$In_xGa_{1-x}N$および$Mg_xZn_{1-x}O$薄膜の偏光XAFS

Polarized XAFS Study for $In_xGa_{1-x}N$ and $Mg_xZn_{1-x}O$ films

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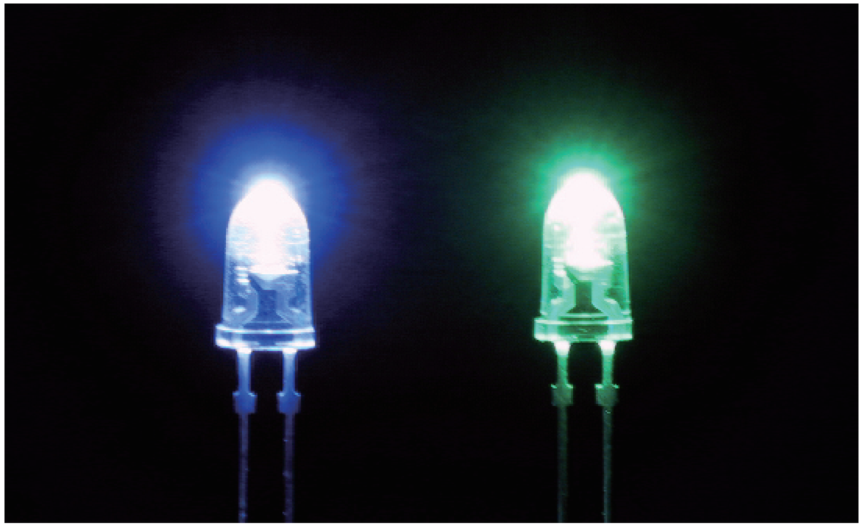

$In_xGa_{1-x}N$ LED

collaborators

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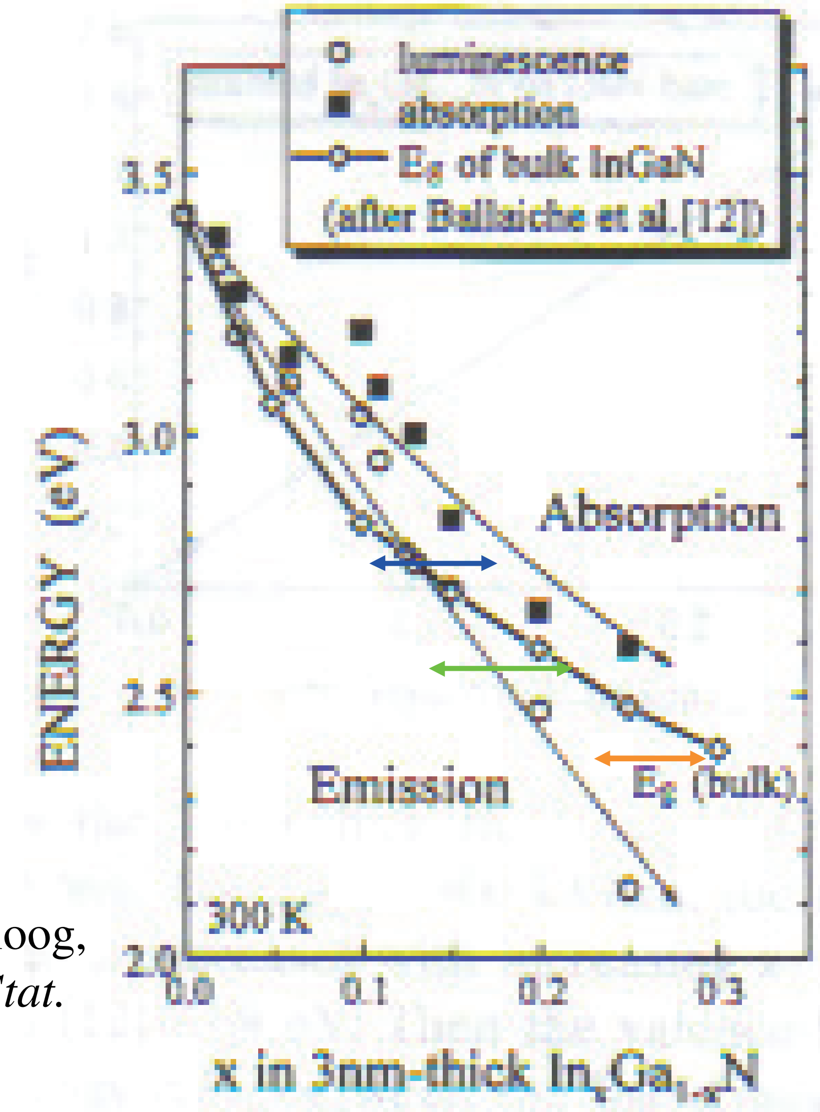
- Tsutomu Yamada (Hirosaki University)
- Shintaro Mikami (Hirosaki University)
- Shigefusa F. Chichibu (Tohoku University)
- Tomoya Uruga (SPring-8)
- Hajime Tanida (SPring-8)
- Kiyofumi Nitta (KEK-PF)
- Yoshinori Kitajima (KEK-PF)

Introduction

- $In_xGa_{1-x}N$ is a key material in high-brightness blue and green LEDs and LD.

Band gap and In concentration x for $In_xGa_{1-x}N$



Chichibu, S.F., Sota, T., Wada, K., Brandt, O., Ploog, K.H., DenBaars, S.P., and Nakamura, S., *Phys. Stat. Sol.(a),* 183, 91 (2001).

- Single Quantum Well (SQW) structure is useful and *c*-plane sample has high quality.

- Although such devices have very high densities of threading dislocations, they show high quantum efficiency in contrast to conventional III-V and II-VI semiconductor based devices.

- The fluctuation of In atom concentration in InGaN active layers has been proposed as its origin.

- → How distributed In atoms are in the InGaN?

On the other hand,

- In the wurtzite (Al, In, Ga)N, the polarization fields along to the *c*-axis causes the quantum confined Stark effects, which reduce the oscillator strength of electron-hole pairs in *c*-plane QWs.
- → *m*-plane $In_xGa_{1-x}N$ is valuable to the next stage

Furthermore,

- $Mg_xZn_{1-x}O$ also has the potential as a useful semiconducting material, because the band gap can be controlled by Mg composition. This is expected to be a new LED and/or LD material in place of InGaN.

- → Mg atom distribution in the $Mg_xZn_{1-x}O$ is also interesting.

Goal

- To reveal the atomic distribution of In atoms are in the Quantum wells. (SQW)
- The relation between the In atom distribution and performance as LED. (SQW)
- The difference in the local structure around In atoms between SQW- and *m*-plane $In_xGa_{1-x}N$.

- To start the XAFS study for Mg *K*-edge in $Mg_xZn_{1-x}O$ analogously to $In_xGa_{1-x}N$.

Outline of this talk

1. $In_xGa_{1-x}N$

(1) Single Quantum Well

T.Miyanaga, T.Azuhata, S.Matsuda, Y.Ishikawa, S.Sasaki, T.Uruga, H.Tanida, S.F.Chichibu, T.Sota, *Phys. Rev. B*, **76**, 035314-1 (2007).

