

Emission channeling with short-lived isotopes (EC-SLI) of acceptor dopants in nitride semiconductors

Proposal INTC-P-489

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**(Emission Channeling with Short-Lived Isotopes,
the EC-SLI collaboration)**

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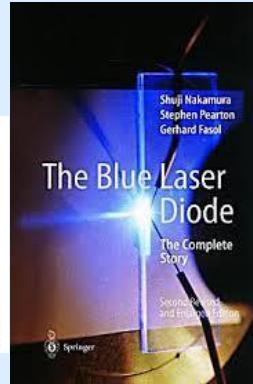
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Spokespersons: U. Wahl and L.M.C. Pereira

Motivation: Mg in nitride semiconductors

- Nitrides are base material e.g. for white LEDs, blue lasers, power devices, voltage transformers



- Mg is the only technologically relevant *p*-type dopant in GaN



- Other group II impurities, e.g. Be, Ca were also tried in GaN but did not succeed as acceptors



- To be electrically active, Mg acceptors (group II) should occupy substitutional Ga (group III) sites

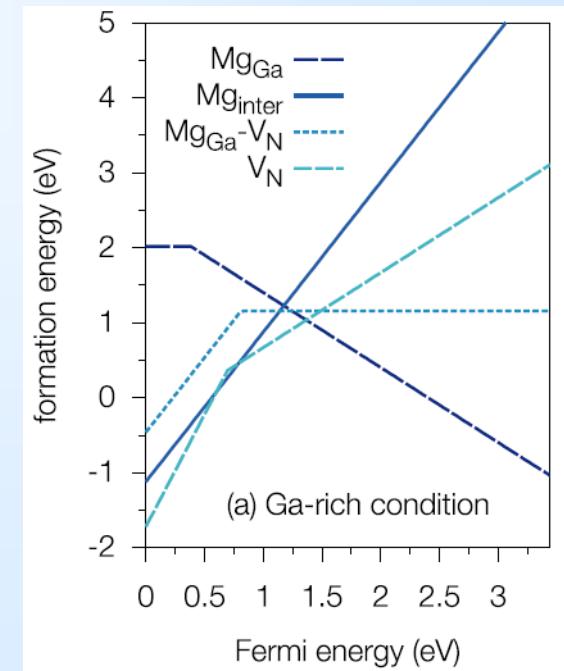
- Mg doping works but not without problems

Nobel prize in Physics 2014
I. Akasaki, H. Amano, S. Nakamura

Doping problems in GaN: limitations at high [Mg]

- Doping limitations: once $[Mg]$ surpasses $\sim 10^{19}$ - 10^{20} cm^{-3} , further introduction of Mg does not lead to an increase in the hole concentration. Reasons?

