

Point defects in nitride-based semiconductors studied by positron annihilation spectroscopy

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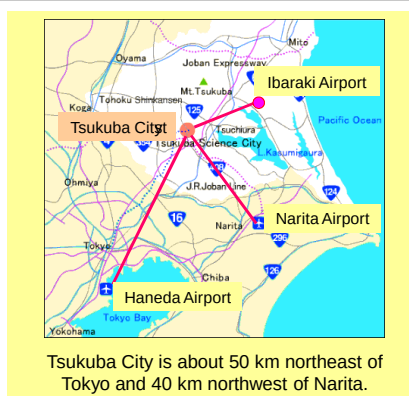
Akira Uedono

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- University of Tsukuba
- Basics of positron annihilation
 - Detection of vacancies in ion-implanted GaN
- Introduction mechanism of vacancies in InGaN and AlGaN alloys
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- Summary



Tsukuba City





Facilities

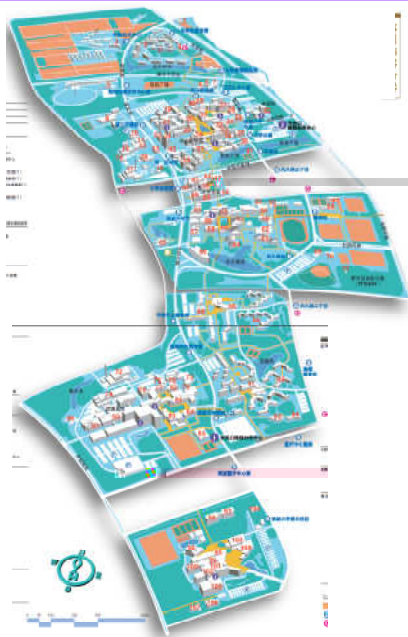
- National research facilities: 32 (1/3 in Japan)
- Private research facilities: 120
- National University: 1 (University of Tsukuba)

Researchers

- 20,000 researchers (10% of city population)
- 8,000 doctoral researchers
- 5,000 overseas researchers



University of Tsukuba (Map)



大学状況

筑波大学的前身 是东京教育大学，1973年10月以更名为契机，在秉承传统与特色的同时，作为一所独具特色的综合性大学而发展起来。主校区位于东京的东北方向60公里处，占地25.8平方公里，校园内绿树成荫，风景秀丽。现在，筑波大学为成为筑波研究学园城市中担负起核心作用的教育研究基地而努力着。

诺贝尔奖



朝永振一郎 (TOMONAGA Shin-iti)
 (东京教育大学) 名誉教授，东京教育大学前校长
 1985 年因在量子电动力学方面取得对粒子物理学产生深远影响的研究成果获得诺贝尔物理学奖。
 [共同获奖者]
 Dr. J. Schwinger (Harvard University, USA) and
 Dr. R.P. Feynman (California Institute of Technology, USA)



江崎玲於奈 (ESAKI Leo)
 名誉教授，筑波大学前校长
 1973 年因发现半导体超导体中的隧道现象获得诺贝尔物理学奖。
 [共同获奖者]
 Dr. I. G. General (General Electric Company, USA) and
 Dr. B. D. Josephson (University of Cambridge, United Kingdom)



白川英树 (SHIRAKAWA Hideo)
 名誉教授
 2000 年因发现导电聚合物 (导电塑料) 获得诺贝尔化学奖。
 [共同获奖者]
 Dr. Alan J. Heeger (University of California, Santa Barbara, USA) and
 Dr. Alan G. MacDiarmid (University of Pennsylvania, USA)
 白川教授已于 1996 年退休。
 白川教授 2009 年 11 月还荣获了日本政府颁发的文化勋章。



国际交流

筑波大学在各领域开展广泛的国际交流，以提高学术研究，培养具有国际视野的人材。这些国际交流包括接纳外国研究员以及与海外大学交流，从而开展交换留学。另外，筑波大学还积极地接纳外国留学生。

