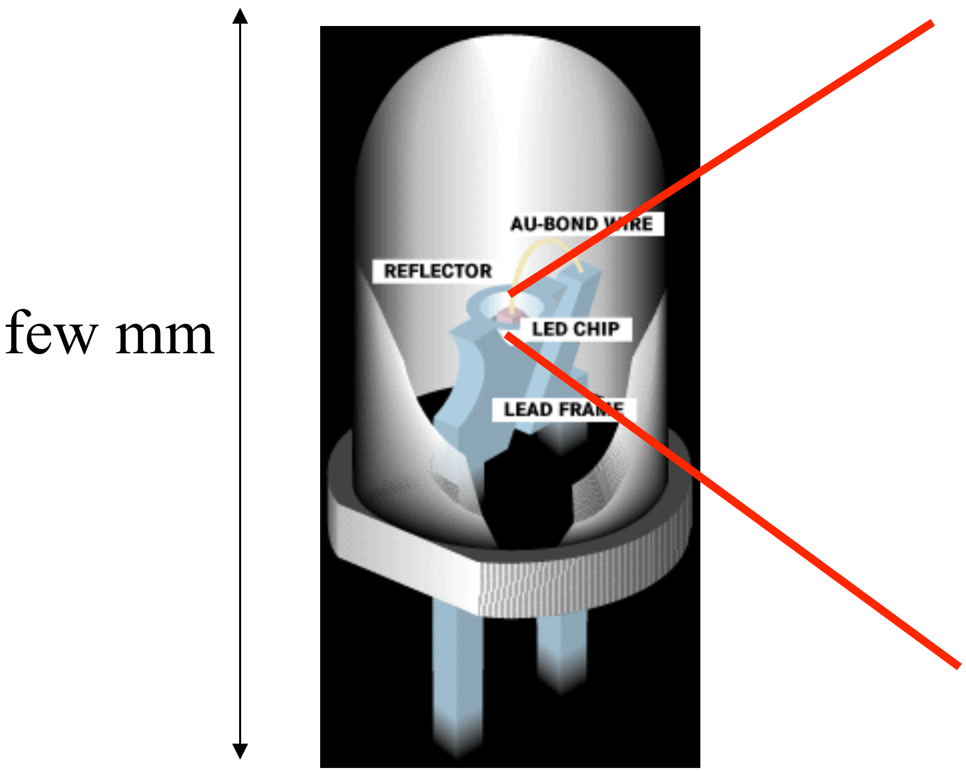
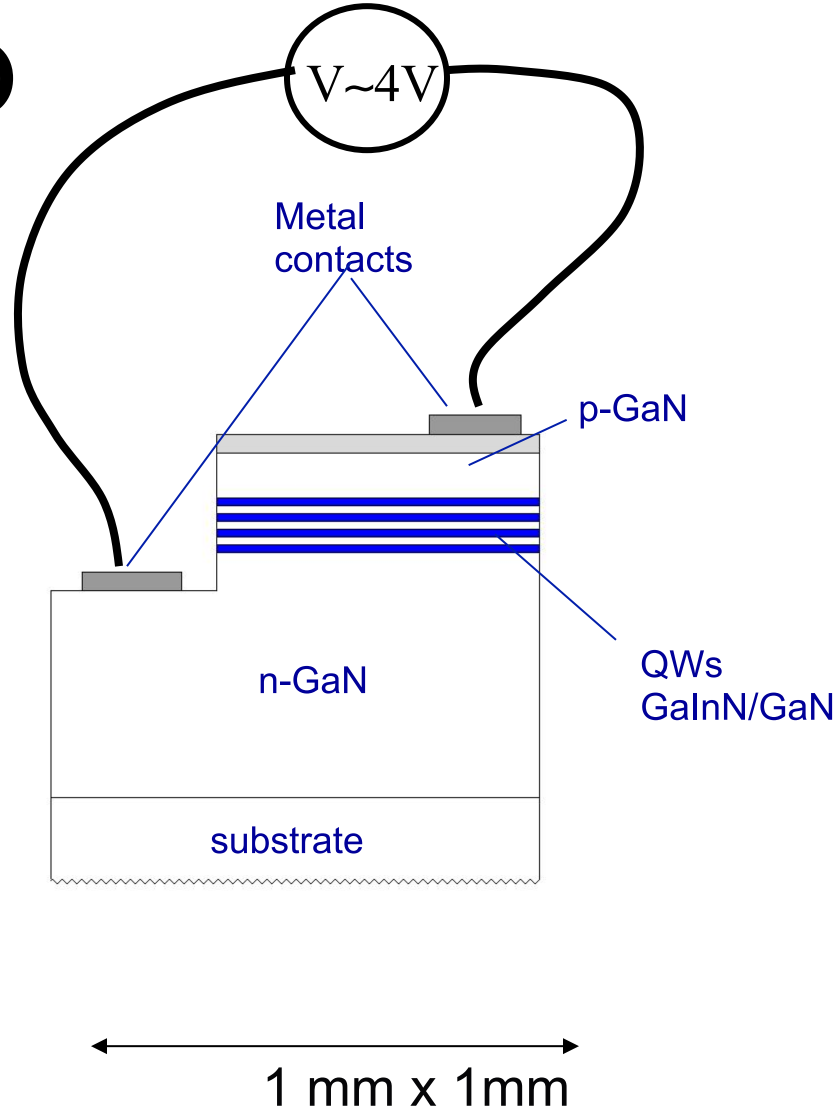
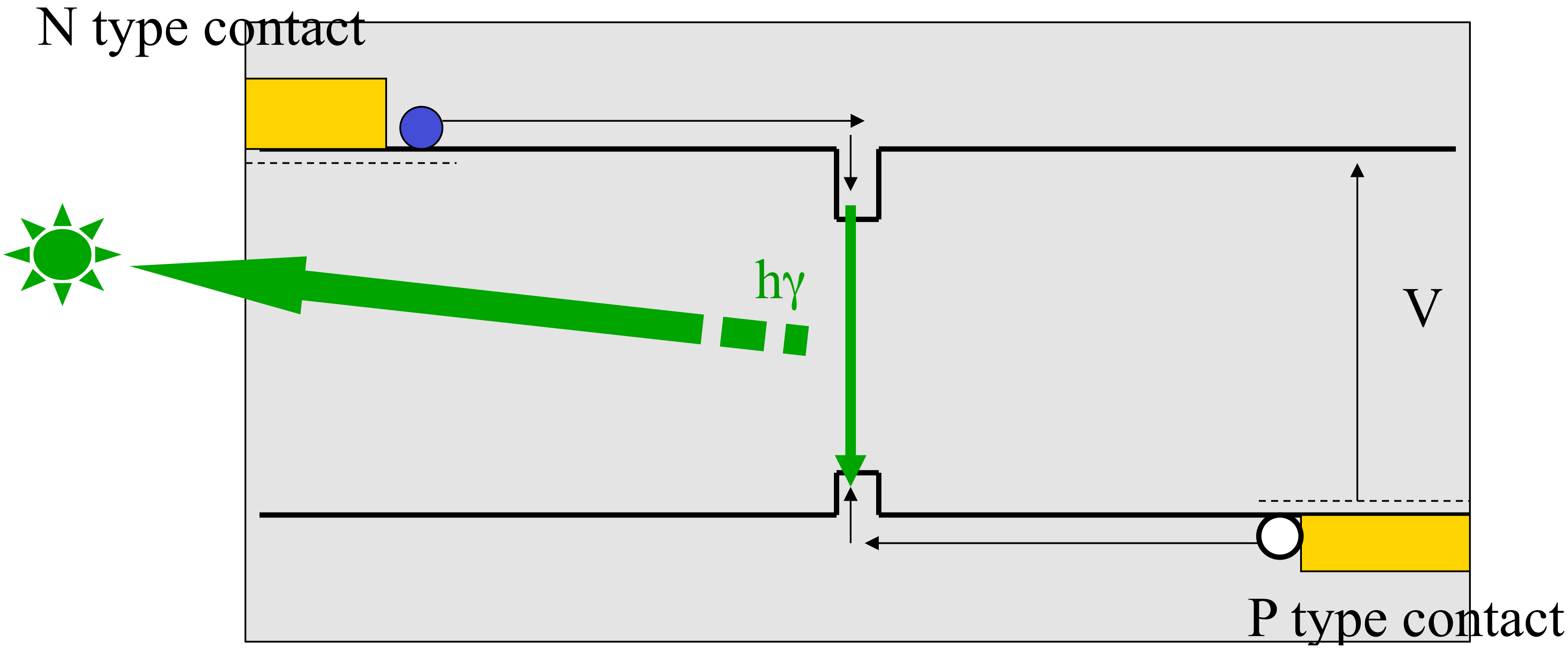
LED



few mm
AU-BOND WIRE
REFLECTOR
LED CHIP
LEAD FRAME



V~4V
Metal contacts
p-GaN
QWs GaInN/GaN
n-GaN
substrate
1 mm x 1mm



1 electron + 1 hole ⇒ 1 photon : Int. Quantum Eff. = 1

Photon escapes from LED: Extraction Eff. = 1

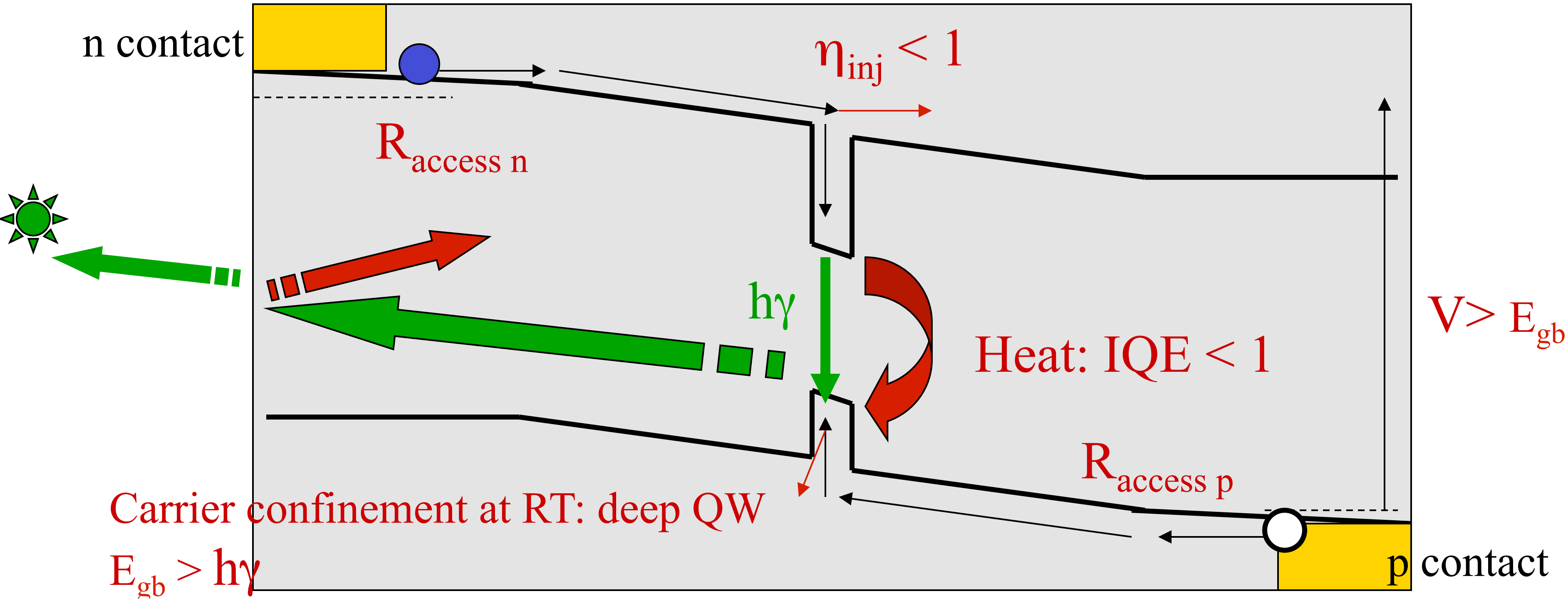
⇒ EQE = 1

Ideal world

$V \sim E_{g\ barrier}$

$P_{elec} = V \times I \sim E_{gb} \times I$

$P_{opt} = h\gamma \times \Phi = h\gamma \times I \Rightarrow WPE = P_{opt} / P_{elec} = h\gamma / E_{gb} \sim 1$



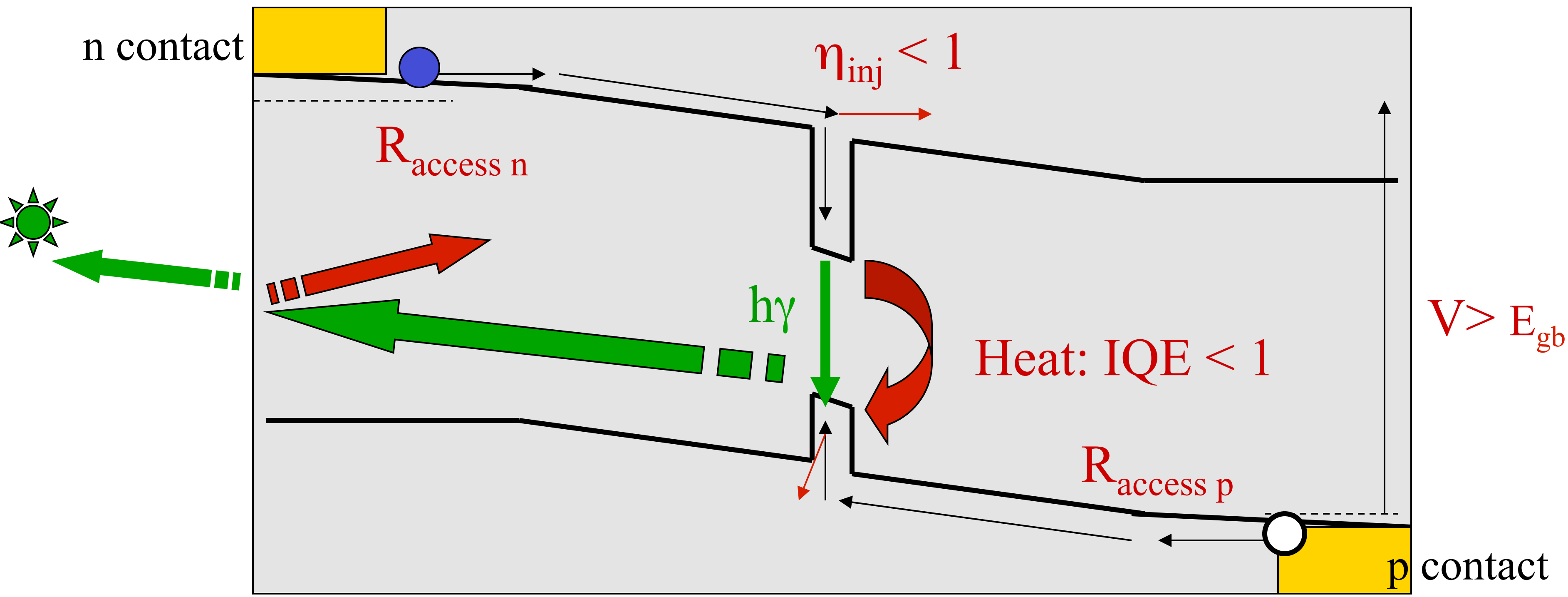
$$V \sim E_{g\ barrier} + R_{access} \times I$$

$$WPE = \underbrace{h\gamma / V}_{<1} \times \underbrace{\eta_{inj} \times IQE \times EE}_{EQE < 1}$$

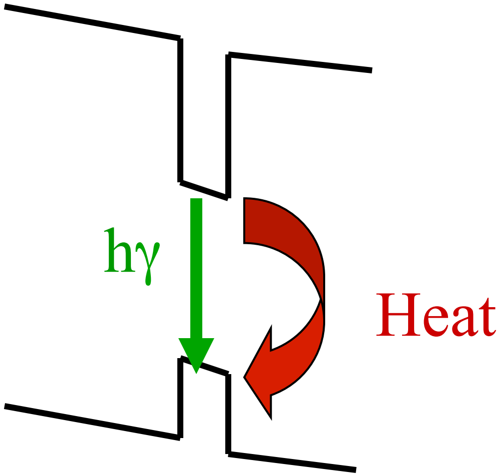
Real world

What can the epitaxy do to address these issues ?

- Almost everything … if processing and design are OK
- Nothing if not !


n contact
$\eta_{inj} < 1$
$R_{access\ n}$
hγ
Heat: IQE < 1
V> E_{gb}
$R_{access\ p}$
p contact

OUTLINE



Radiative transitions described by a radiative time τ_R

Non radiative recombinations described by τ_{NR}

$$IQE = \frac{1/\tau_R}{1/\tau_R + 1/\tau_{NR}} = \frac{\tau_{NR}}{\tau_R + \tau_{NR}}$$

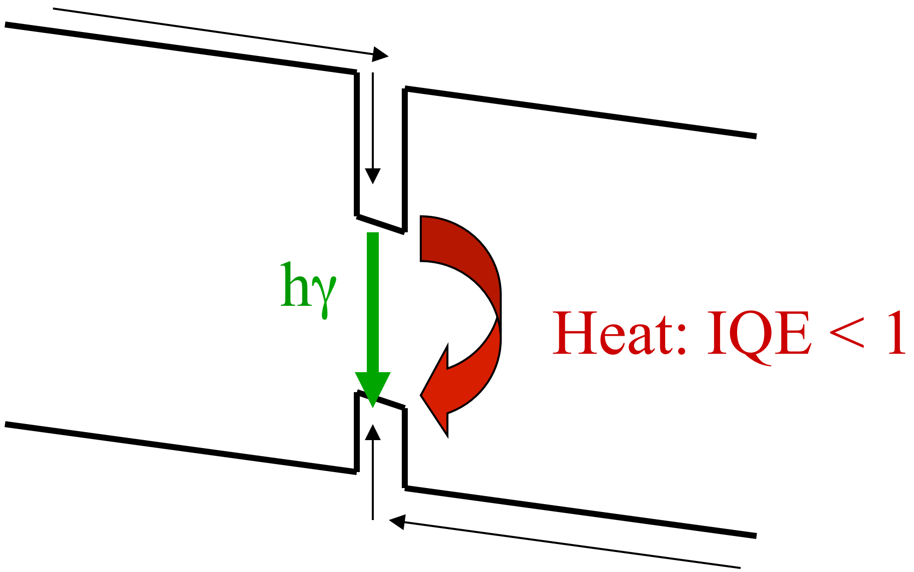
Minimize τ_R

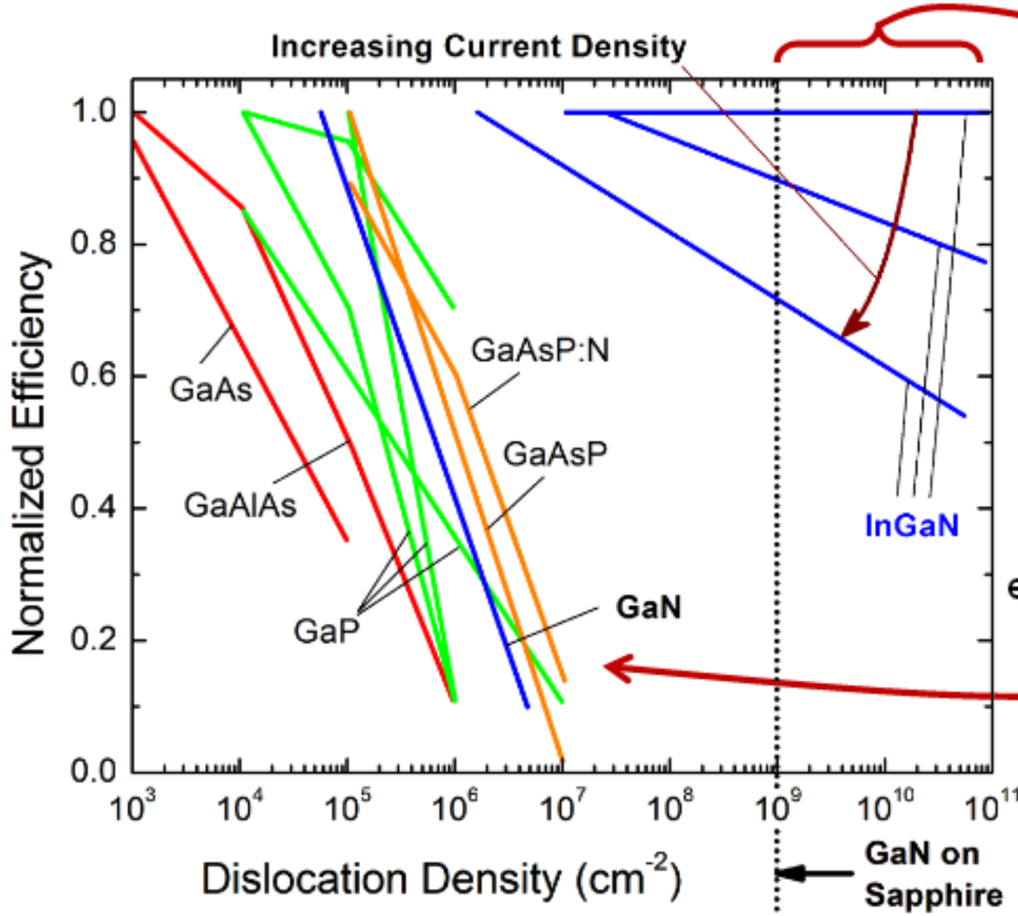
Maximize τ_{NR}

NB: some non linear phenomena and non exponential transients in particular at high injection. See later.