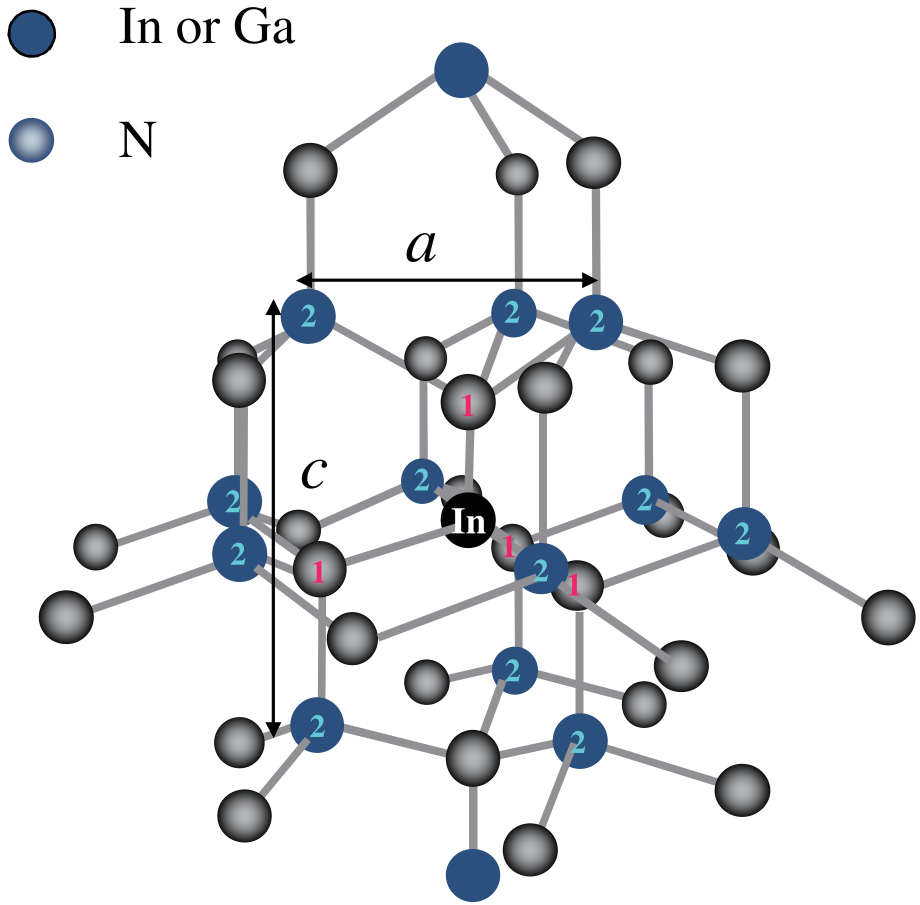
(2) *m*-plane $In_xGa_{1-x}N$

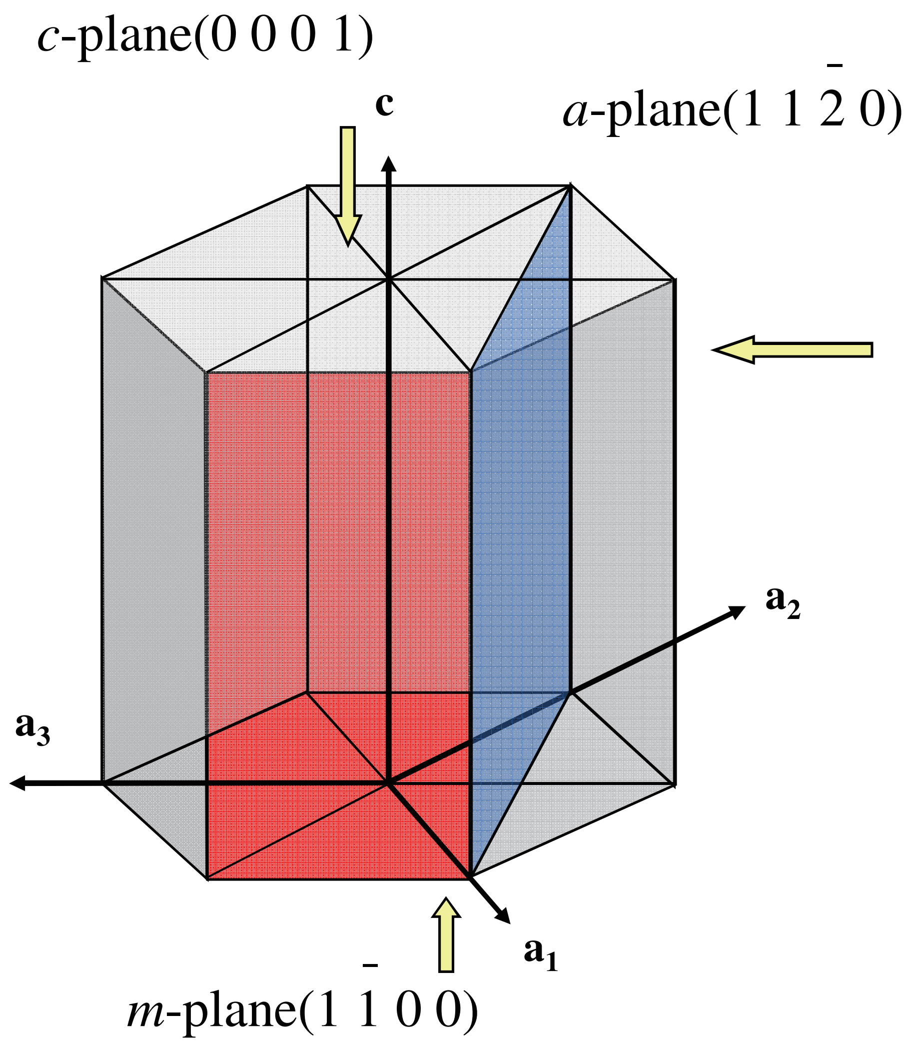
unpublished

2. $Mg_xZn_{1-x}O$ film

T.Yamada, T.Miyanaga, T.Azuhata, T.Koyama, S.F.Chichibu, Y.Kitajima, e-J. Surf. Sci. Nanotech., **7**, (2009) in press.

Wurtzite Structure of InGaN

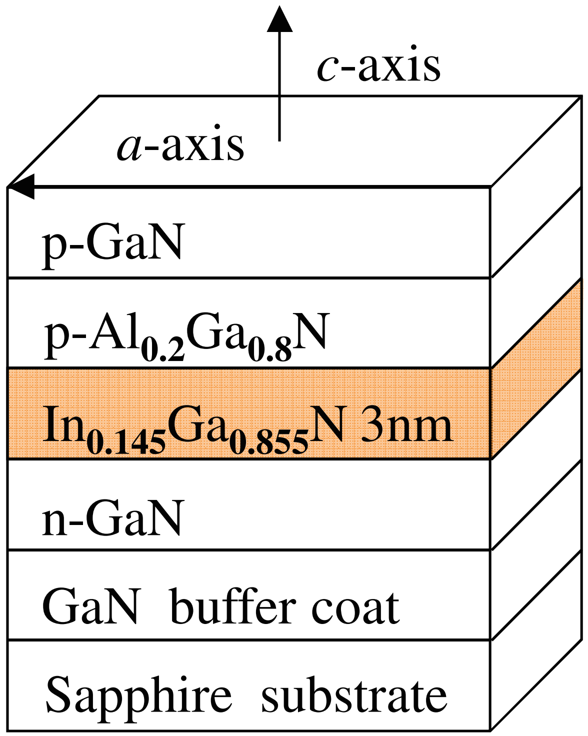




Experimental

Sample preparations:

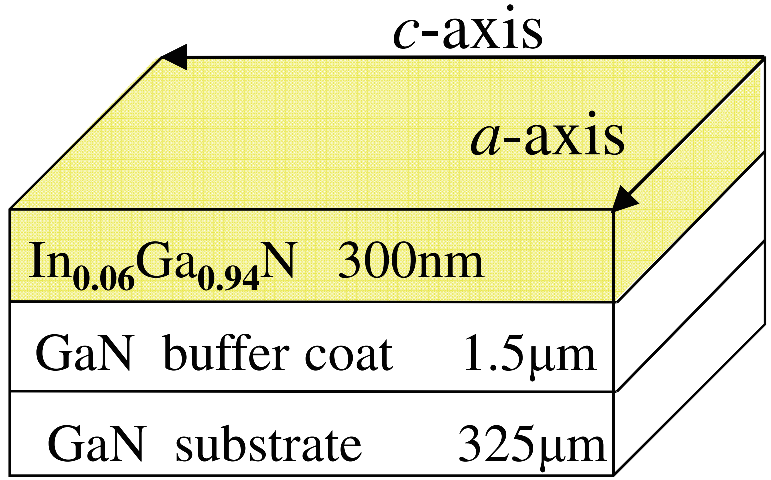
(1) $In_xGa_{1-x}N$
(x=0.145 blue, 0.20 green, 0.275 amber)
3nm SQW
grown by metal organic chemical vapor deposition(MOCVD) on GaN and sapphire 0001 substrates



SQW $In_xGa_{1-x}N$

(2) *m*-plane $In_xGa_{1-x}N$ (x=0.06) 300nm

grown using a metal organic vapor phase epitaxy (MOVPE) on *m*-plane GaN



m-plane $In_xGa_{1-x}N$

Measurement:

(1) $In_xGa_{1-x}N$ SQW

SPring-8: BL01B1, BL38B1, BL10XU

Si (111) Monochromator

(2) *m*-plane $In_xGa_{1-x}N$

PF-AR NW10A

Si(311) Monochromator

Fluorescence EXAFS

19-SSD(Ge)

In *K*-edge (27.9keV)

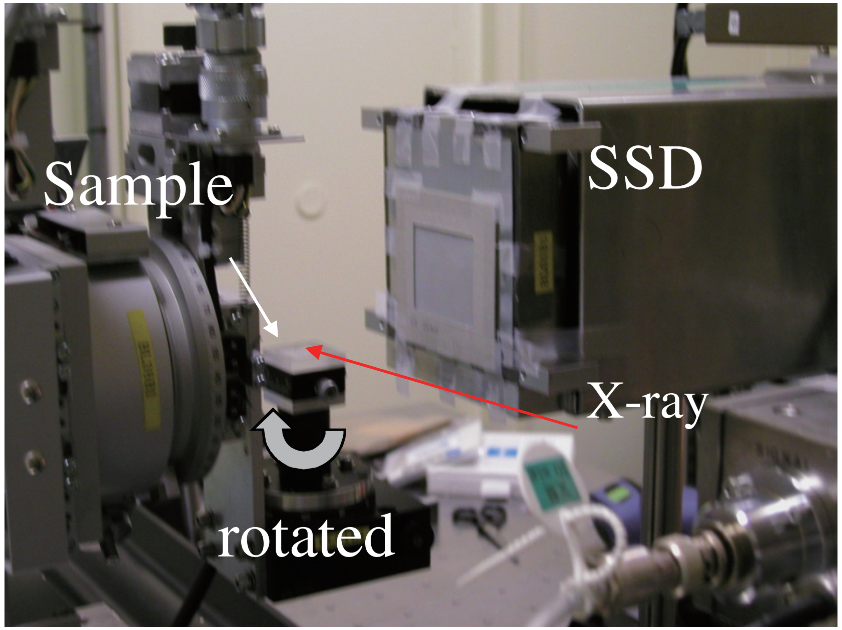
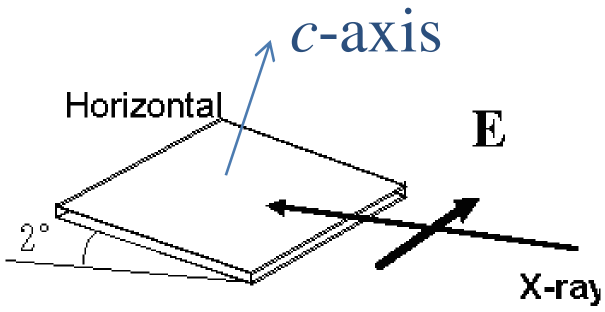
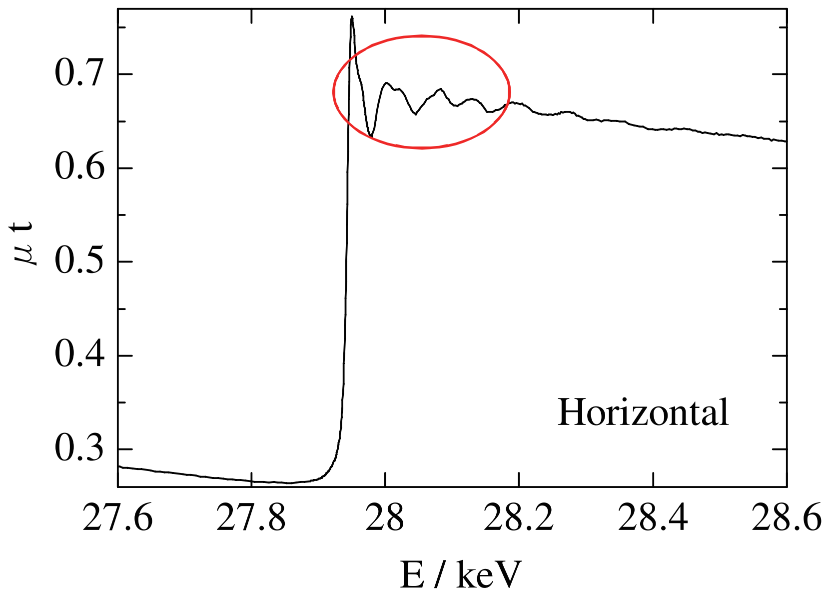


