Emission Channeling Lattice Location Experiments with Short-Lived Isotopes

Status report and 2nd addendum

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ISOLDE

Major physics cases of the previous (2010) addendum to IS453

- **lattice location of transition metals in semiconductors (contaminants in Si, dilute magnetic semiconductors, oxides)**

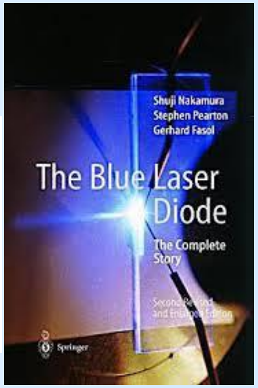
  ... is the only subject of our new experiment IS580 approved by INTC in Oct. 2013.

- **lattice location of ^{27}Mg in nitride semiconductors**

  INTC decided not to incorporate this topic in IS580.
  Since IS453 still has 4.5 shifts of ^{27}Mg left and no new experiments can be applied for before June 2014, we opt for asking for a 2nd addendum to IS453.

  Lattice location of ^{27}Mg and ^{11}Be in nitrides is hence the only physics case of this addendum.

Physics case: Lattice location of Mg and Be 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
- Mg and Be candidates for acceptors in AlN

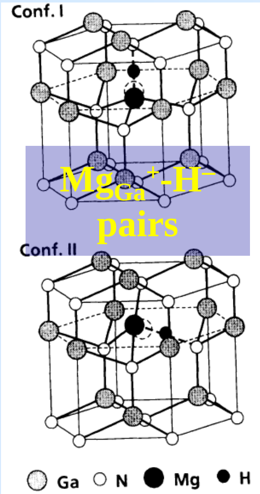
- Mg+Be acceptors (group II) should occupy substitutional Al, Ga (group III) sites

- Are there any other lattice sites for Mg and Be?

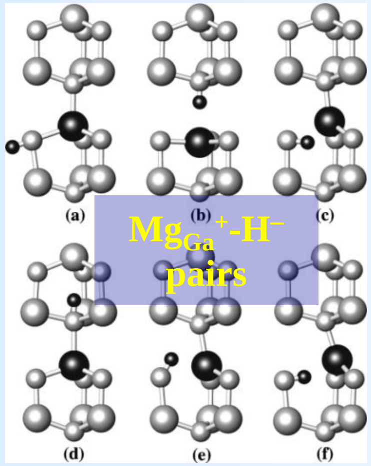
$\Rightarrow$ Lattice location of (implanted) Mg will help to answer this question

No other experimental technique than emission channeling can characterize structural properties of Mg and Be in nitrides!

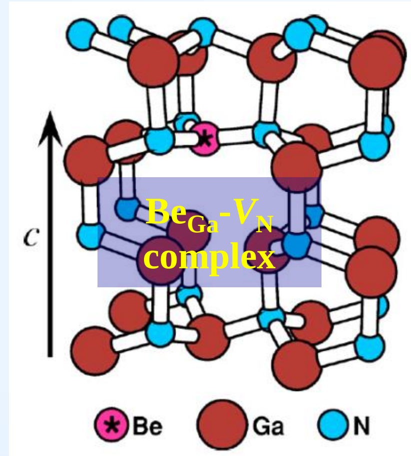
Mg+Be in GaN: 20 years of rich theory playground with little experimental data…



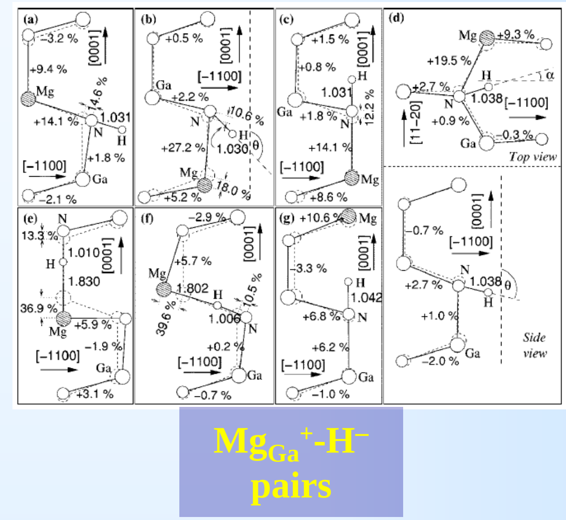
Brandt *et al*, *PRB* (1994)