Non radiative recombinations

τ_{NR} decreases with defect density (point defects, dislocations)





Inhomogeneous: (InGaN)

Bright (!) despite high defects

Higher currents mask inhomogeneity effects (valleys fill up)

Homogeneous: (GaN,AlGaN)

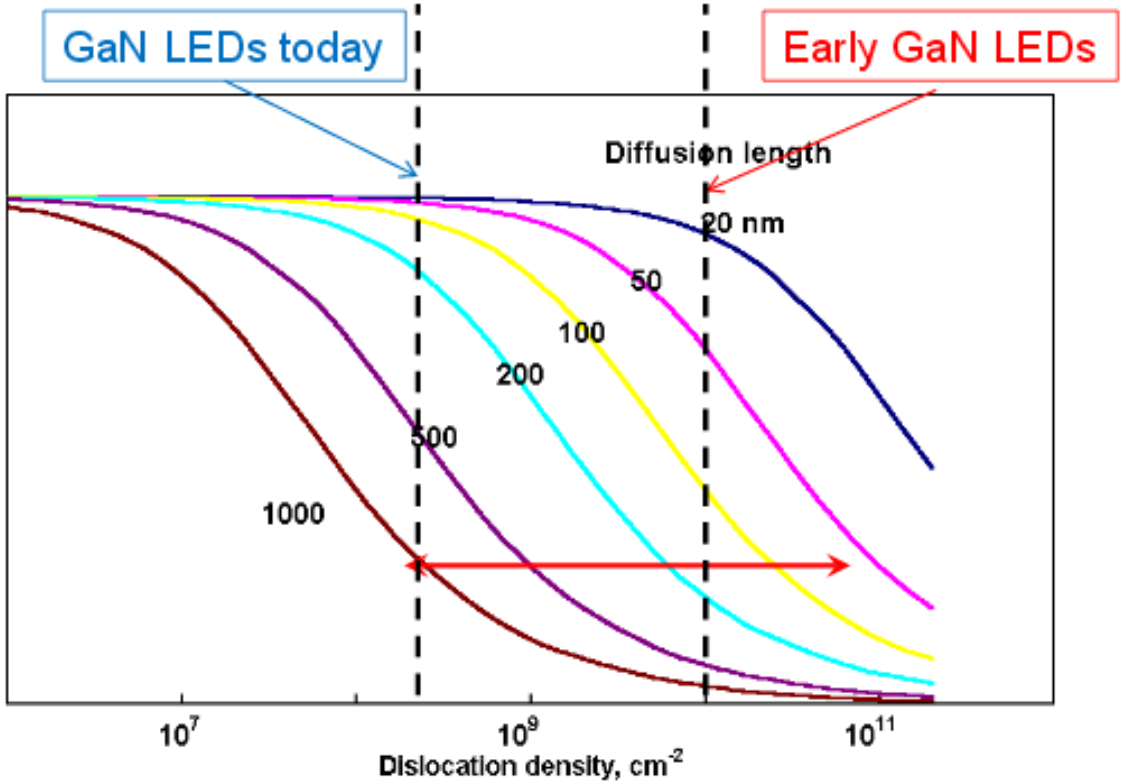
Dim as defects “swallow” electrons **without** producing light

Nitrides more defect tolerant than other SC !!!

source: S. Nakamura, Nobel lecture

Dislocations and diffusion length

IQE



S. Speck and S.J. Rosner, Physica B274. 24 (1999)

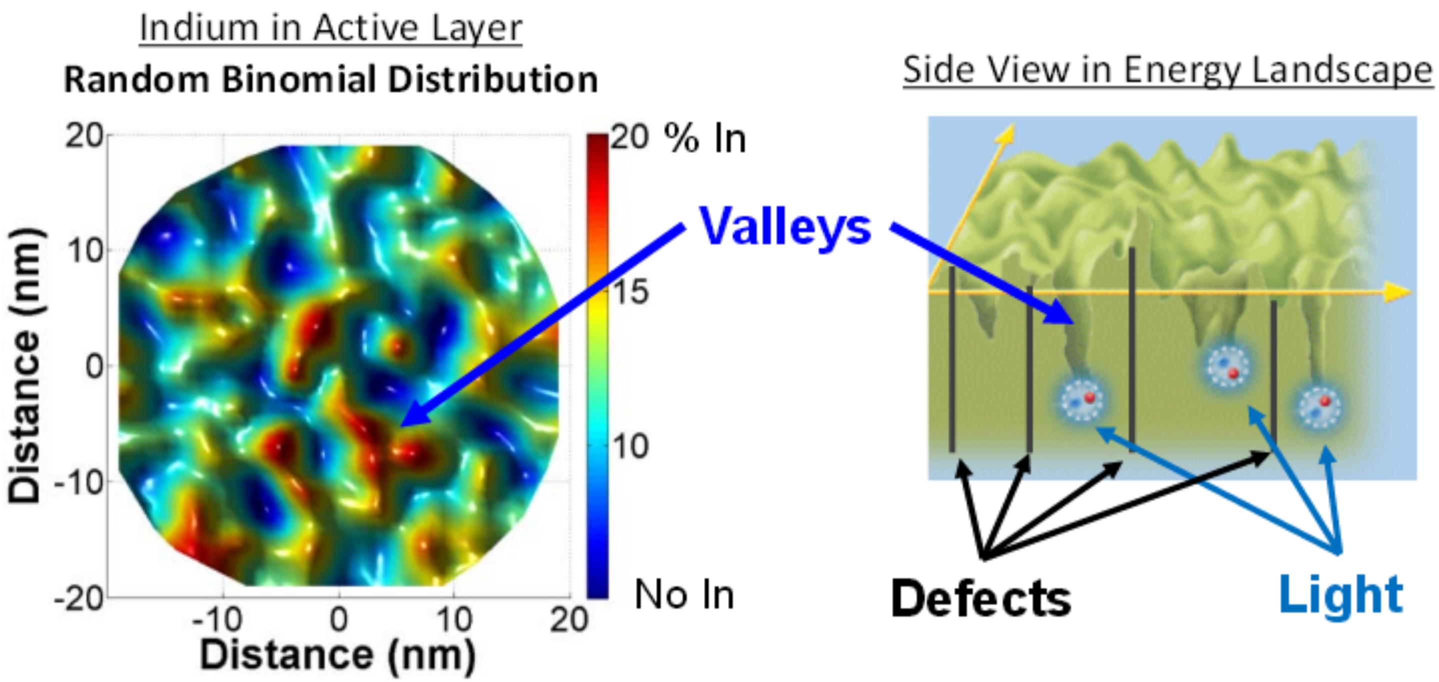
Mean distance between dislocations = $DD^{-1/2}$

EH pairs do not see dislocations if L_{dif}< disloc distance

$DD=10^8$ cm^{-2}, distance =1 μm

What can epitaxy do on diffusion length ?

Lateral potential fluctuations in QWs (In fluctuation) limit the diffusion length. QW epitaxy is crucial !

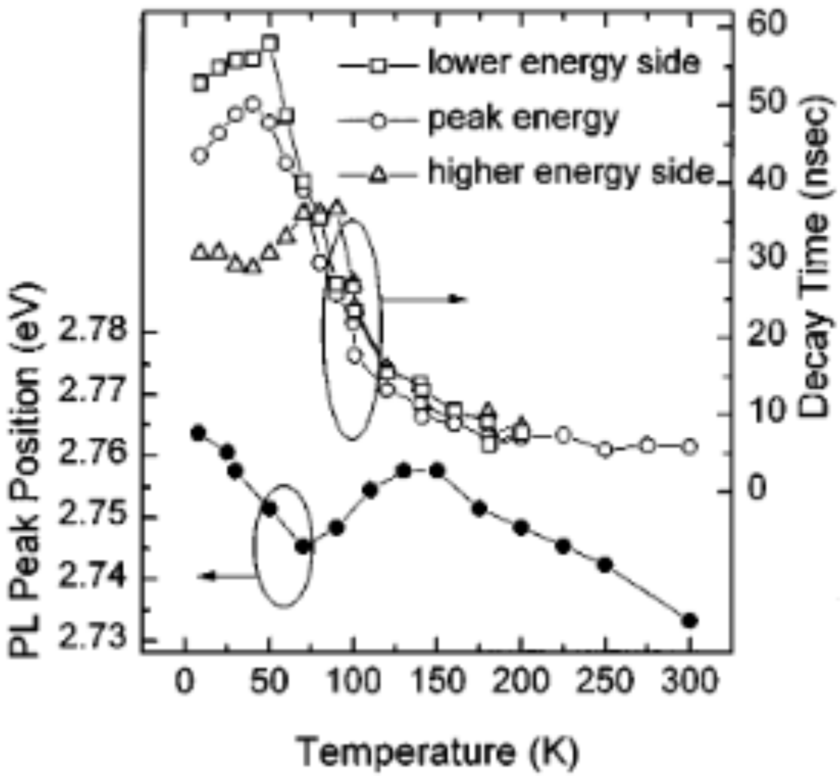


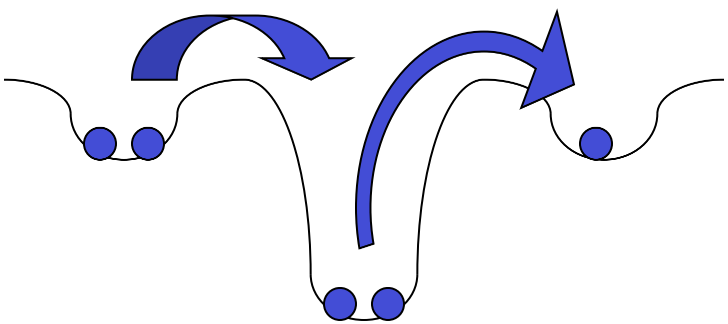
S. Nakamura, Nobel lecture. Chichibu, Nakamura et al., Appl. Phys. Lett., 69(1996) 4188; Nakamura, Science, 281(1998) 956.

Many studies on In fluctuations, localization, S shape in PL versus T, In spinodal decomposition, In Quantum Dots …

Patent issues: are InGaN LEDs based on Q Dots ?

Exciton localisation and S-shape PL

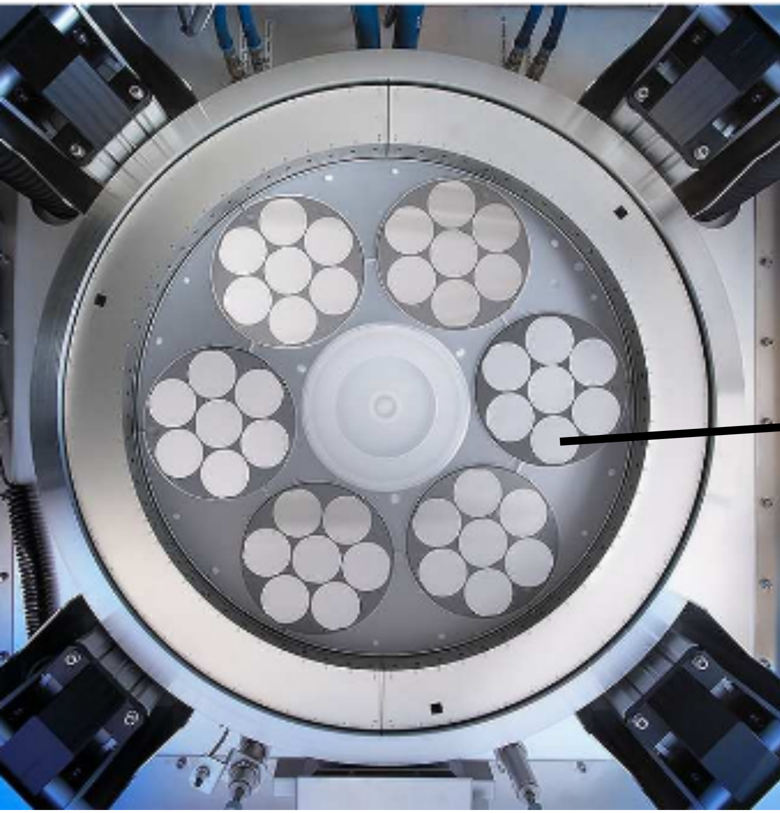




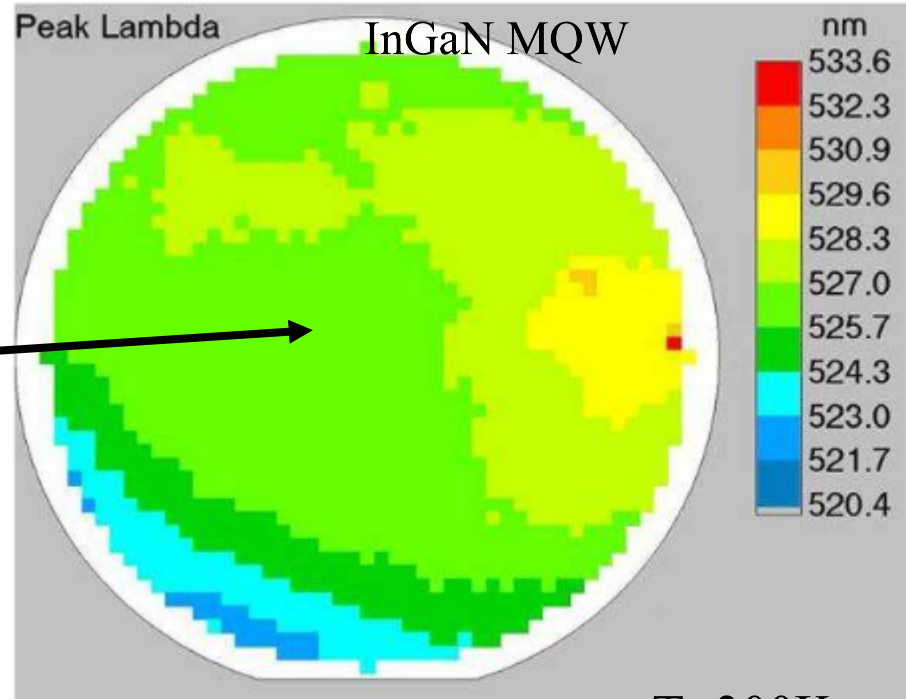
S. Chichibu, T. Azuhata, T. Sota, and S. Nakamura, APL 69, 4188 (1996)

Y-H Cho, G. H. Gainer, A. J. Fischer, J. J. Song, S. Keller, U. K. Mishra, and S. P. DenBaars, APL 73, 1370 (1998)

Control on In content



42x2-inch Planetray Reactor



T=300K

Average wavelength = 527 nm

Standard deviation = 1,2 nm ⇔ **5 meV**.

Source INDOT (STREP 2008) final activity report by Aixtron

InGaN now very uniform and high IQE ! Different localization scale ? Still an open question !!

What can epitaxy do on the dislocation density ?

GaN substrates grown at equilibrium (2530 °C, 45 atm) or even close to, are extremely difficult to obtain : efforts by Unipress, Poland for 2 decades have led to cm^2 samples

- Heteroepitaxy is unavoidable
- No lattice matched substrate (sapphire lattice mismatch 16%, …)
- Need for a transition layer (buffer)
- **Thousands of studies, papers, conferences on dislocation density reduction. Nobel prize !**
- High performance LED are currently fabricated on GaN with a DD ~ 10^8 cm^{-2} with IQE >90 %.

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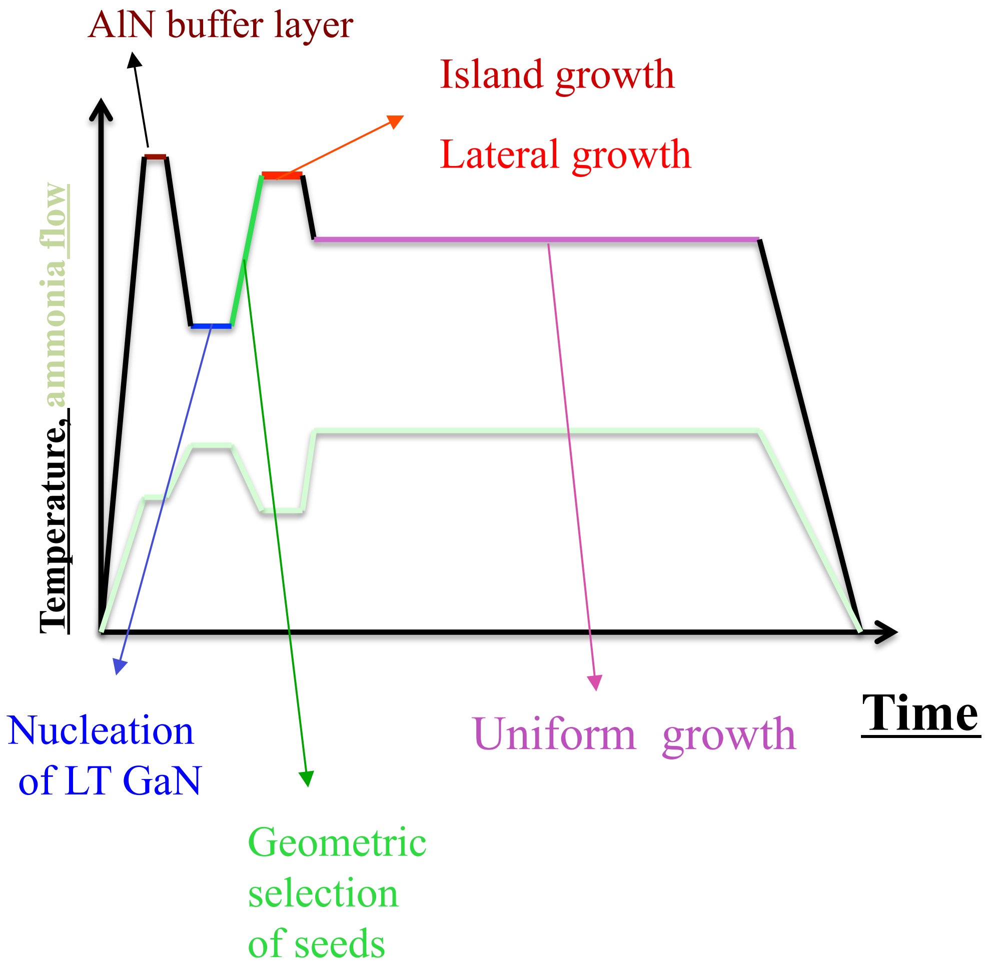
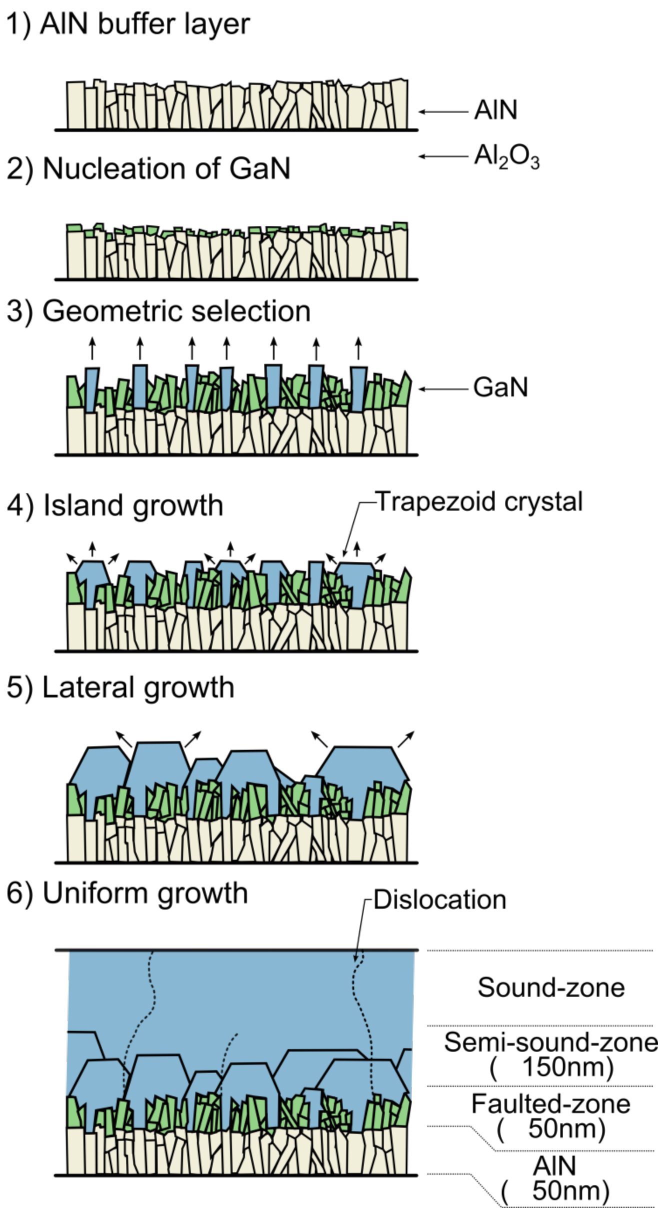
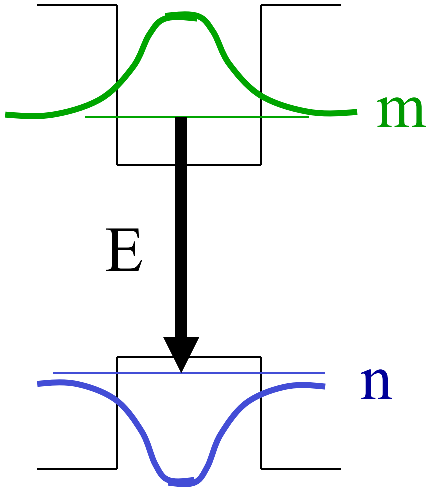
Multi step growth on sapphire

Yoshida et al, Akasaki et al. , Hiramatsu et al. , Nakamura et al., ….. 1986 to 2014





From B. Gil, GaN school 2015



Radiative transitions described by a radiative time $\tau_R \sim 1 / G_{mn}$

$$G_{mn} = \frac{e^2}{2h}\left|\vec{E}.\vec{r}_{vc}\right|^2 \frac{m_r}{\hbar^2}\left|\langle nv|mc\rangle\right|^2 H(\hbar\omega - E_g - E_n^v - E_m^c) f_m^c(\hbar\omega)(1 - f_n^v(\hbar\omega))$$

Transition dipole	Wave function overlap	Energy conservation	Carriers in the QW : injection

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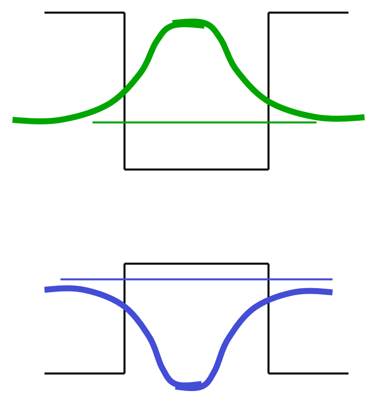
$$G_{mn} = \frac{e^2}{2h}\left|\vec{E}.\vec{r}_{vc}\right|^2 \frac{m_r}{\hbar^2}\left|\langle nv|mc\rangle\right|^2 H(\hbar\omega - E_g - E_n^v - E_m^c) f_m^c(\hbar\omega)(1 - f_n^v(\hbar\omega))$$

Material properties

Epitaxy (and design) can have an impact on transition selection rules: remains limited for visible LEDs

$$\left|\langle nv|mc\rangle\right| = \int \zeta_{nv}(z)\zeta^*_{mc}(z)dz$$

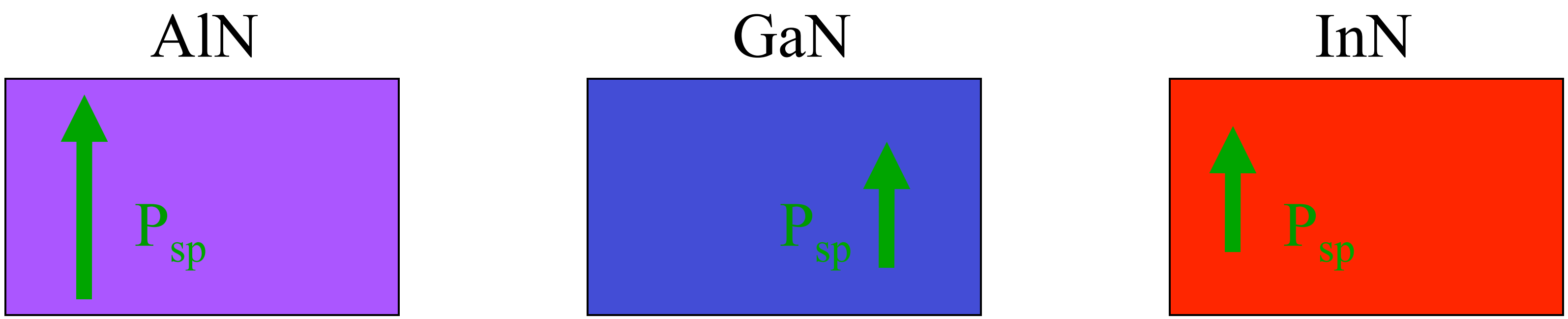


Envelope functions

Not a critical issue in ” normal” semiconductors (GaAs) but very critical in GaN !