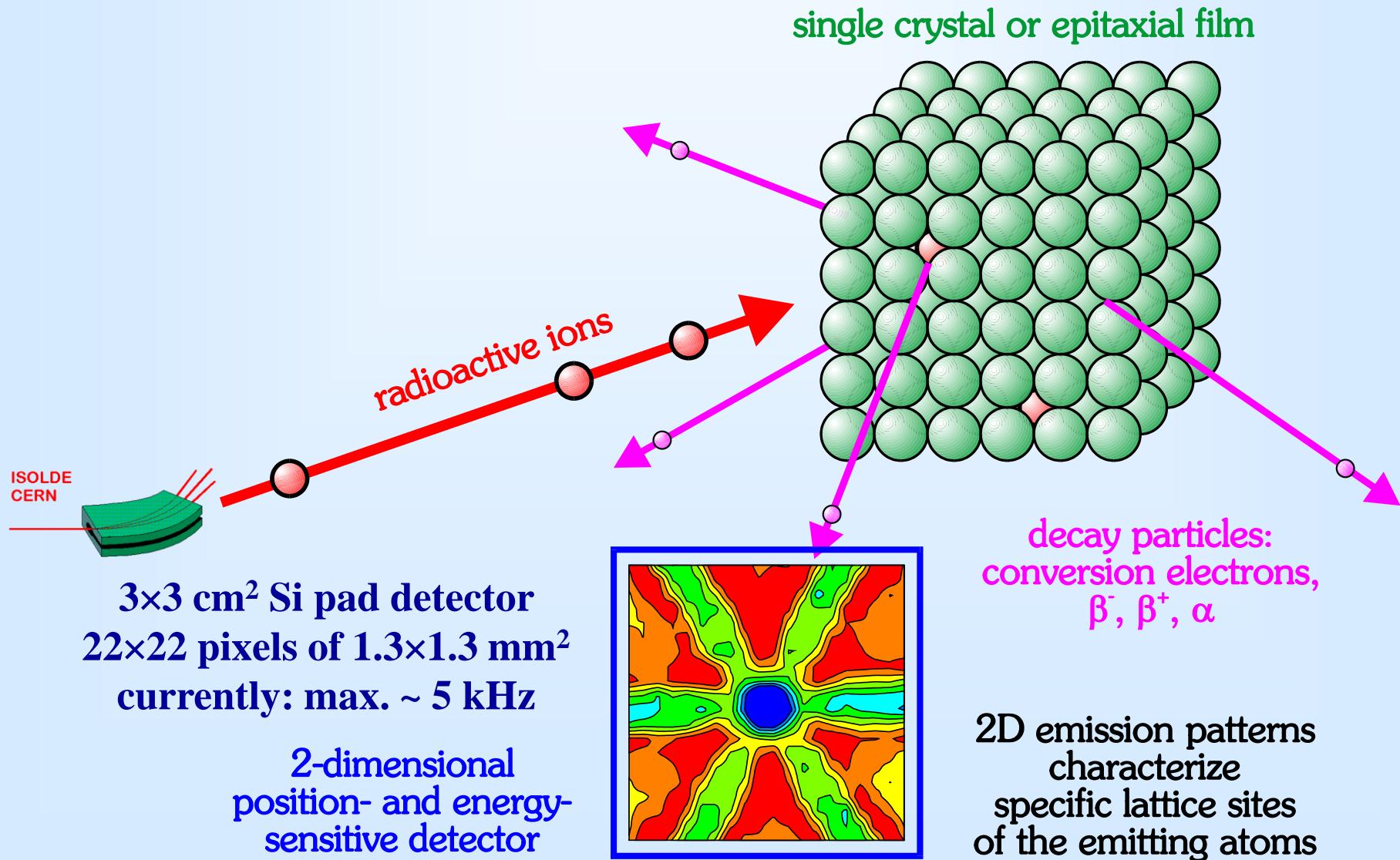
- Passivation of Mg_{Ga} acceptors by H
- Compensation by native defects: V_N^+
- Solubility limit: formation of Mg_3N_2 precipitates.
- Formation of Mg_i interstitials (double donors) also predicted by theory, but previously never experimentally observed!



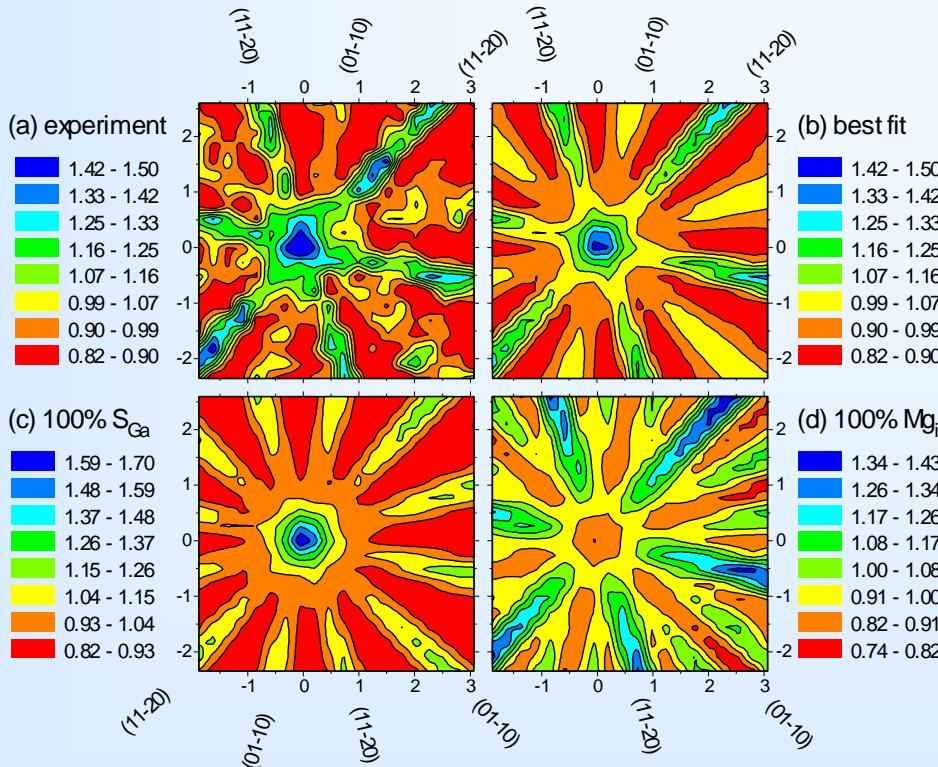
G. Miceli, A. Pasquarello,
PRB 93 (2016) 165207