中国科学院研究生院

浙江大学

南开大学

西安交通大学

吉林大学

北京航空航天大学

厦门大学

中山大学

中国科学技术大学

东北师范大学

华南师范大学

湖南大学

上海交通大学

中国海洋大学

北京大学信息管理系

北京师范大学

上海图书馆

北京大学环境科学与工程学院

复旦大学

中国农业大学

西北农林科技大学

清华大学建筑学院

清华大学核能与新能源技术研究院

清华大学环境科学与工程系

西南交通大学

中国原子能科学研究院

沈阳农业大学

吉林农业大学

中国科学院地理科学与资源研究所

中国地质大学(北京)

郑州大学

河南科技大学

大连大学

云南大学

南京大学环境学院

中国美术学院

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中国科学院

国立中山大学

国立清华大学

国立台湾大学

国立台湾艺术大学

国立政治大学

国立台湾科技大学

国立台北大学

国立交通大学

国立台湾师范大学



Student exchange in Tsukuba and Wuhan University



Positron annihilation



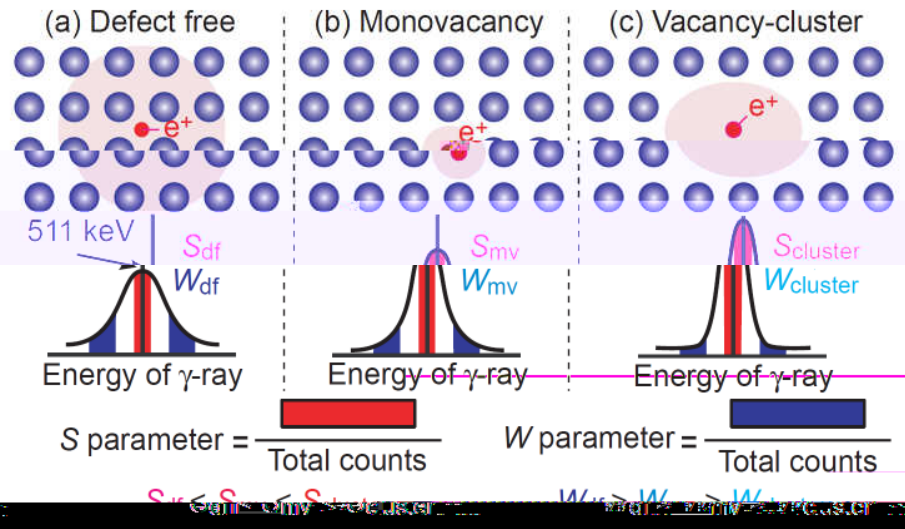
A positron annihilates with an electron and emits two γ -rays.

From measurements of the energy distribution of γ -rays and the positron lifetime, we can detect vacancy-type defects.

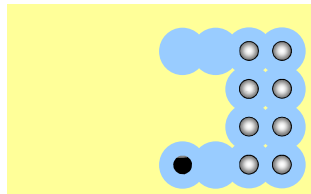
✓ Detectable defect: monovacancy - open pore ($<100 \text{ nm}^3$)

Trapping of positrons by vacancy-type defects

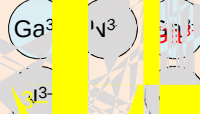
A freely diffusing e^+ may be localized in an open space because of the Coulomb repulsion from ion cores.



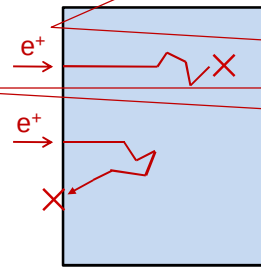
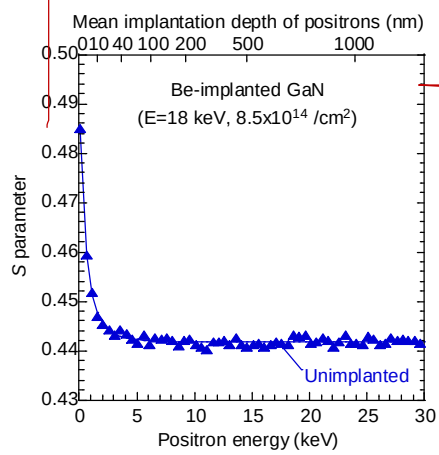
Trapping of positrons by vacancy-type defects