Polarization in wurzite nitrides

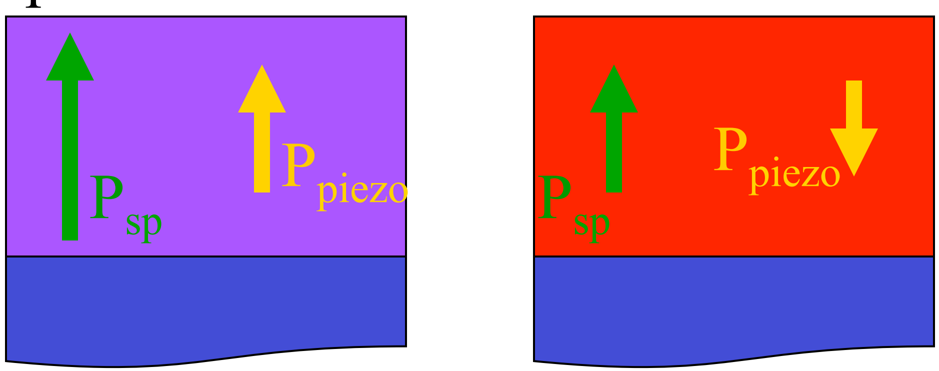
- Spontaneous polarisation :



	AlN	GaN	InN
P_{spont} (C/m2)	-0.081	-0.029	-0.032

- Piezoelectric polarisation due to strain:

AlN (AlGaN) in tension on GaN



InN (InGaN) in compression on GaN

Polarization in heterostructures

$$div\vec{F} = \frac{\rho}{\varepsilon} - \frac{1}{\varepsilon} div\vec{P}$$

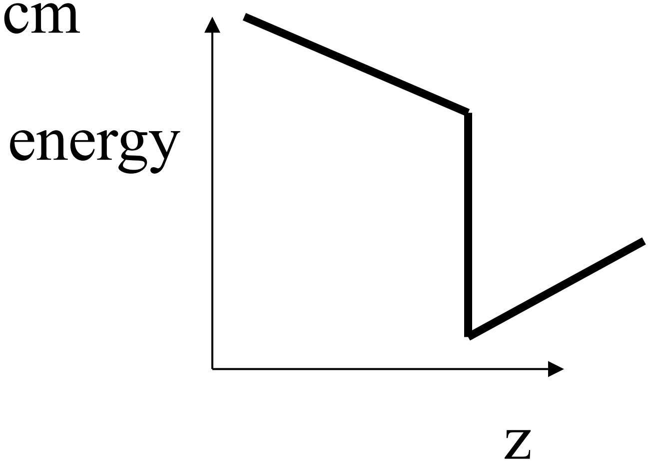
$$\frac{\partial F}{\partial z} = \frac{\rho(z)}{\varepsilon} - \frac{1}{\varepsilon}\frac{\partial P}{\partial z}$$

Across an interface along z : $\Delta F = -\frac{1}{\varepsilon_0 \varepsilon_r}\Delta P$

$\Delta P = P_{AlN} - P_{GaN} \approx$ 0.05-0.1 C/m^2

$\Delta F = F_{AlN} - F_{GaN} \approx \Delta P / \varepsilon_0 \varepsilon_r \approx$ 6-12 MV/cm

Enormous internal field discontinuity at the interface !



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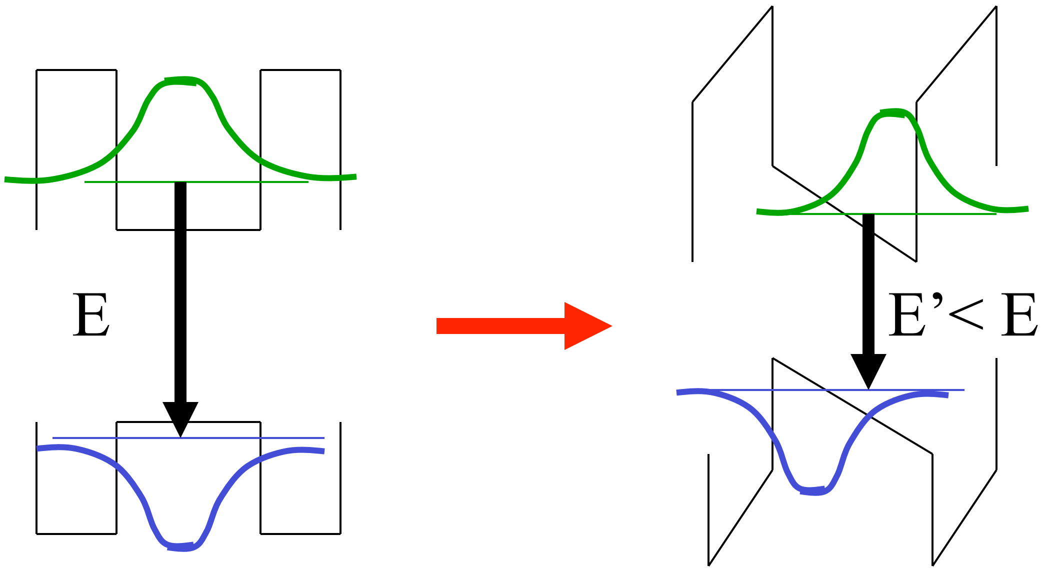
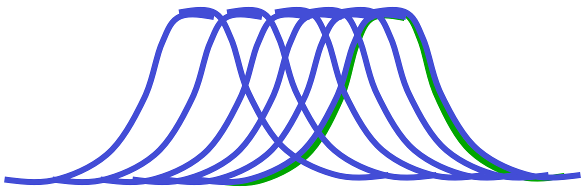
Polarization in wurzite nitrides

In quantum wells:

Quantum Confined Stark Effect





The energy redshifts and the wavefunction overlap decreases:

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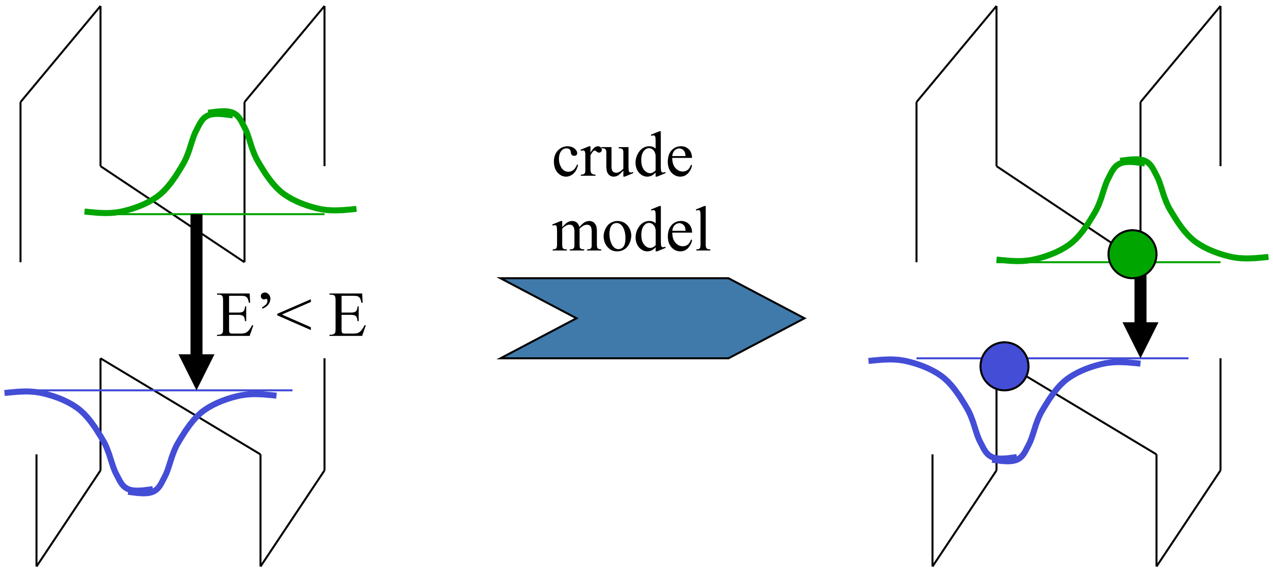
Polarization in wurzite nitrides

Quantum Confined Stark Effect



$$E = E_0 - eFW_{qw}$$

hole wavefunction decreases exponentially towards the electron wavefunctions or vice versa

$$\left|\langle nv | mc \rangle\right| = \int \zeta_{nv}(z)\zeta^*_{mc}(z)dz \approx e^{-W_{QW}/W_0}$$

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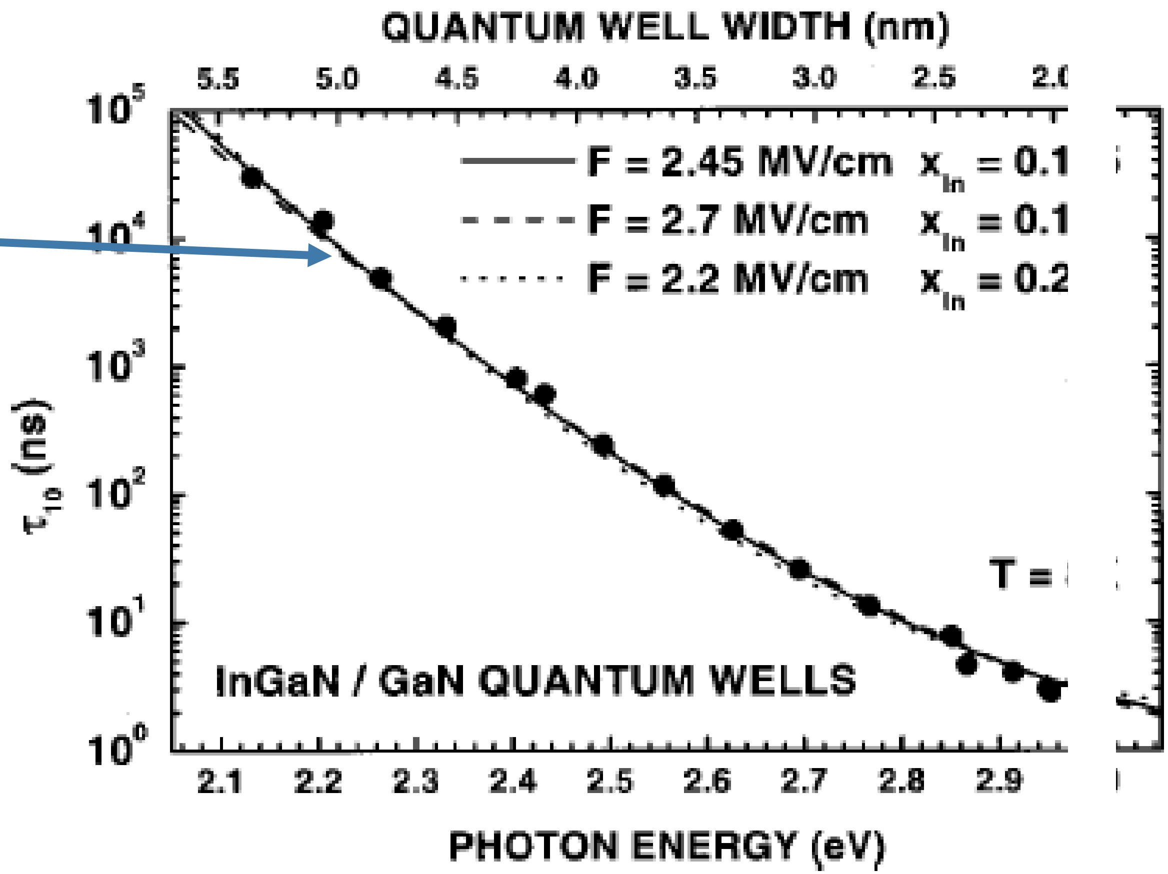
Polarization in wurzite nitrides

Radiative lifetime measured in InGaN OWs

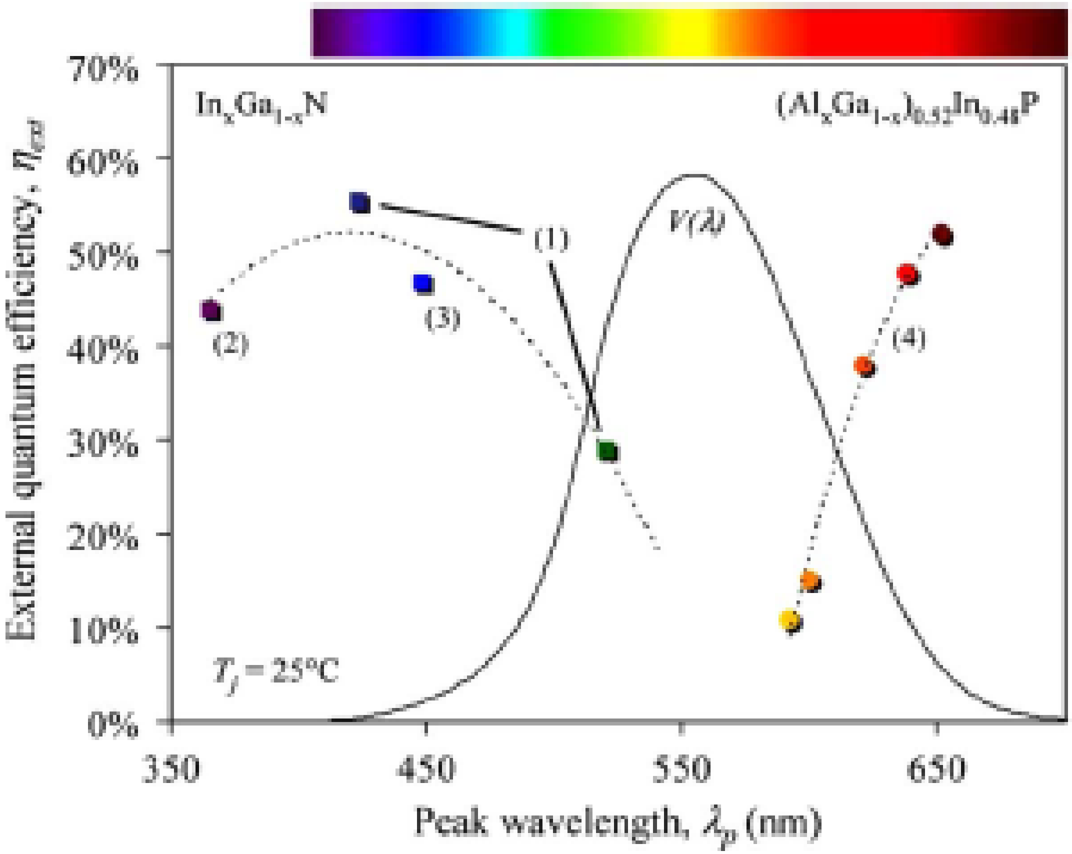
Exponential decrease in large QWs



P. Lefebvre et al, APL 78, 1252 (2001)

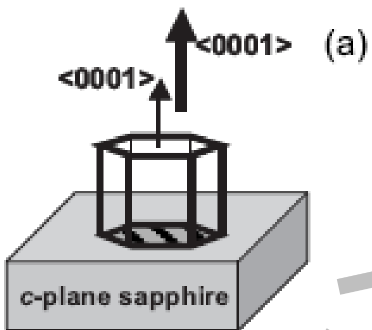
Polarization in wurzite nitrides

Stark effect is one of the reasons why green LEDs and lasers are less efficient than blue ones (green gap)

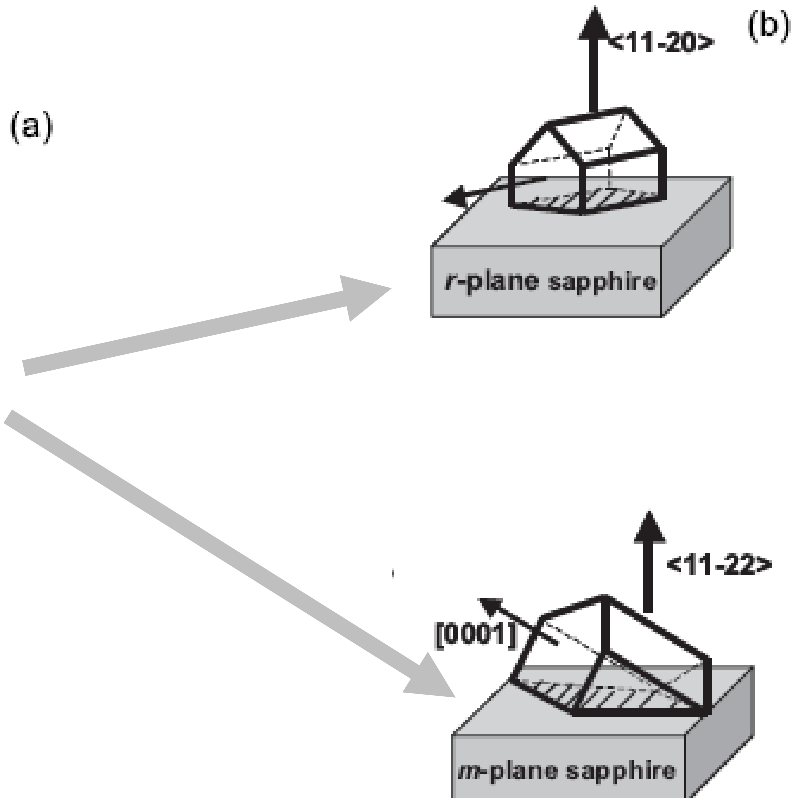


M. Crawford, IEEE J. OF SELECTED TOPICS IN QUANTUM ELECTRONICS, 15, 4, (2009)

Non/semi polar materials



Growth along c: polar

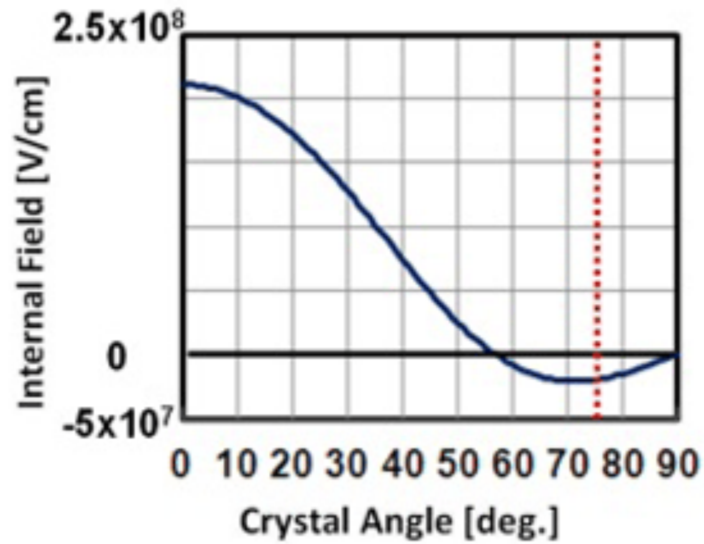


Growth ⊥ c: non polar

F = 0

Growth ≠ c: semipolar

F weak



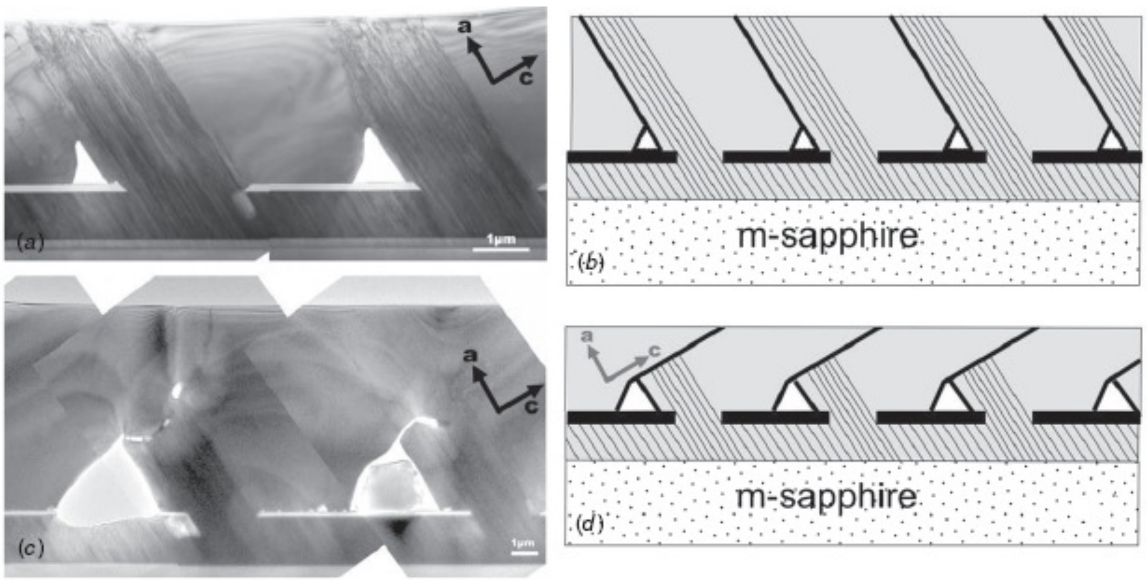
Non/semi polar materials

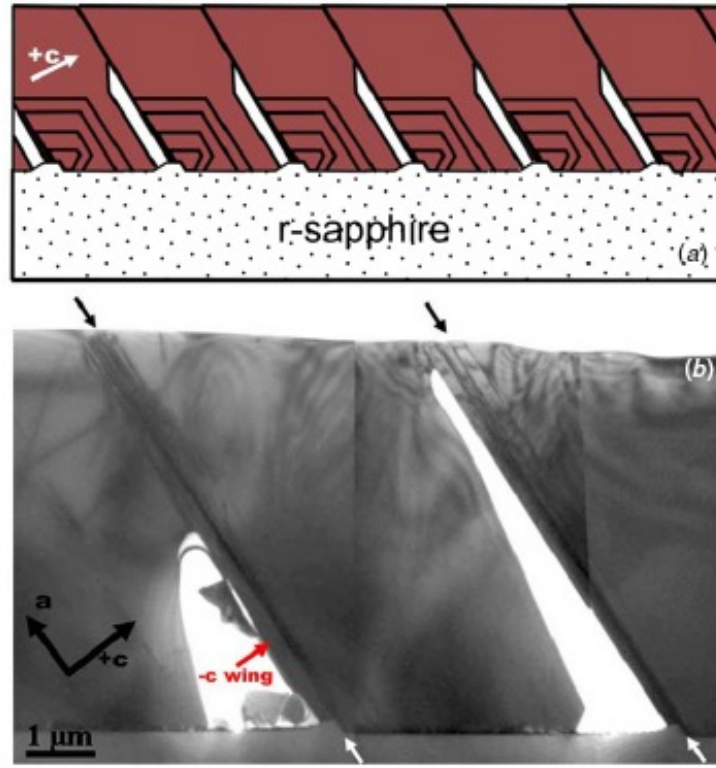
Approach	Result and problems	Solutions
Substrates with various cuts (Si, SiC, sapphire…)	Large surface Dislocations (>10^9 cm^{-2}) and stacking faults (10^5 cm^{-1})	Try new substrates. Optimize growth conditions
GaN crystal grown along c and cut in oblique direction	High quality material (Mitsubishi, Sumitomo) High performance LEDs and lasers (UCSB…) Small size	Increase initial thickness
Localized epitaxy on inclined facets	High quality Small size or problems of coalescence	Be smart to filter defects during lateral growth

SP GaN

Localized + lateral epitaxy

Differents steps with varied growth conditions





Start up project from CRHEA

F. Tendille

CRHEA

Semicond. Sci. Tech. 27 (2012) 024004

Epitaxy choice

- Non/semipolar material
  - Short τ_R is good if τ_{NR} remains long
- Polar material with thin QWs ⇒ large confinement energy ⇒deeper QWs needed for the same transition energy ⇒ more Indium ⇒ new problems:
  - Strain, possible plastic relaxation, dislocations
  - Spinodal decomposition of InGaN (thermodynamic instability).

