Defects in Nitride Semiconductors Materials and their relevance to electrical devices

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Outline

1) Short introduction to technology of nitride semiconductor crystal growth

- Distinguishing between bulk crystal growth and epitaxy

2) The real structure of semiconductor crystals

- Defects in Semiconductors
  - Point defects
  - Extended defects
  - Where do defects in crystals come from?
  - Vizualisation and identification of defects

4) Properties of dislocations

- Electrical nature of defects

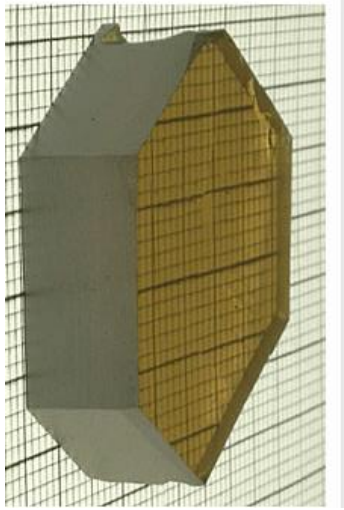
5) Why are dislocations relevant to an electronic device?

3) Problems associated to heteroepitaxy, especially extended defects

6) Why we would need native nitride substrates.

Short introduction to technology of nitride semiconductor crystal growth

Amongst all solid materials, pure crystals have extraordinary properties, which only exist in an perfectly ordered lattice



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Short intro to technology of nitride semiconductor crystal growth

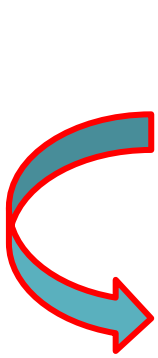
What does crystal mean?

Ideal crystal :

→ Strict geometric, infinite, perfect, periodic arrangement of atoms,

→ By definition no defects

- Crystal structure → crystal lattice
- One individuum → single crystal, volume crystal



- Single crystal with defects
- Two individuals with geometrical orientation relation → twin
- Many individuals→ poly crystal

Real crystal

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Short introduction to technology of nitride semiconductor crystal growth

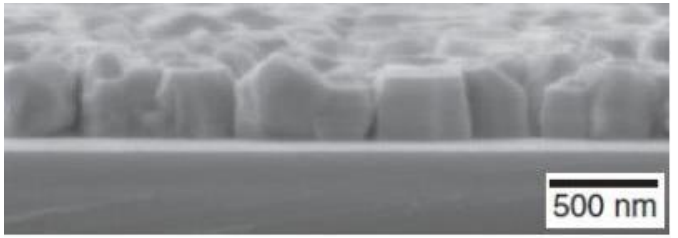
Single crystal
Bulk crystal
Volume crystal

One large individuum of a solide material with a crystal lattice

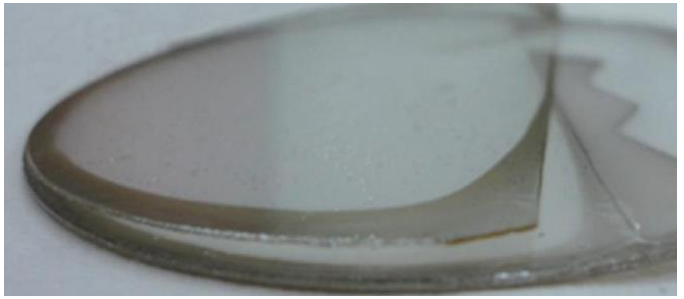
Crystal layer
Epitaxial layer

Important for building up a device

Polycrystalline or nearly single crystalline layer eventually strong preferential orientation



One large individuum of a solide material with a crystal lattice as layer



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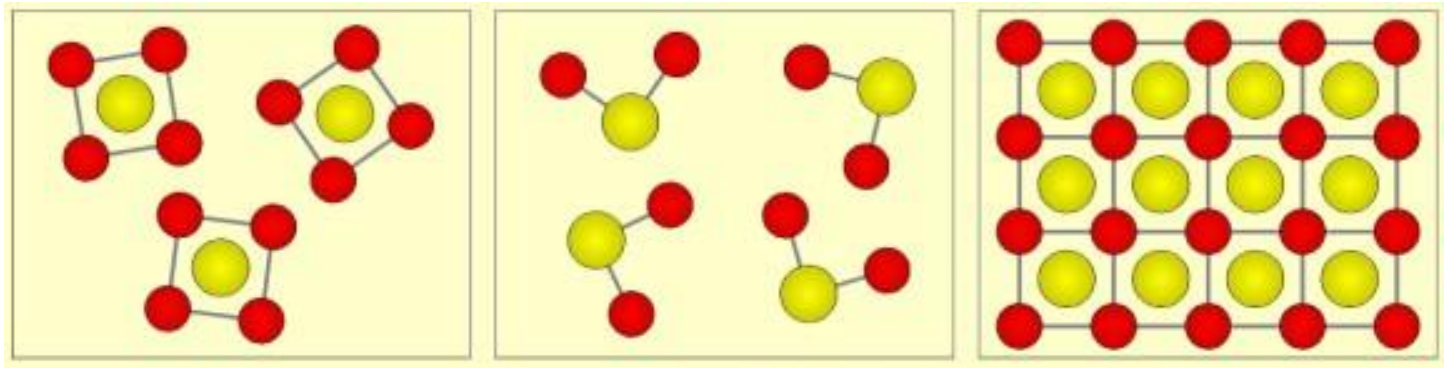
Basics of crystal growth of semiconductor crystals



Raw material, powder

Mobilization of building blocks, atoms

Ordered crystal with perfect lattice

Raw material	evaporate →	Gas	condens →	Crystal
Raw material	melt →	Melt	freeze →	Crystal
Raw material	Solve →	Solution	deposite →	Crystal

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Choose the right crystal growth process

Meltable materials

Melt growth:

Si: Czochralski growth,
GaAs: VGF-Technique
Sapphire: Kyropoulus

Materials that can be evaporated

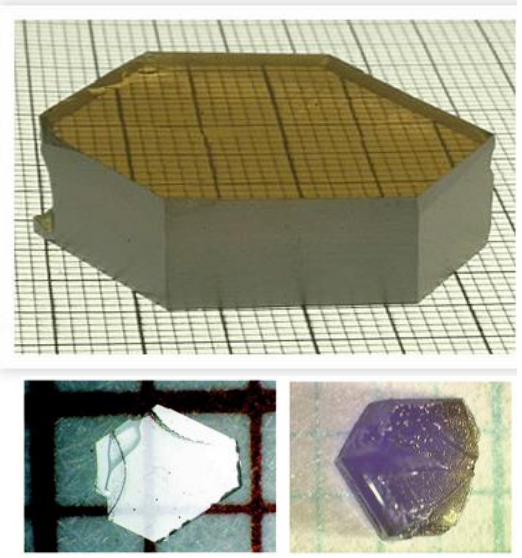
Gas phase growth:

PVT: AlN, SiC
HVPE: GaN

Non- meltable Not evaporatable

Solution growth:

Flux growth: GaN
HP solution growth: GaN
Ammonothermal-growth: GaN



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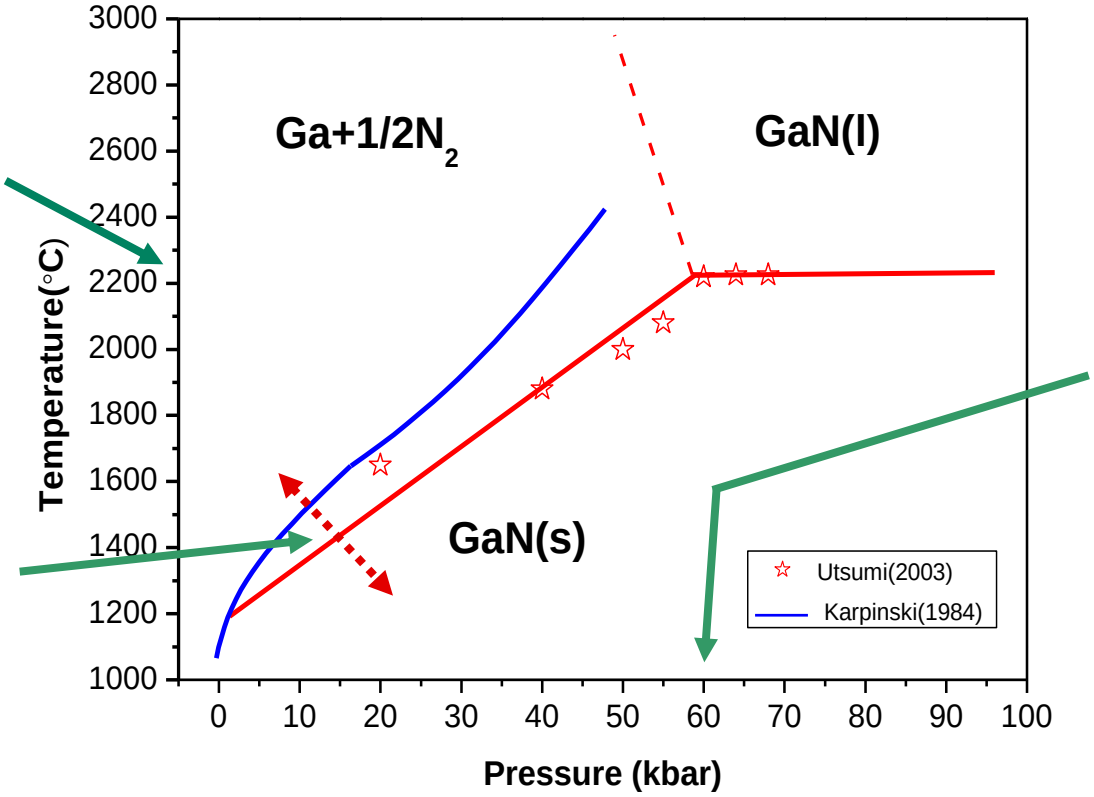
What is the problem with GaN Crystal Growth?
Why is it so difficult to grow as a crystal?

Extrem high melting point, ~2200°C



Very high equilibrium partial pressure ~60 kbar

Below T_m : dissociation

incongruent

→ **Classical melt growth is not possible for GaN, except at very high pressure**

→ **Classical gas phase process like PVT growth not favorable**

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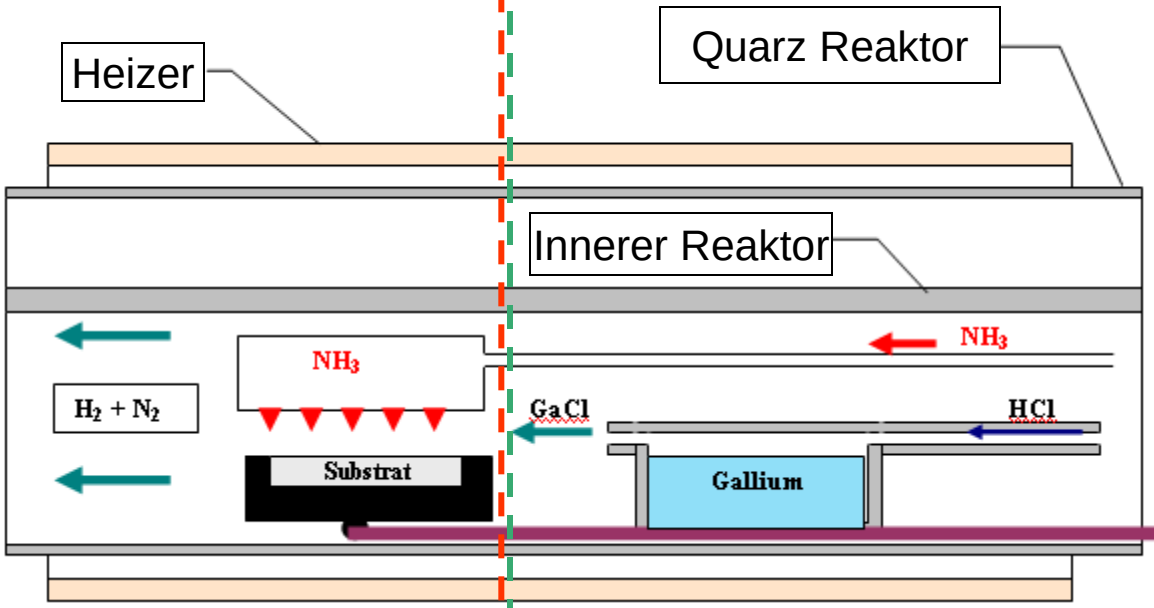
Hydride Vapour Phase Epitaxy – HVPE
„Chemical assisted“ gas phase growth



$GaCl + NH_3 \longrightarrow GaN + HCl + H_2$

$GaN \longleftrightarrow Ga + 1/2\ N_2$

$Ga + NH_3 \longleftrightarrow GaN + 3/2\ H_2$

$Ga + HCl \longrightarrow GaCl + 1/2\ H_2$

Ca. 900-1100 °C

Ca. 700-900°C

Thick layers or crystal bodies up to 5-10 mm in lentgh

Growth rates : ~100µm/h

Problems:

- Stability of the process for longer process times
- Parasitic reactions
- Deposits on reactor parts, downfalls, …