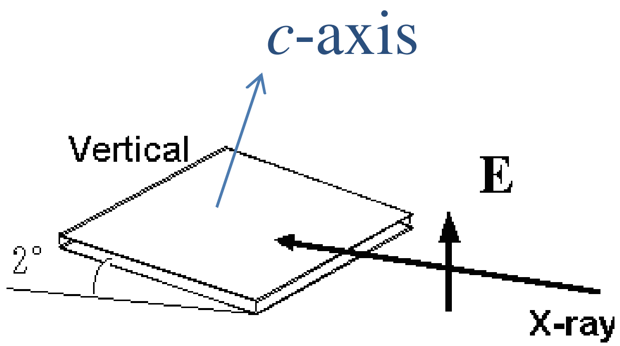
Photo at SPring-8

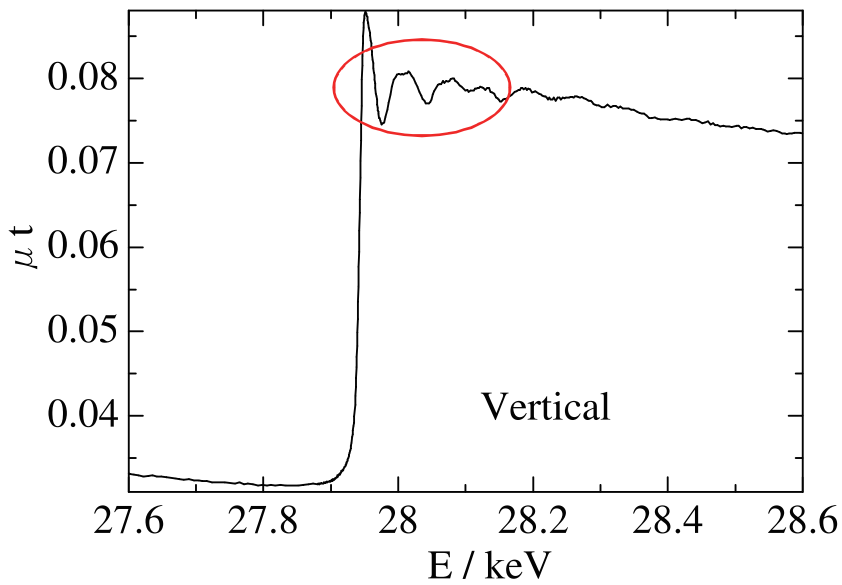
I. Results for SQW $In_xGa_{1-x}N$

XAS of $In_{0.20}Ga_{0.80}N$ SQW

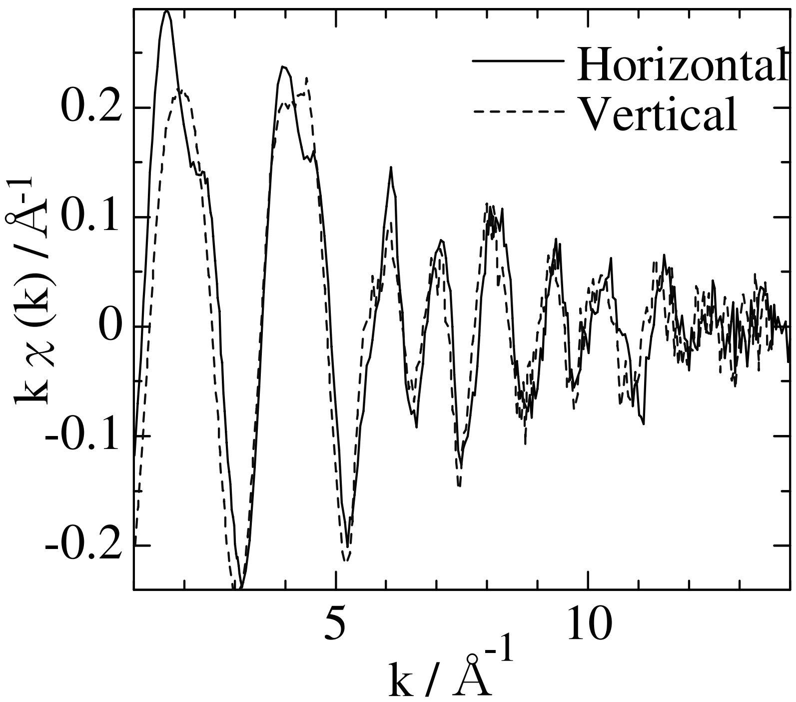


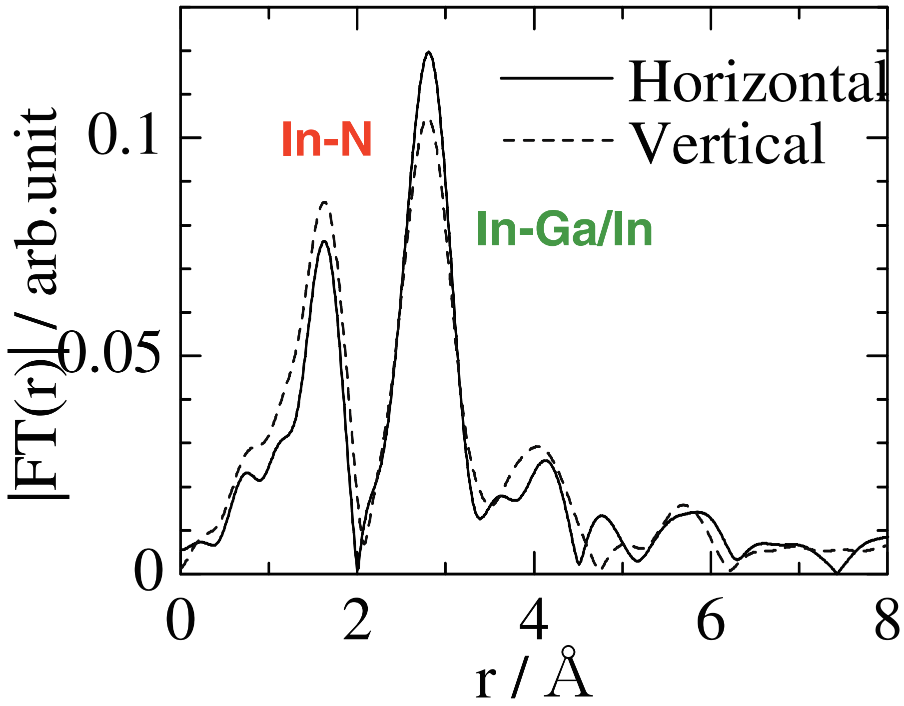




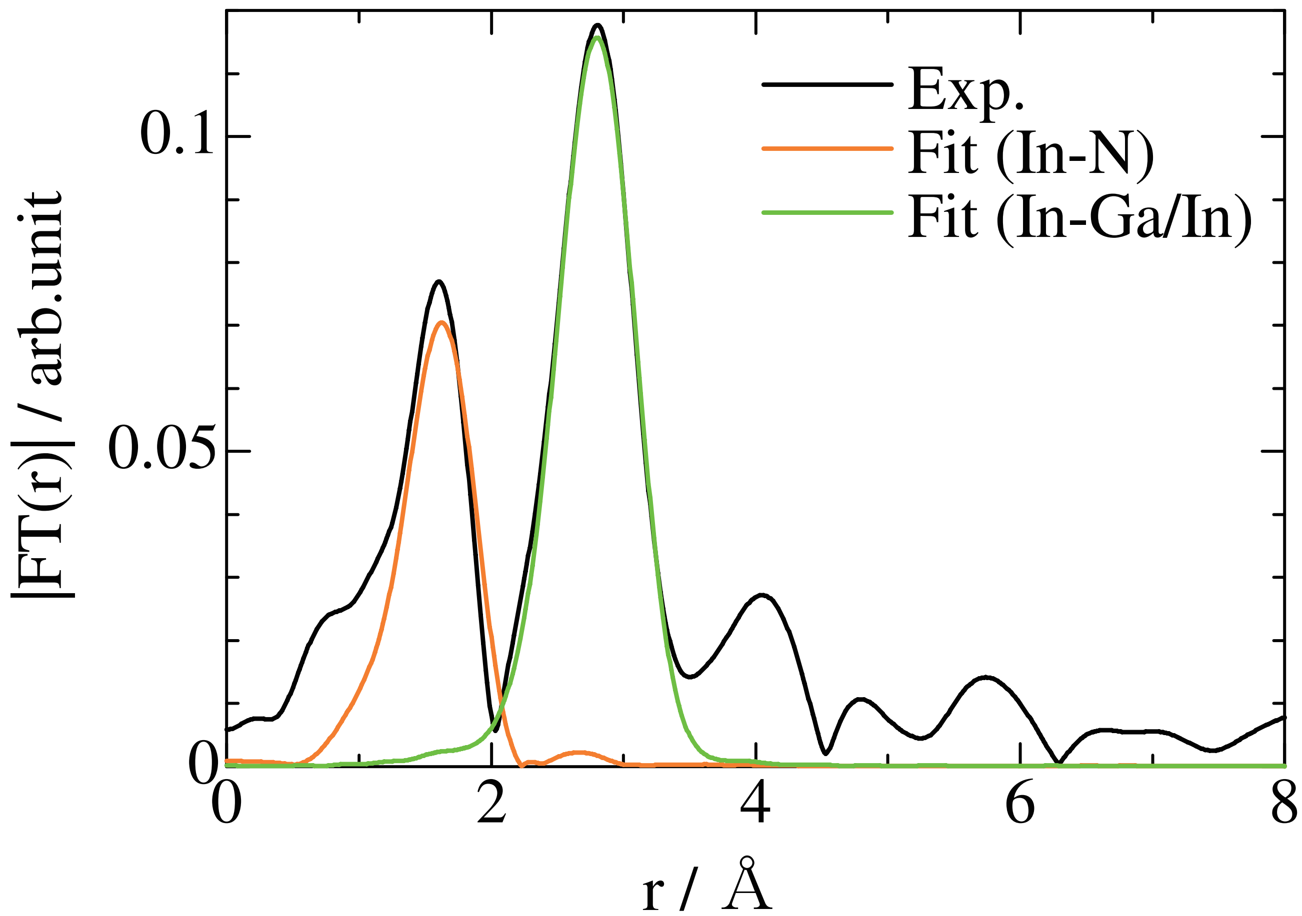


In *K*-edgeEXAFS , $k\chi(k)$ and Fourier transform of horizontal and vertical direction for $In_{0.20}Ga_{0.80}N$ SQW





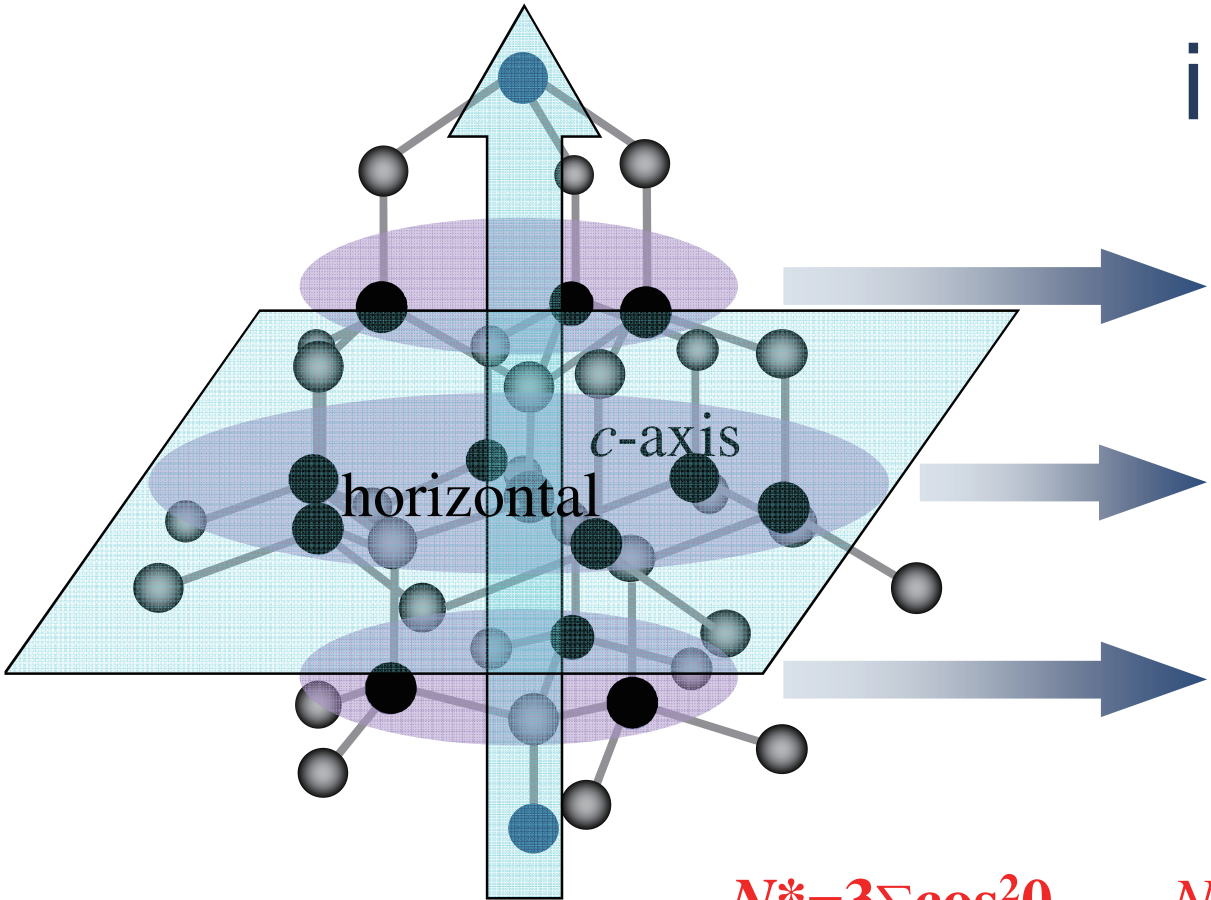
Curve-fitting of EXFS for $In_{0.20}Ga_{0.80}N$ SQW（horizontal）



Structural parameters from curve-fitting for 1st nearest N atom

		In-N	
x	h/v	r (Å)	σ (Å)
0.145	h	2.10	0.047
	v	2.11	0.047
0.20	h	2.10	0.052
	v	2.12	0.059
0.275	h	2.10	0.050
	v	2.10	0.052

Effective coordination number (CN) in 2^{nd} NN



2-1 nearest neighbor (out of plane)

2-2 nearest neighbor (in plane)

2-1 nearest neighbor (out of plane)

$N^*=3\sum\cos^2\theta$ N^*: effective CN

	N	N^* horizontal	N^* c-axis
2-1 NN	6	3.04	11.96
2-2 NN	6	9.00	0.00

Structural parameters from curve-fitting for 2nd nearest In and Ga atom

		In-Ga			In-In		
x	In/out	r (Å)	N^*	σ (Å)	r (Å)	N^*	σ (Å)
0.145	In	3.22	7.6	0.079	3.22	1.4	0.064
	Out	3.25	9.8	0.087	3.30	2.2	0.114
0.20	In	3.21	7.2	0.075	3.23	1.8	0.061
	Out	3.27	7.9	0.073	3.29	4.1	0.086
0.275	In	3.22	6.6	0.072	3.23	2.4	0.081
	Out	3.26	8.7	0.080	3.30	3.3	0.082