- EC-SLI experiments have given first clear evidence for the existence of Mg interstitials and its coupling to the Fermi level \Rightarrow amphoteric nature of Mg

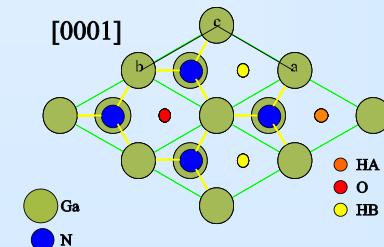
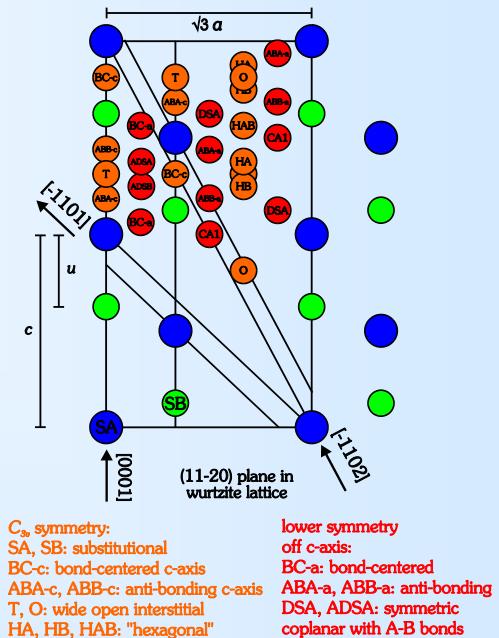
Emission channeling: basic principle



β^- emission channeling patterns from ^{27}Mg ($t_{1/2}=9.5$ min) in p -GaN:Mg



High-symmetric sites in wurtzite structure



fit results:

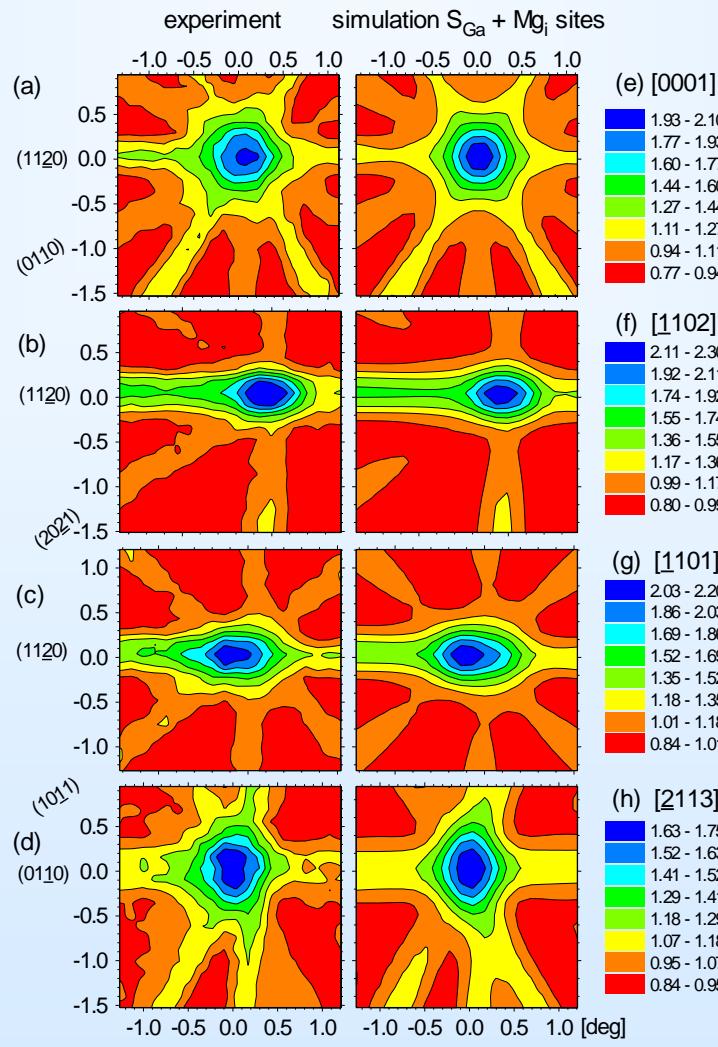
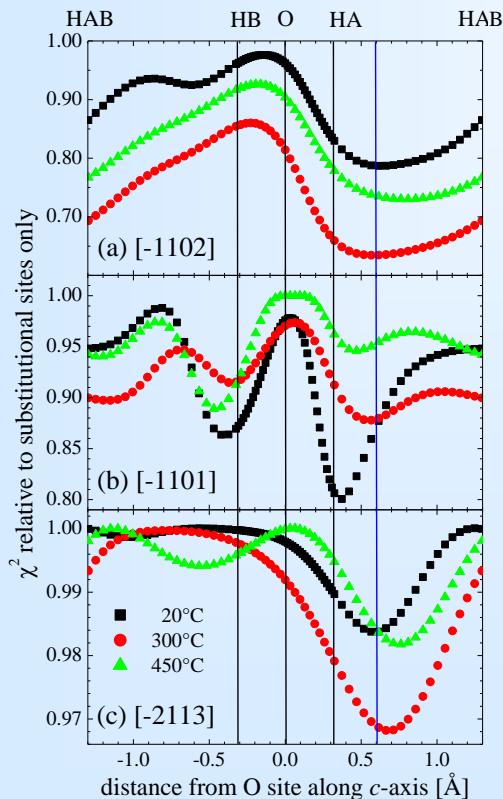
200°C: ~72% ^{27}Mg aligned with c -axis, ~33% on interstitial sites

0.20 pA implantation current, total fluence $1.1 \times 10^{11} \text{ cm}^{-2}$

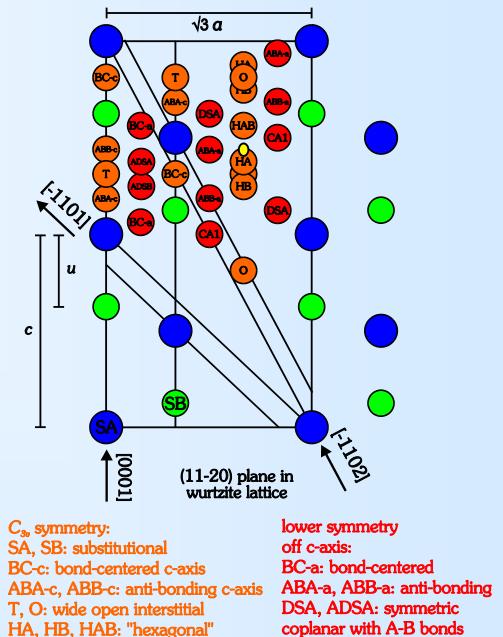
Lattice location precision of ^{27}Mg in p -GaN:Mg

High angular resolution
(small solid angle)