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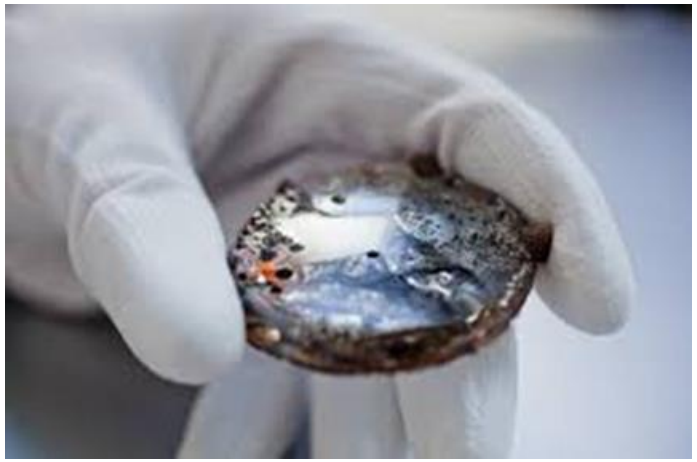
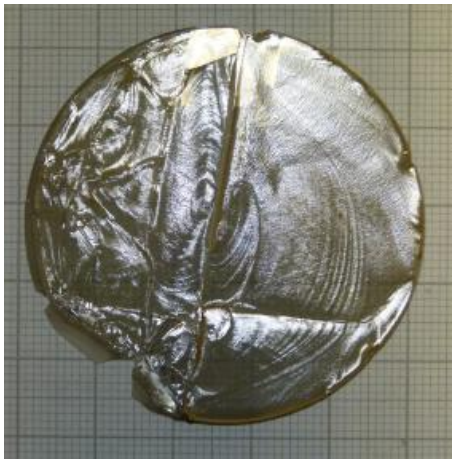
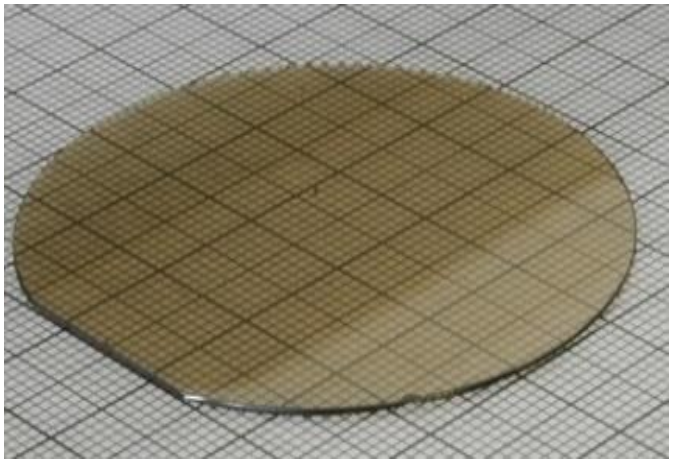
GaN crystals from HVPE







- Crystals are 2“, larger diameters 3“ up to 100mm visible attempts
- Costs are high app. 2000$ per 2“ substrate wafer, available in small numbers
- Crystals have many growth defects like cracks or pits
- Process yields are currently very low, crystal bodies are short (max. 10mm)
- No native seeds are available for crystal growth
- Dislocation density is $10^6/cm^2$ → much lower than that of epi layers

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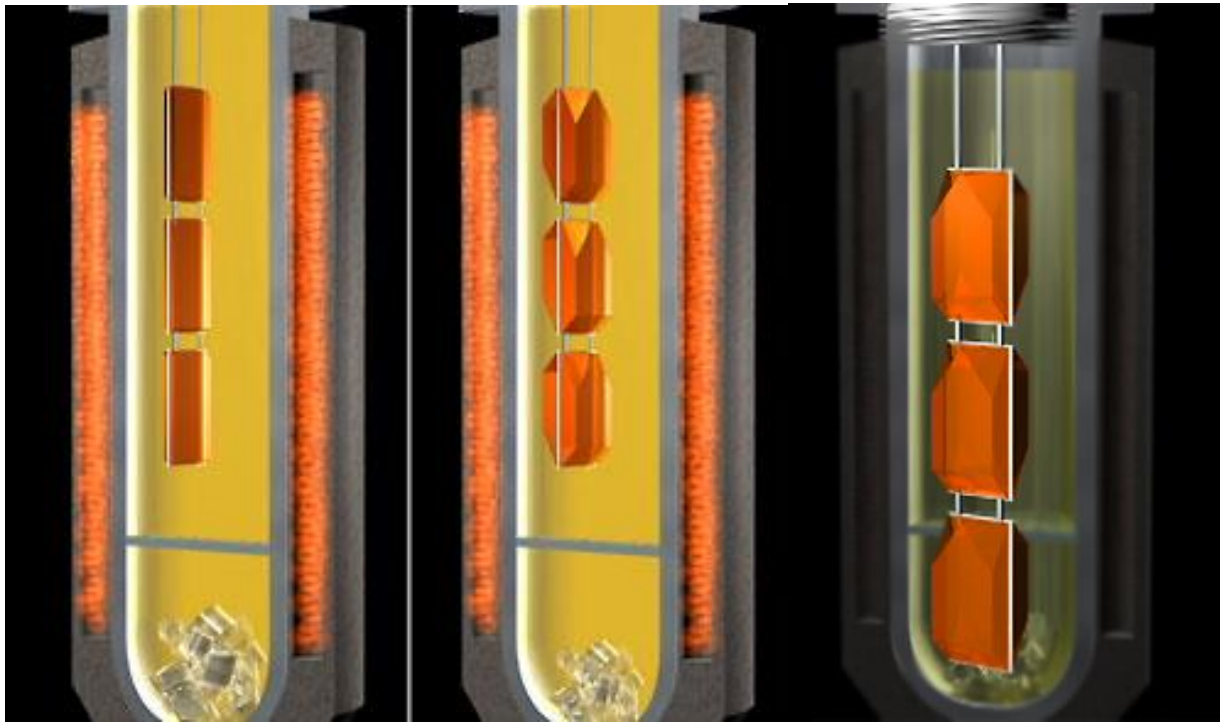
GaN crystal growth – Ammonothermal Method – solution growth



- Solution growth method
- High pressure method
- Moderat temperatures
- Uses supercritical ammonia

→ Comparable to hyrothermal growth that is used for the production of many tons of Quarz crystals every year

- Temperatures 300-600°C, pressures 3000-6000bar
- Supercritical ammonia → highly corrosive
- Difficult technology actual still under developement

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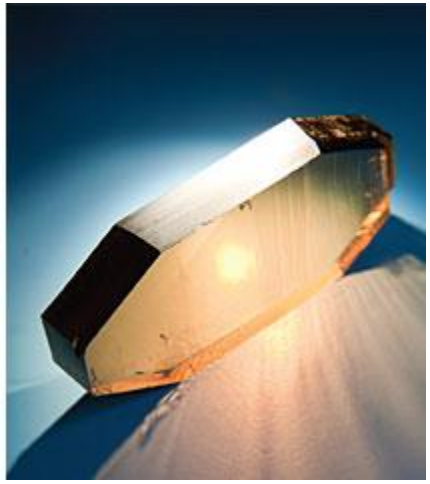
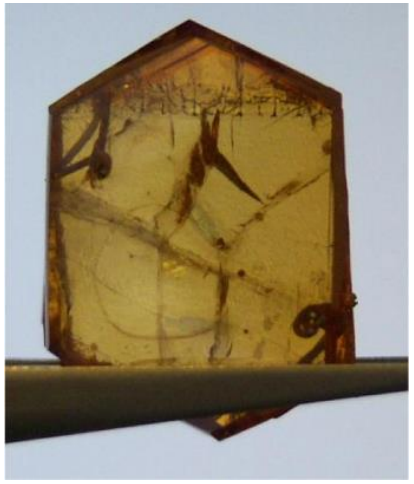
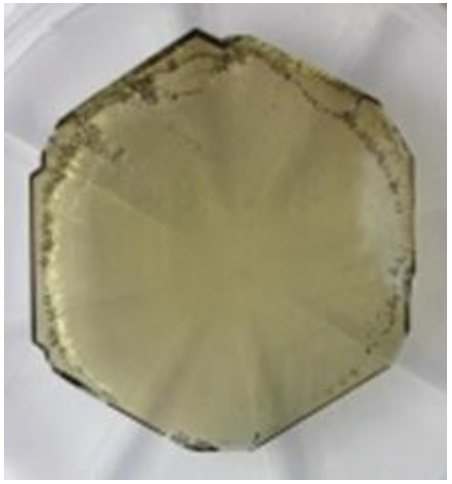
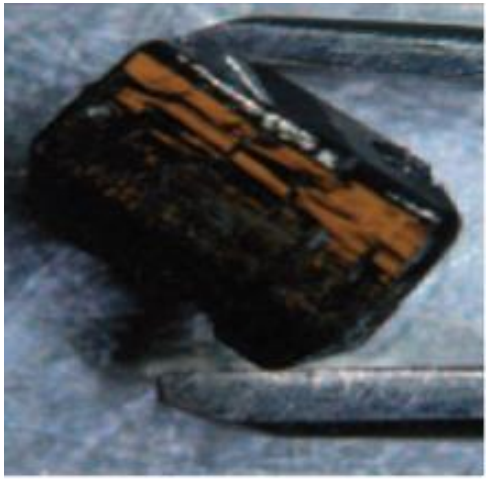
Quality of GaN crystals from Ammonothermal growth

- Results of ammonthermal GaN growth is quite diverse
- Structural quality is very good, DD $10^4/cm^2$ or even lower
- Lowest dislocation density of GaN compared to other growth techniques
- No larger diameters are in sight, availability poor
- Diversity of optical and electrical properties and lattice constants

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Silicon crystal growth after J. Czochralski

Wafers for GaN on Si heteroepitaxy

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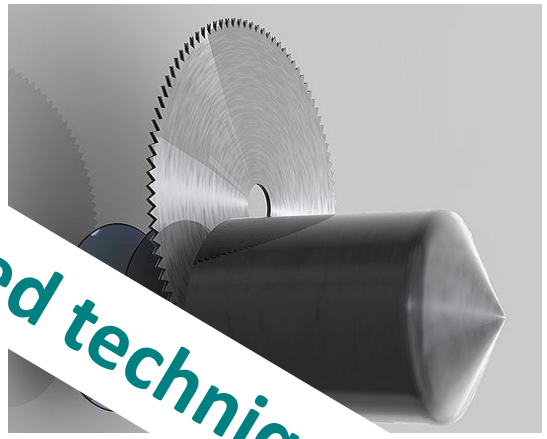
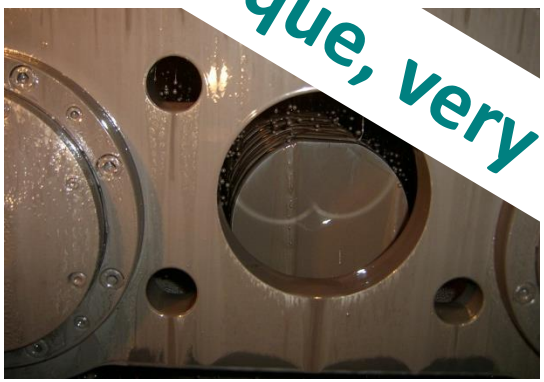
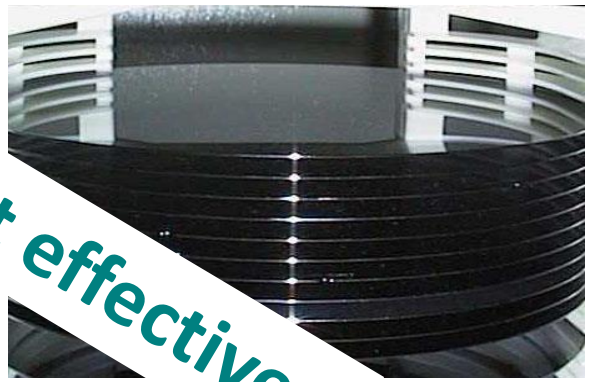
Production of a Silicon wafer

Crystal growth





Wafering



Po…ing

Very established technique, very cost effective

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The real crystal

Real crystal:

Any deviation from the infinite, 3D periodic crystal lattice

= Atomic arrangement in a crystal lattice with imperfections

Any real crystal has defects:

0-D: point defects

vacancy, interstitials, doping atoms, impurity atoms

1-D: line defects

dislocations

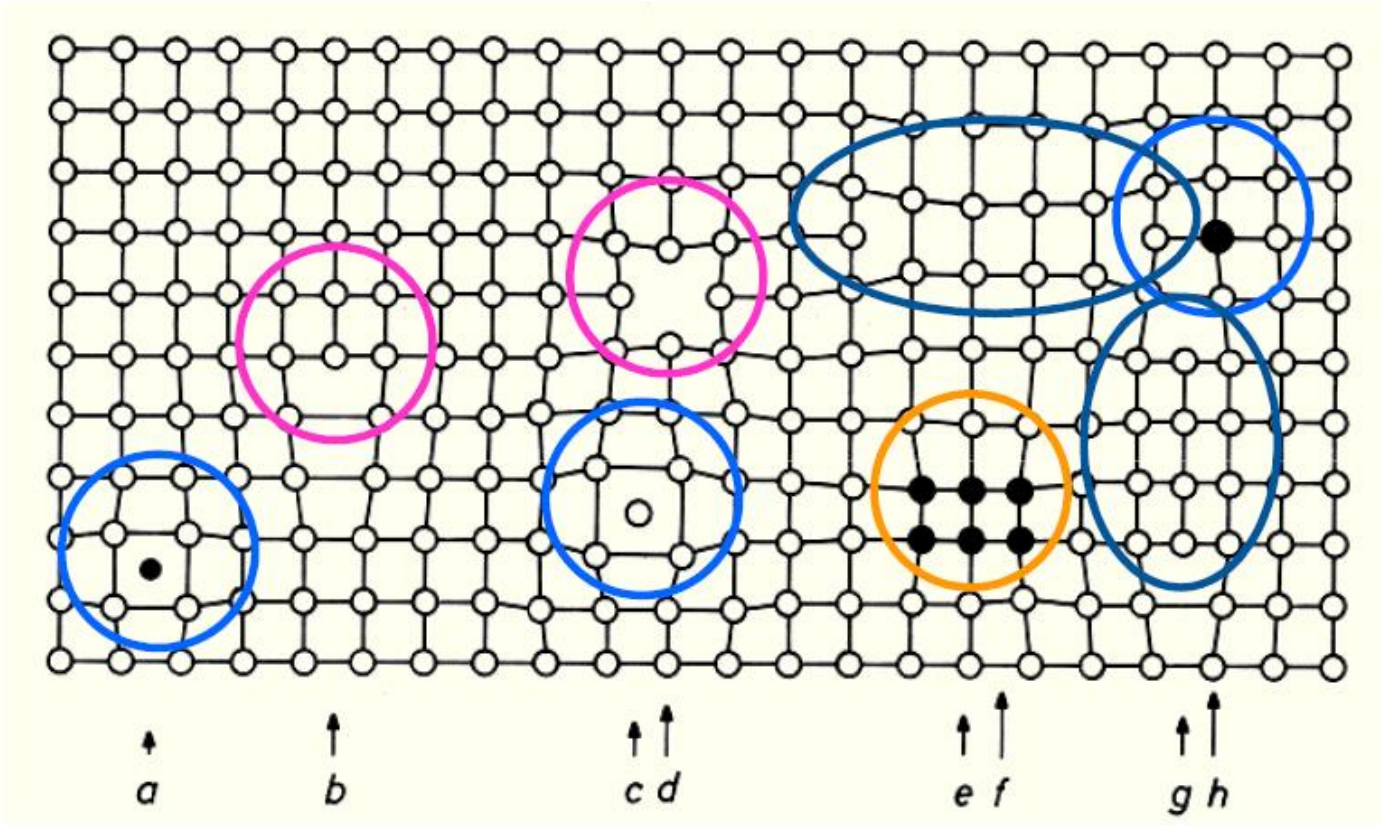
2-D: planar defects

surface (!), grain boundary, twin, stacking fault

3-D: volume defects

precipitates, voids, twin lamellae, non-uniformity, strain region

Types of defects in semiconductors crystals



a – interstitial impurity atom
b – edge dislocation
c – self interstitial atom
d – vacancy
e – precipitate of impurity atoms
f – vacancy type dislocation loop
g – interstitial type dislocation loop
h – substitutional impurity atom