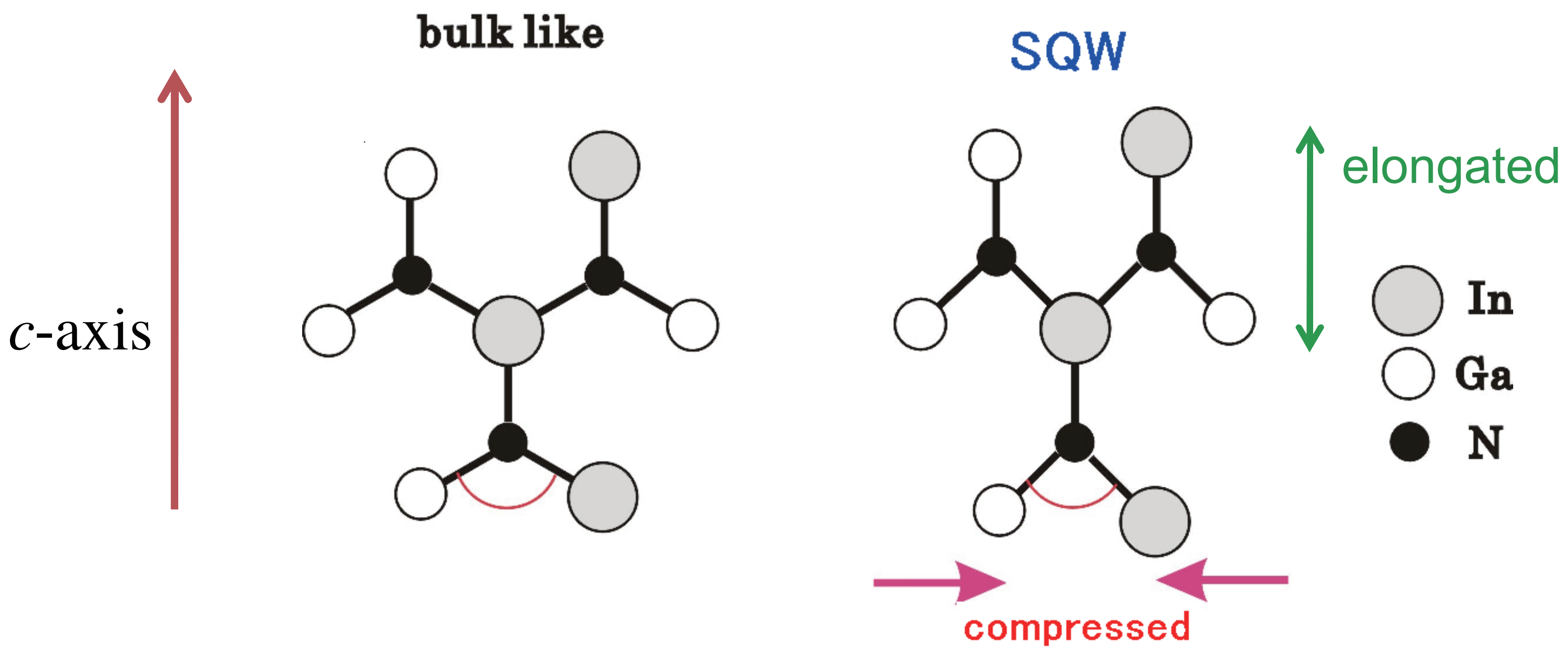
Result 1

Interatiomic diatnce

(1) **In-N:** Horizontal ~ Vertical (2.10A)

(2) **In-In**: out of plane (3.30A) > in plane (3.23A)

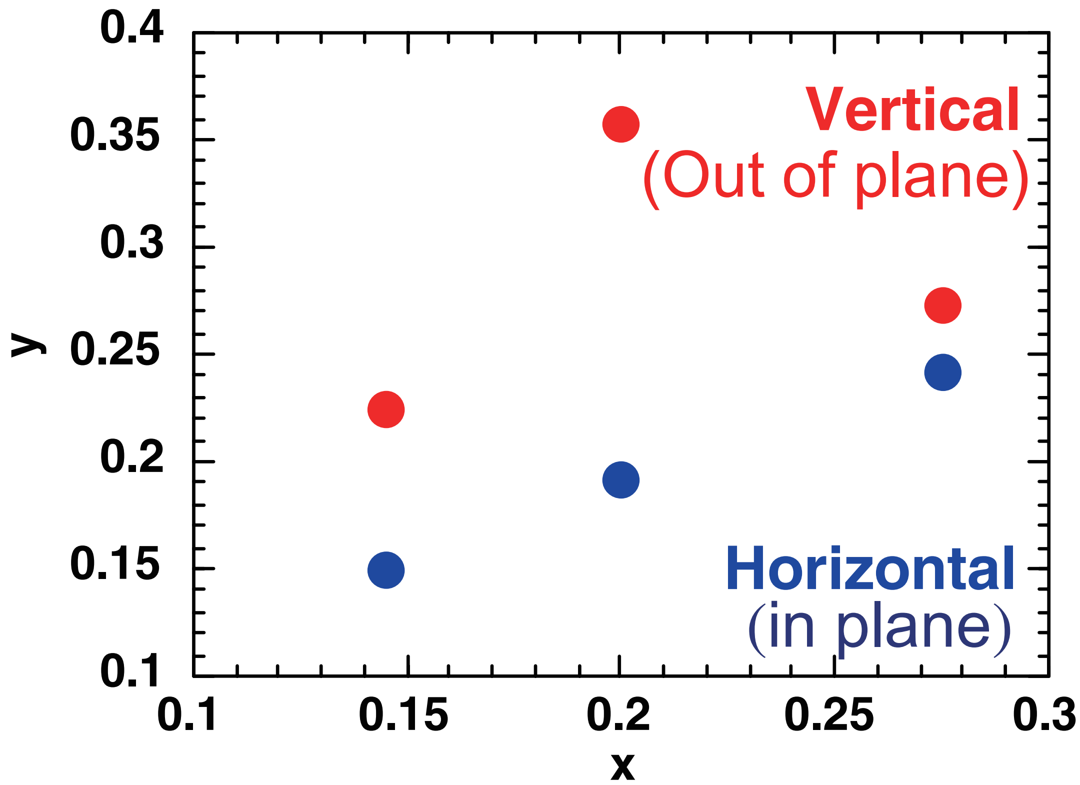
→ **compressed in the *a*-*b* plane** → **elongated to *c*-axis**