Detection of ... PAS



S-E curve for unimplanted GaN (MOVPE)



$$S_{\text{surface}} > S_{\text{bulk}}$$

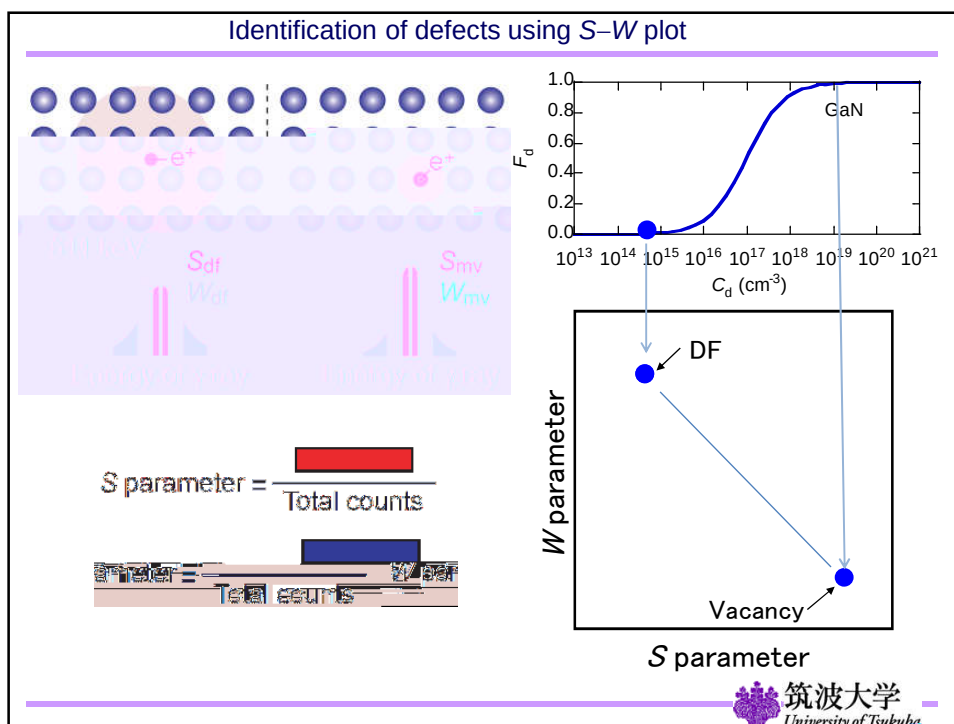
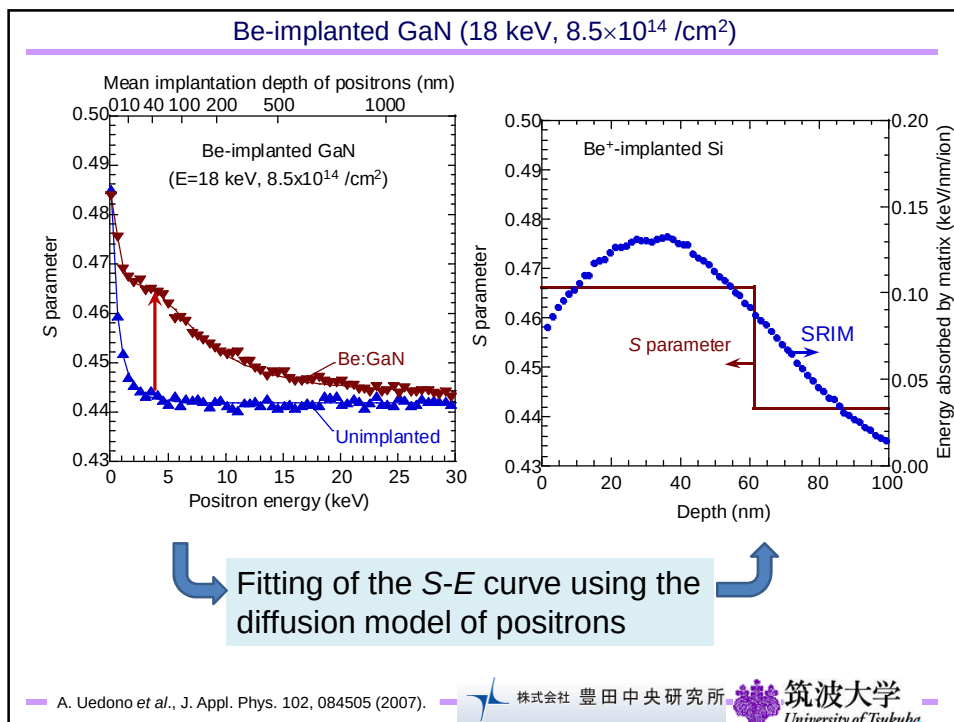
A. Uedono *et al.*, J. Appl. Phys. 102, 084505 (2007).