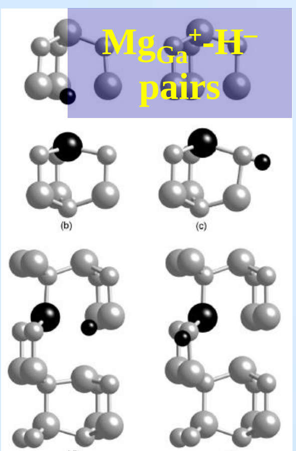
Wright *et al*, *JAP* (2003)



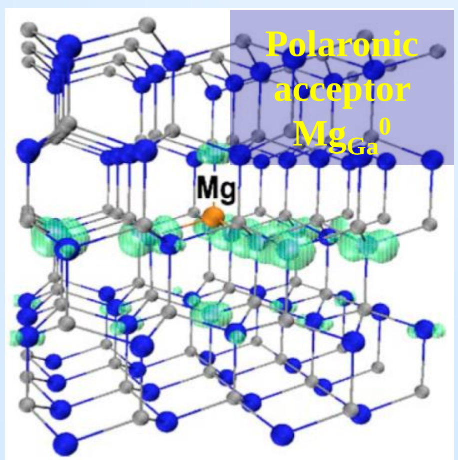
Latham *et al*, *PRB* (2003)



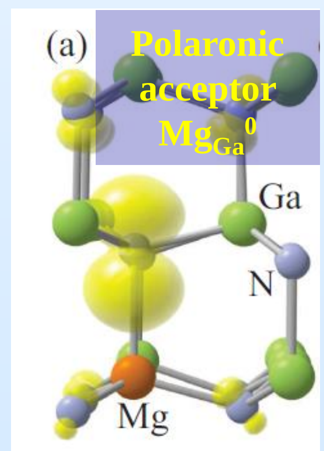
Limpijungjong *et al*, *PRB (2003)*



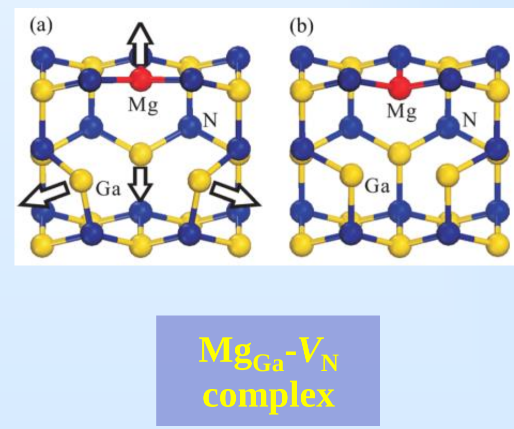
Myers *et al*, *JAP* (2006)



Lany *et al*, *APL* (2010)