Coordination number

$y = N_{\text{In-In}} / (N_{\text{In-In}} + N_{\text{In-Ga}})$

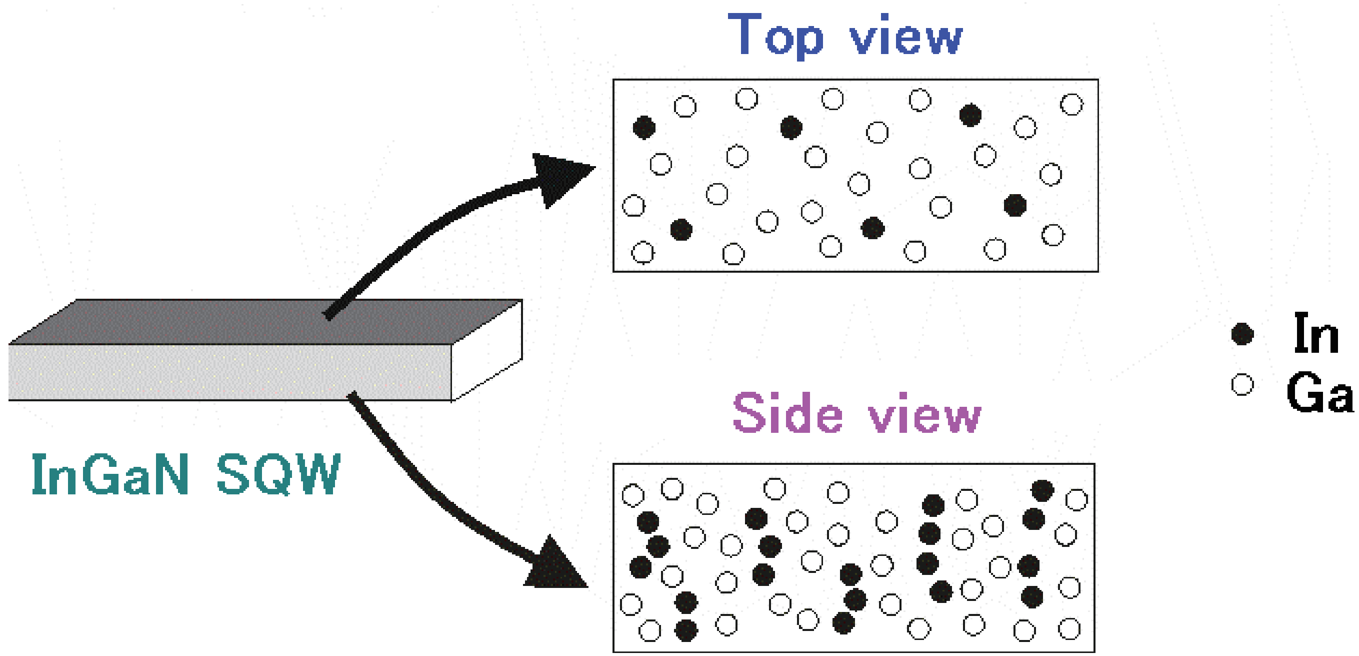
x : average concentration of In



Result 2

(1) ***c*-plane**: In atoms are distributed randomly

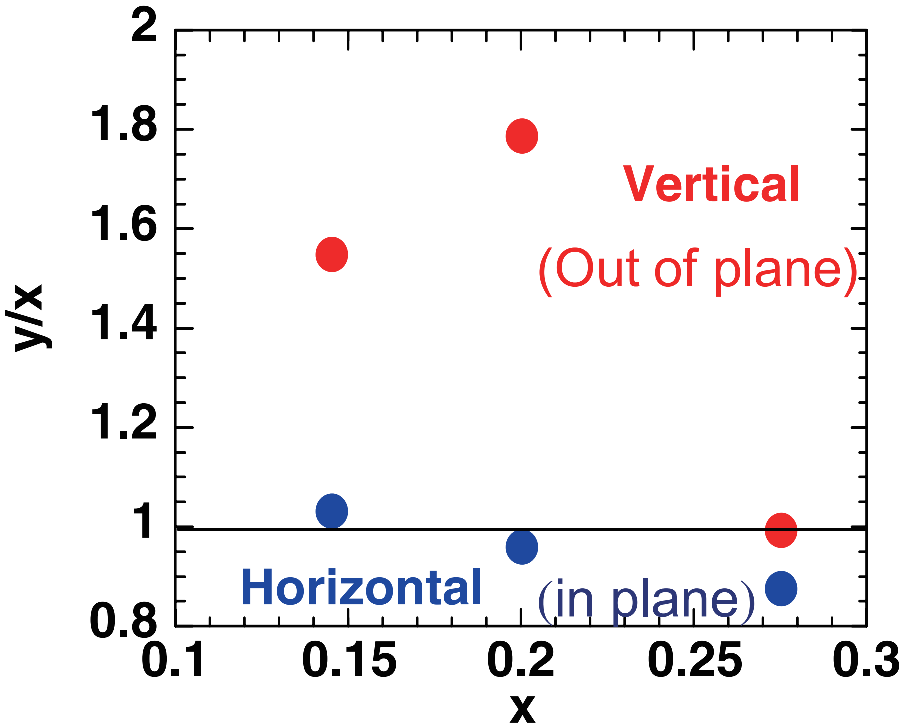
(2) ***c*-axes**: In atoms are localized top and down



In atom fluctuation !

In atom fluctuation and quantum efficiency

Localization of In atoms



External quantum efficiency

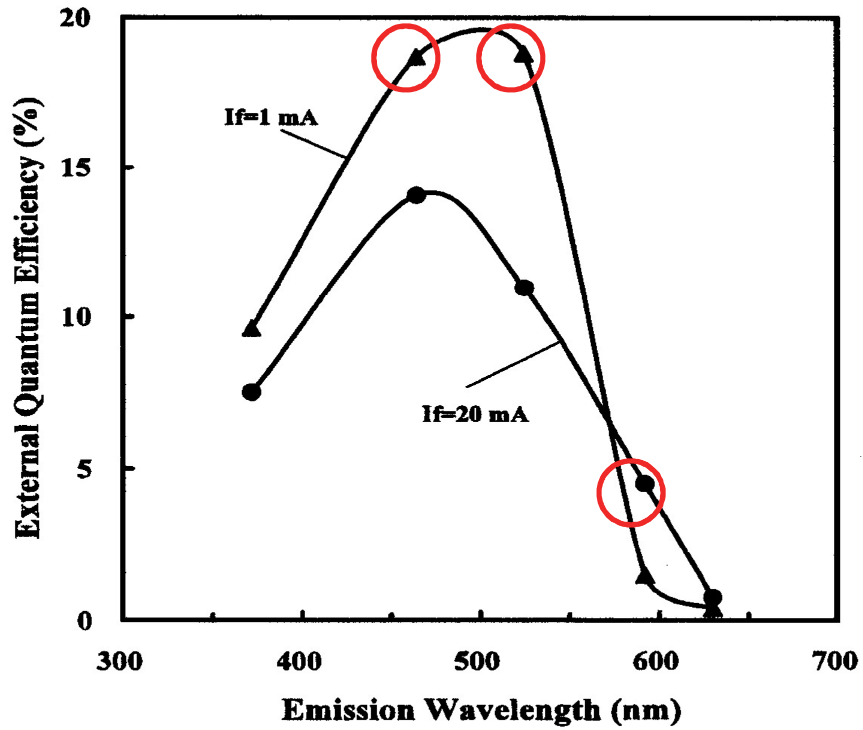


Fig. 7. External quantum efficiency as a function of the emission wavelength of InGaN-based UV, blue, green, amber and red LEDs.

T. Mukai, M. Yamada, and S. Nakamura, Jpn. J. Appl. Phys. **38**, 3976 (1999).

Conclusion 1 (InGaN SQW)

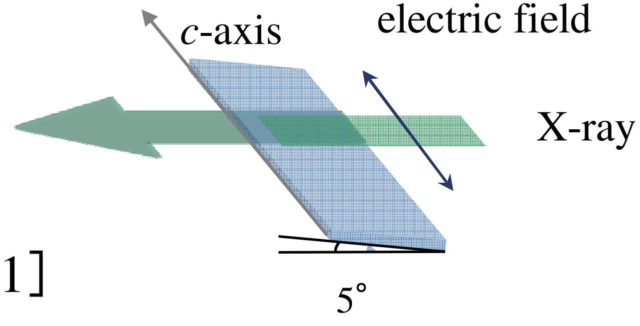
◆The interatomic distance of In-In in the out of plane of SQW is longer than that in plane. SQW is compressed in plane and elongated out of plane.

◆In atoms are aggregated out of plane and randomly distributed in plane of $In_{0.20}Ga_{0.80}N$ SQW

◆Correlation between the In atom aggregation and the higher quantum efficiency of LEDs was suggested.