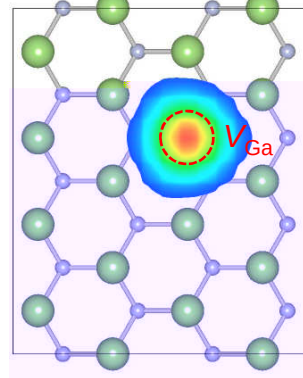
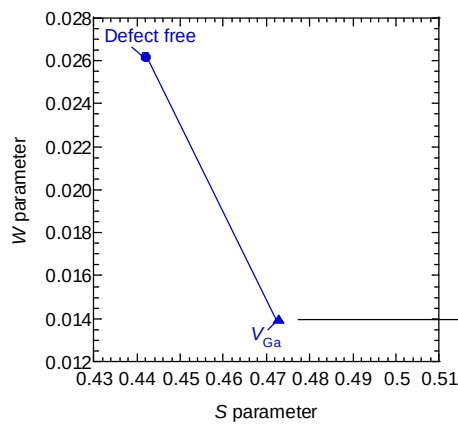
株式会社 豊田中央研究所



筑波大学
University of Tsukuba



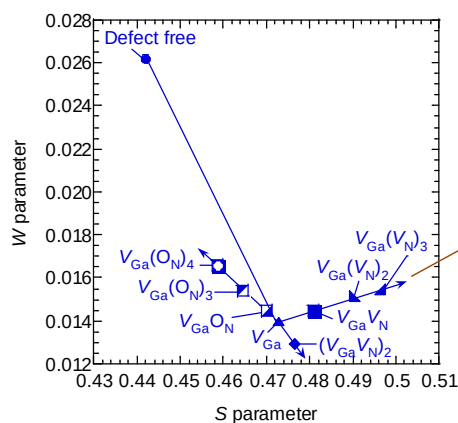
S-W plot for defects in GaN (Projector Augmented-Wave method)



Localized positrons in V_{Ga}

The blue symbols were obtained by the first principle calculations.

S-W values for vacancy clusters in GaN



V_{Ga} with multiple V_N s

Increase in the number of V_N coupled with V_{Ga} causes right-hand side shift.

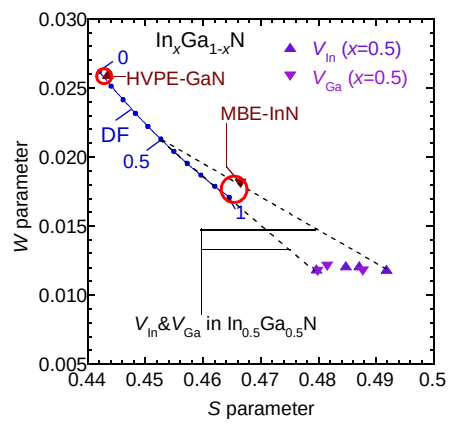
The blue symbols were obtained by the first principle calculations.

S-W plot for Be-implanted GaN

FWHM of XRD & PL, and, S for $\text{In}_x\text{Ga}_{1-x}\text{N}$



S–W plot for GaN and InN (experiments)



Conclusion

- (i) The bond-length/angle distortions
- (ii) the decrease in E_F of V_N (due to strong In-In interaction) introduce vacancy clusters at mid In content.

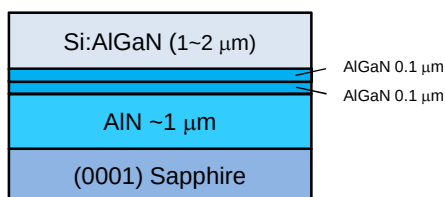


For fabrication of high-quality InGa_N, it seems that we cannot escape from the **intrinsic** defect introduction mechanism.