Drawing from lecture Prof. G. Müller, Erlangen

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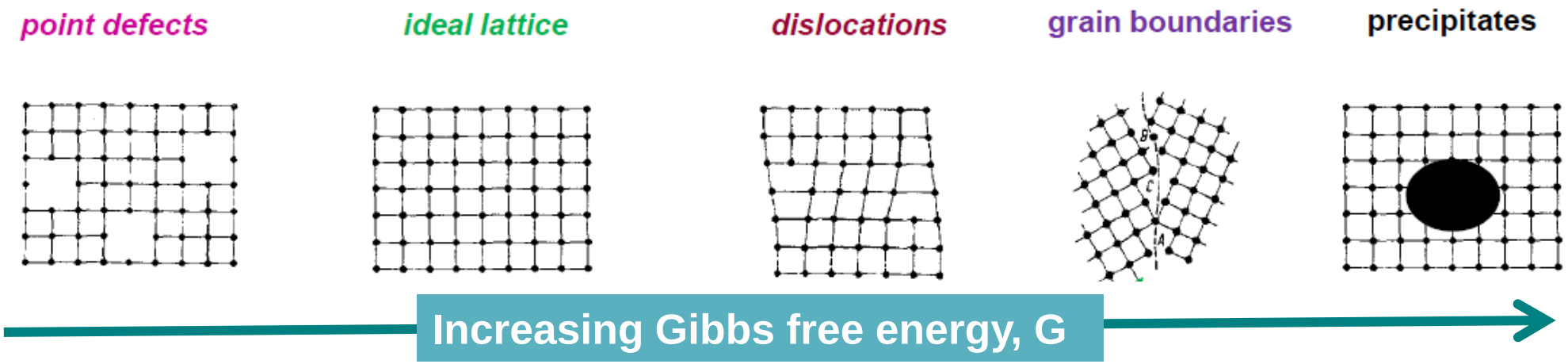
Where do defects come from ?

Thermodynamic driving force for the formation of defects

- Gibbs free energy, as G or ΔG is one of the most fundamental properties of matter
- G defines kind of a „potential“ state of a crystal, considering entropy and energy
- Minimisation criterion → any matter tends to minimise its free energy
- The Gibbs free energy of a crystal depends on its defect content



Some concentration of point defects cause higher entropy ⇒ lowers G ⇒ no crystal without point defects

Extended defects can be avoided in principle, due to thermodynamic reasons

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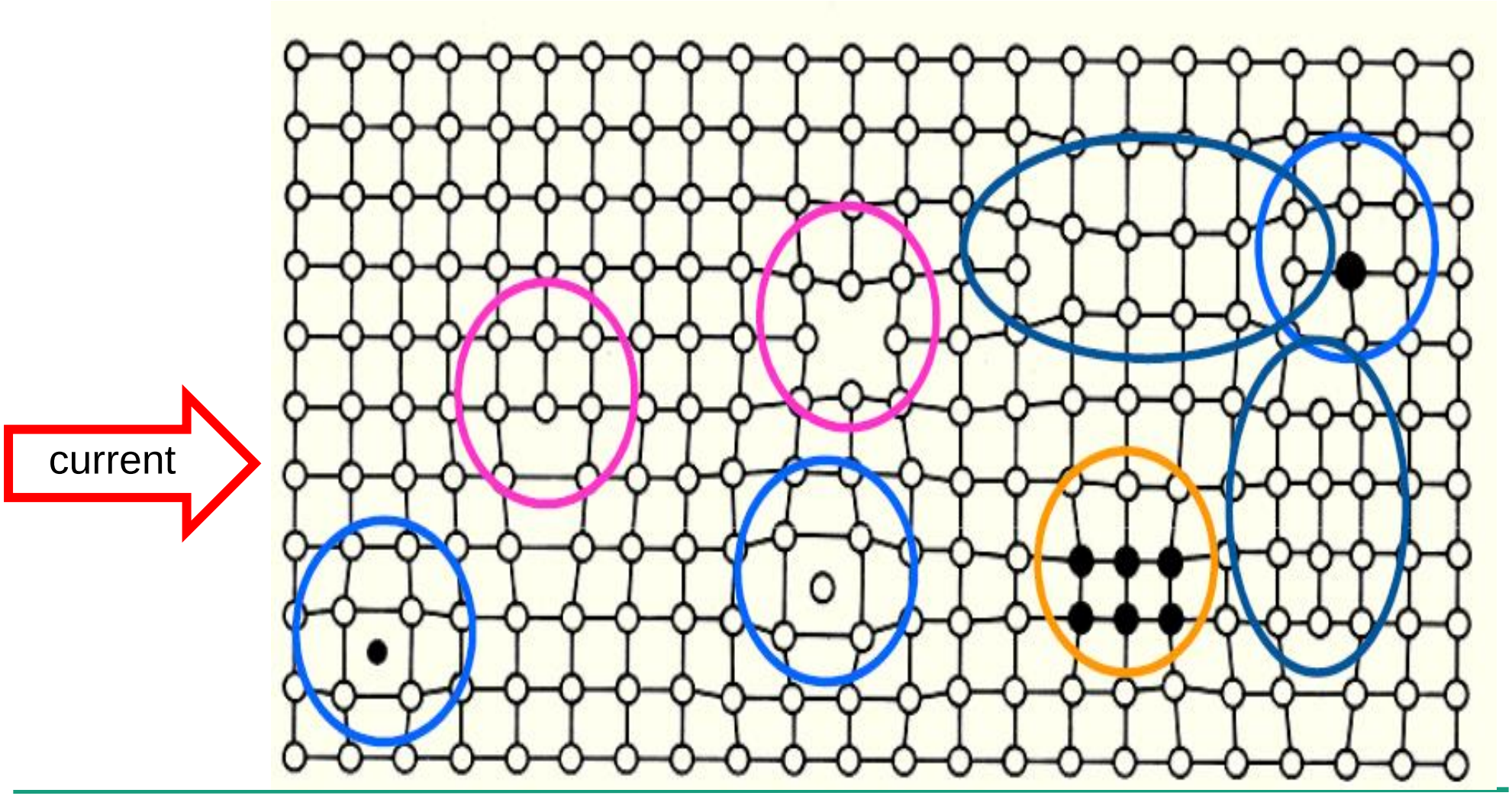
Semiconductor crystals



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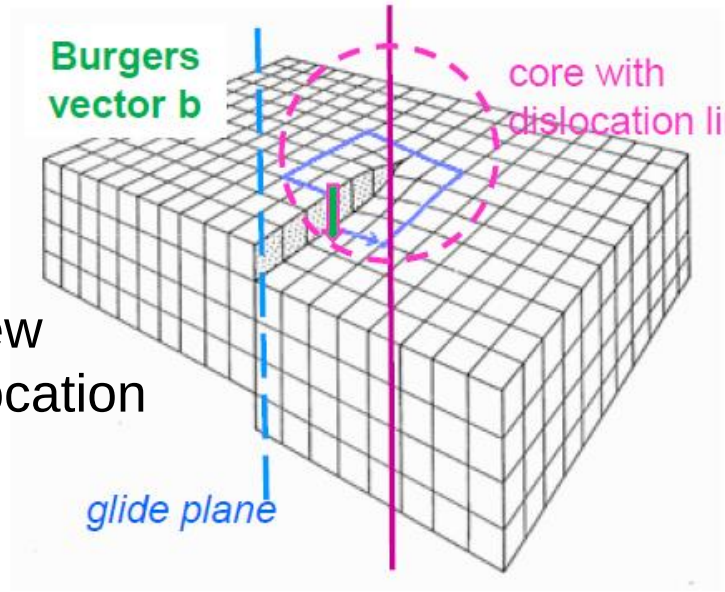
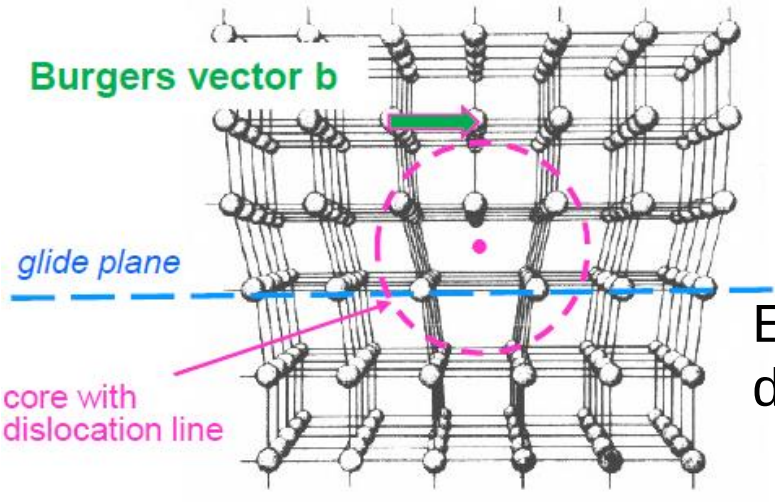
Important types of extended defects in crystals

Screw dislocation





Edge dislocation

Burgers vector is parallel to the **dislocation line**

- A screw dislocation can move out of the plane
- Moving a screw dislocation needs climb or glide effort

Burgers vector is perpendicular to the **dislocation line**

- An edge dislocation moves in one glide plane (or a set of equivalents)
- It does not move out of plane

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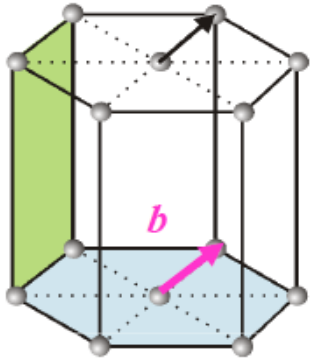
Dislocations in hexagonal, Wurzit-type lattices (GaN)

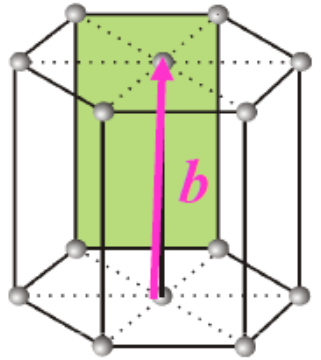
Glide systems in wurtzite crystals
Perfect dislocations on:

- basal plane {0001}
- prismatic planes {1$\bar{1}$00}

b=1/3 <11$\bar{2}$0>



b=<0001>



Dislocation type	Threading Edge Dislocation (TED)	Basal Plane Dislocation (BPD)		Threading Screw Dislocation (TSD)
Burgers vector	$\langle 11\bar{2}0 \rangle$	$\langle 11\bar{2}0 \rangle$		$\langle 0001 \rangle$
Line vector	$\langle 0001 \rangle$	$\langle 11\bar{2}0 \rangle$	$\langle 1\bar{1}00 \rangle$	$\langle 0001 \rangle$
Glide plane	$\{1\bar{1}00\}$	$\{0001\}$		

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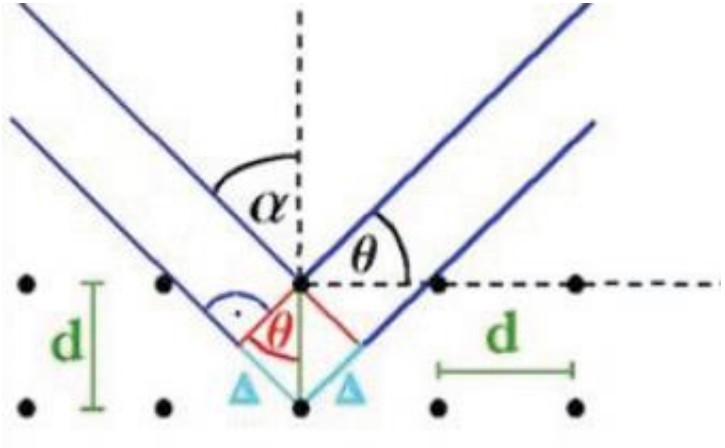
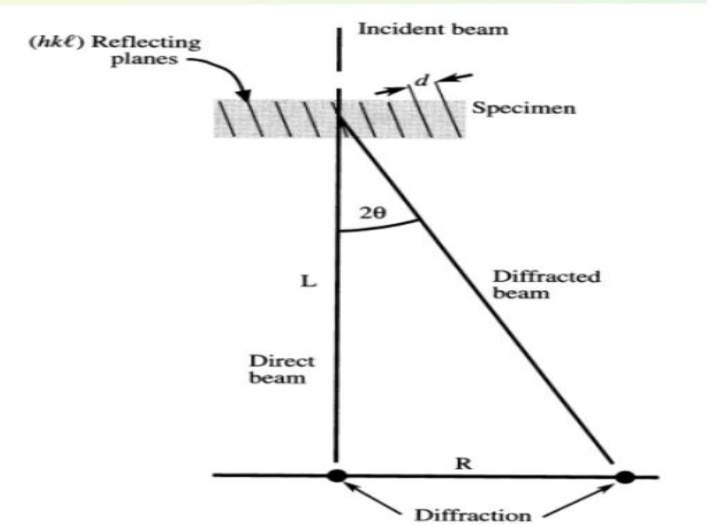
Investigation and visualization of defects