1.5-3 pA
 $1.5 \times 10^{12} \text{ cm}^{-2}$ per pattern

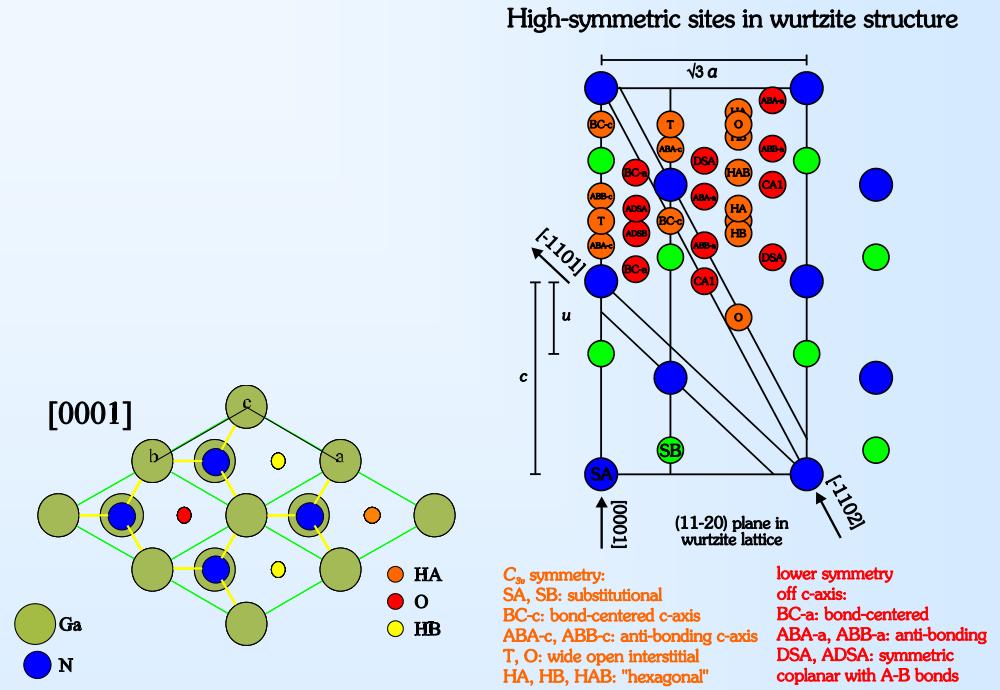
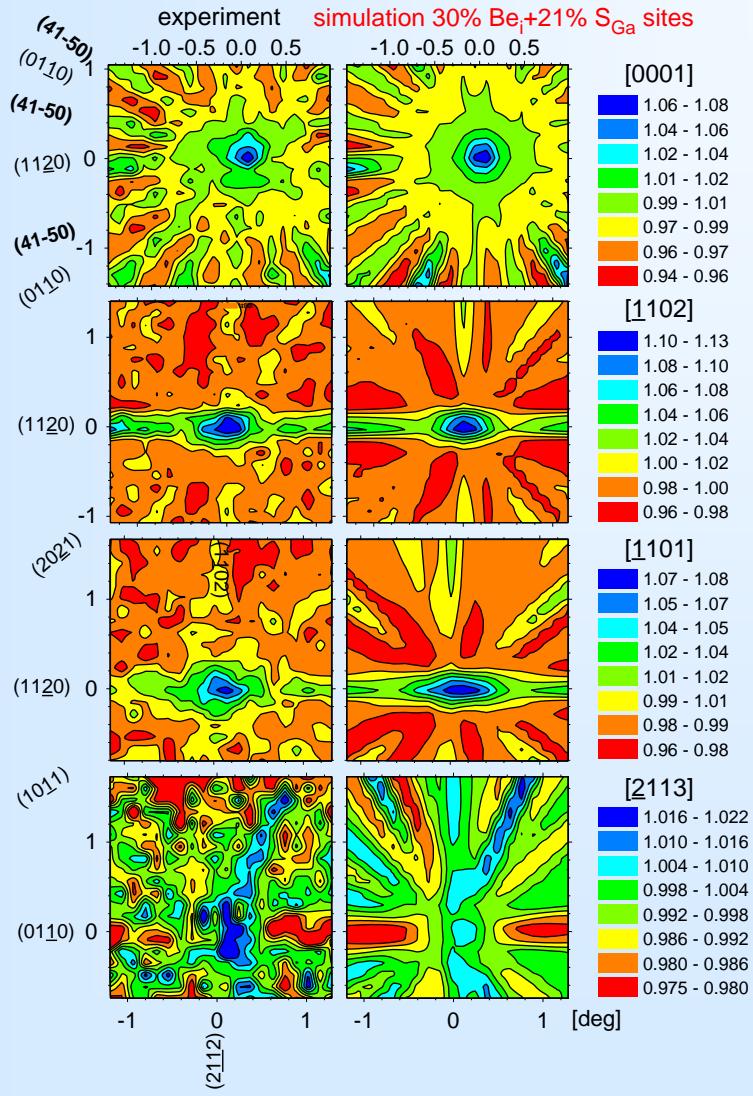