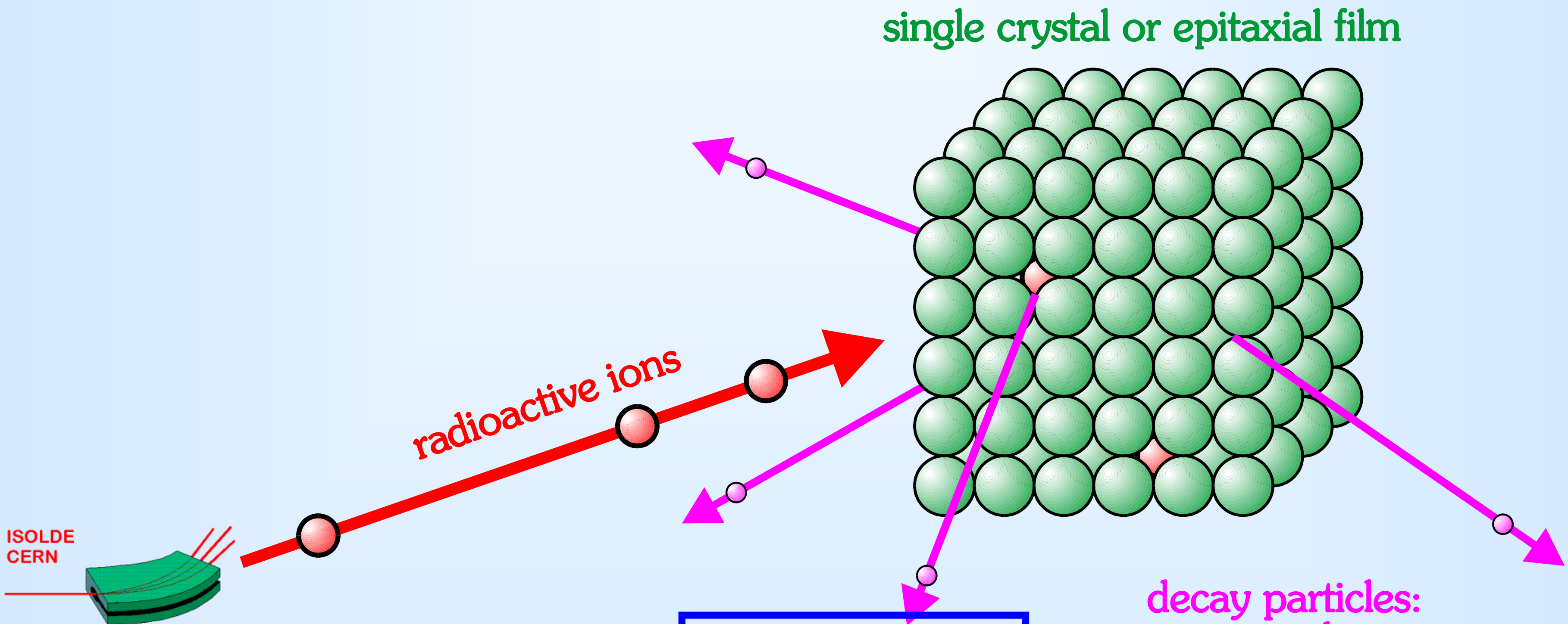
Lyons *et al*, *PRL* (2012), JAP (2014)



Yan *et al*, *APL* (*2012*)

Some of the predicted structures involve significant relaxation of Mg/Be

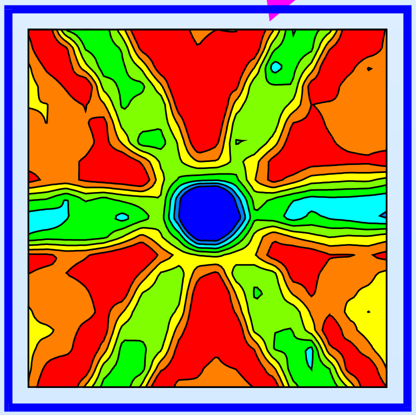