- Defects can be imaged by microscopic techniques
- Size and type of defects determine the method and technique of choice
- Point defects can not be visualized
- Defects can be investigated by x-ray or electron diffraction techniques, based on Bragg‘s law





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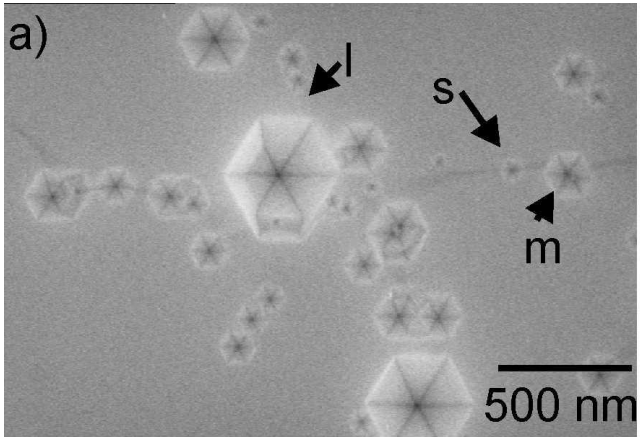
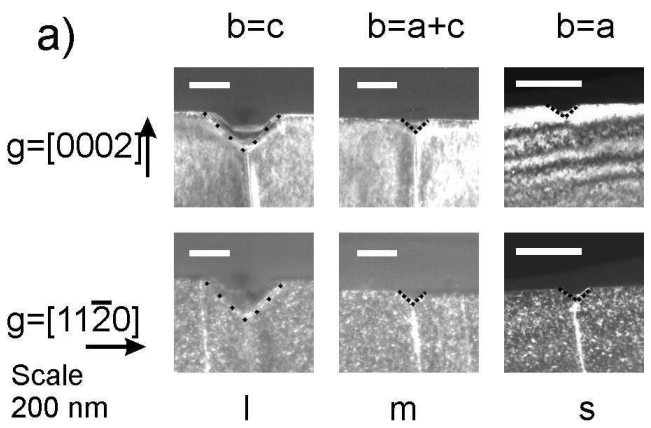
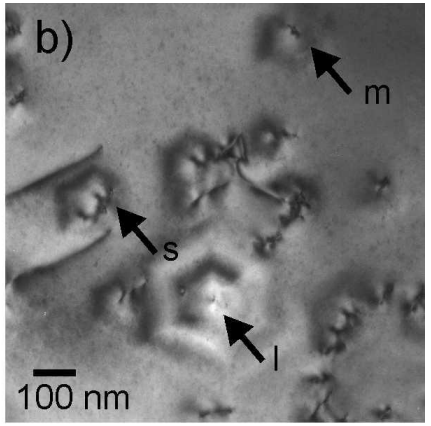
Identification of dislocations in GaN







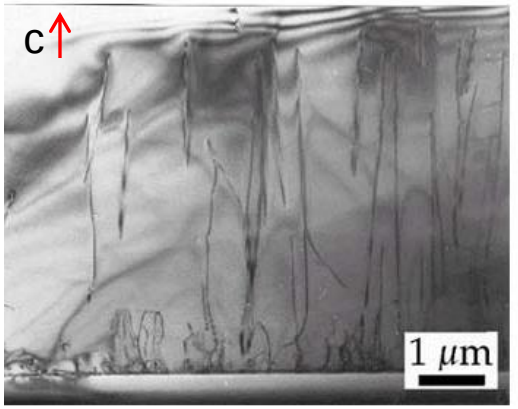
Defect selective etching

Transmission electron microscopy

Dislocations in GaN layers are to the majority threading dislocations along the growth direction, [0001]:

- Pure screw dislocations
- Pure edge dislocations
- Mixed type dislocations

→ *Line vector is along c-direction but Burgers vector is different* →



I.Y. Knoke, E. Meissner et al.,JCG, 312, 20, 3040-3045 (2010)

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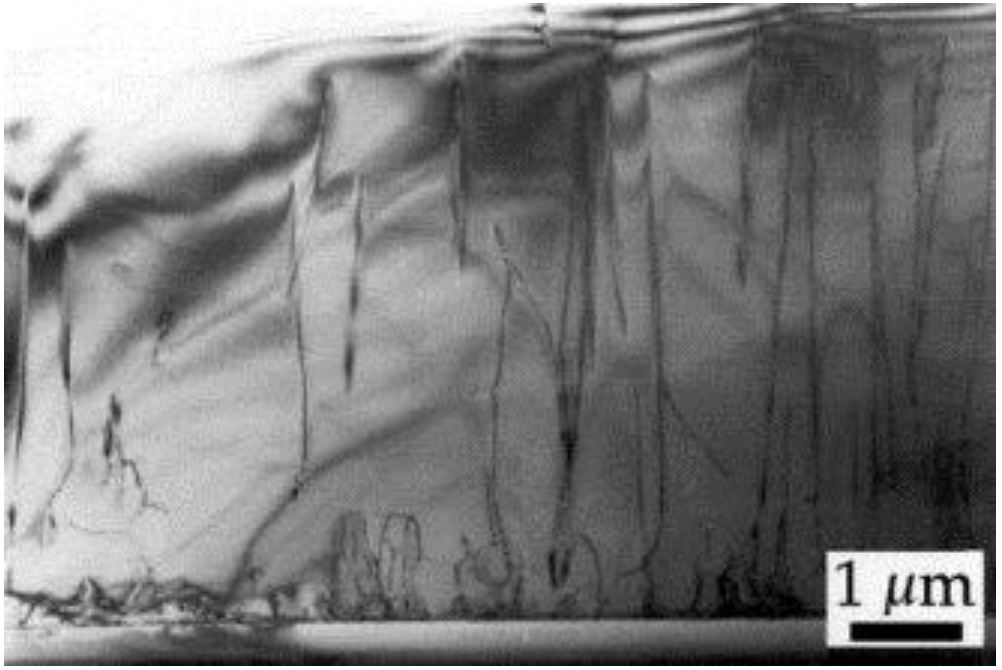
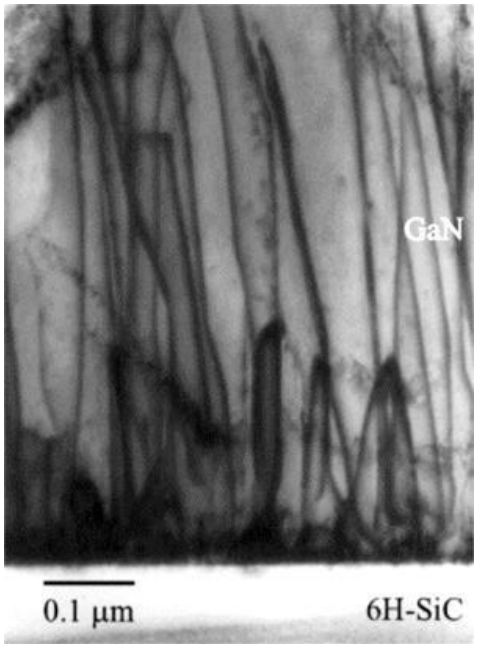
TEM Images of dislocations in GaN





A dislocation cannot just stop or disapear in a crystal lattice, it has to do something:

- React with another dislocation
- Move to a crystal surface
- Getting rid of dislocations requires actions related to the structure and energy of the system

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Something typical for dislocations, general rules

- Dislocations have a strain field around them
- Changes to that strain field are energetic actions

Total energy of a dislocation : $E_{ul} = E_{el} + E_{core}$

The total energy of a dislocation is proportional to it‘s length:

$$U = E_{ul} \cdot L = L \cdot (E_{el} + E_{core})$$

<u>The consequence of the energy minimisation prinziple is:</u>

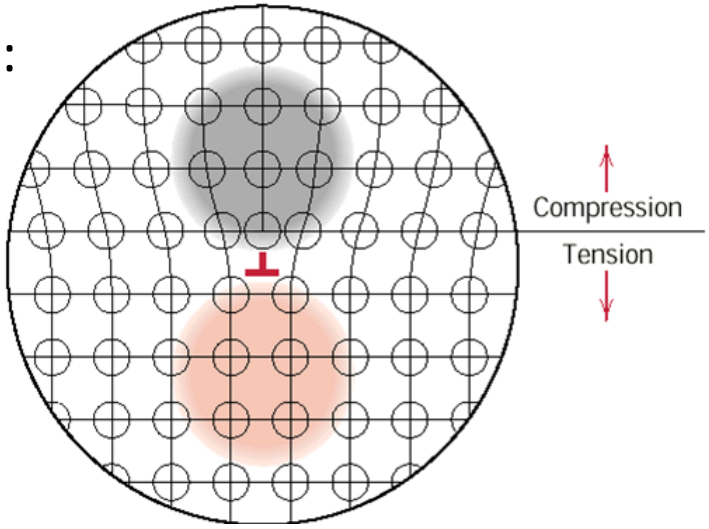
→ Any dislocation tends to be straight
→ Dislocations want to have a short as possible dislocation line and the smalles possible burges vector
→ Edge dislocations always have larger line energies than screws

Actions of dislocations

A movement of dislocations towards each other creates two basic cases:

a) The combined strain is larger than the strain around each single dislocation:
→ energy is higher → repulsive action

b) The combined strain is lower than the single ones:
→ energy is lower → attractive action



- Attraction is obvious if a tensile region and a compressive region overlap
- Opposite burgers vectors in the same plane are always attractive
- Same direction burgers vectors are always repulsive

Dislocations can anihilate, form clusters, change nature due to interactions

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Interactions of dislocations with point defects

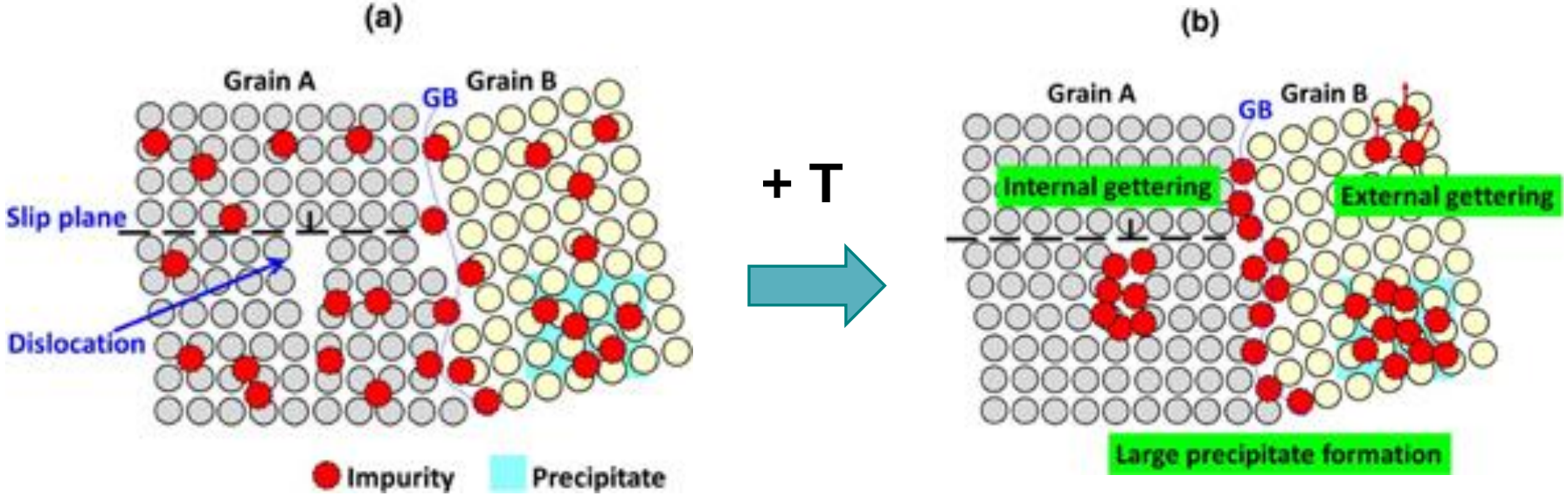
Dislocations can getter point defects or impurities:

- The interaction is through the strain field or the core
- Impurities are supersaturated and the dislocation acts as a nucleation site for precipitates
- Dislocation cores offer special energetic places, charges, dangling bonds that are attractive for foreign atoms
- Dislocations are a perfect energetic sink for metal atoms

→ **Dislocations decorated with foreign atoms change their electrical nature**
→ **The neigboured material changes it‘s properties due to a depletion of e.g. doping atoms**
→ **The properties of a crystal with many dislocations can be non homogeneous on a microscopic scale**

Movement of impurities to a dislocation

- Activation of impurity gettering by thermal energy
- Collecting impurities at dislocations can be wanted or unwanted
- Collecting dopant atoms at dislocations is always unwanted

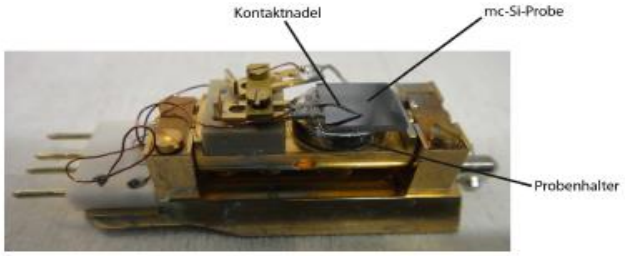


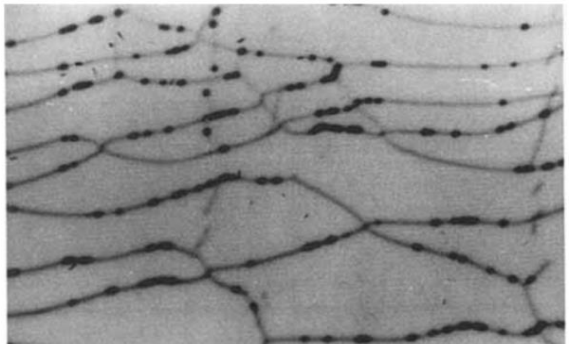
Supawan Joonwichien, Isao Takahashi, Japanese Journal of Applied Physics, Volume 54, Number 8S1, 2015