High-symmetric sites in wurtzite structure



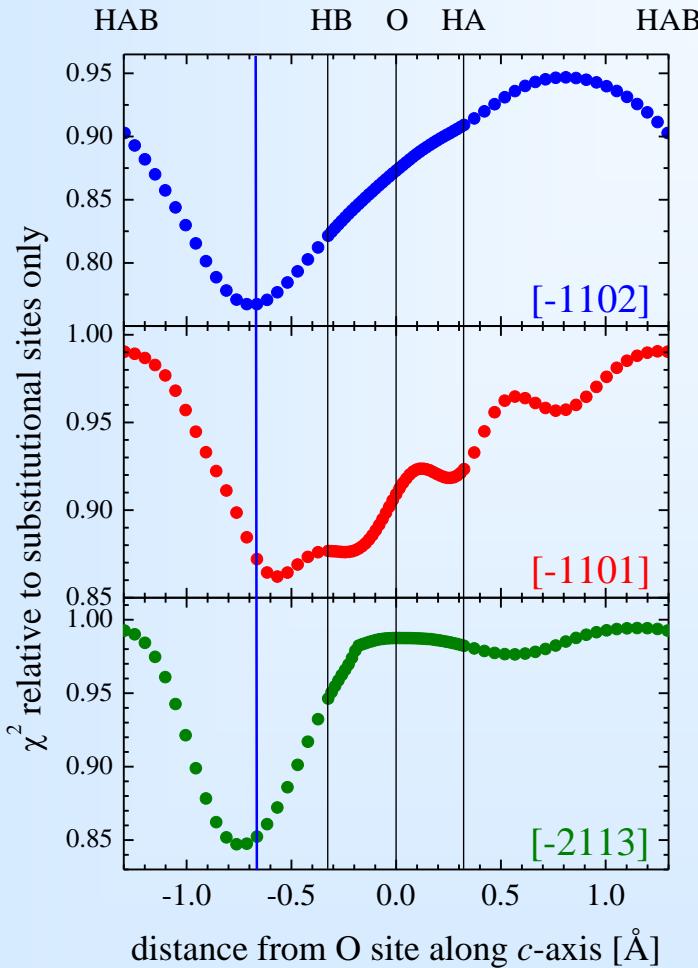
- Location of interstitial Mg_i in between HA and HAB site ($+0.60 \pm 0.14$ Å from ideal O sites, but only 13% Mg_i at RT)

β^- emission channeling patterns from ^{11}Be ($t_{1/2}=13.8$ s) in n-d-GaN

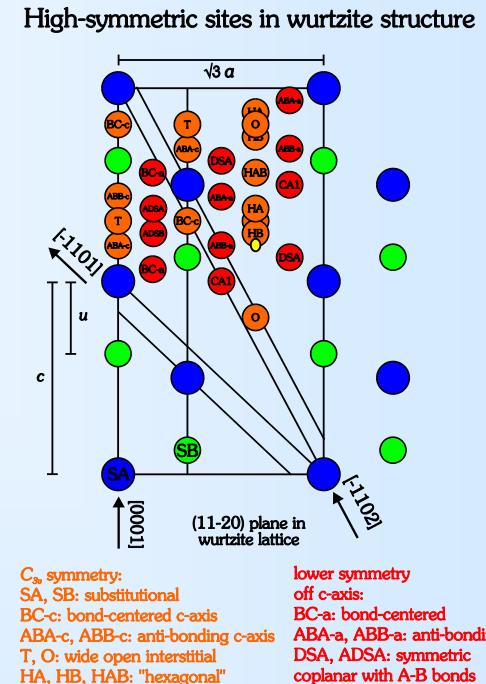
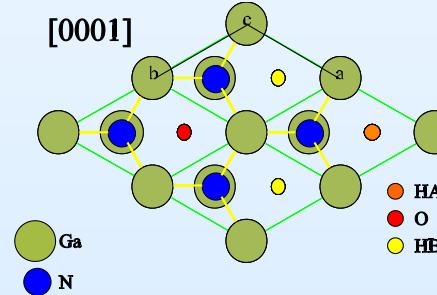


RT, fit results
(not yet corrected for background):
 ~21% ^{11}Be on S_{Ga} sites,
 ~30% near interstitial O sites
 majority of ^{11}Be on interstitial sites!