Emission channeling: basic principle



decay particles:
conversion electrons,
β^-, β^+, α

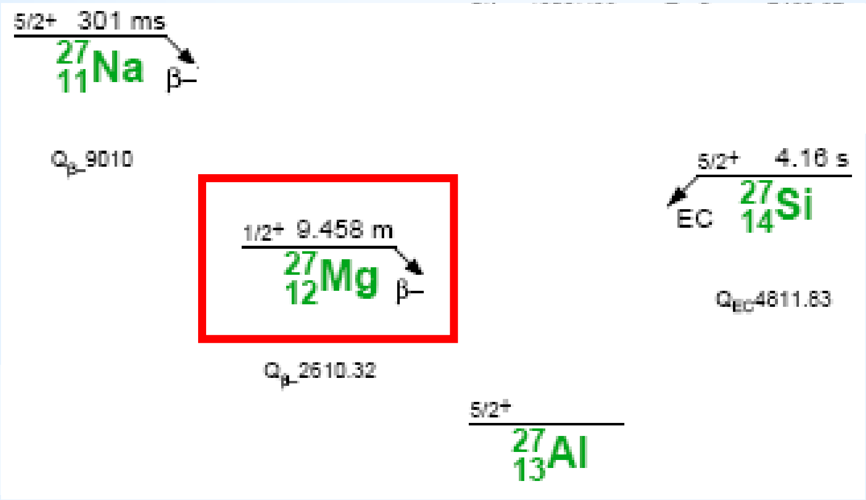
3×3 cm^2 Si pad detector
22×22 pixels of 1.3×1.3 mm^2
currently: max. ~5 kHz