Fraunhofer IISB

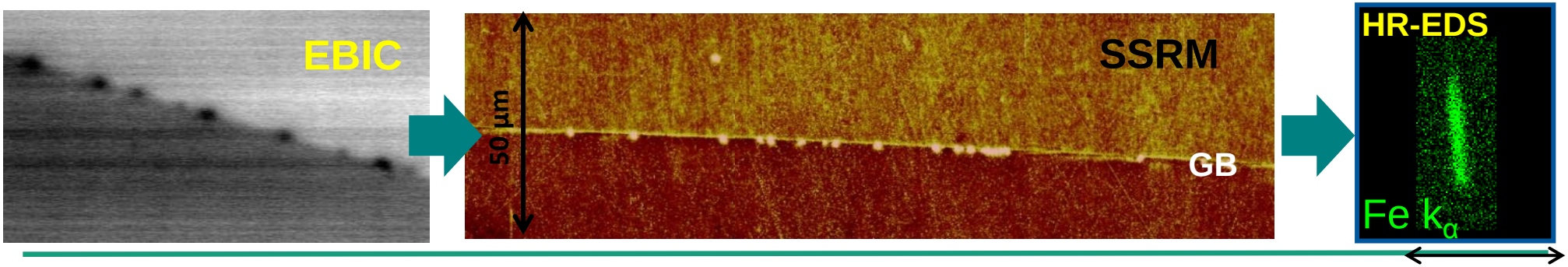
Investigating structural disruptions for electrical action
EBIC= Electron Beam Induced Current + EDS

- EBIC imaging reveals places of carrier recombination
- Can be performed lateral or vertical
- On material or devices
- Need for electrical contacts (Schottky and Ohm type)
- Combined analysis: EBIC+SSRM+EDS
  - Identification of recombination centers
  - local electrical properties
  - Chemical information





EBIC Image of Fe precipitates in Si intentionally contaminated and annealed at 450°C



Fraunhofer IISB

Electrical properties of dislocations in GaN

Effect of a dislocation depends on the :

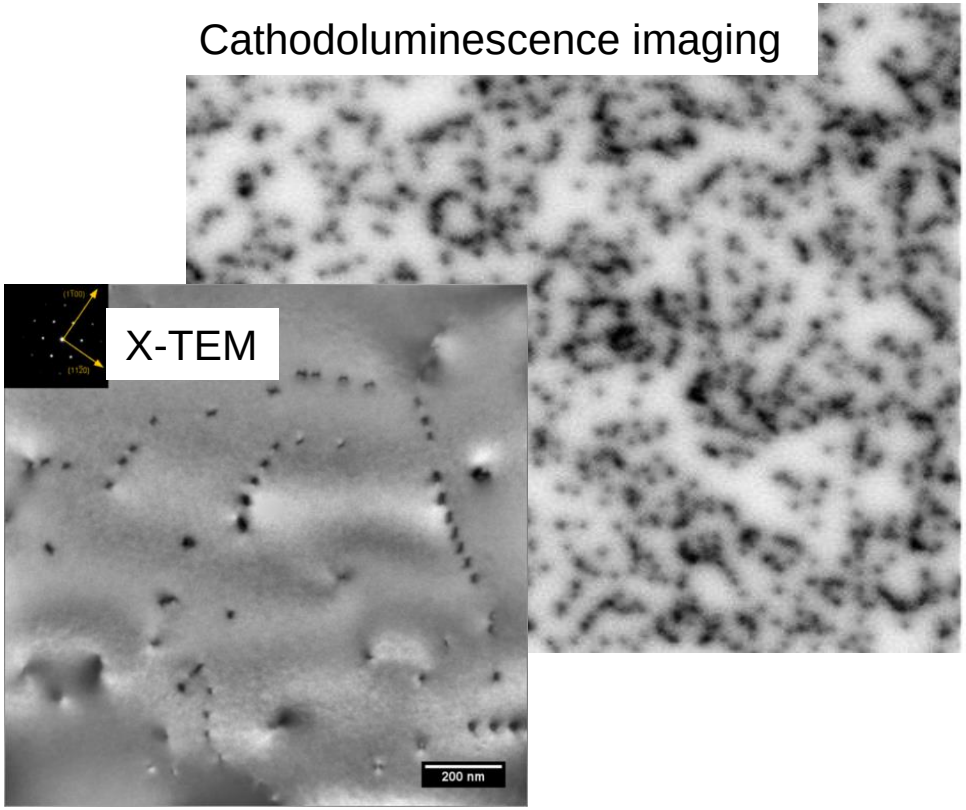
- Orientation of the dislocation with respect to the current flow
- The nature/type of the dislocation
- The charge of the dislocation → the core structure

Note:

Properties of „pure“ dislocatios can change due to gettering effects or segregation of atoms along the dislocation core

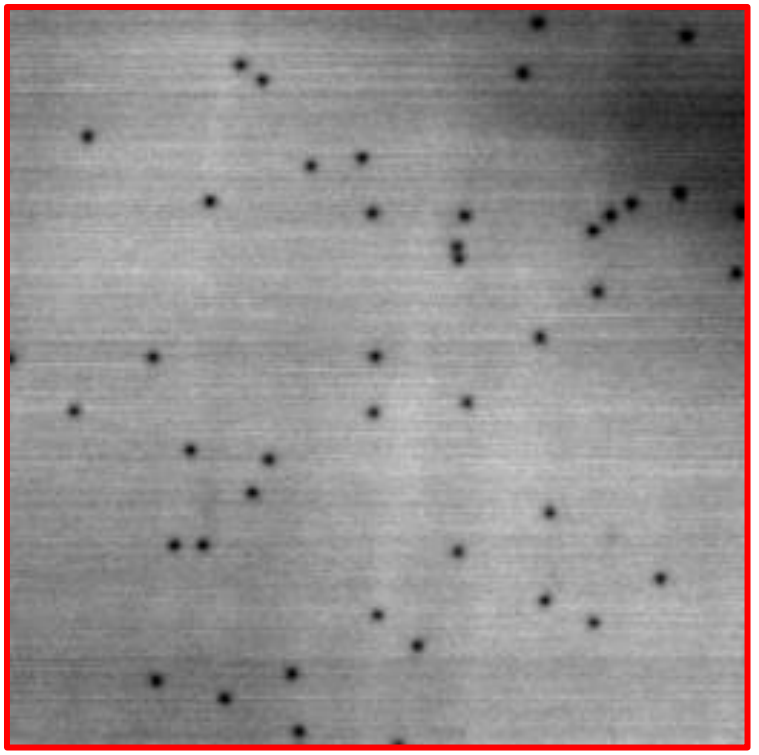
Clusters, arrangements, cells etc can have different effects compared to a single, locally isolated dislocation

Defect microstructure of GaN on Silicon vs. native GaN (HVPE)



GaN on Si , DD $10^9/cm^2$

Clustering of dislocations



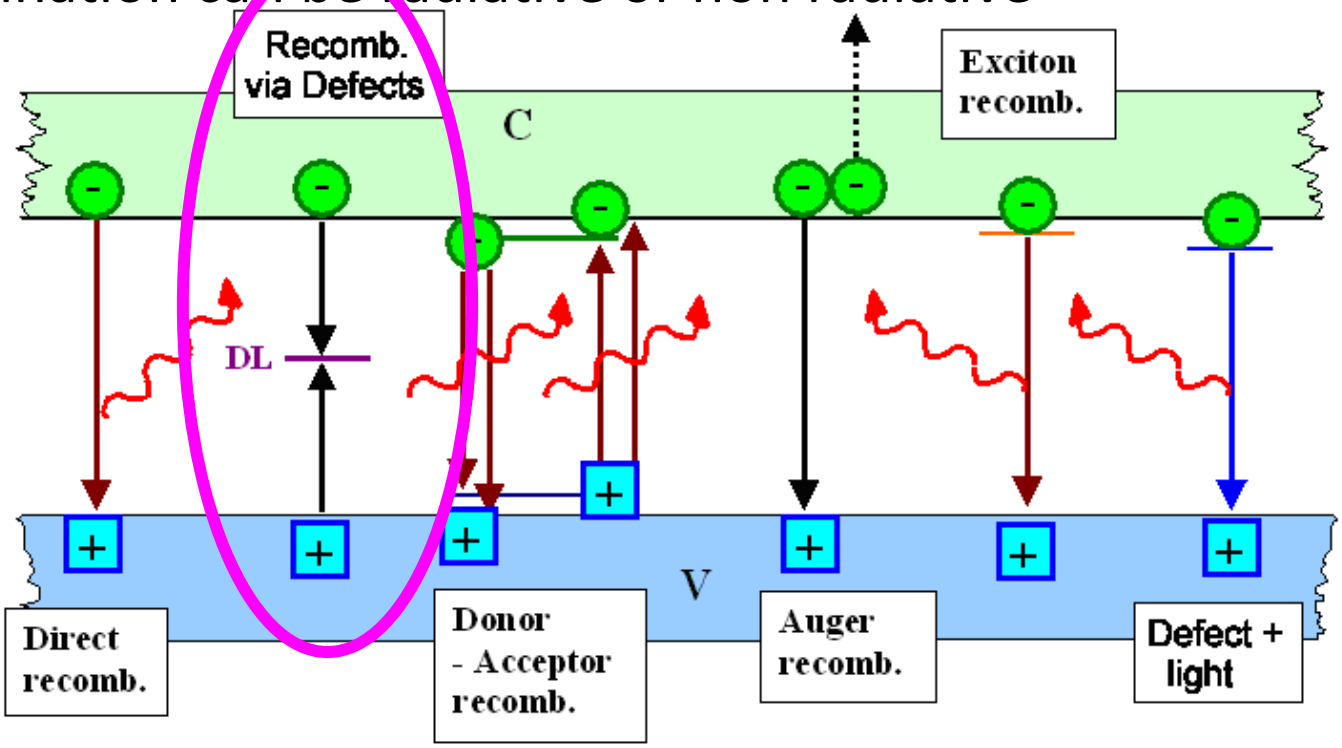
Free standing GaN crystal , DD $10^6/cm^2$

Randomly distributed dislocations

Fraunhofer IISB

Electrical relevance of dislocations

- Any energetic level existing in the band gap of a semiconductor (forbidden region) can act as recombination path and recombine carriers
- The recombination can be radiative or non radiative



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Electrical properties of dislocations in GaN

- Different core structures of screw dislocations are theoretically possible
- Most configurations create negatively charged pure screw dislocations
- At least two configurations are thought to be neutral
- Electrical properties of egde dislocations are under debate

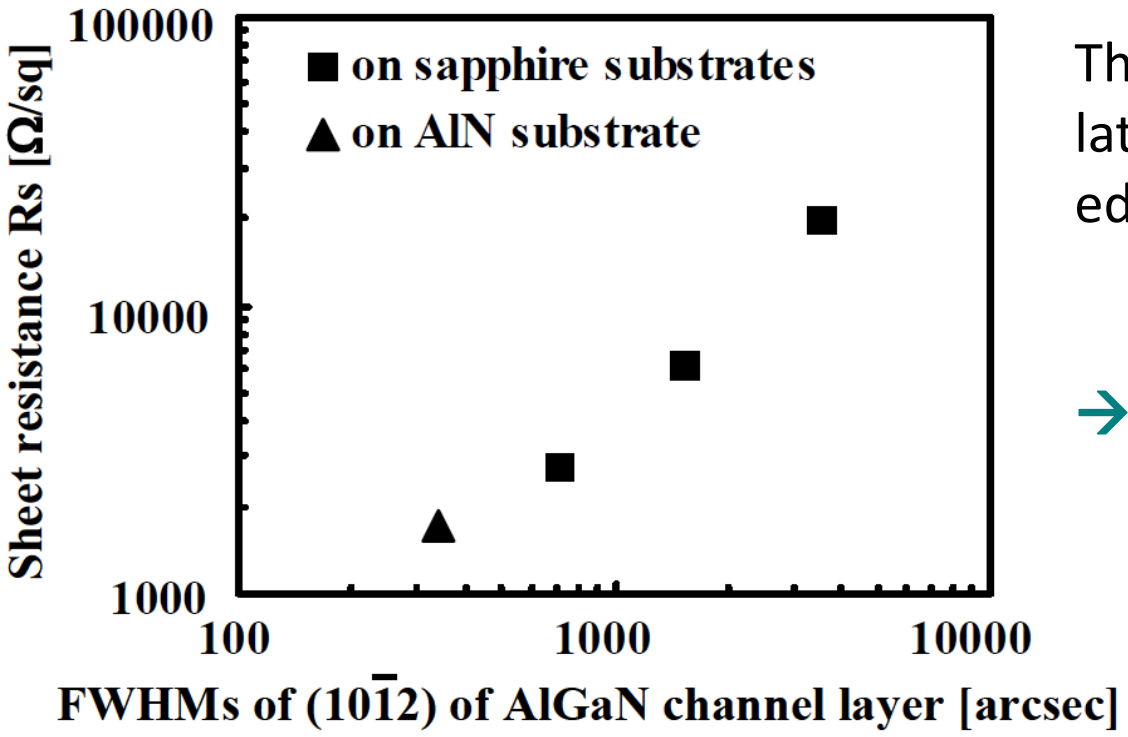
- Published experimental data does not correlate clearly with theoretical assumptions

→ **Different properties of dislocations - depending on:**

- the substrate, the growth process, the device process

→ **So all actions of dislocations described before are possible in GaN**

Electrical action of dislocations with respect to dislocation types



S. Hashimoto et al., PSS (C) 7, (2010)

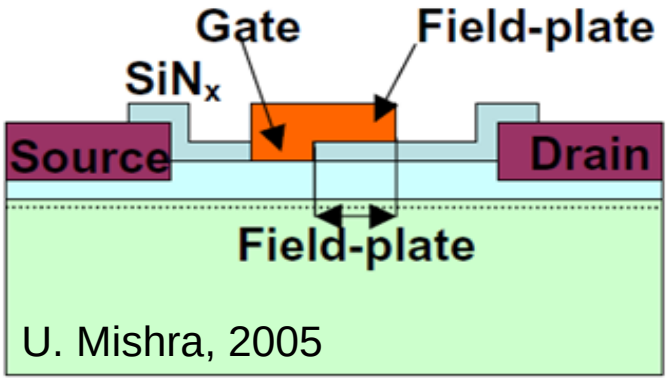
The FWHM values of the asymmeric lattice reflex are related to threading edge dislocations