Lattice location precision of ^{11}Be in n-d-GaN

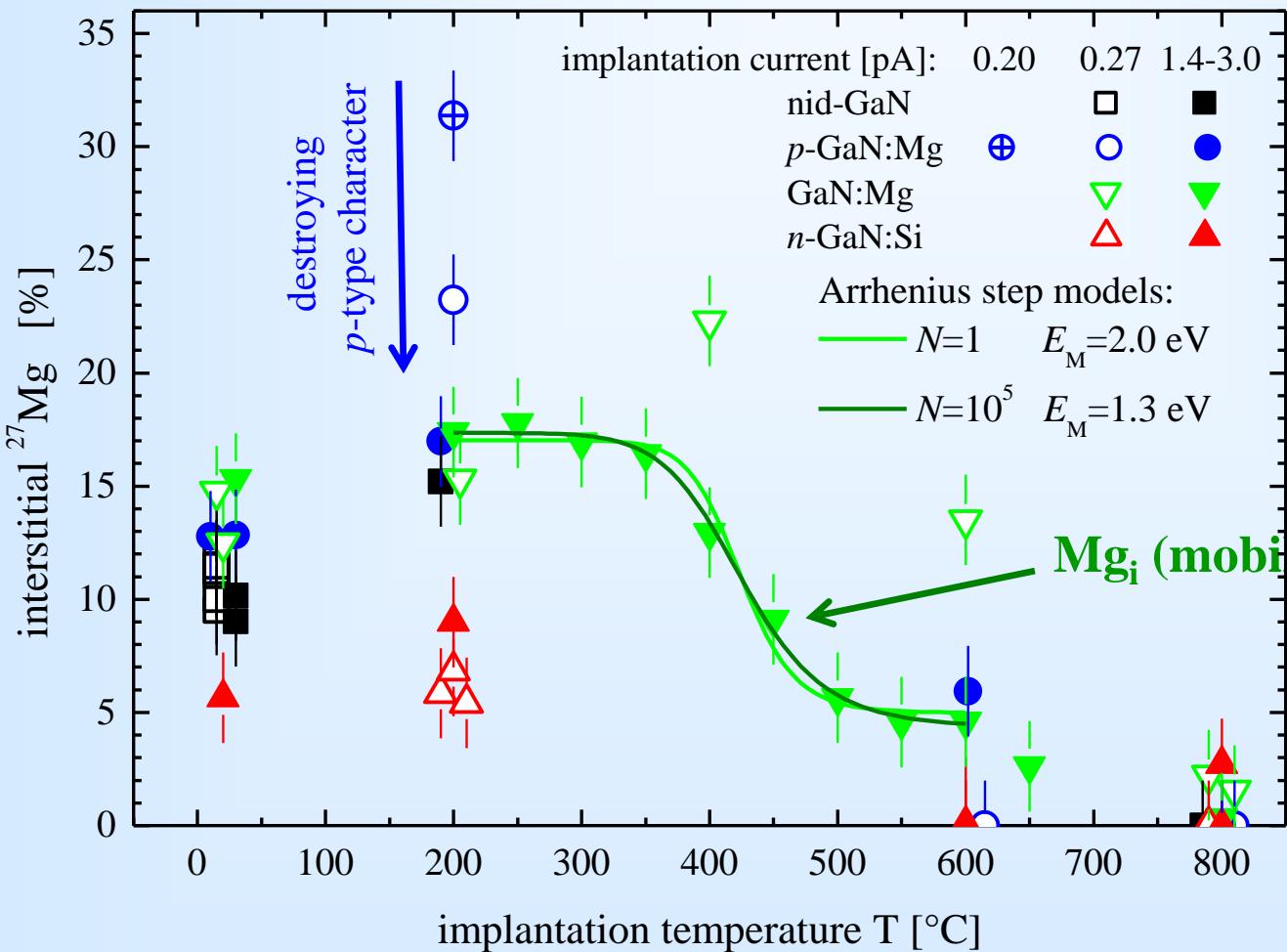


High angular resolution
(small solid angle)
0.15 pA
 $4.7 \times 10^{11} \text{ cm}^{-2}$ per pattern