If In is the matter, how about AlGa_N?

Experiments (Hiramatsu Miyake / Mie university)

Sample structure



Growth condition

Substrate temp. (°C)	1100-1200
TMG flow rate (sccm)	15~25
TMA flow rate (sccm)	15
NH ₃ flow rate (slm)	1.4
CH ₃ SiH ₃ (sccm)	1~5
V/III ratio	970~1480

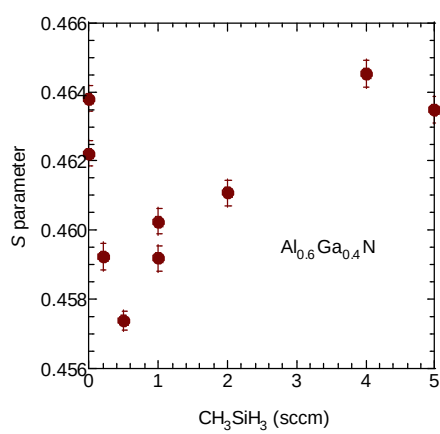
Characterization

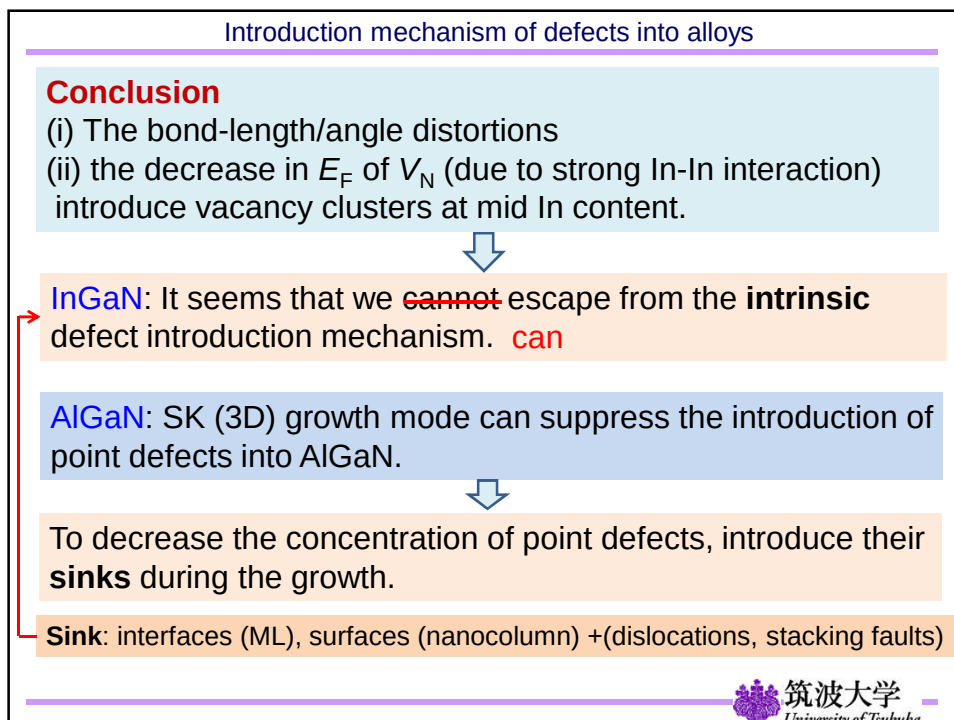
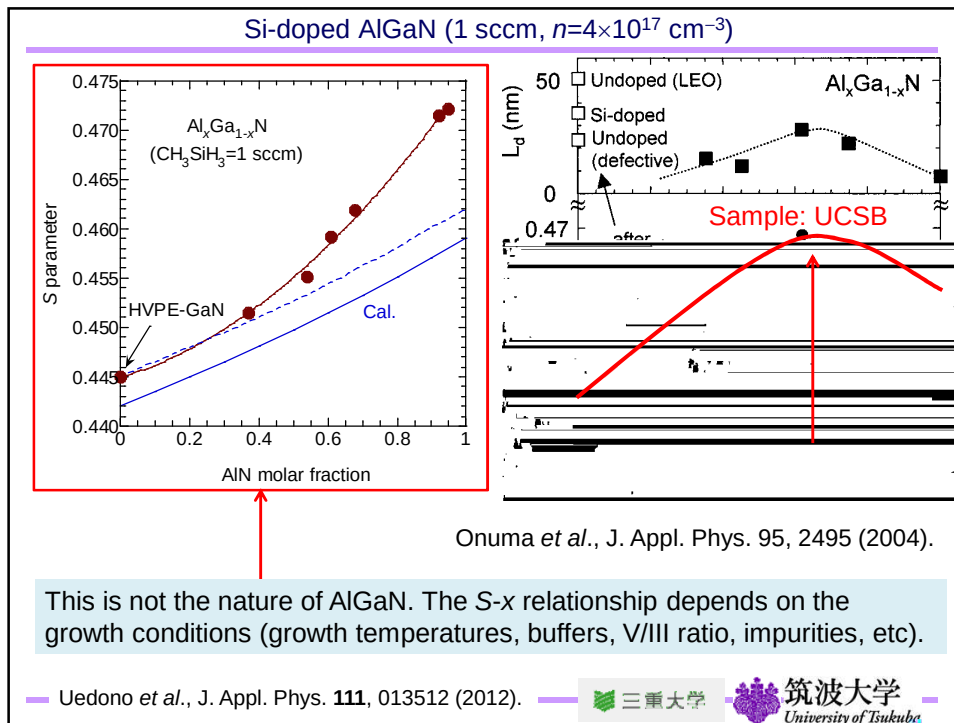
- Stress measurements, XRD, STM, PL, CL, SIMS, Hall measurements
- Monoenergetic positron beam line & PPMA
- First-principles calculation