→ **Though, the sheet resistance variation is not due to screw but to edge dislocations in this case**

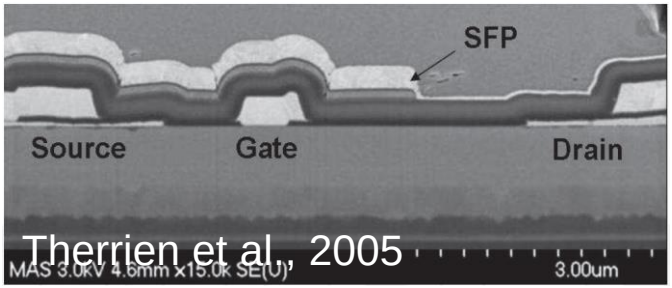
Effect on lateral devices & any lateral current flow

Fraunhofer IISB

Fabrication of a nitride semiconductor device

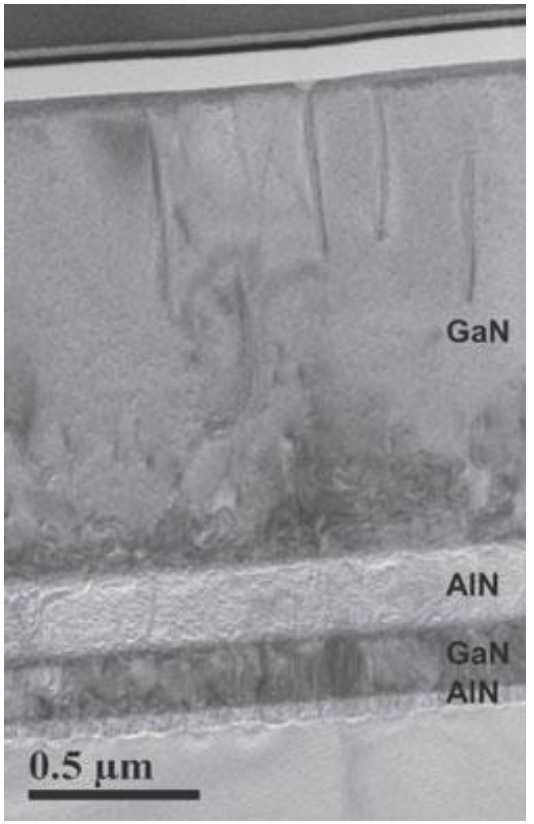


Fix design and technological steps



Device:
A sequence of epitaxial layers deposited on a substrate wafer

Properties and quality of the epilayers determine performance and reliability of the device



→ **Substrate wafer determines the quality of the subsequent epilayers**

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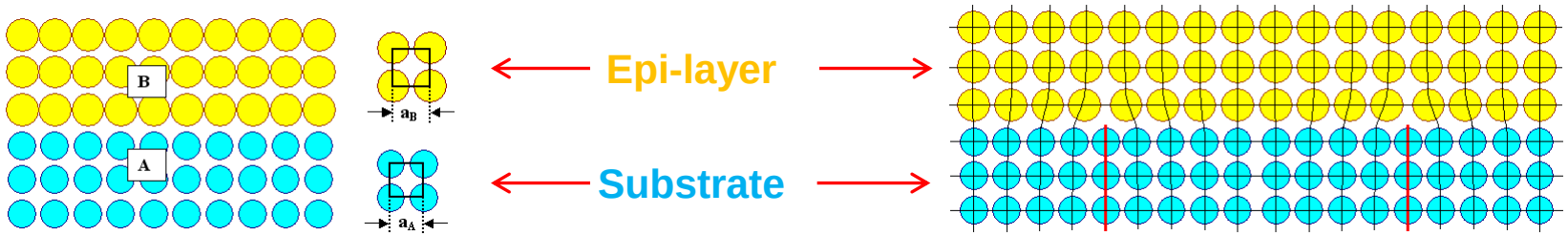
Epitaxy and requirements for the substrate

Aim: the crystal layer should have no defects



Perfect structural match
between substrate & layer
→ *Native substrate case*

Structural mismatch
between substrate & layer
→ *Foreign substrate case*

The substrate must:

- **fit as perfect as possible to the structure of the epitaxial layer match as good as possible „thermally“ (thermal expansion coefficients)**

→ **native substrates**

Fraunhofer IISB

Choice of the ideal substrate

For epitaxial layers with defect-free, perfect crystal structure we need:

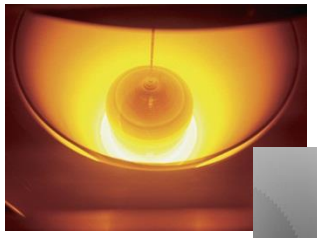
→ Homoepitaxy

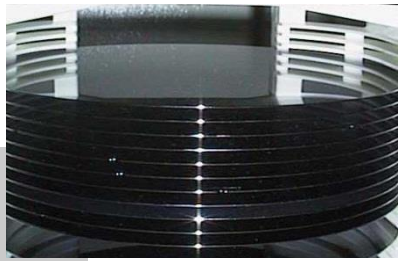
→ Native, epi-ready substrates

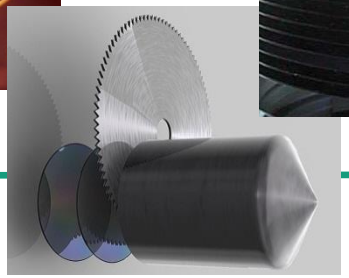
Technology	Substrates	Crystal growth	Availability
Silicon	Silicon	CZ Si	Very good, very cheap, up to 450 mm
GaAs	GaAs	VGF GaAs	Good, cheap, up to 200mm
SiC	SiC	PVT SiC	Good, expensive, up to 150mm
GaN	Si, SiC, Sapphire	Not established, trials various	Few, some 2“ freestanding, majority templates, extremly expensive

→ Problem: Availability of substrates depends on :

- available semiconductor crystals
- availability of crystal growth technology
- technological solutions for wafering and polishing







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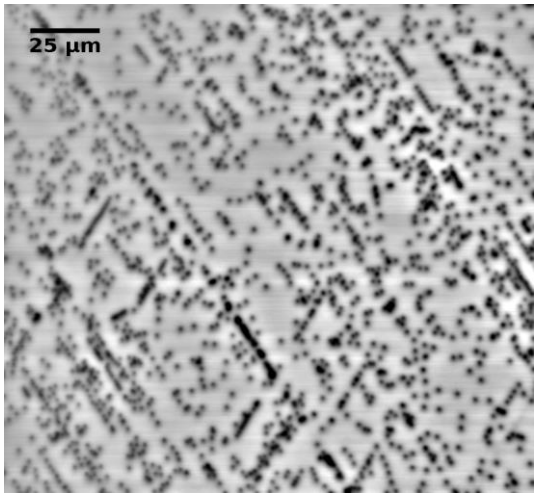
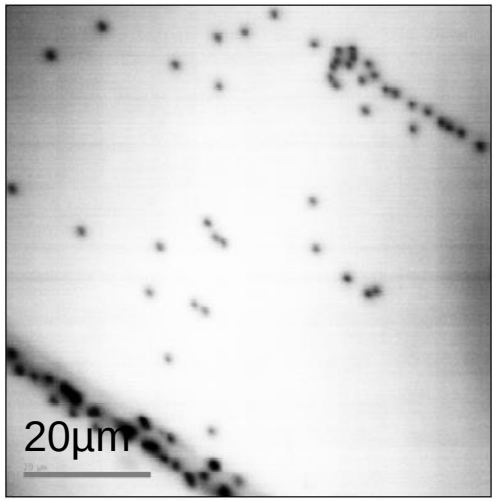
Why we would need native crystals

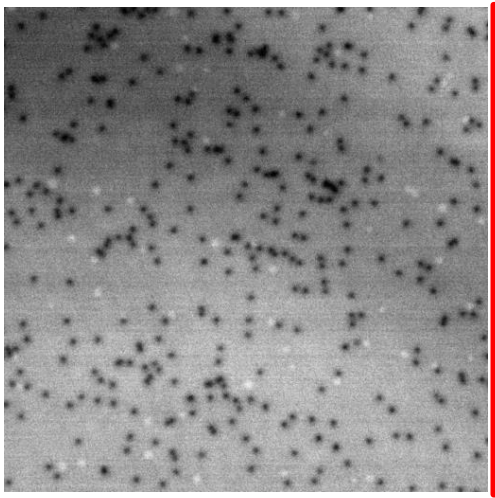
How does a „better“ GaN crystal look like (CL-dark-spot imaging)



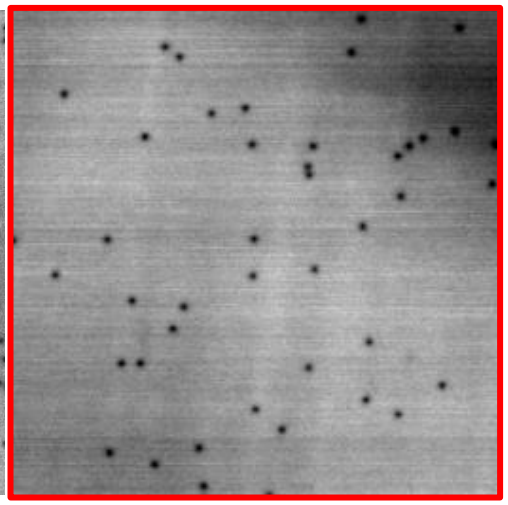
$1x10^9$ cm^{-2} alignments



$1\text{-}5x10^8$ cm^{-2} clusters



$0.5\text{-}1x10^8$ cm^{-2}



$1x10^6$ cm^{-2}

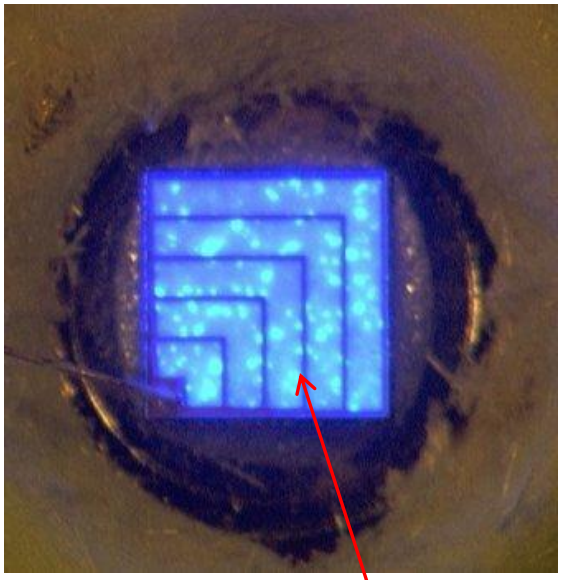
- Decrease of total dislocation density by improved growth conditions and reduced strain
- Reduced formation of cell structure respectively growth with small sized columns
- Reduce presence of sub-grain boundaries
- Avoide dislocation cluster formation

→ **Low total number of randomly distributed dislocations**

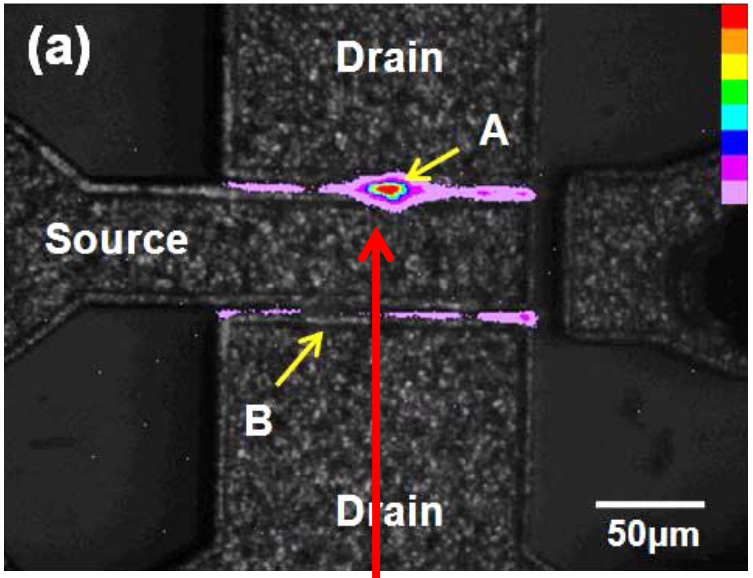
→ **Dislocation microstructure in heteroepitaxy is a problem → *native substrates***

Fraunhofer IISB

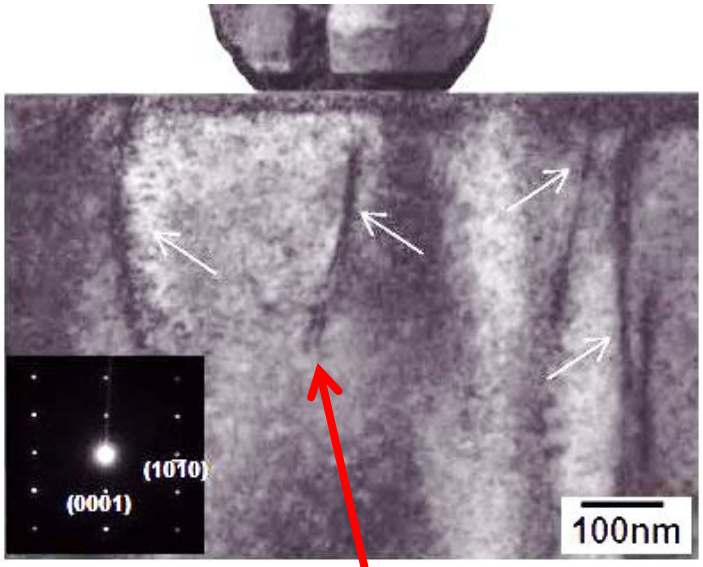
Influence of dislocations on reliability of a GaN power device