2-dimensional
position- and energy-
sensitive detector



2D emission patterns
characterize
specific lattice sites
of the emitting atoms

Problems with mass 27 beams: ^{27}Al + ^{27}Na contaminations

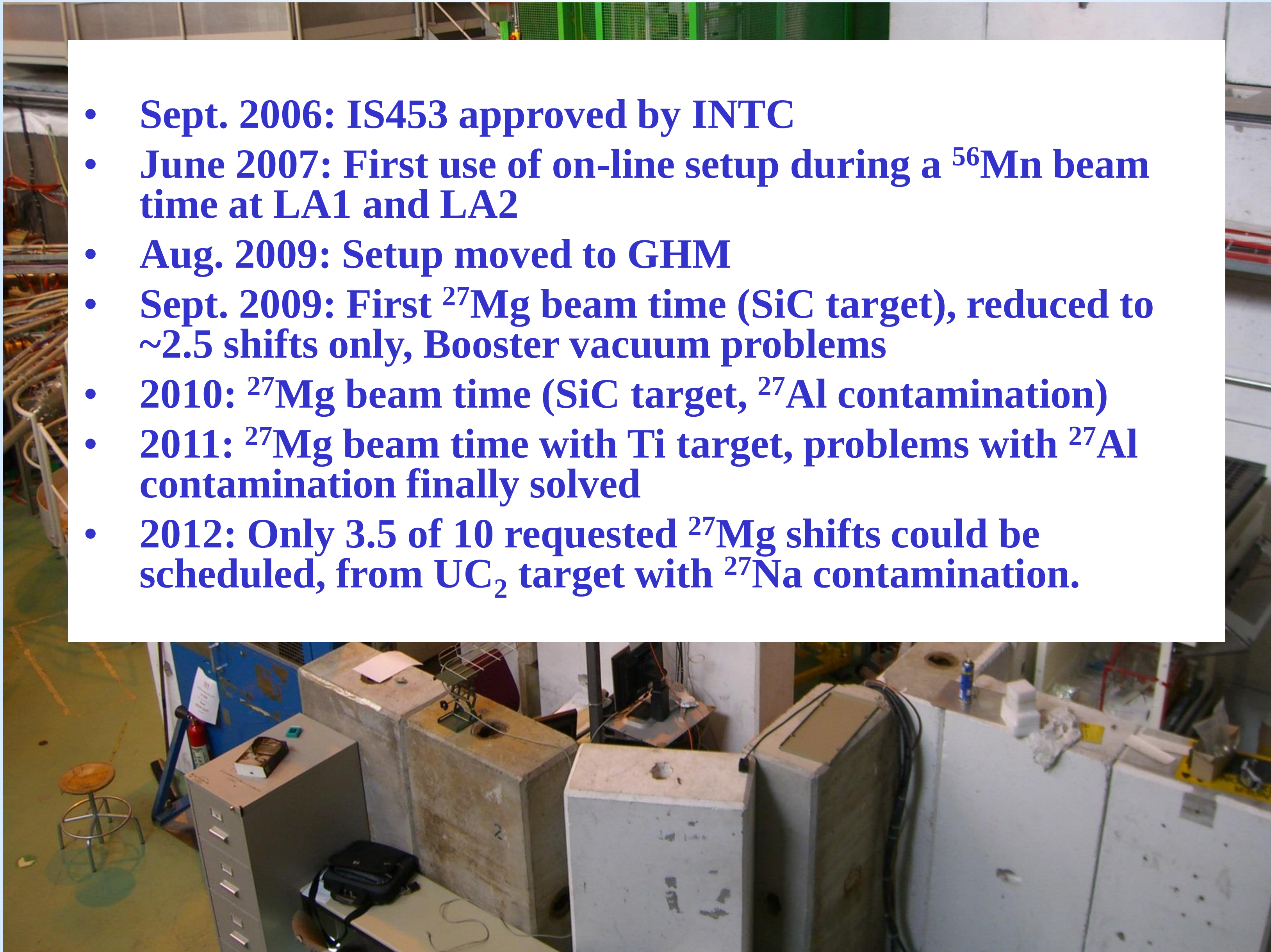


- Considerable contaminations of ^{27}Al (SiC) or ^{27}Na (UC_2) make experiments from SiC or UC_2 targets impossible or very inefficient.

- Following the approval of our ^{27}Mg experiments in 2006, it took 5 years for ISOLDE target development to solve these problems:
- Only the use of a Ti target avoids the contaminations.

- However, only 1 run with a Ti target could be scheduled so far in 2011.
- The Ti target still exists and can be re-used.

Use of EC-SLI on-line @ GHM for ^{27}Mg



- Sept. 2006: IS453 approved by INTC
- June 2007: First use of on-line setup during a ^{56}Mn beam time at LA1 and LA2
- Aug. 2009: Setup moved to GHM
- Sept. 2009: First ^{27}Mg beam time (SiC target), reduced to ~2.5 shifts only, Booster vacuum problems
- 2010: ^{27}Mg beam time (SiC target, ^{27}Al contamination)
- 2011: ^{27}Mg beam time with Ti target, problems with ^{27}Al contamination finally solved
- 2012: Only 3.5 of 10 requested ^{27}Mg shifts could be scheduled, from UC_2 target with ^{27}Na contamination.

First results on ^{27}Mg in AlN are published:

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Precise lattice location of substitutional and interstitial Mg in AlN