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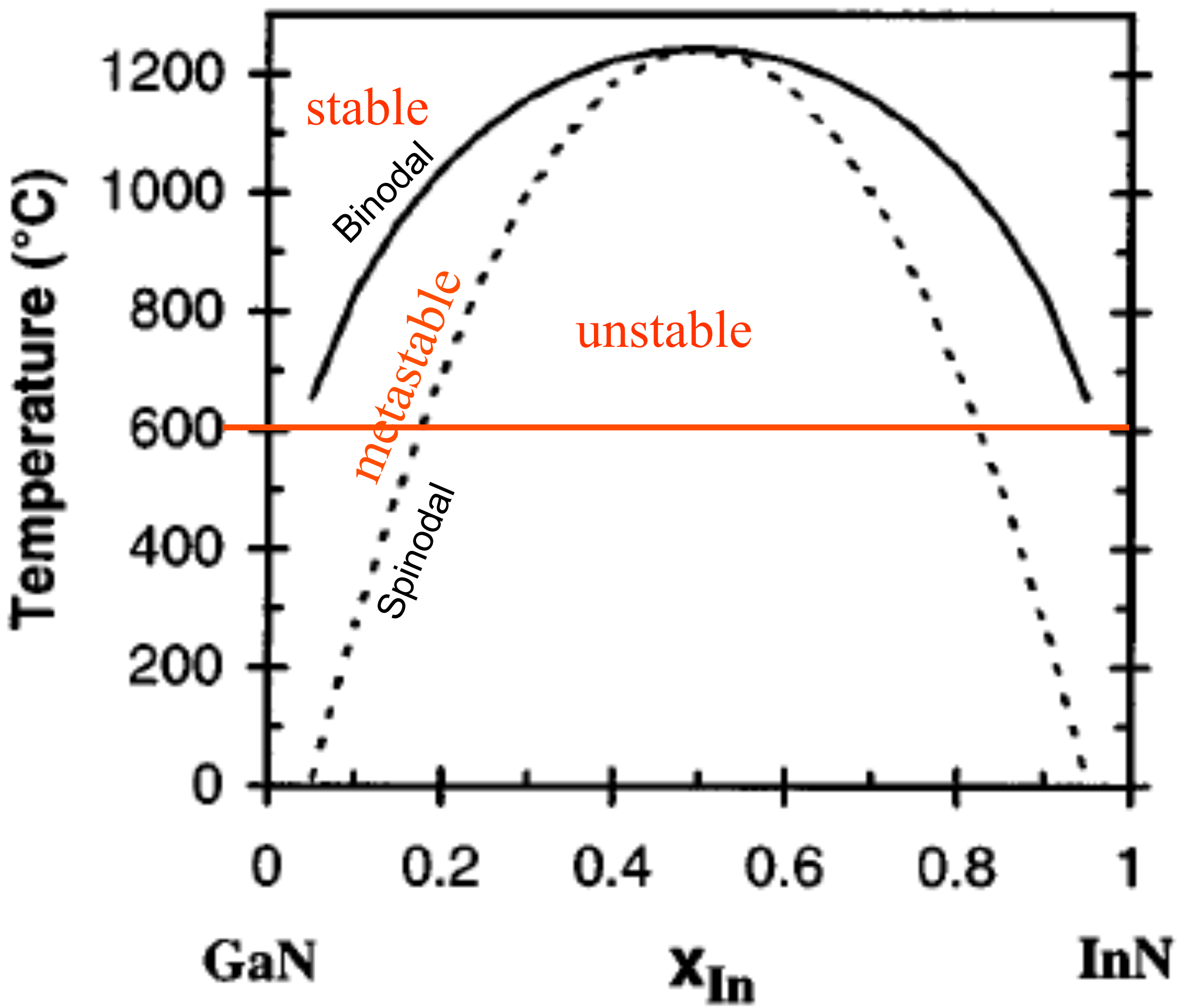
Decomposition of $Ga_{1-x}In_xN$

GaN and InN have very different atomic radii ➔Phase separation

Very low solubility of InN in GaN

Dynamics of phase separation is thermally activated : InGaN can be grown at low temperature

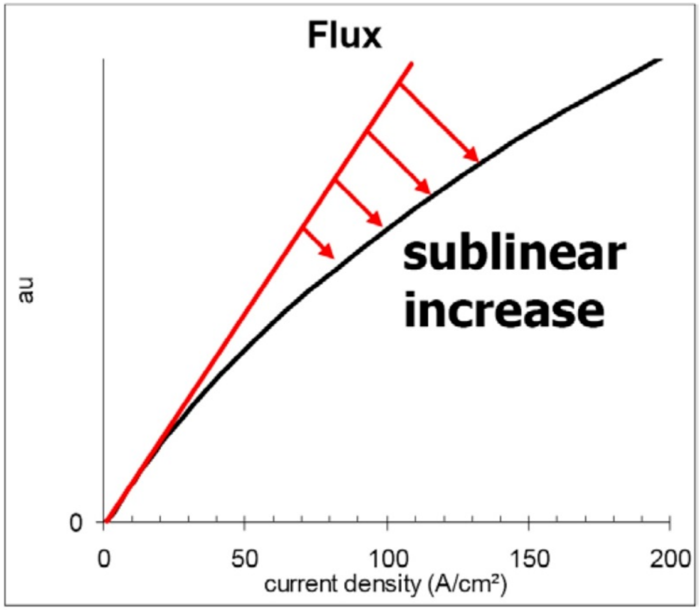
Calculated GaInN alloy phase diagram

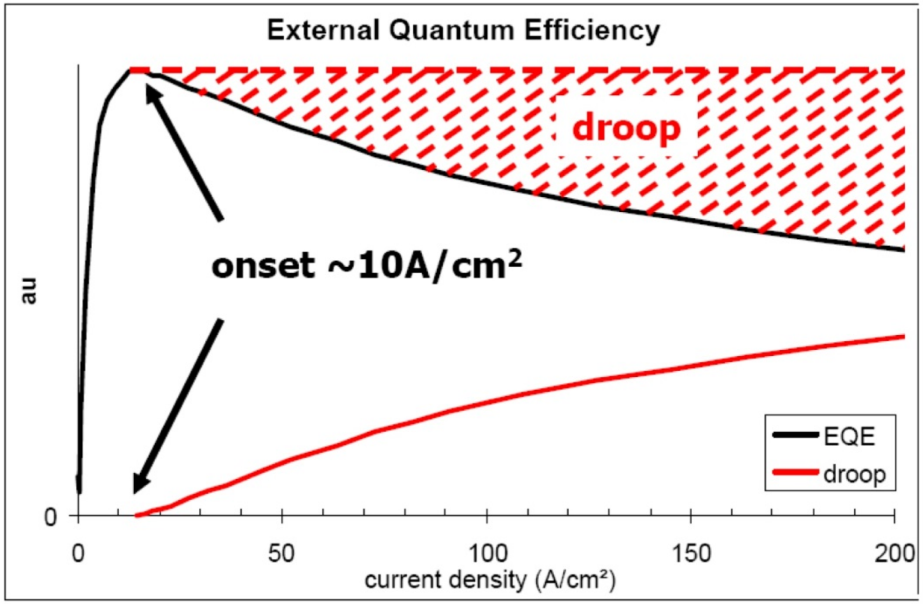


Ho and Stringfellow APL 69 2701 (1996)

Ultimate problem : droop

Reduction of the quantum efficiency at high injection





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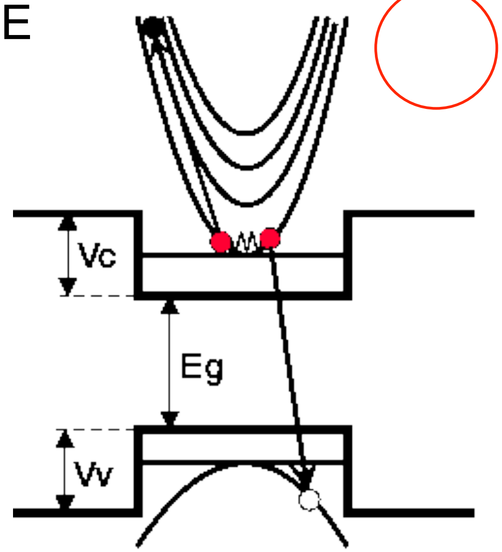
Origins of the efficiency droop

Auger recombination processes

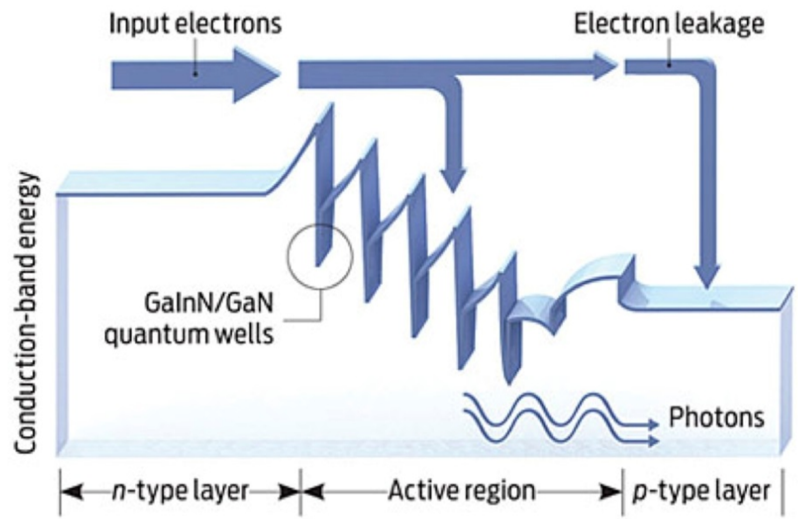
$$\eta = \frac{\eta_{inj} B N^2}{AN + BN^2 + CN^3}$$

IQE



rate ~ n^2p

Carrier overshoot



J. Iveland, L. Martinelli, J. Peretti, J.S. Speck, and C. Weisbuch, Phys. Rev. Lett. ***110****, 177406 (2013).*

Solutions to the droop

Auger recombination processes

Non radiative rate $\sim C\,n^3$

Reduce n for a constant I

Increase well width

Increase well number

- **QCSE**
- **Strain issues**

Strain issues

Epitaxy !!

$$G_{mn} = \frac{e^2}{2h}\left|\vec{E}.\overrightarrow{r_{vc}}\right|^2 \frac{m_r}{\hbar^2}\left|\langle nv|mc\rangle\right|^2 H(\hbar\omega - E_g - E_n^v - E_m^c) f_m^c(\hbar\omega)(1 - f_n^v(\hbar\omega))$$

Epitaxy (and design) can have an impact: remains limited for LEDs

Many epitaxial parameters:

- Polar / non polar
- Strain
- Barrier composition and thickness
- QW composition and thickness

Carrier injection

Large hole and electron densities in the QW

Doping

AlGaInN

Tableau périodique des éléments

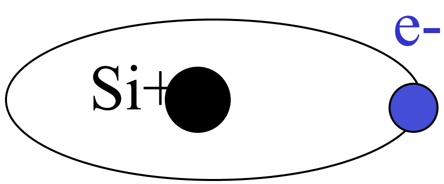
Masse atomique relative, donnée avec deux décimales → M_r
Symbole de l'élément → X
Nombre atomique → Z

1 (Ia)	2 (IIa)		3 (IIIb)	4 (IVb)	5 (Vb)	6 (VIb)	7 (VIIb)	8 (VIIIb)	9 (VIIIb)	10 (VIIIb)	11 (Ib)	12 (IIb)	13 (IIIa)	14 (IVa)	15 (Va)	16 (VIa)	17 (VIIa)	18 (VIIIa)
1,01 **H** 1																		4,00 **He** 2
6,94 **Li** 3	9,01 **Be** 4												10,81 **B** 5	12,01 **C** 6	14,01 **N** 7	16,00 **O** 8	19,00 **F** 9	20,18 **Ne** 10
22,99 **Na** 11	24,31 **Mg** 12												26,98 **Al** 13	28,09 **Si** 14	30,97 **P** 15	32,07 **S** 16	35,45 **Cl** 17	39,95 **Ar** 18
39,10 **K** 19	40,08 **Ca** 20		44,96 **Sc** 21	47,88 **Ti** 22	50,94 **V** 23	52,00 **Cr** 24	54,94 **Mn** 25	55,85 **Fe** 26	58,93 **Co** 27	58,69 **Ni** 28	63,55 **Cu** 29	65,39 **Zn** 30	69,72 **Ga** 31	72,61 **Ge** 32	74,92 **As** 33	78,96 **Se** 34	79,90 **Br** 35	83,80 **Kr** 36
85,47 **Rb** 37	87,62 **Sr** 38		88,91 **Y** 39	91,22 **Zr** 40	92,91 **Nb** 41	95,94 **Mo** 42	**Tc*** 43	101,07 **Ru** 44	102,91 **Rh** 45	106,42 **Pd** 46	107,87 **Ag** 47	112,41 **Cd** 48	114,82 **In** 49	118,71 **Sn** 50	121,75 **Sb** 51	127,60 **Te** 52	126,90 **I** 53	131,29 **Xe** 54
132,91 **Cs** 55	137,33 **Ba** 56	**57-70**	174,97 **Lu** 71	178,49 **Hf** 72	180,95 **Ta** 73	183,85 **W** 74	186,21 **Re** 75	190,21 **Os** 76	192,22 **Ir** 77	195,08 **Pt** 78	196,97 **Au** 79	200,59 **Hg** 80	204,38 **Tl** 81	207,21 **Pb** 82	208,98 **Bi** 83	**Po*** 84	**At*** 85	**Rn*** 86
Fr* 87	**Ra*** 88	**89-102**	**Lr*** 103	**Rf*** 104	**Db*** 105	**Sg*** 106	**Bh*** 107	**Hs*** 108	**Mt*** 109	**Uun*** 110	**Uuu*** 111	**Uub*** 112						

138,92 **La** 57	140,12 **Ce** 58	140,91 **Pr** 59	144,24 **Nd** 60	**Pm*** 61	150,36 **Sm** 62	151,97 **Eu** 63	157,25 **Gd** 64	158,93 **Tb** 65	162,50 **Dy** 66	164,93 **Ho** 67	167,26 **Er** 68	168,93 **Tm** 69	173,04 **Yb** 70
Ac* 89	232,04 **Th** 90	231,04 **Pa** 91	238,03 **U** 92	**Np*** 93	**Pu*** 94	**Am*** 95	**Cm*** 96	**Bk*** 97	**Cf*** 98	**Es*** 99	**Fm*** 100	**Md*** 101	**No*** 102

* : Eléments n'ayant pas de nucléide (isotope) de durée de vie suffisamment longue et n'ayant donc pas une composition terrestre caractéristique.

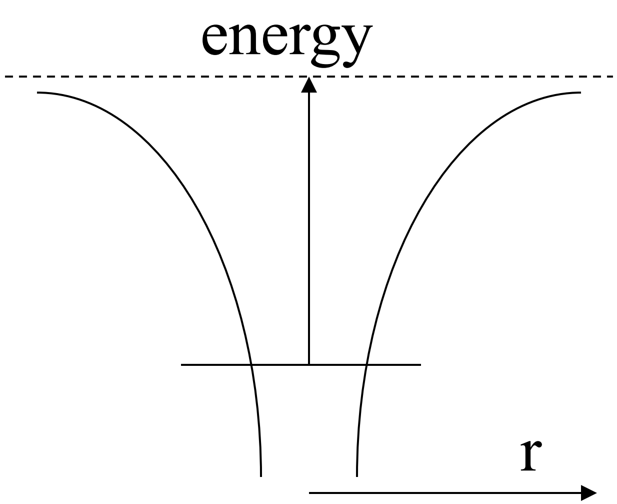
Donors

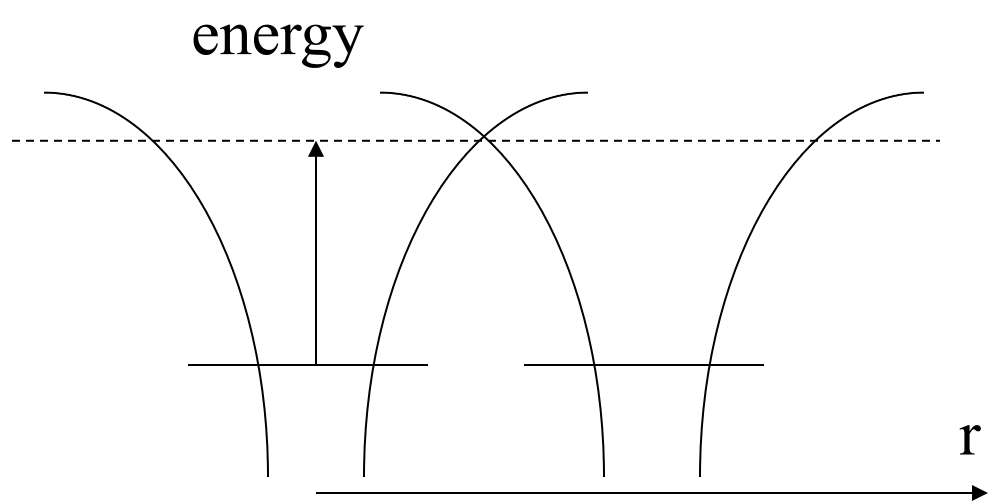


$$E = \frac{m_e}{m_0}\frac{1}{\varepsilon_r^2}R_y$$

Large donor energies are expected in nitrides (37 meV)

$1/\mu = 1/m_e + 1/m_{Si} \approx 1/m_e$





Donor energy renormalized at high concentration

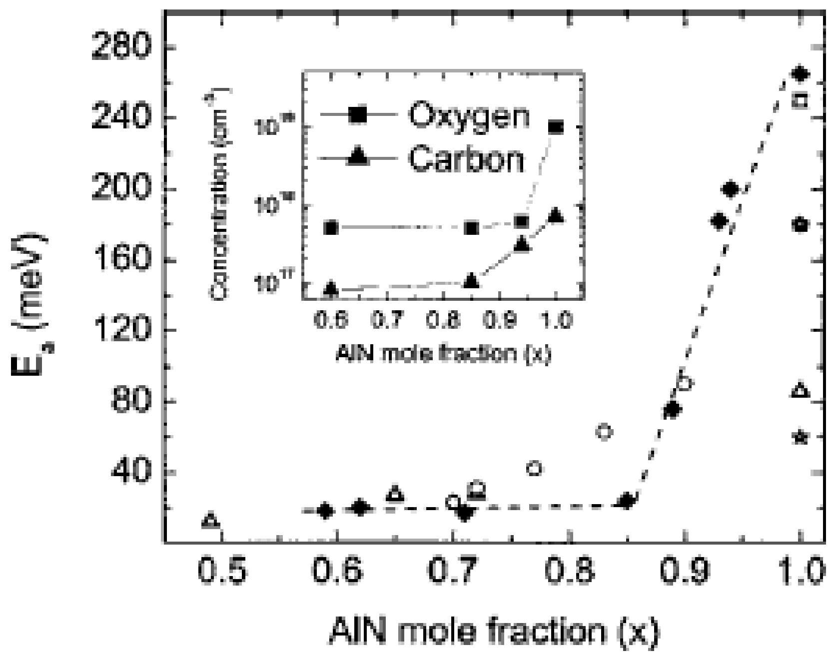
$E = E_0 - \beta n^{1/3}$ with $\beta = 10^{-8}$ eV/cm

Donors in GaN - AlGaN

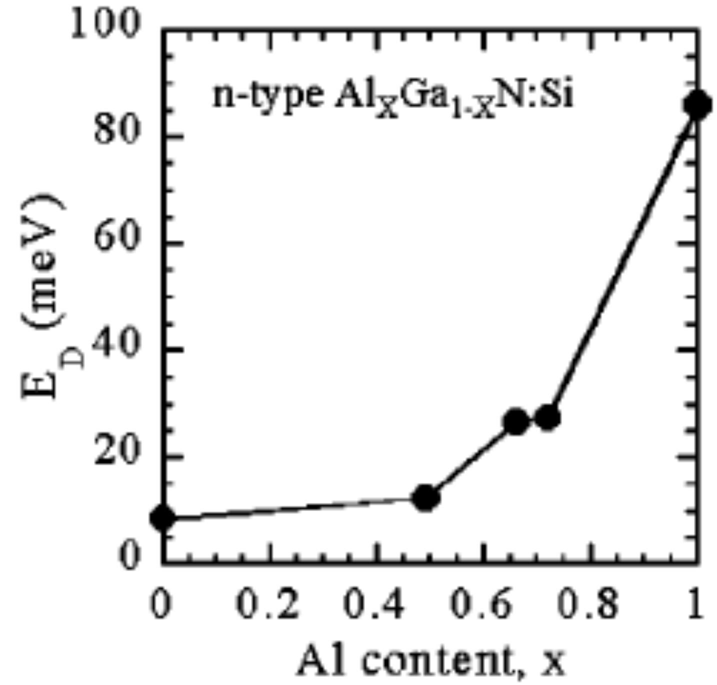
O : shallow donor in GaN (26 meV) but deep level in AlGaN

Si: shallow donor in GaN (25 meV), deeper in AlGaN (250 meV)

B. Borisov, APL 87,132106 (2005)

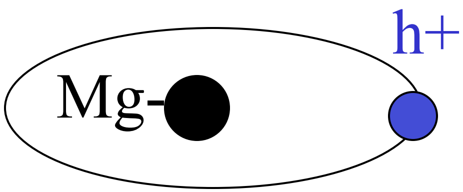


Taniyasu, APL 81, 1255 (2002)



Conclusion: n-doping by Si (Ge for reducing strain, not used for LEDs)

Acceptors: Mg



$1/\mu = 1/m_h + 1/m_{Mg} \approx 1/m_h$

$$E = \frac{m_e}{m_0}\frac{1}{\varepsilon_r^2}R_y$$

Very large acceptor binding energies are expected in nitrides (168 meV with m_h=1): not hydrogenoid !