Radiative or non-radiative recombination at dislocations



Local warming



JJAP, 2015

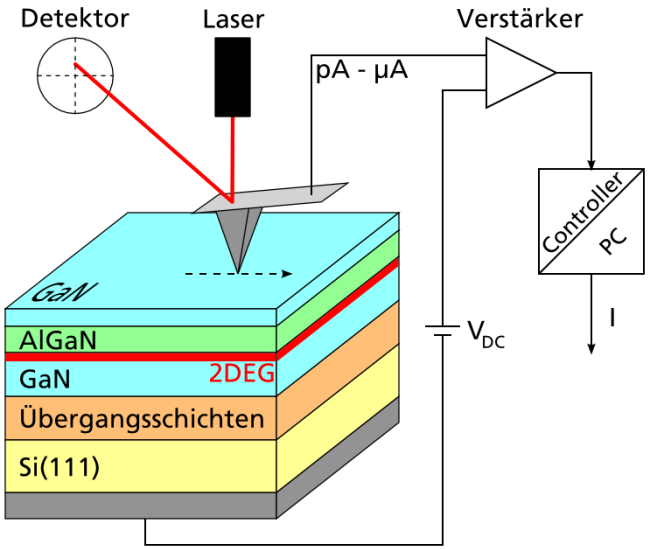
Dislocation lines

→ Dislocations directly in the region of the device contacts or in the active area can cause catastrophic device failure

→ Dislocations can reduce the performance of a device

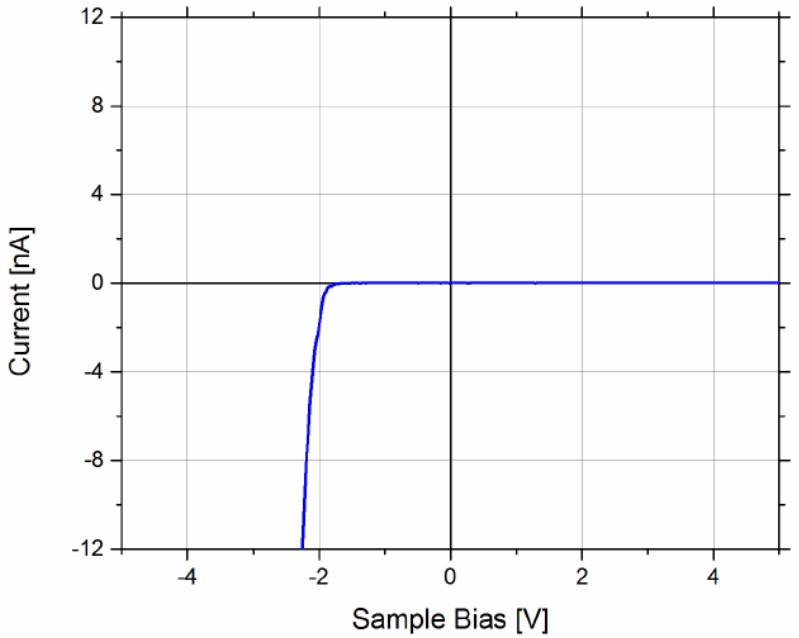
Fraunhofer IISB

Identification of vertical conductive defects



- Scanning of surfaces of a device structure
- Topography imaging
- Mapping of vertical or lateral current flows
- IV-curves

C-AFM good possibility to characterize el. properties of AlGaN/GaN-HEMT heterostructures on µm-scale



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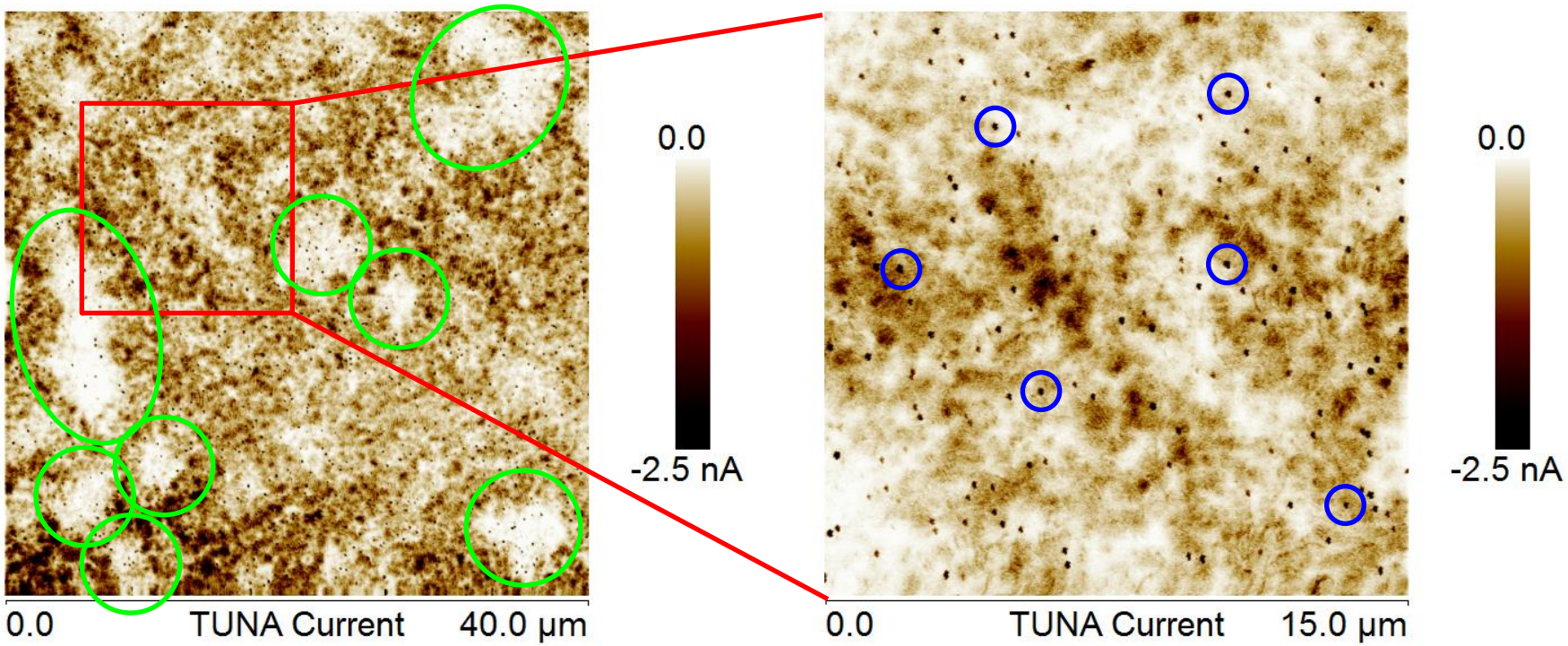
Identification of electrical action of structural disruptions

Mapping of vertical current flow



Current at constant sample bias is distributed inhomogeniously

- Large regions (~10µm) of very low current (○)
- Discrete spots of higher current (spot density ~$10^8 cm^{-2}$) (○) → dislocations

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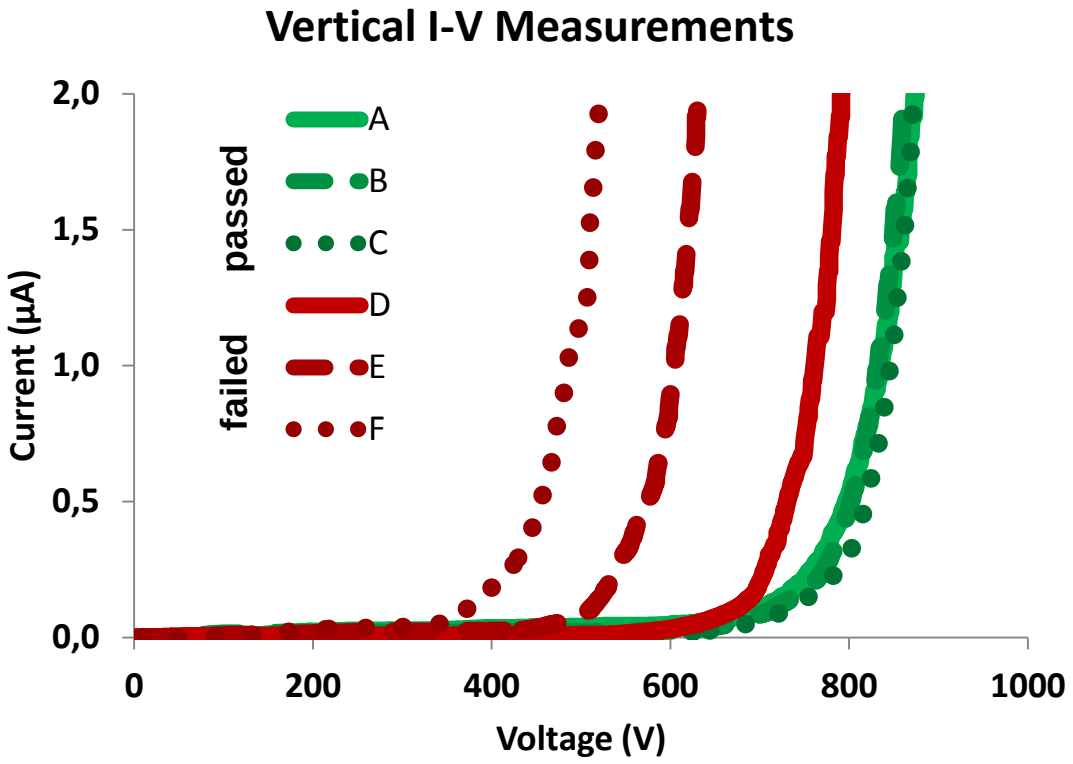
Understanding the defects responsible for vertical breakdown of HEMTs:

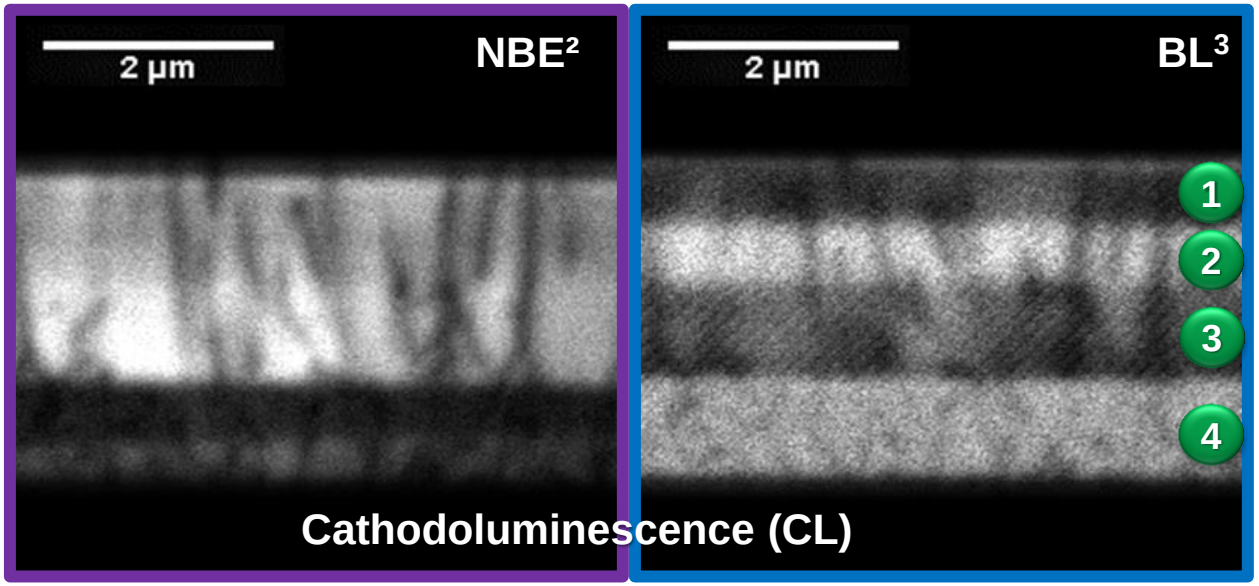
Six Samples from the same wafer, with differences in vertical breakdown voltage

- Two groups of I-V-Curves
- **Samples A,B,C** → passed ($V_{BD,vert}$ = 850V)
- **Samples D,E,F** → failed: ($V_{BD,vert}$ = 720, 570, 450 V)

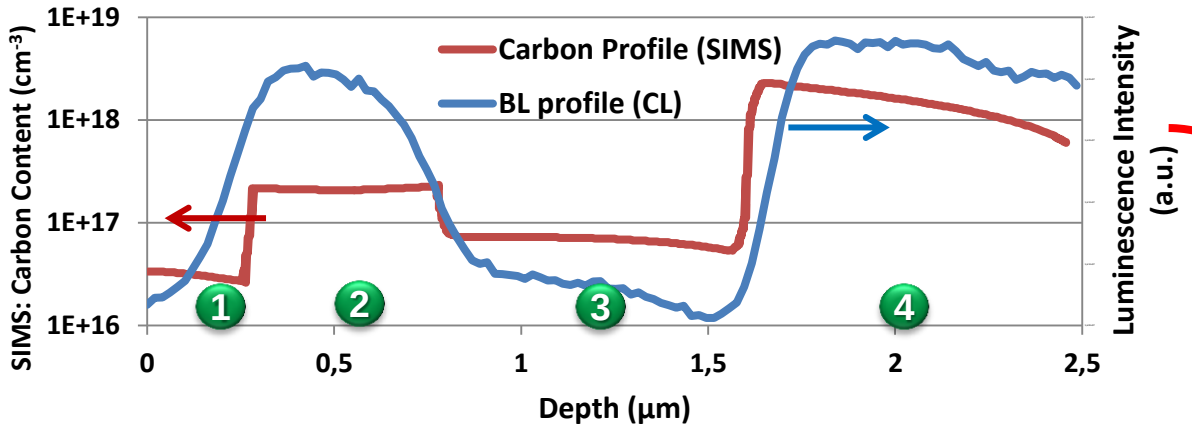


Basis for structural investigations, to determine critical defects

Correlating Carbon Content (SIMS) with Blue Luminescence (BL)



- Carbon is used as dopant for semi-insulating GaN
- BL stems from carbon
- NBE does not correlate with carbon content



→ Use BL intensity to visualize local differences in carbon concentration

Effect on electrical breakdown resistance of the insulating HEMT layer?