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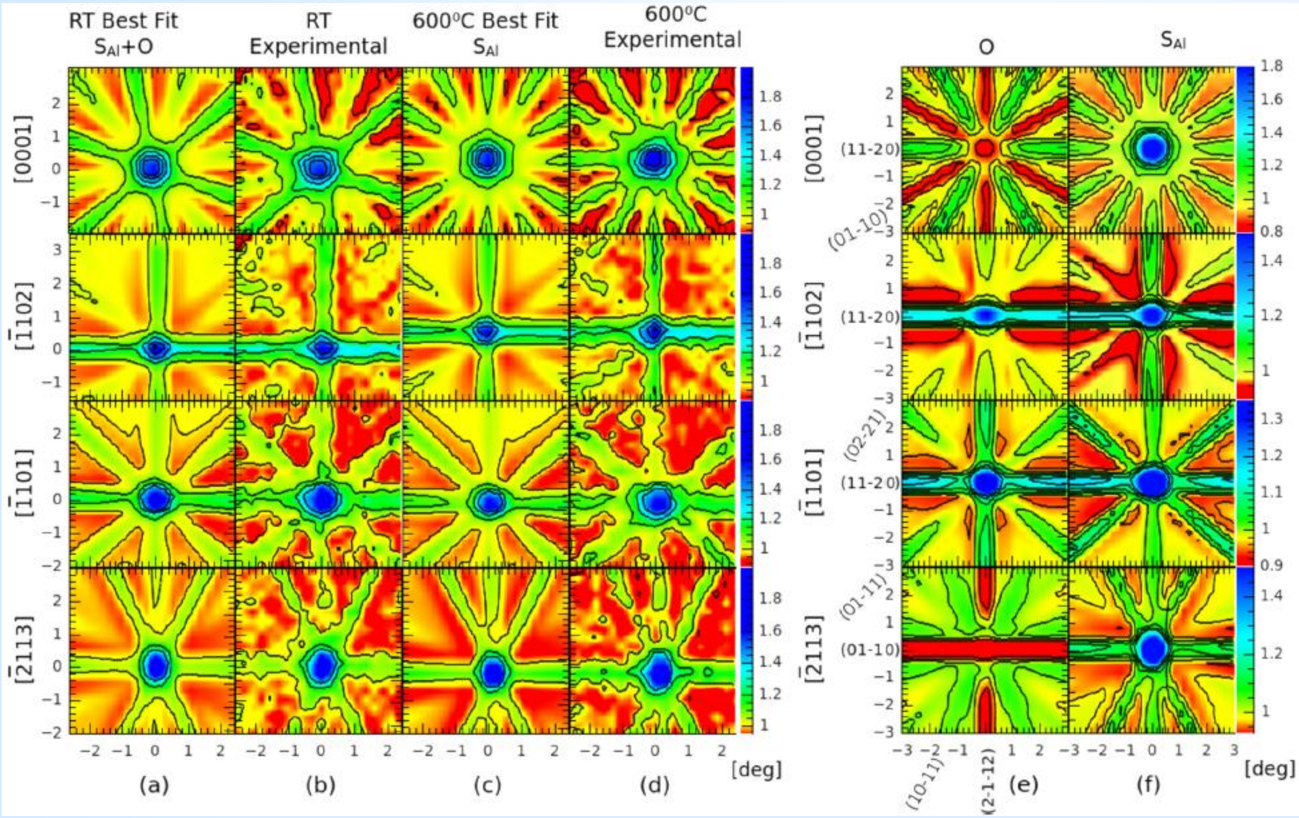
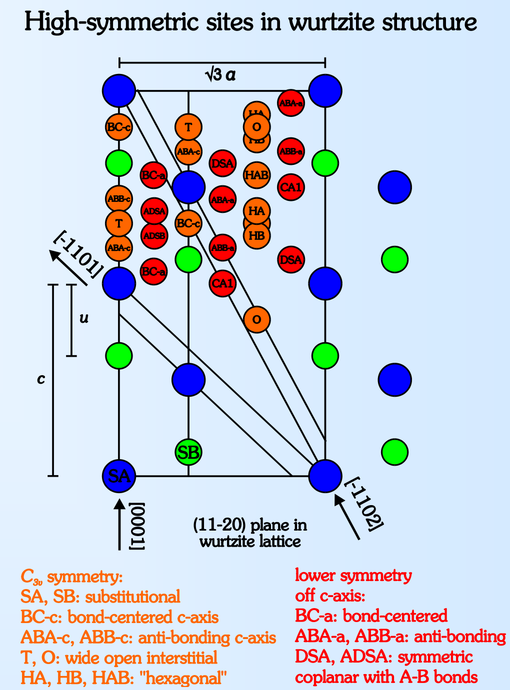
L. Amorim *et al*, *APL 103 (*2013) 262102

β⁻ emission channeling patterns from ^{27}Mg in AlN





fit results:

RT: ~70% ^{27}Mg on substitutional Al sites, ~30% on interstitial O sites

600°C: ~100% ^{27}Mg on substitutional Al sites

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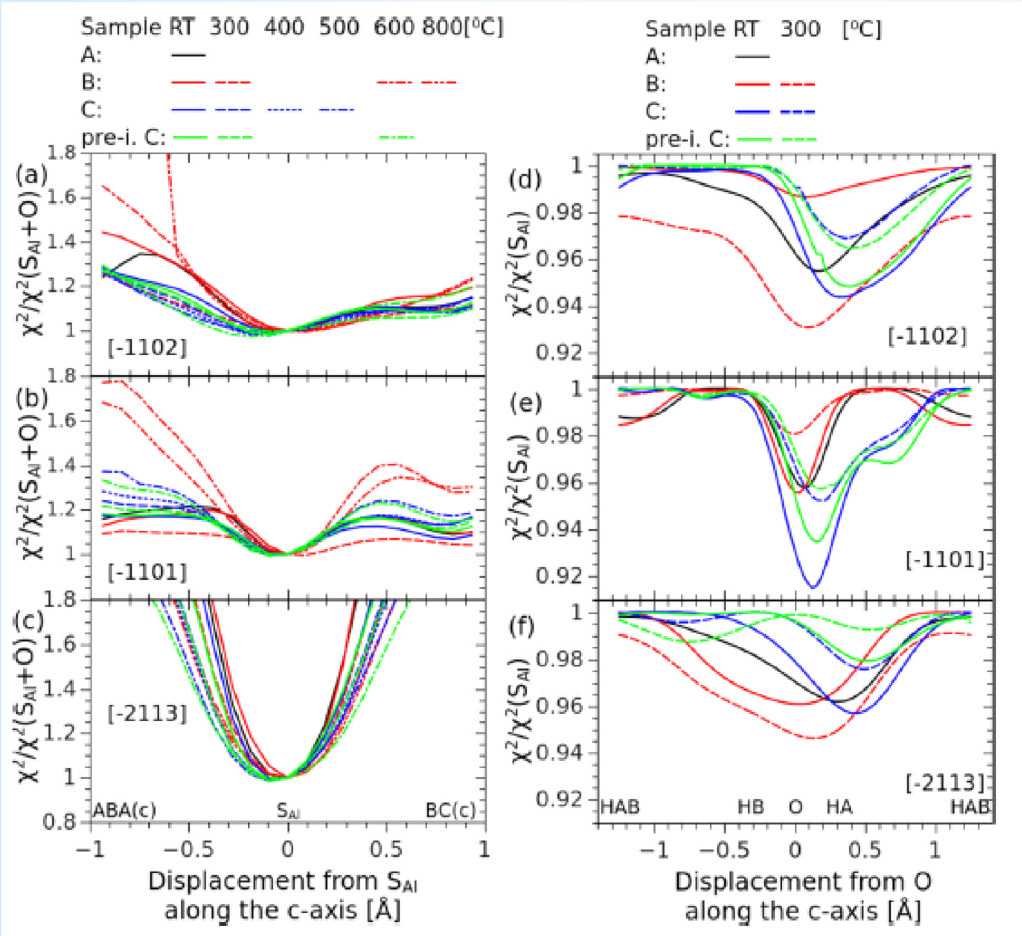
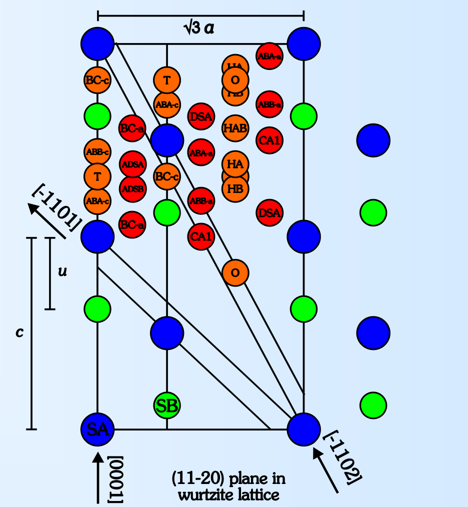
Lattice location precision of ^{27}Mg in AlN



High-symmetric sites in wurtzite structure



C_{3v} symmetry:
SA, SB: substitutional
BC-c: bond-centered c-axis
ABA-c, ABB-c: anti-bonding c-axis
T, O: wide open interstitial
HA, HB, HAB: "hexagonal"

lower symmetry off c-axis:
BC-a: bond-centered
ABA-a, ABB-a: anti-bonding
DSA, ADSA: symmetric coplanar with A-B bonds

χ^2 of fit: Majority of ^{27}Mg located less than 0.1 Å from S_{Al}

Location of interstitial Mg between O and HA site (determined with ~0.3 Å precision)