Sample fabrication: Shimahara *et al.*, JJAP **50**, 095502 (2011).

Optical properties: Chichibu *et al.* PR6-2 (next talk!!)

Impact of CH_3SiH_3 (methylsilane) flow rate on defects in $\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$



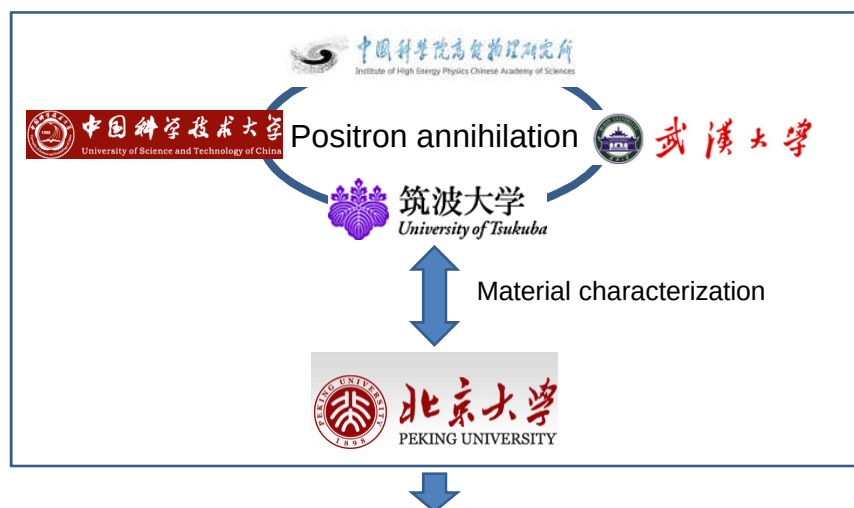


Summary

Positron annihilation spectroscopy (PAS) can be used to study vacancies in nitride-based semiconductors.

- **I/I-GaN**: the defect species was $V_{\text{Ga}}V_{\text{N}}$, where their depth distributions were well predicted by the SRIM code.
- **InGaN**: the vacancy concentration reached the maximum at mid In content. The major defect species was identified as cation vacancies coupled with multiple nitrogen vacancies.
- **AlGaN**: the vacancy clusters started to be introduced above mid Al content. This could be attributed to the growth mode transition to FM(2D) from SK(3D), suggesting that SK(3D) growth mode suppress the introduction of point defects.

Summary



For better understanding of condensed matter
and material science