[2] **N**ear **B**and **E**dge luminescence

[3] **Blue L**uminescence

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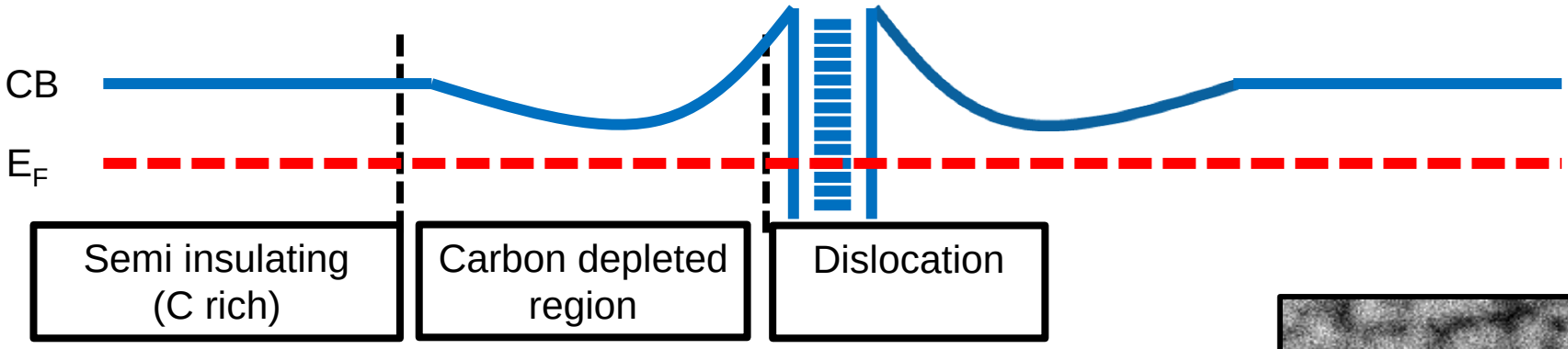
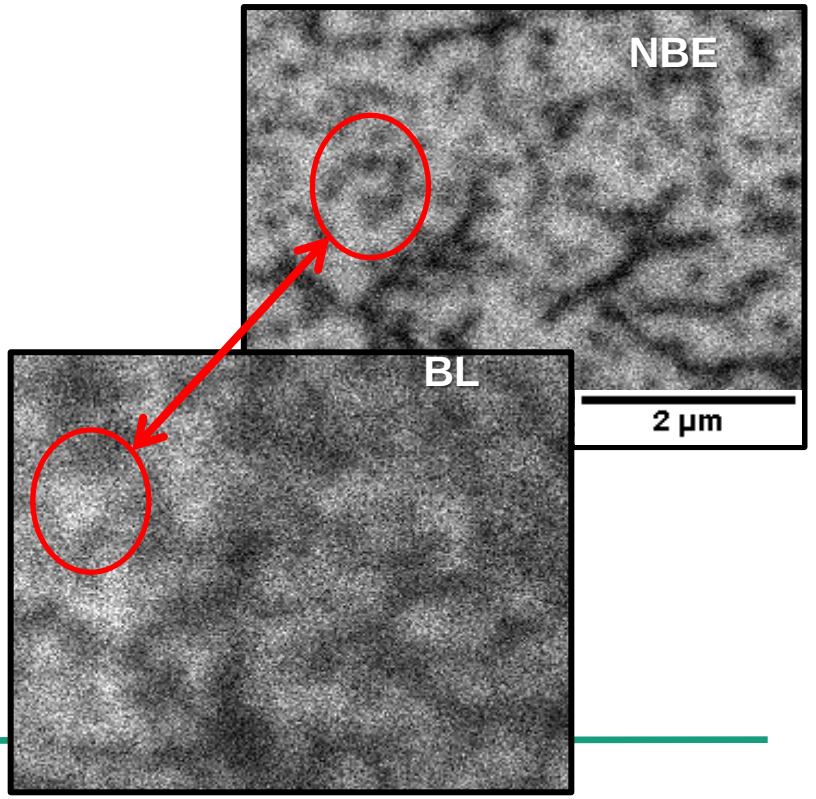
Explanation Model: Carbon depletion around a dislocation



- A dislocation **getters carbon**, thus **deplete** the region around it
- Gettered carbon stays in the dislocation core



→ **Depleted regions change conduction type**
→ **Dislocations may develop highly conductive**

[1]Kim et al. *Appl. Phys. Lett.* 104 (2014)
[2]Krtschil et al. *Appl. Phys. Lett.* 82 (2003)

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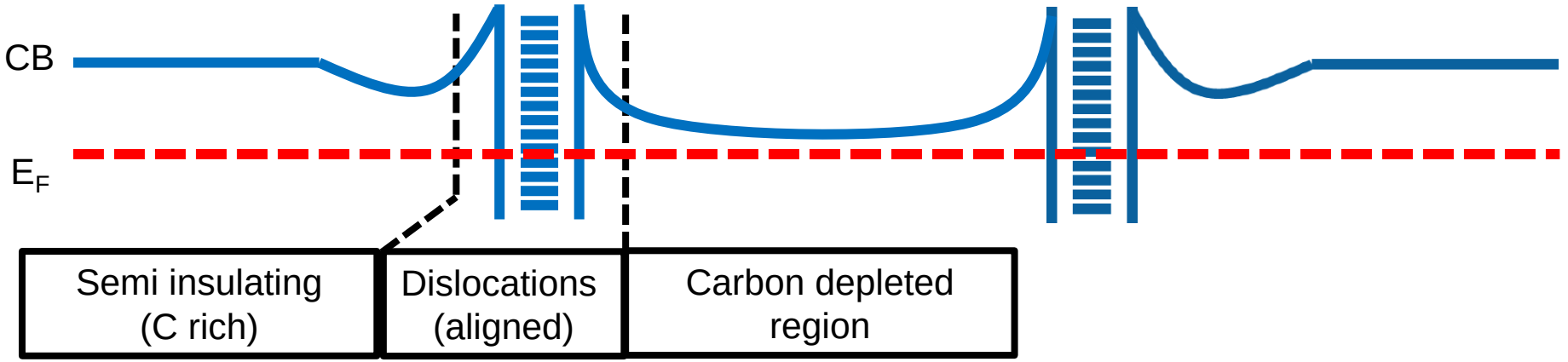
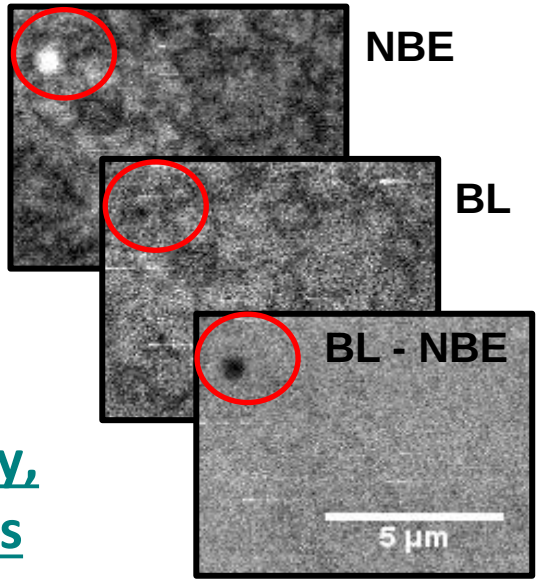
Carbon Depletion at Clustered / Aligned Dislocations



- Dislocation alignments form a cluster or a cell
- Average distance of dislocations at a density of 10^9 cm^{-2} : 300 nm
- Interaction distance of a dislocation: 150 nm
- Size of a carbon depleted region : 350 nm



→ Overlapping of carbon depleted regions quite likely, dislocation clusters are more harmful than single ones

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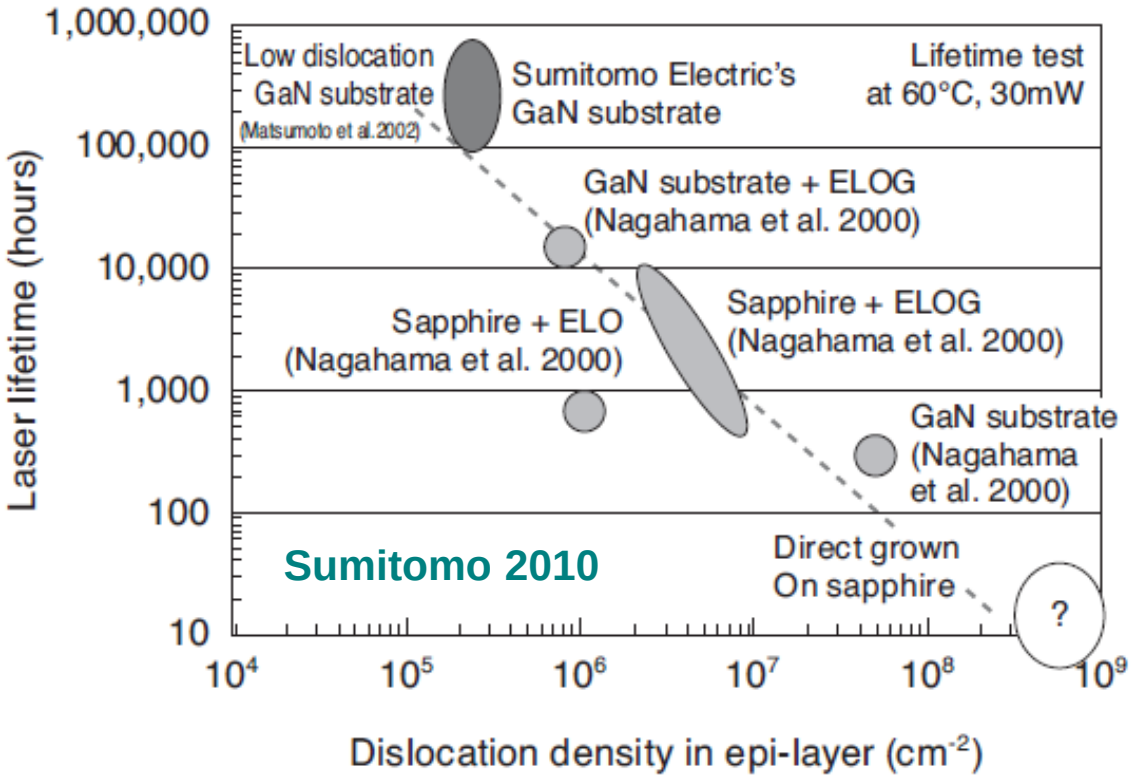
Effect of dislocations on the life time of a device



- Lifetime of LDs depend strongly on total dislocation density
- Reliability of transistors is affected by dislocations
- Heteroepitaxy is difficult in this sense

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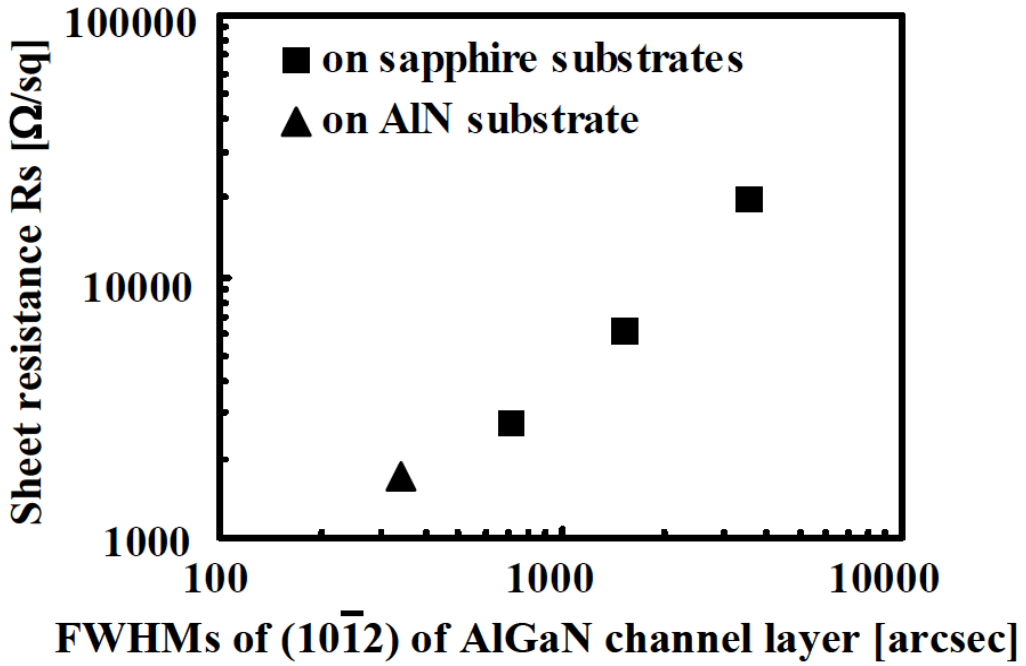
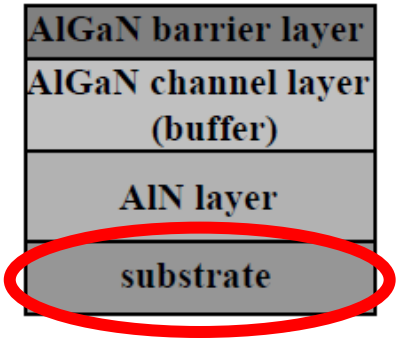
Effect of dislocations on sheet reistance of AlN layers



S. Hashimoto et al., PSS (C) 7, (2010)

→ **The better the quality of the AlGaN layer – the lower it‘s sheet resistance**

- Investigation of the influence of structural qualtity of the active epitaxial layers on the electrical performance of a device
- Investigation of the quality of the 2DEG in Al-rich HEMT structures
- Growth on Sapphire and AlN native substrates



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Conclusions

- A semiconductor must be as perfect as possible, but no crystal exists without at least point defects
- Extended defects must be avoided as much as possible
- Heteroepitaxy has strong consequences for the semiconductor microstructure
- In the case of GaN heteroepitaxy works but with many defects
- Defects do influence the electrical properties of a semiconductor device
- In the case of native substrates the amount of defects is small
- The availability of the substrates and respective growth technique for the bulk crystals are is an issue

Defects in Nitride Semiconductors Materials and their relevance to electrical devices

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