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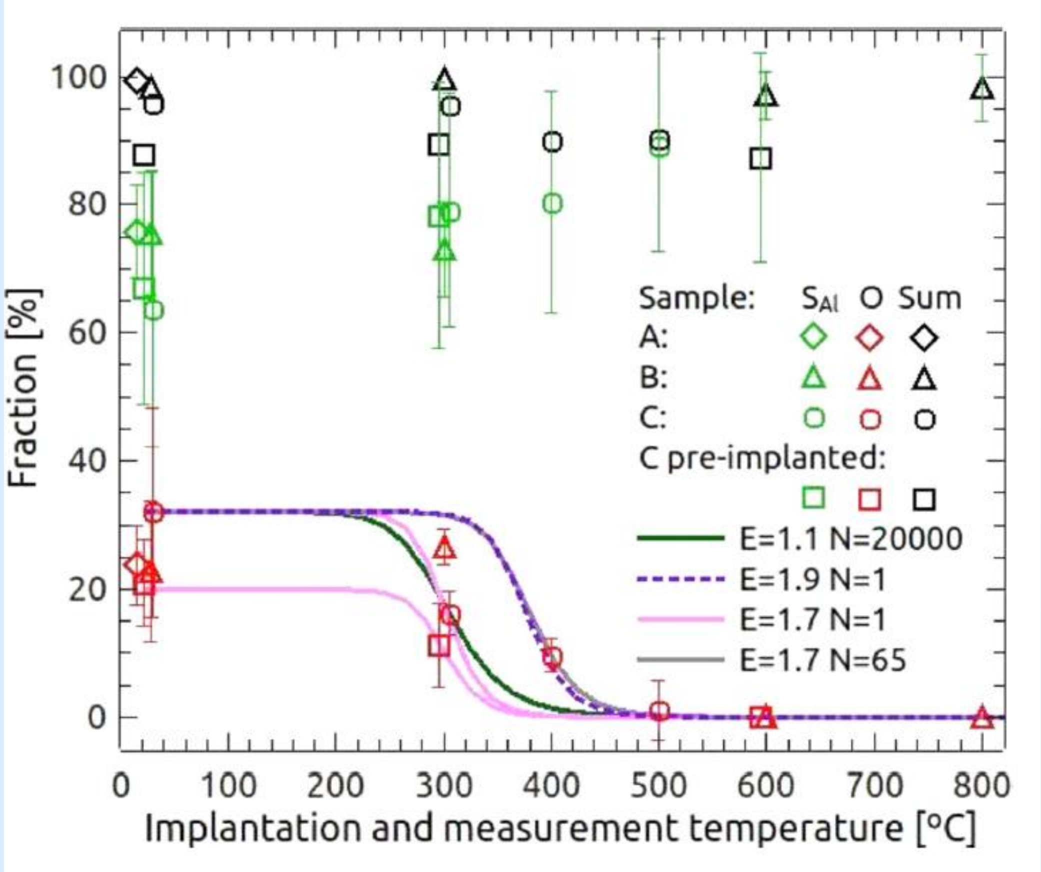
Thermally activated site change of ^{27}Mg in AlN



Site change of ^{27}Mg from interstitial O to substitutional Al sites as function of implantation temperature allows to estimate activation energy for migration of Mg_i as 1.1–1.7 eV

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Beam request

isotope	shifts	target	ion source	yield [at/s/μA]
^{27}Mg (9.5 min)	12	Ti-W	RILIS Mg	1×10^{7}
^{11}Be (838 ms)	3	UC_2-W or Ta-W	RILIS Be	6×10^{6}

Total requested shifts: 15 **(4.5 still existing, 10.5 new)**

Foreseen experimental program

- **Study of lattice sites of ^{27}Mg in GaN and AlN from RT to 50 K**
- **Lattice sites of ^{27}Mg in *p*-GaN (doped with stable Mg during growth)**
- **Lattice sites of ^{27}Mg in hydrogenated GaN**
- **Compared to previous ^{27}Mg data, the angular resolution will be doubled by moving the detector further away from the sample.**
- **Lattice location of ^{11}Be in GaN and AlN from RT to 800°C**