E_{Mg} = 220 meV

⇒Low ionization ratio

⇒Large Mg densities necessary: 5×10^{19} cm^{-3} for p=5 $\times10^{17}$ cm^{-3}

⇒Large energy renormalization:

$E=E_0-\beta n^{1/3}$=180 meV ($\beta=10^{-8}$ eVcm)

Acceptors: alternatives to Mg ?

Time-resolved spectroscopy of Zn- and Cd-doped GaN

P. Bergman, Gao Ying,[a] B. Monemar, and P. O. Holtz
Department of Physics and Measurement Technology, Linköping University, S-581 83 Linköping, Sweden

(Received 27 October 1986; accepted for publication 22 December 1986)

Journal of Applied Physics 61, 4589 (1987)

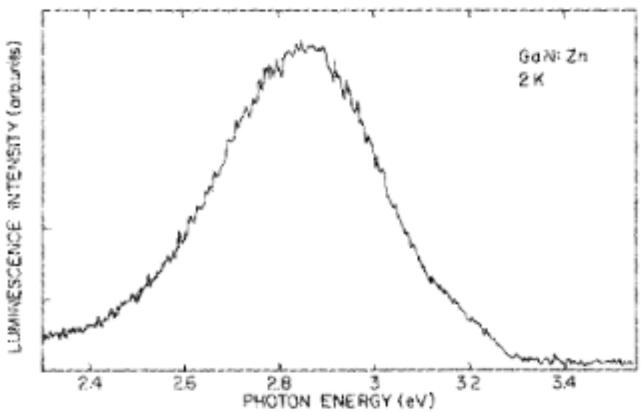
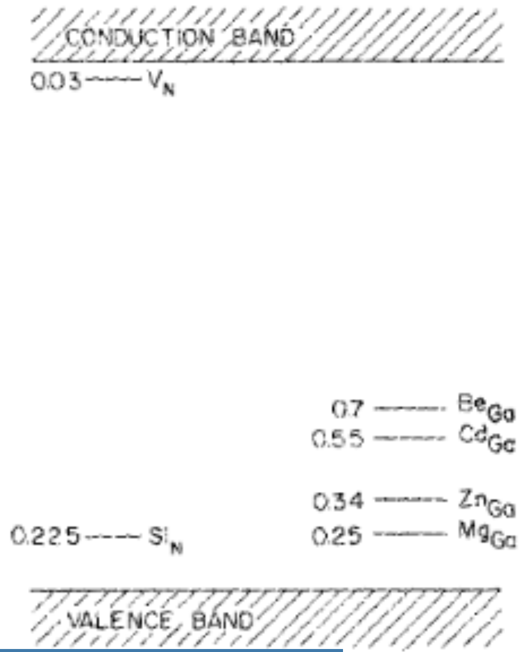


FIG. 1. Photoluminescence from Zn-doped GaN at 2 K, using pulsed nitrogen laser excitation. The spectrum shows a broad blue-violet emission band, peaking at ≃2.89 eV.



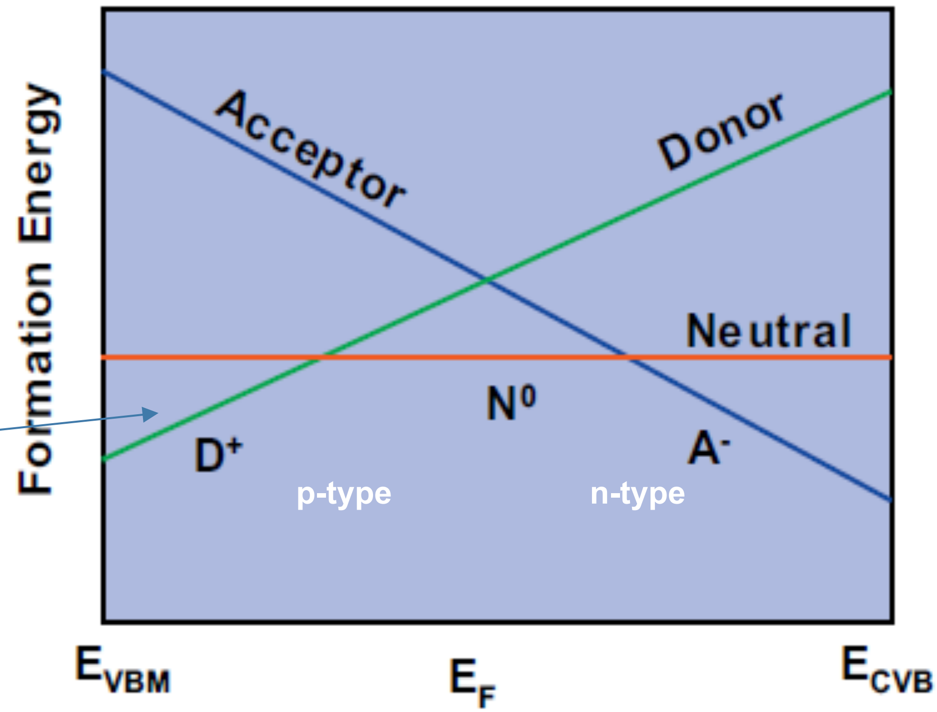
Conclusion: p-doping by Mg

Mg acceptor: other problems

Thermodynamic ionised defect formation energy and compensation mechanism

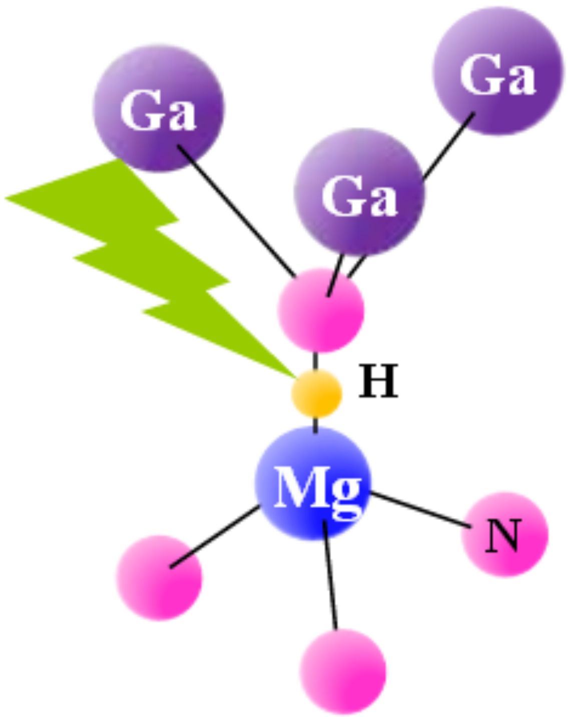
Donor case	**Acceptor case**
$Ef(d,q) = E_t(d) - E_t(0) + \mu_{i\,d} + q\,E_{Fermi}$	$Ef(d,q) = E_t(a) - E_t(0) + \mu_{i\,a} - q\,E_{Fermi}$

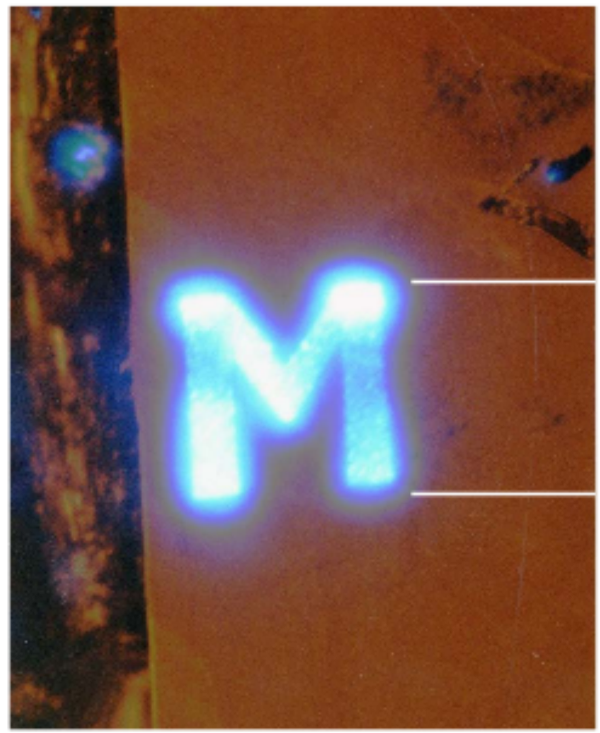
In p type materials, the Ga/Mg substitution becomes more difficult: other insertion sites where Mg is not active



Yan et Wei phys. stat. sol. (b) 245, No. 4, 641–652 (2008); Zunger 2004

The solution: with H, Mg is not active during epitaxy, better Mg incorporation in Ga substitution. H is eliminated afterwards (LEEBI or annealing)





50 µm

H. Amano et al., JJAP 28(1989)L2112.

1992 Thermal annealing

S. Nakamura et al., JJAP 31(1992)1258.

From Amano Nobel lecture

Electron and hole densities in GaN

Si doping:

n=10^{17}-10^{20} cm^{-3}

Mg doping

P ~ 5×10^{17} cm^{-3} for Mg= 5×10^{19} cm^{-3} MOCVD

P ~ 10^{18} cm^{-3} MBE : less compensation as less thermodynamic because lower temperature (which is good for InGaN QWs), less H_2

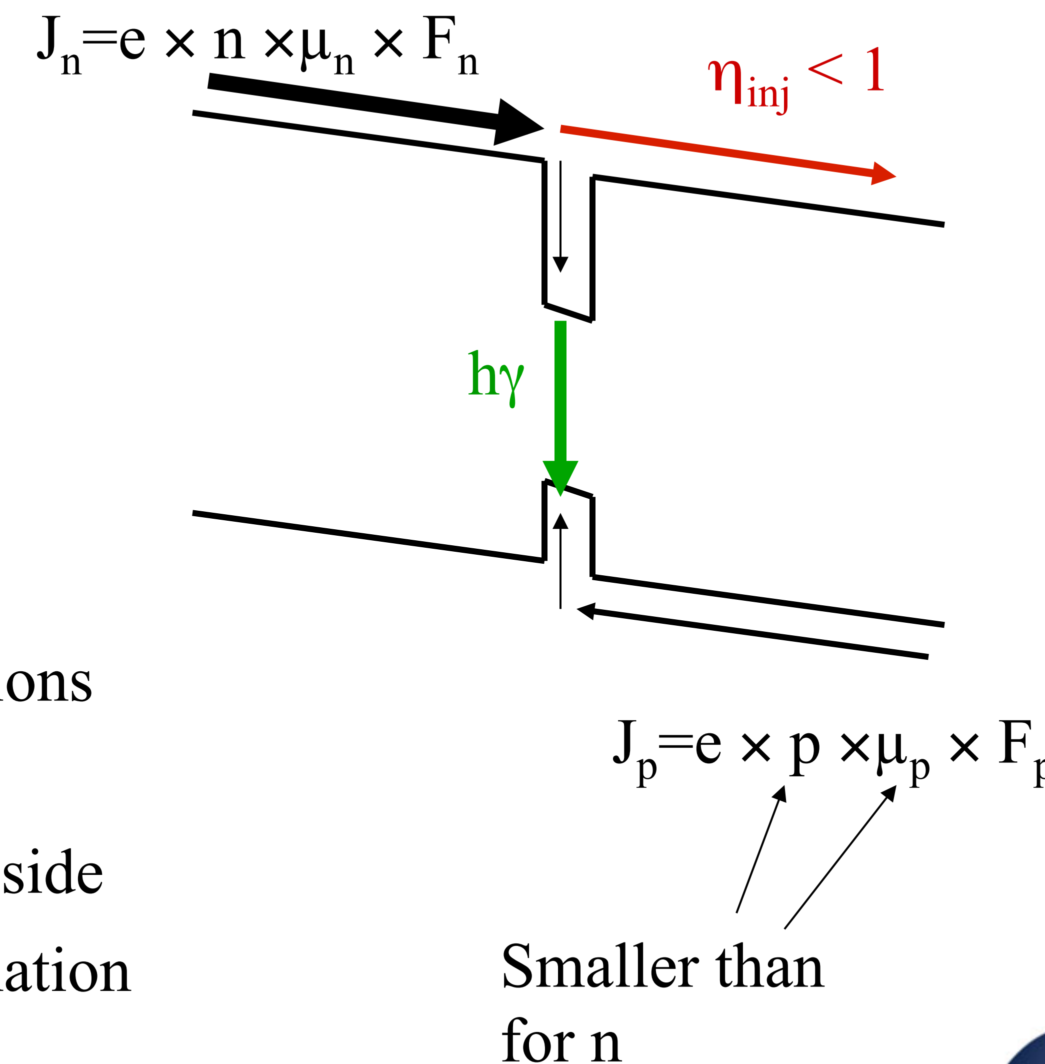
Carrier injection

Under high injection, the carrier densities close to the QW are proportional to the densities in the doped layers: $J = e \times n \times \mu \times F$

In the barrier: $J_n > J_p$

In the QW, if recombinations are radiative only, $J_n = J_p$

$\Rightarrow$Electrons injected in p side with non useful recombination



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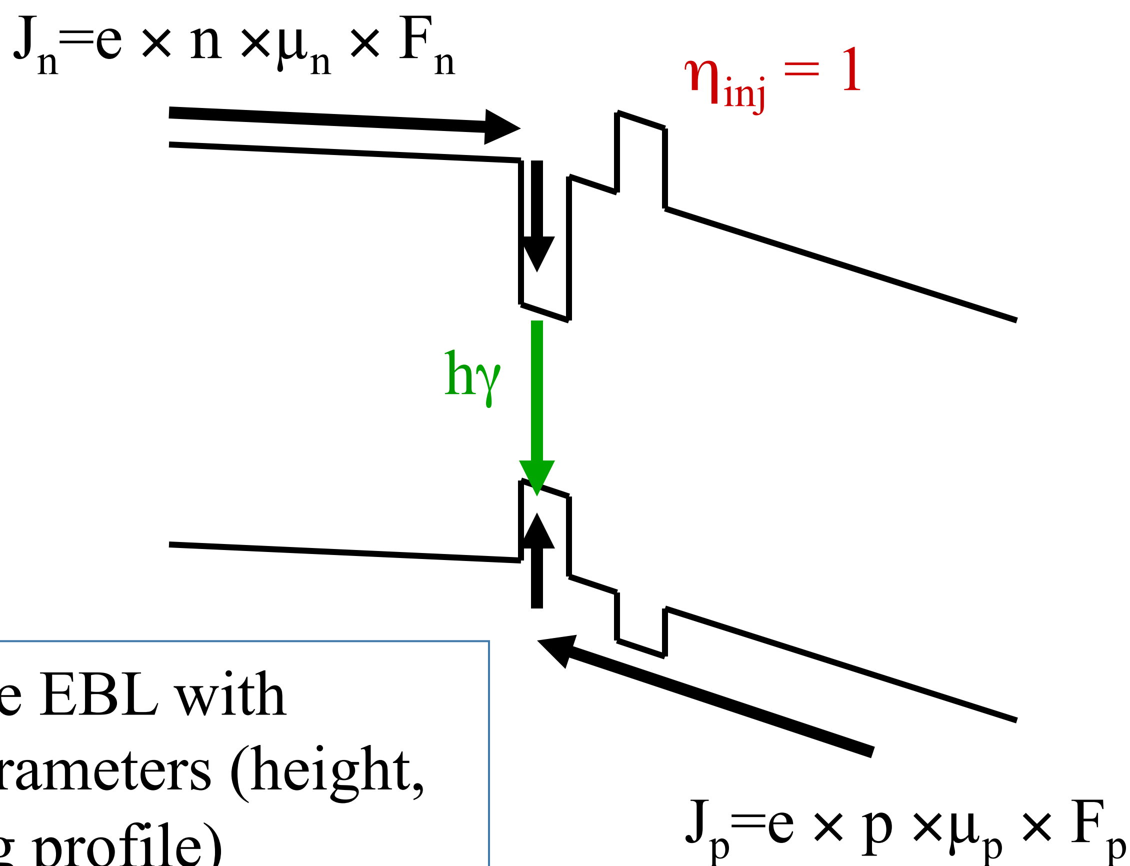
Carrier injection

Electrons are blocked (EBL), accumulate in the QW. The field redistribute, is larger on p side, the hole current increases. The electron current decreases

Finally, $J_n = J_p$ in the whole structure



Epitaxy of the EBL with optimized parameters (height, width, doping profile)

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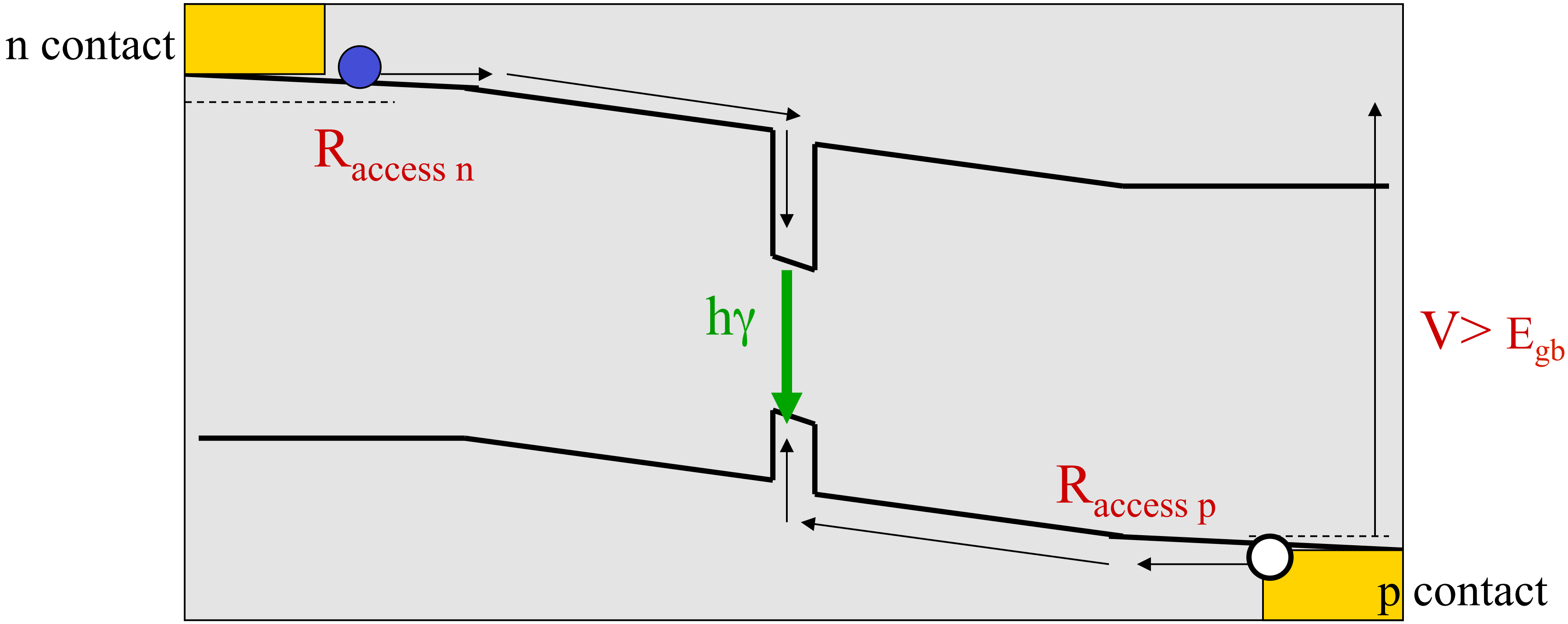
Access resistance



n type contact: $\rho \sim 10^{-5}\ \Omega cm^2$

p type contact: $\rho \sim 10^{-3}\ \Omega cm^2$ (epitaxy optimized close to the surface): @ 100 Acm^2, $\Delta V = 0.1V$

Crucial for the WPE

Substrates for LEDs

All major players on sapphire:

•The MOVPE process is now well mastered

•Transparent but is removed sometimes (thermal, backside contact)

•Price is decreasing and size increasing

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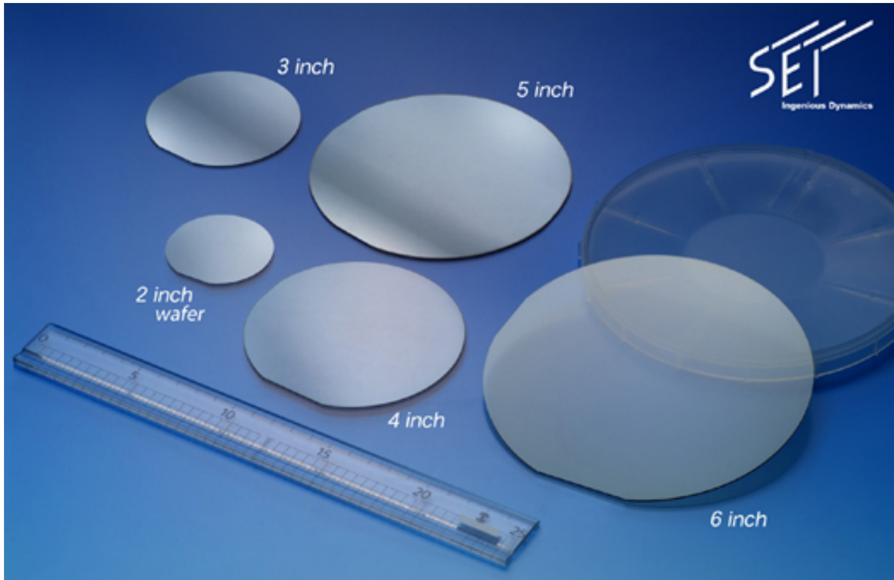
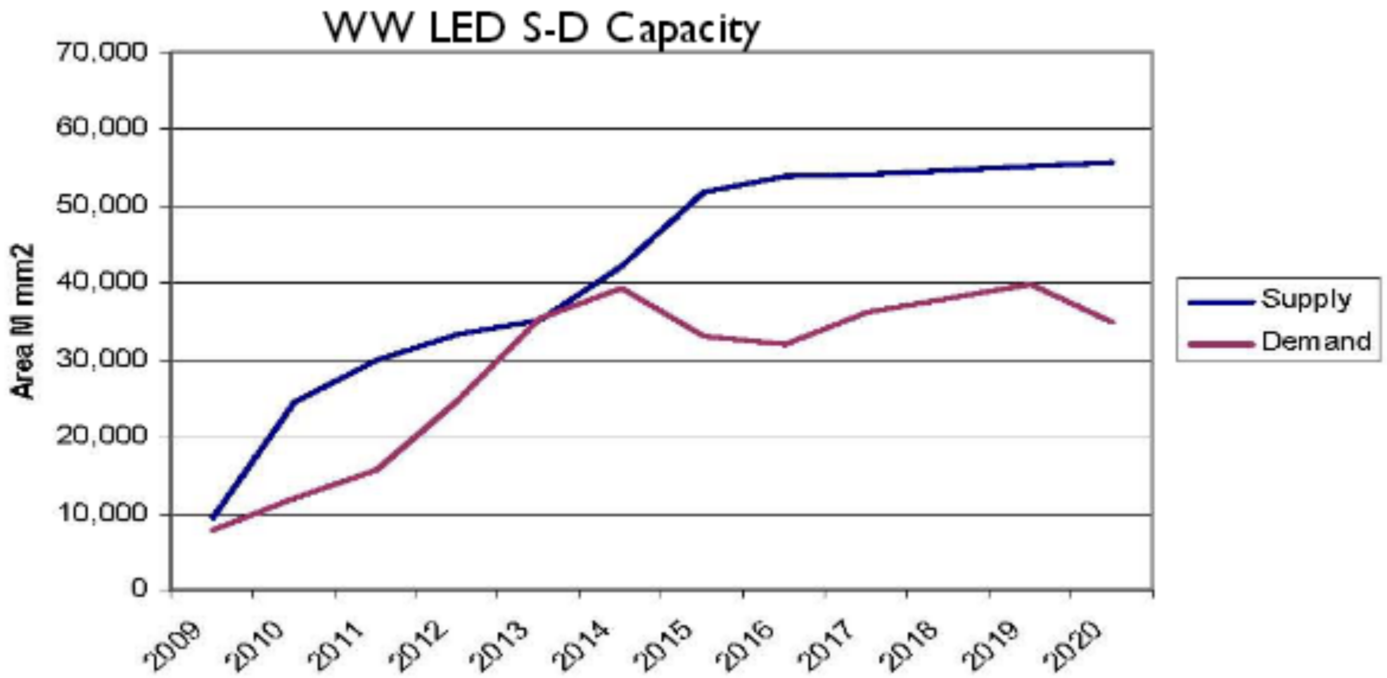