- Location of interstitial Be_i in between HB and HAB site (-0.66 ± 0.13 \AA from ideal O sites).
- In comparison to Mg, Be sits on the opposite side from O

Interstitial ^{27}Mg in different doping types of GaN



- Interstitial Mg_i enhanced in $p\text{-GaN}$ and suppressed in $n\text{-GaN}$.
- Site change of ^{27}Mg from interstitial to substitutional Ga sites as function of implantation temperature allows to estimate activation energy for migration of Mg_i as $E_{\text{M}} \approx 1.3\text{--}2.0 \text{ eV}$.

Comparison: site changes of interstitial Li, Be, Na, Mg in nitrides

Material	Interstitial ion	Ionic radius (Å)	Temperature $T_{O \rightarrow S}$ (°C)	Migration energy experim. $E_{M,exp}$ (eV) [Ref]	Migration energy theoretical $E_{M,theo}$ (eV) [Ref]
GaN	Li ⁺	0.59	~ 427	~1.7 [Dalmer JAP 1998, Ronning JAP 2000]	1.4 (⊥) 1.55 () [Bernardini PRB 2000]
	Be ²⁺	0.27	? (> 20)	[this work]	1.2 (⊥) 2.9 () [Van de Walle PRB 2001]
	Na ⁺	0.99	~ 900	2.2 – 3.4 [Ronning JAP 2000 PhD thesis L.Amorim 2016]	
	Mg ²⁺	0.57	~ 400	1.3 – 2.0 [this work]	0.15 (⊥) 0.68 () [Harafuji PSSC 03, Harafuji JJAPL 04]
AlN	Li ⁺	0.59	~ 427	~1.7 [Ronning JAP 2000]	
	Na ⁺	0.99	600-900	2.0 – 2.6 [Ronning JAP 2000, PhD thesis L. Amorim 2016]	
	Mg ²⁺	0.57	300-400	1.1 – 1.7 [Amorim APL 2013]	

- Interstitial → substitutional site changes observed for light alkalis and alkaline earths, but not for Ca and Sr [B. De Vries et al, JAP (2006)]
- Interstitial migration energy is correlated with ionic radius of diffusing ion
- Migration energies tend to be lower in AlN

Proposed further experiments:

- **^{27}Mg :**
- Detailed mapping of site change $\text{Mg}_i \rightarrow \text{Mg}_{\text{Ga}}$ in all doping types:
does site change temperature depend on doping type?
 \Rightarrow If yes, $E_M(\text{Mg}_i)$ or $[\text{V}_{\text{Ga}}]$ depend on doping type
- Fluence dependence of $[\text{Mg}_i]$ at various implantation temperatures:
 \Rightarrow Introduction rates of compensating defects by implantation.
- GaN:Mg: can its *p*-type activation be observed around 400-500°C?
- Lattice location of ^{27}Mg in hydrogenated GaN samples
 \Rightarrow New insights in electrical activation mechanisms of Mg
- **^{11}Be :**
- So far only results in **nid-GaN** at RT.
Site changes $\text{Be}_i \rightarrow \text{Be}_{\text{Ga}/\text{Al}}$ of ^{11}Be in **nid-GaN**, ***p*-GaN:Mg** and **AlN** as function of implantation temperature
 \Rightarrow Experimental insights why Be is not an active dopant + $E_M(\text{Be}_i)$

Beam request

isotope	yield [atoms/ μ C]	target – ion source	shifts [8h]
^{27}Mg	1×10^7	Ti-W - RILIS Mg	16
^{11}Be	6×10^6	UC _x -W or Ta-W - RILIS Be	8
		Total	24

- We welcome sharing beam times with other users.
- However, for ^{27}Mg runs use of Ti-W targets is a must, since e.g. SiC or UC_x targets suffer from ^{27}Al and ^{27}Na contamination.

EC-SLI Publications + theses:

- **Detailed list available on INDICO**
- **2012-2016: 19 papers published**
- **2017: 1 paper accepted, 3 submitted**
- **2012-2016: 3 PhD theses + 2 Masters theses completed**
- **2017: 4 PhD theses ongoing**