LED production

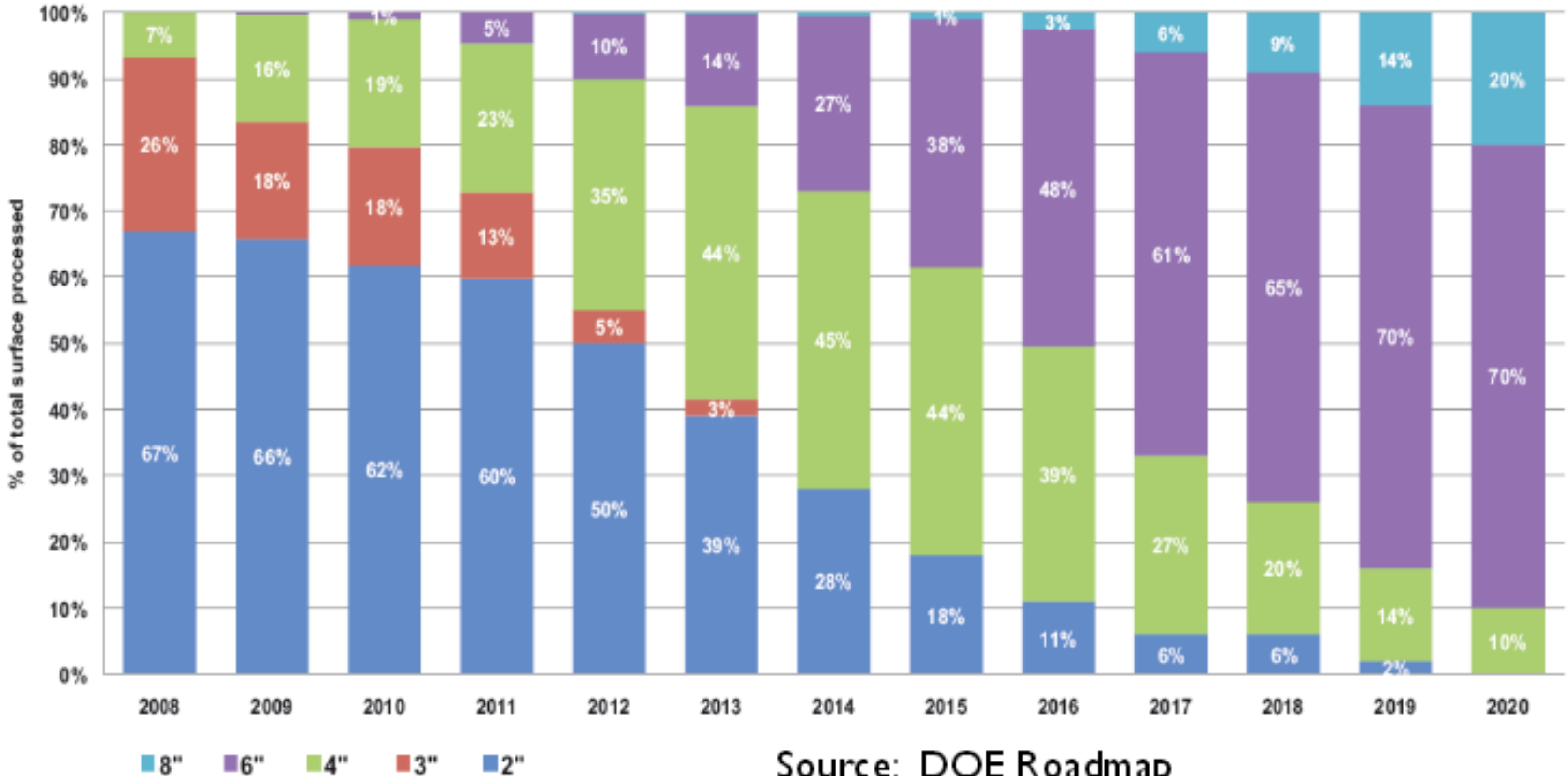


- 40 Bmm^2=8 soccer fields / year
- 5 Million substrates (4 inch)
- Installed capacity is large enough

Source: Canaccord, estimate model.

Presentation by Semi

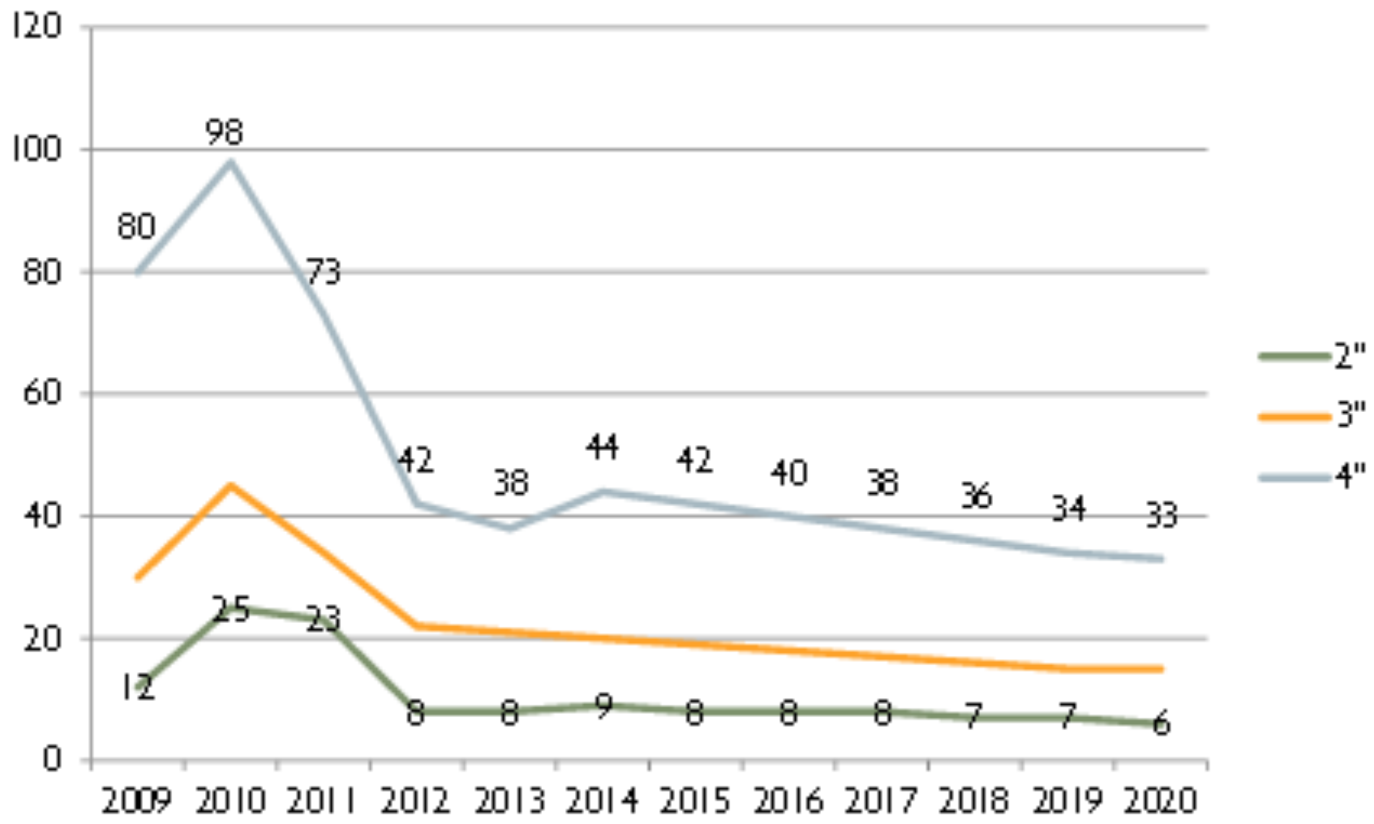
Sapphire Substrates for LEDs: Diameter trends to 2020



Source: DOE Roadmap

Wafer size increases

Sapphire wafer price forecast ($)



Source: Canaccord, estimate model.

Presentation by Semi

Substrates for LEDs

Some players on Si (111): Plessey (UK), Toshiba (JP), Lattice power (Ch), Samsung (Kr), OSRAM (Ge), LG (Kr), Epistar (Kr), Novagan (Sw)

- Large area (lower epitaxy and processing costs)
- Easy back process : Si is removed
- Epitaxy is more tricky but almost similar performance can be reached

Source: OSRAM & Yole

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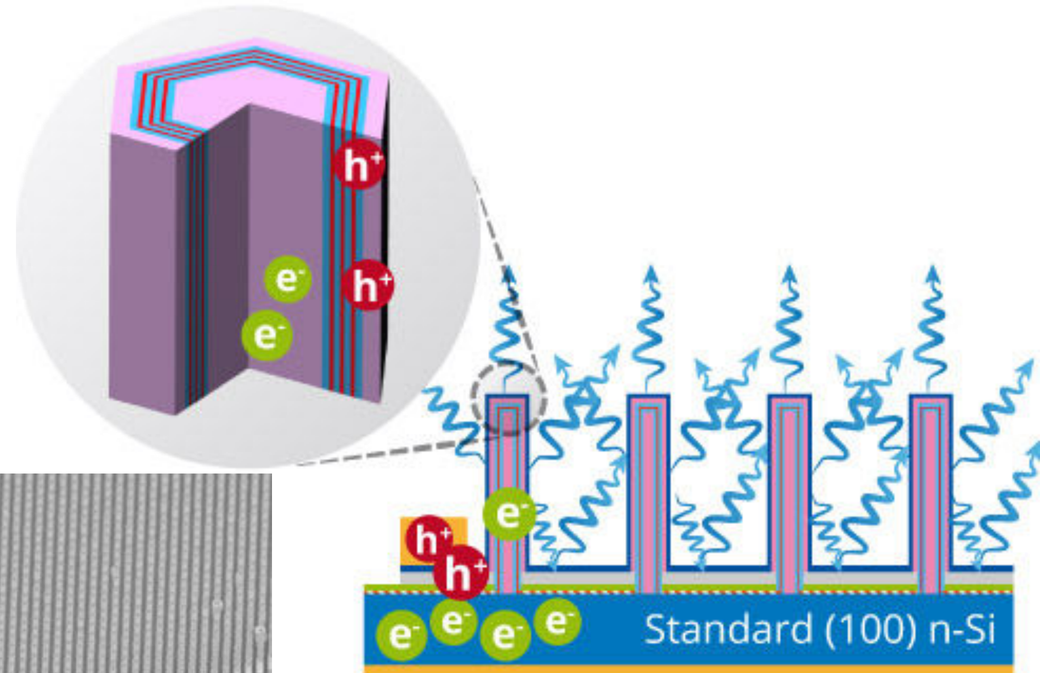
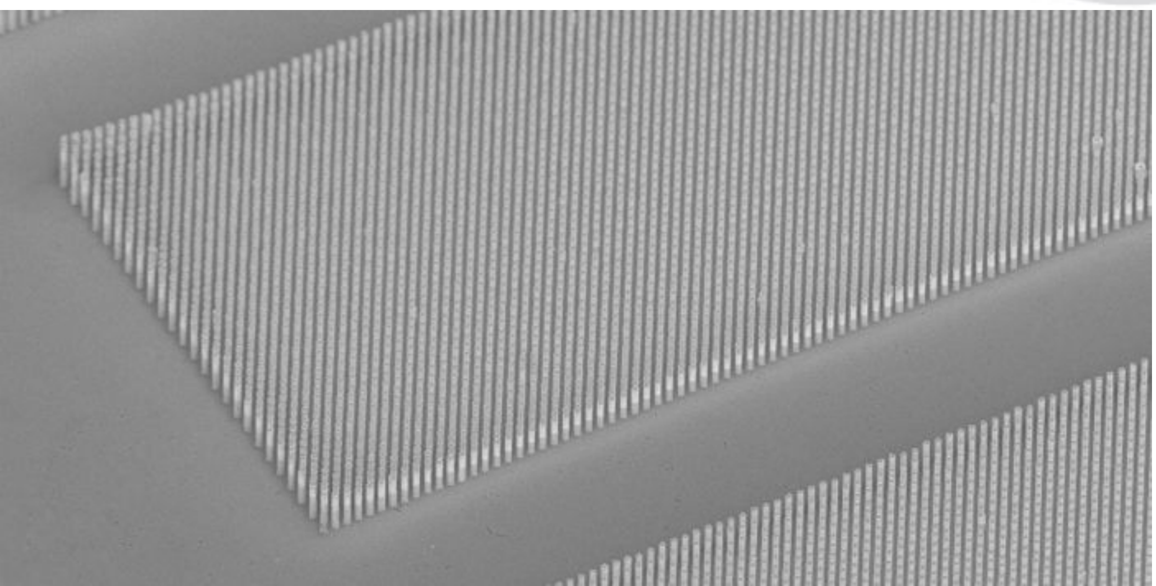
Substrates for LEDs

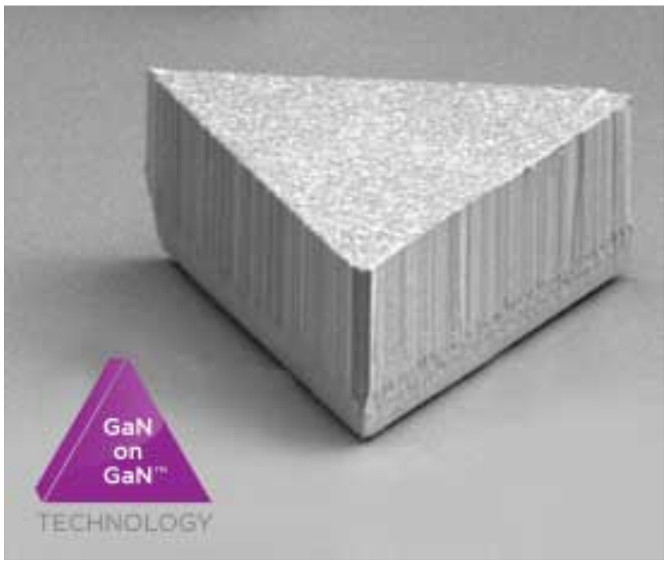
Si (100): : epitaxy difficult for 2D layers as the square surface symmetry induces two domains of wurzite material twisted by 90°. OK for nanowires ⇒ ALEDIA (Grenoble): Si (100) 8 inch





Substrates for LEDs

GaN substrate (Soraa): better cristalline quality, higher efficiency, light extraction by simple process (triangular shape)



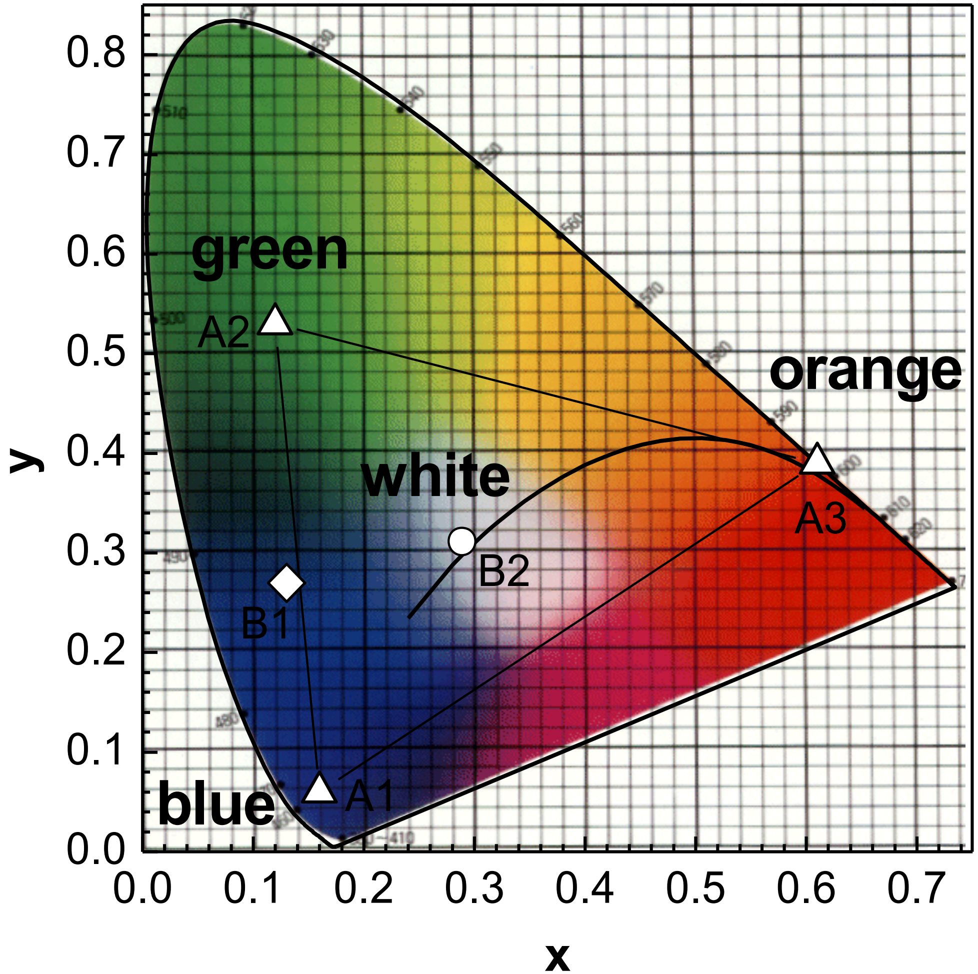
WPE=84% @ 1 A/cm2

⇒All individual η close to unity !

Growth technique

	MBE	MOVPE
Point defects		Higher T_g
Dislocations		Lateral growth
N doping	OK	OK
P doping	Less H problem Lower $T_{g\,:}$ less compensation, better for QW grown below	
InGaN		More localisation ? Less point defects ?
InN	Low T_g (P-MBE)	
Throughput		Developed large systems

White from color mixing



Black body equivalent temperature : warm white (red) = lower T. Cold white (blue) = higher temperature

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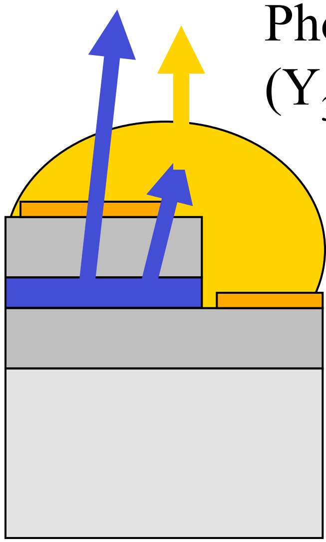
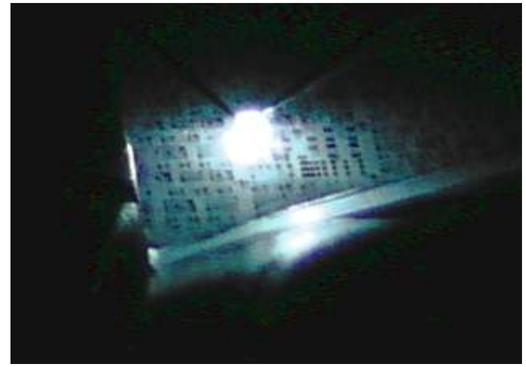
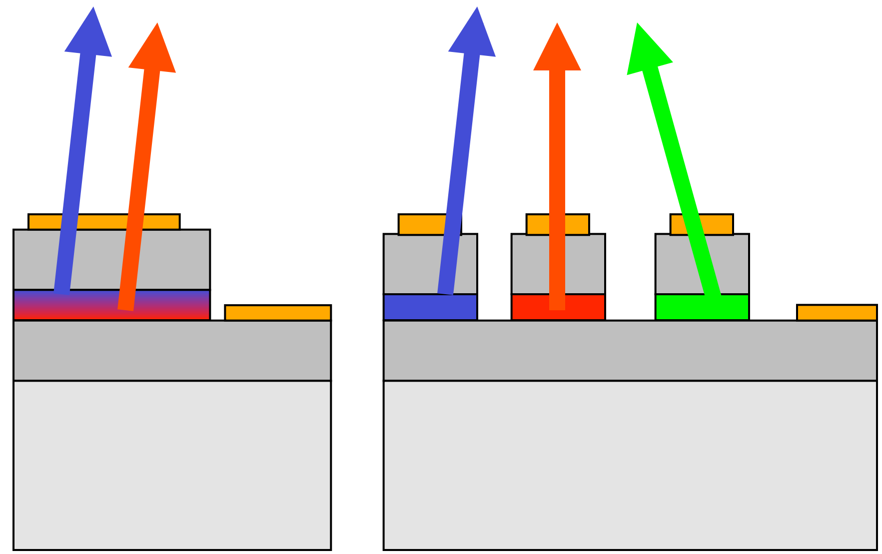
Phospors versus RGB

Usual approach: Blue/ yellow conversion



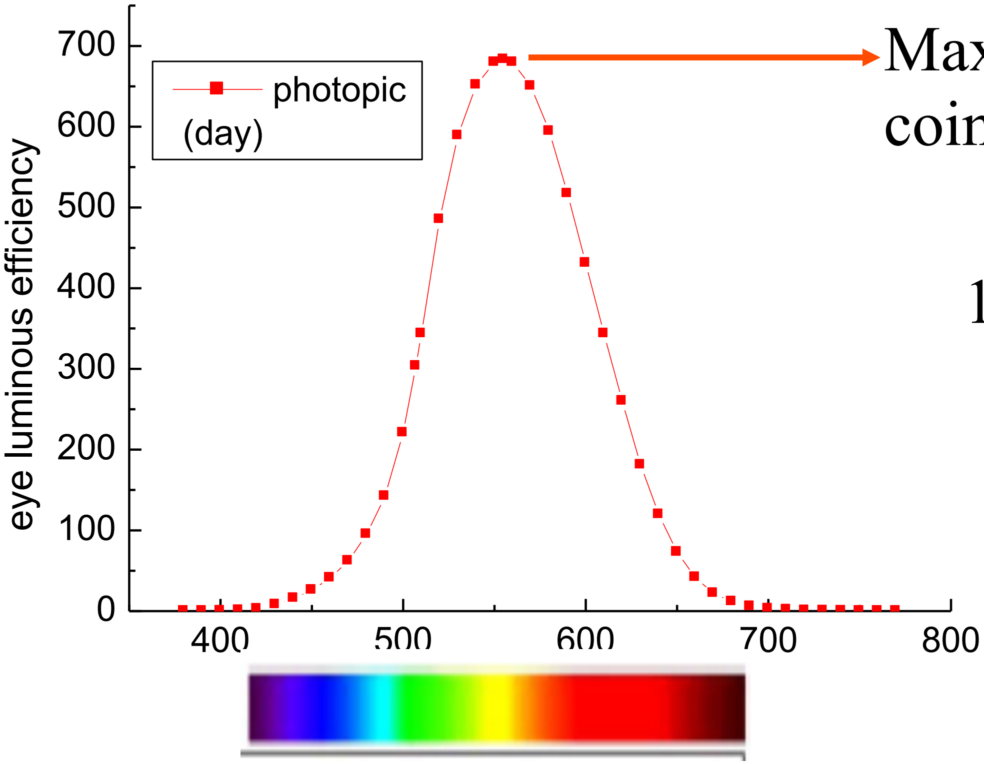
Phosphore ($Y_3Al_5O_{12}:Ce^{3+}$)





Integrated approach (epitaxy): ideal solution but still less efficient and more complicated

Eye perception of light and lumen



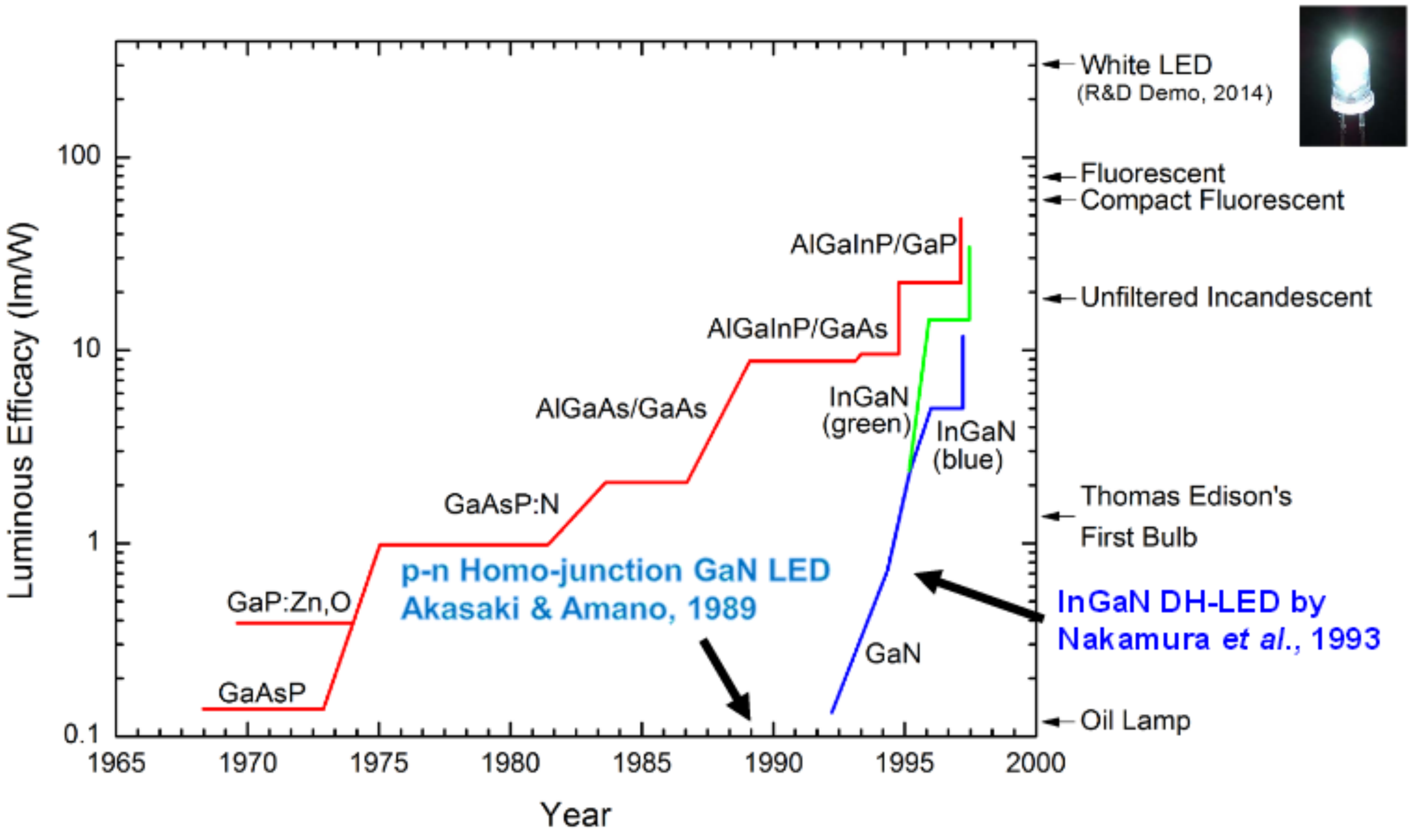
Maximum at 555nm (not a coincidence !!)

1 lumen is the luminous flux of a monochromatic source at 555 nm with a power = 1/683 W

Average value from 430 to 630 nm : 350 lum / W

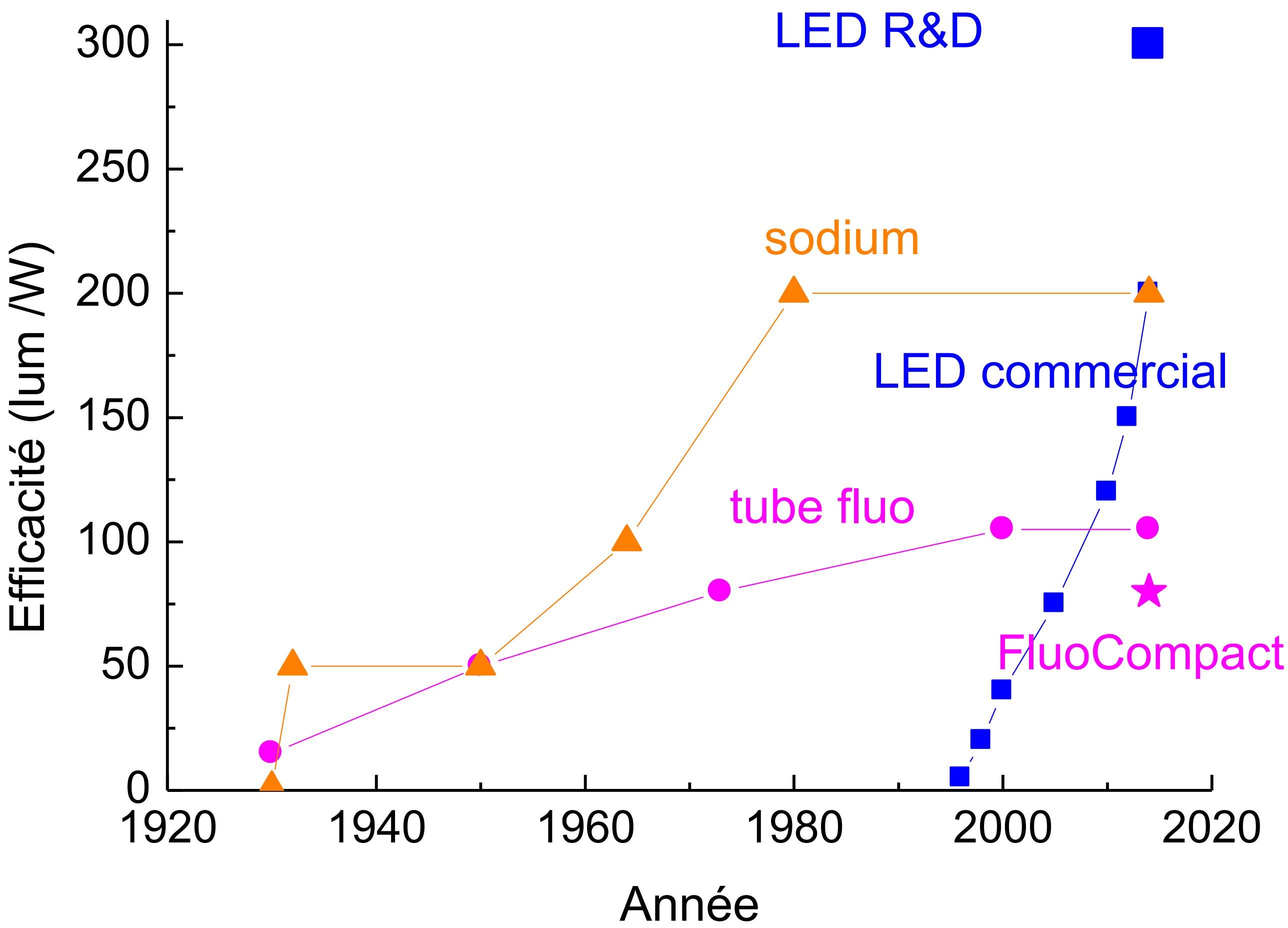
~ Ideal lighting source for humans

Historical perspective on LED efficacy



Source: Amano Nobel lecture

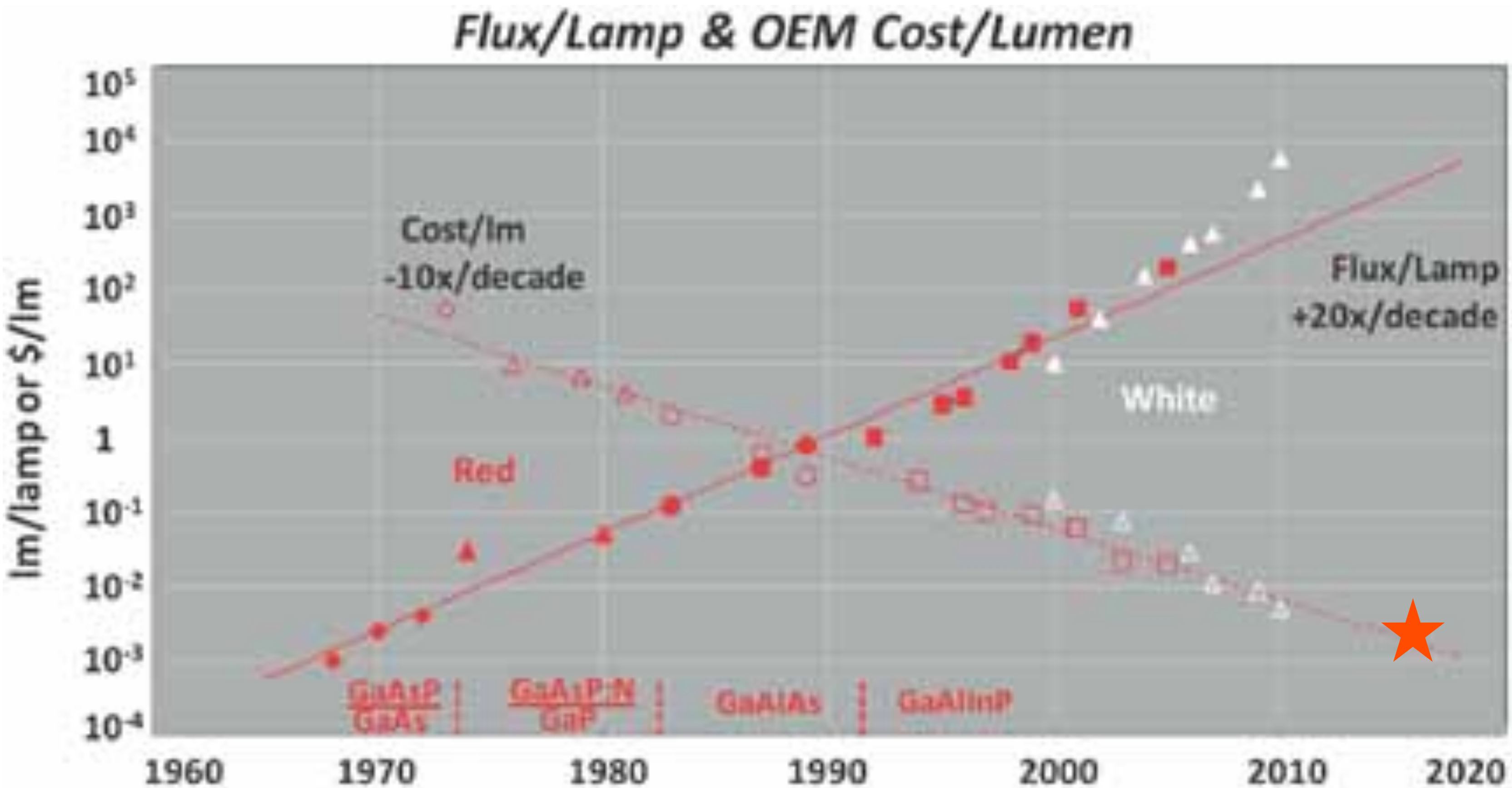
Historical perspective on efficacy for lighting



Revolution rather than evolution !

Best LEDs close to the limit !

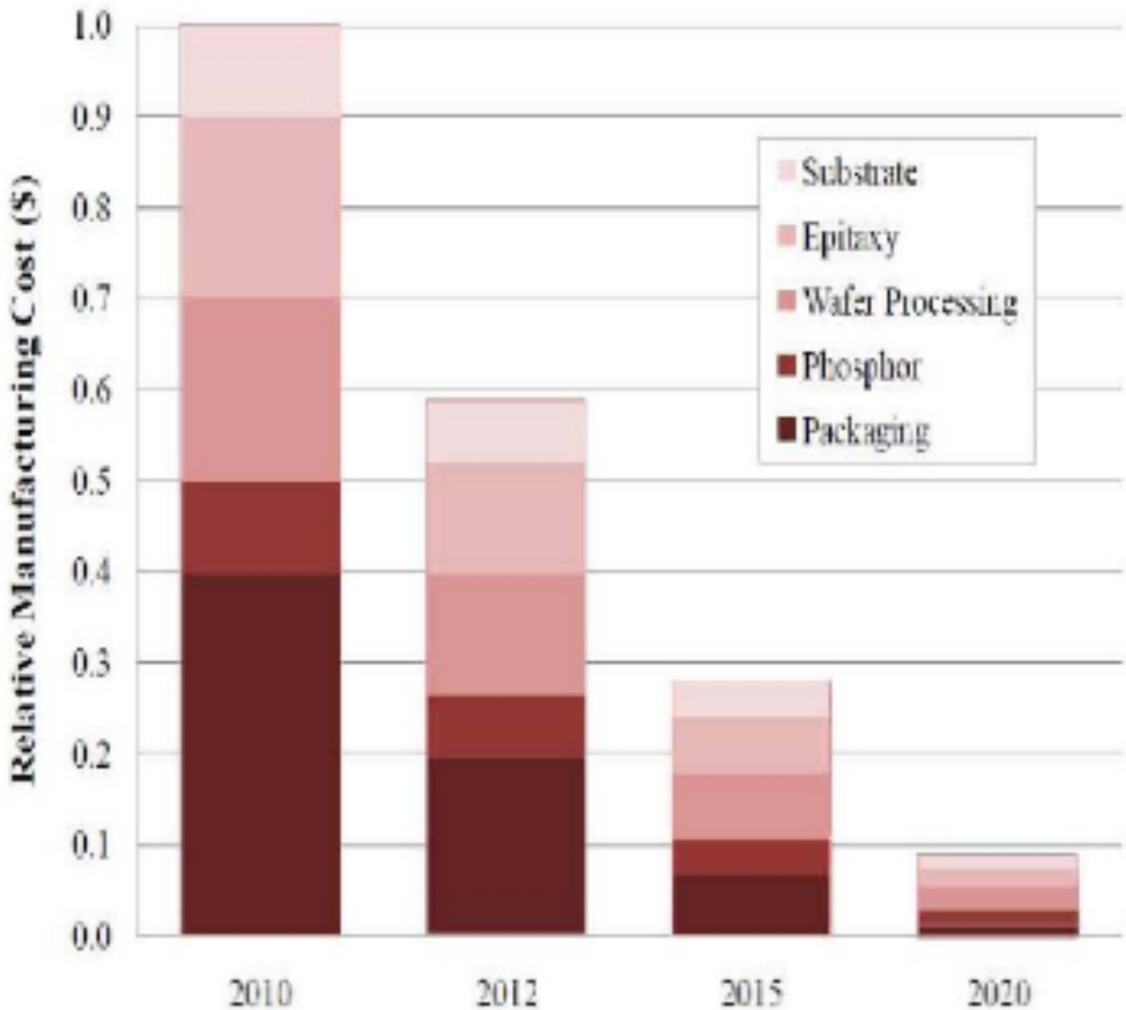
Haitz' Law: Cost ↓10x & Performance ↑20x per decade.



About $2/klm in 2015 (1 klum is the output of former 60W incandescent bulbs)

Roland Haitz and Jeffrey Y. Tsao, **physica status solidi (a),** Volume 208, Issue 1, pages 17–29, (2011)

Epitaxy is the enabling technology but is only part of the cost



Source US DOE 201107

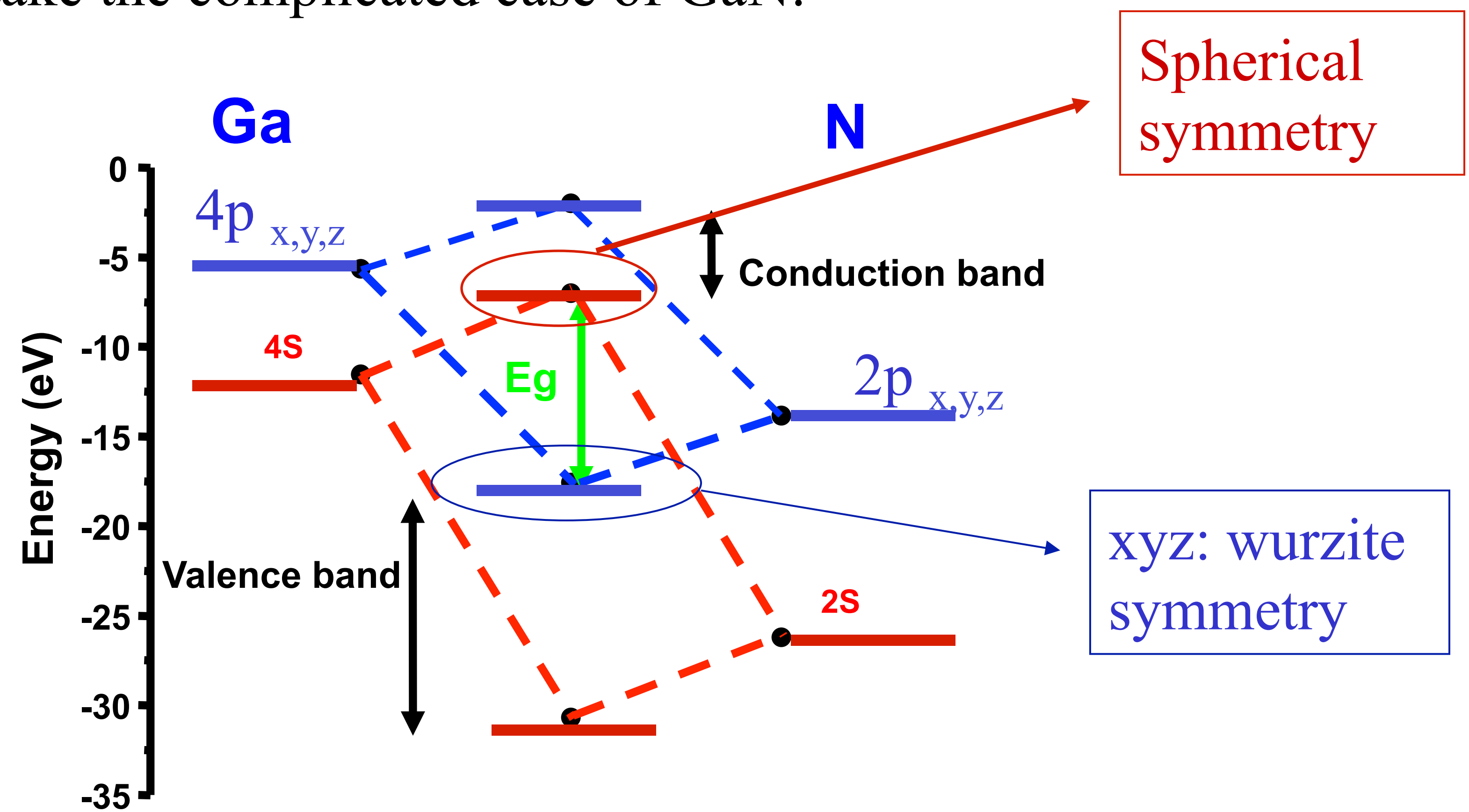
CONCLUSION

- Tremendous efforts in academic and industrial R&D have been dedicated to epitaxy for LEDs
- But epitaxy is only part of the game: design, process, packaging…and economic issues

$$\left|\vec{E}.\vec{r_{vc}}\right|^2$$

Dipolar matrix element r_{vc} : Intrinsic parameter which depends on the band structure of the QW material

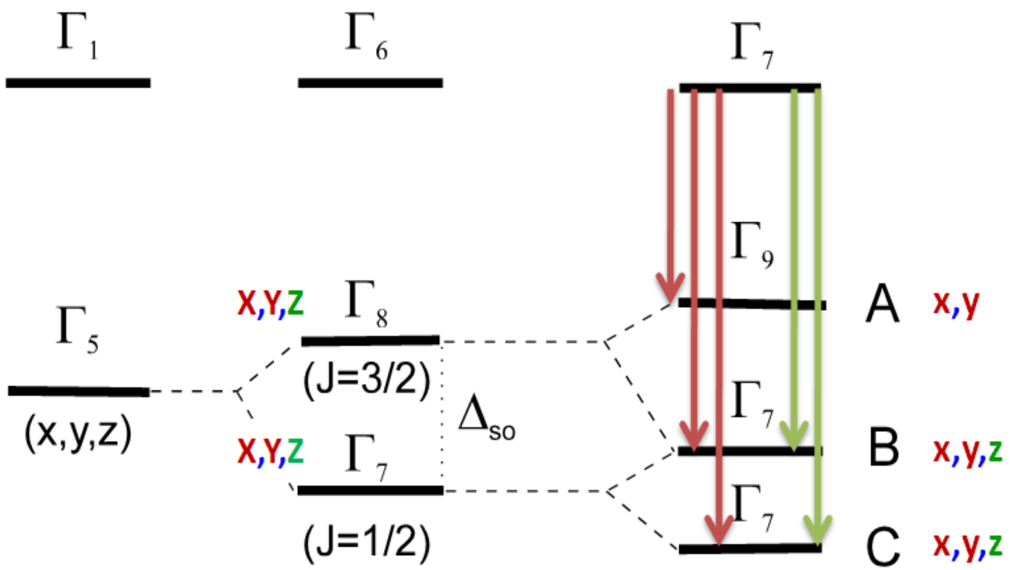
Let us take the complicated case of GaN:



Valence band structure of GaN:

- x,y and z not equivalent in wurtzite (crystal field)
- spin orbit coupling small (light atoms)

Similar value

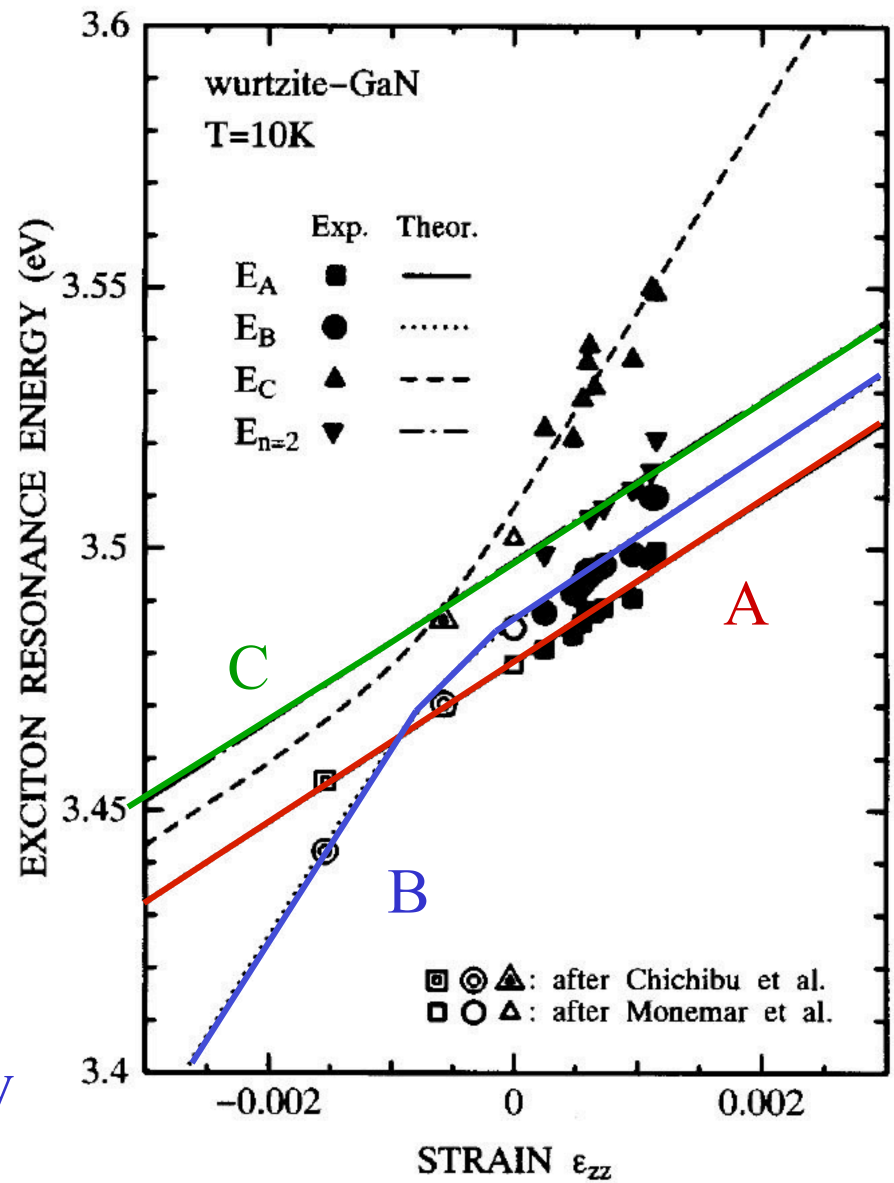


wavefunctions

Transition polarisation:

- A (x,y) ⇒ **E** in x,y plane, ⊥c
- B,C (xyz) ⇒ any **E**, amplitude depends on z/x,y ratio

Strain modifies the crystal field and the valence band structure: energy and change



Wavefunctions:

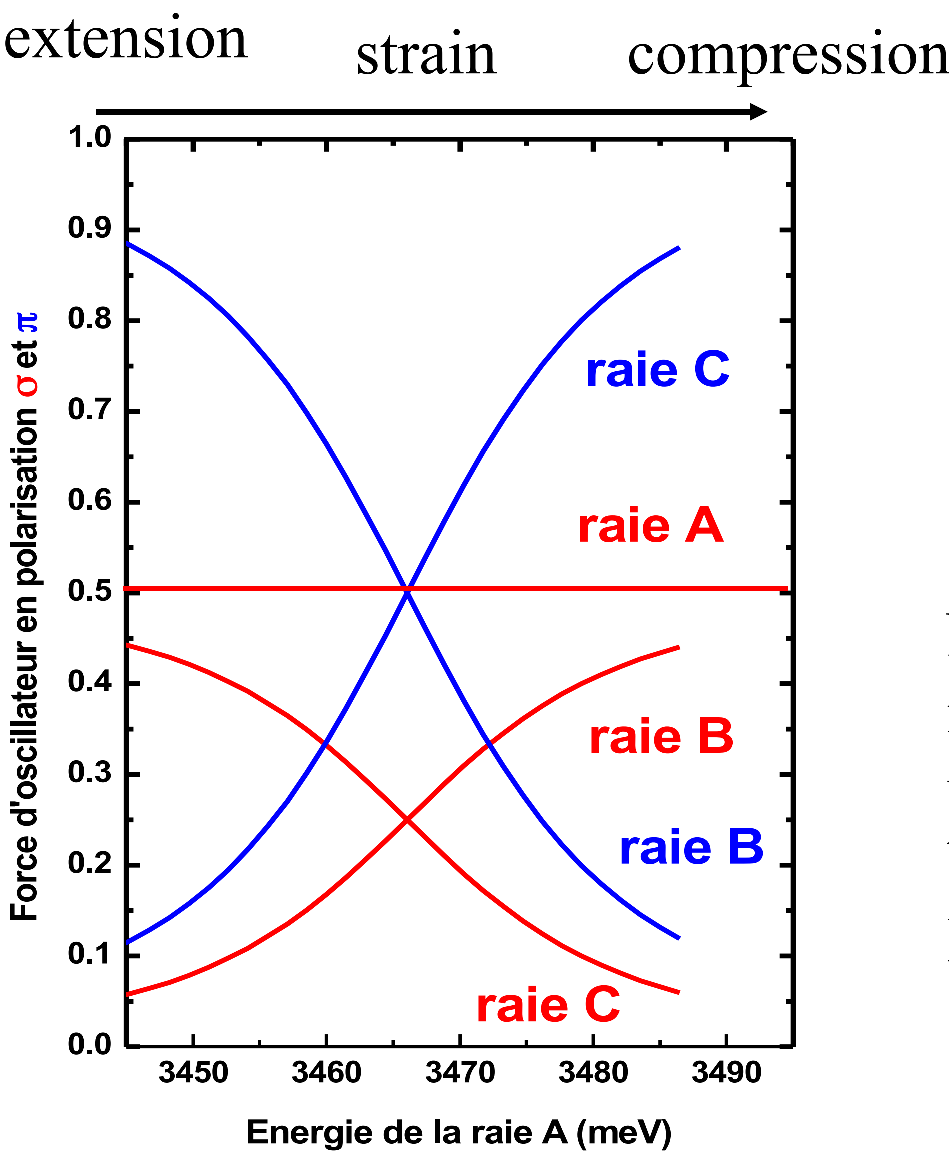
C⇒xy

B⇒z

Wavefunctions:

C⇒xy

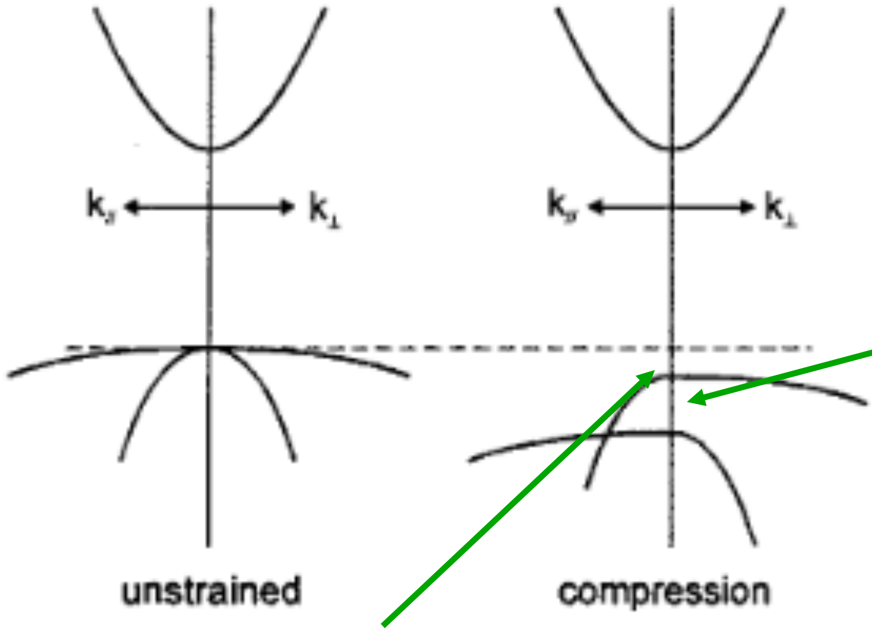
B⇒xy



There is some choice (substrate, buffer layer, growth conditions…) on the strain state during the epitaxy to favor one transition or another.

Not so important for GaN, but more important for AlGaN where the top valence band become A (emitting along z) + B (emitting in the xy plane)

Another famous example: strained InGaAs laser



InGaAs the VB degeneracy is lifted.

The in plane effective mass becomes smaller

⇒ the effective density of states decreases

⇒ the threshold decreases

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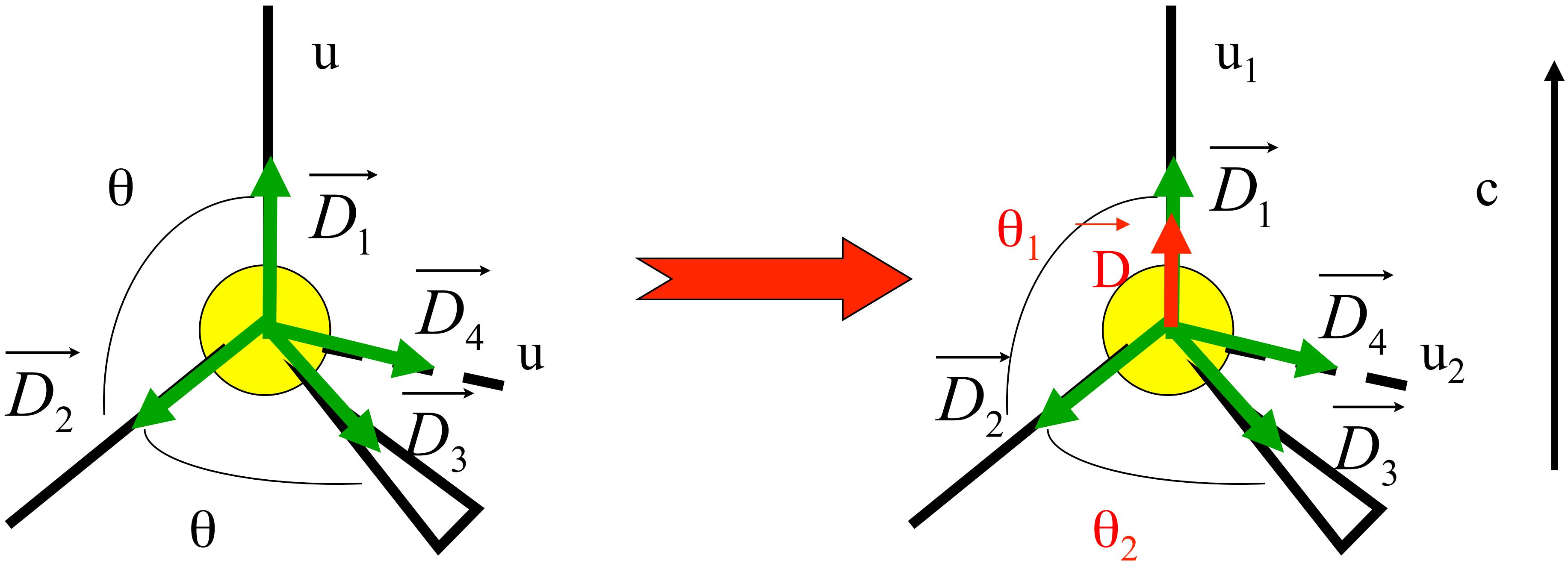
Polarization on the atomic level

Ideal tetrahedron | Real distorted tetrahedron*



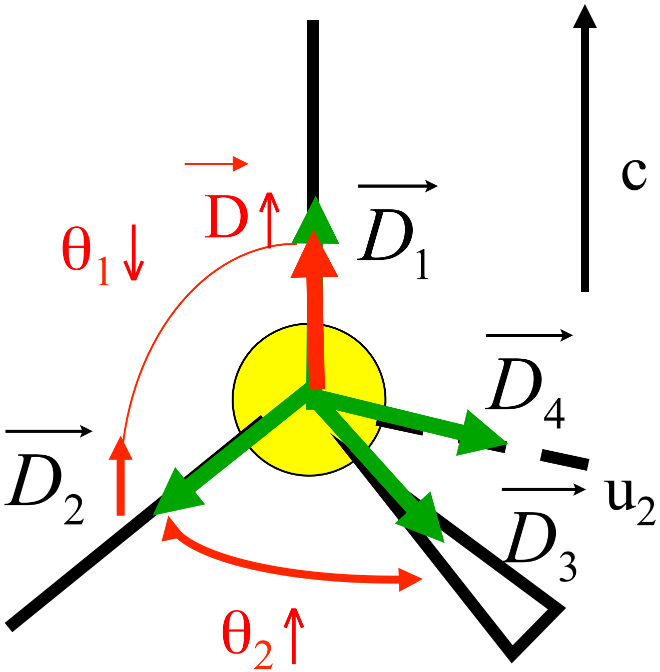
$$\vec{D_1} + \vec{D_2} + \vec{D_3} + \vec{D_4} = \vec{0}$$

$$\vec{D_1} + \vec{D_2} + \vec{D_3} + \vec{D_4} = \vec{D}$$

$$and\,\vec{D} // c$$

*picture should include the electron cloud and not the atoms only (not marbles !): the distorsion comes from third neighbours environment

Wurzite nitrides

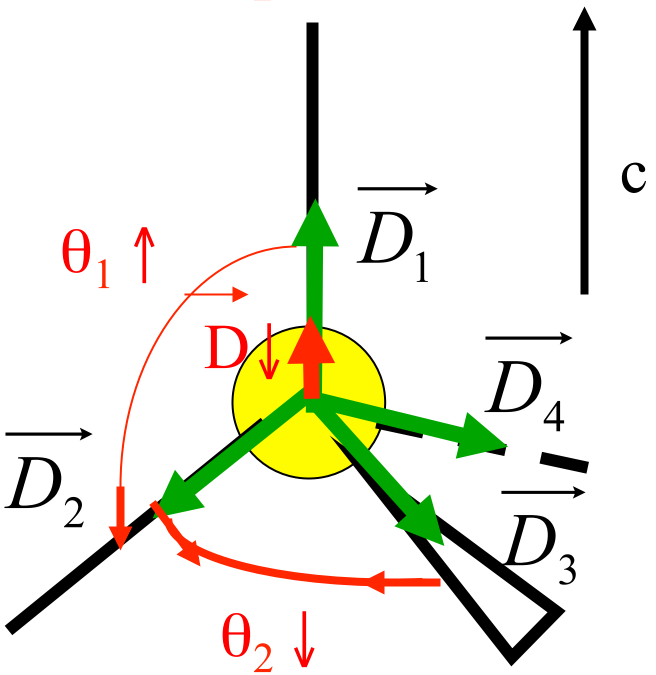


Spontaneous polarization: distorsion of the cell / ideal structure (c shorter, c/a <1.633)

Growth on a substrate with a larger a

⇒ tensile stress, deformation of the cell, increase of a and decrease of c

⇒ piezoelectric polarization added to the spontaneous polarization



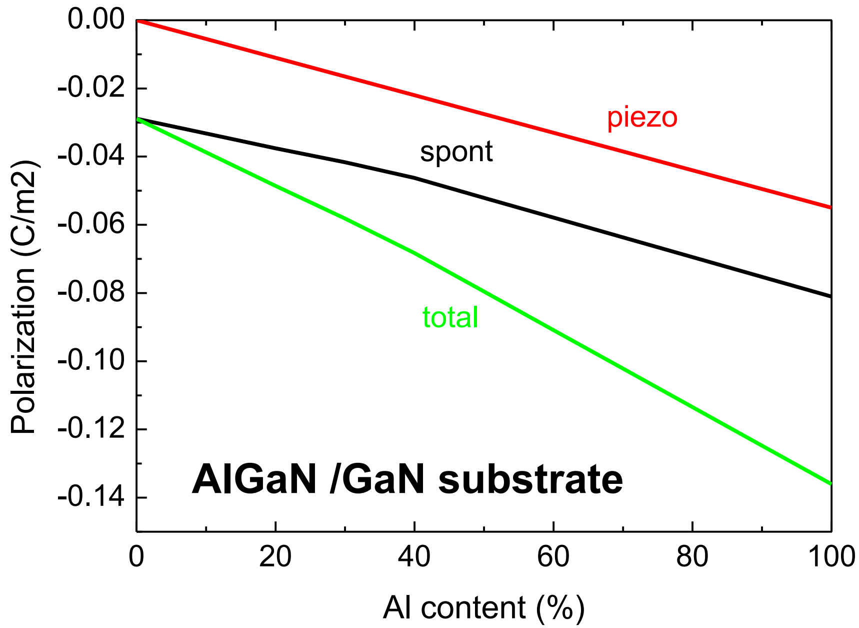
Growth on a substrate with a smaller a

⇒ Compressive stress, deformation of the cell, decrease of a and increase of c

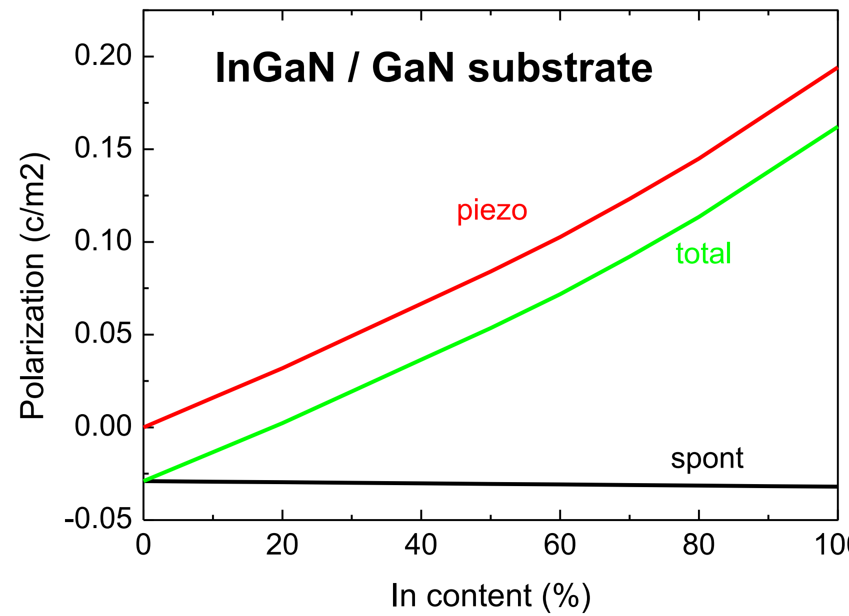
⇒ piezoelectric polarization opposite to the spontaneous polarization

Polarization in wurzite nitrides

Polarization in AlGaN



Polarization in InGaN



For strained heterostructures :

$P_{AlGaN} < P_{GaN} < P_{InGaN}$

Jpn. J. Appl. Phys. Vol. 31 (1992) pp. 3662–3663
Part 1, No. 11, November 1992

Short Note

Defeating Compensation in Wide Gap Semiconductors by Growing in H that is Removed by Low Temperature De-Ionizing Radiation

James A. Van VECHTEN*, J. David ZOOK[1], Robert D. HORNING[1] and Barbara GOLDENBERG[1]
Center for Advanced Materials Research, Oregon State University, Corvallis, Oregon 97331-3211, USA
[1]*Sensor and System Development Center, Honeywell Inc., Bloomington, Minnesota 55420, USA*

(Received April 27, 1992; accepted for publication July 18, 1992)

We propose a general method to obtain high conductivity of either type in wide gap semiconductors where compensation normally limits conductivity of one or both types. We suggest that the successes of Amano *et al*. and of Nakamura *et al*. in obtaining more than 10^{18} cm^{-3} holes in GaN are particular examples of the general process that we propose.

KEYWORDS: hydrogen, compensation, GaN, conductivity, wide gap semiconductors

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cnrs advancing the frontiers

Lattice location of hydrogen in Mg doped GaN

Wampler et al, JAP 90, 108 (2001)

Measurements by ion channeling to examine the lattice configuration of hydrogen in Mg doped GaN

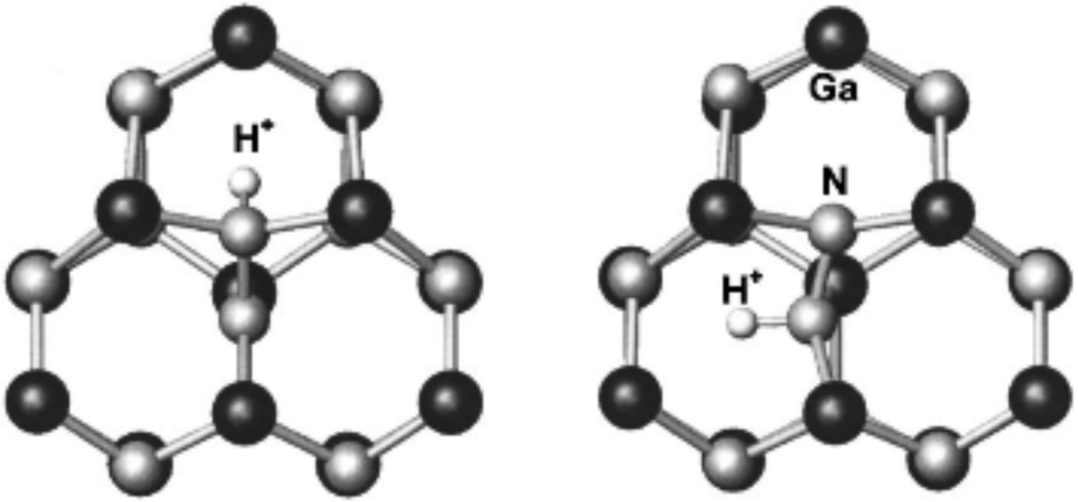

FIG. 1. Configurations for H bound to nitrogen split interstitial (viewed along the *c* axis) calculated by the density functional theory. The H is near the center of the trigonal channel in both cases.