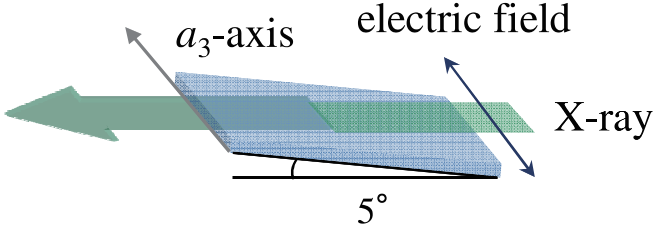
II. Results for *m*-plane $In_xGa_{1-x}N$

(1) : *c*-horizontal



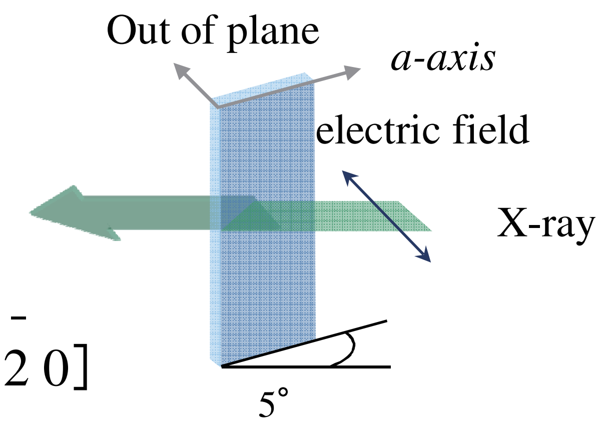
c-axis [0 0 0 1]

(2) : *a*-horizontal

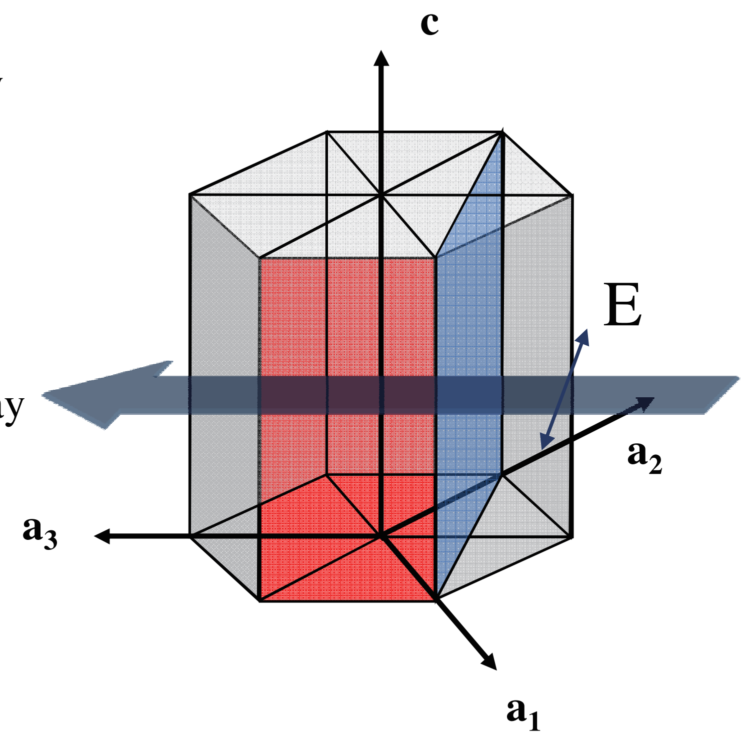


a_3-axis $[0\ 0\ \bar{1}\ 0]$

(3) : *a*-vertical



Out of plane $[1\ \bar{1}\ \bar{2}\ 0]$



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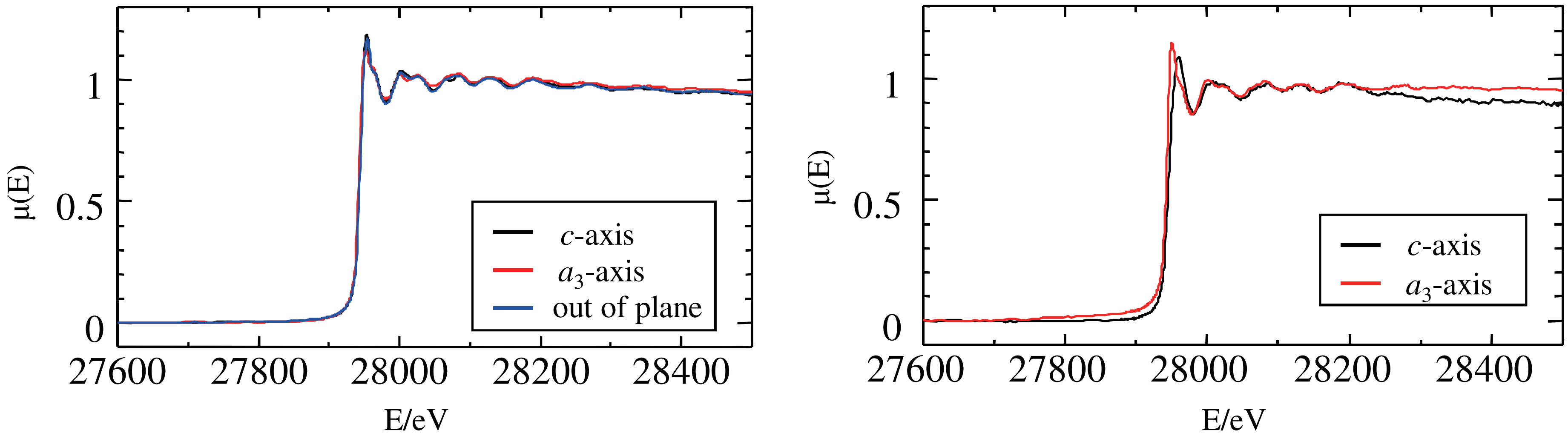
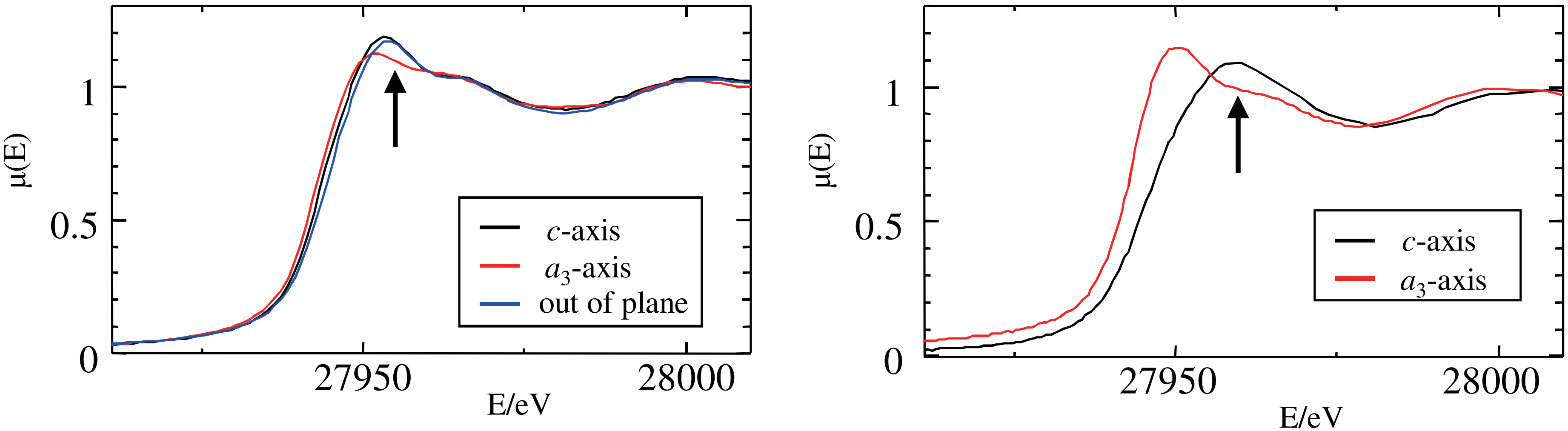
XAS and XANES



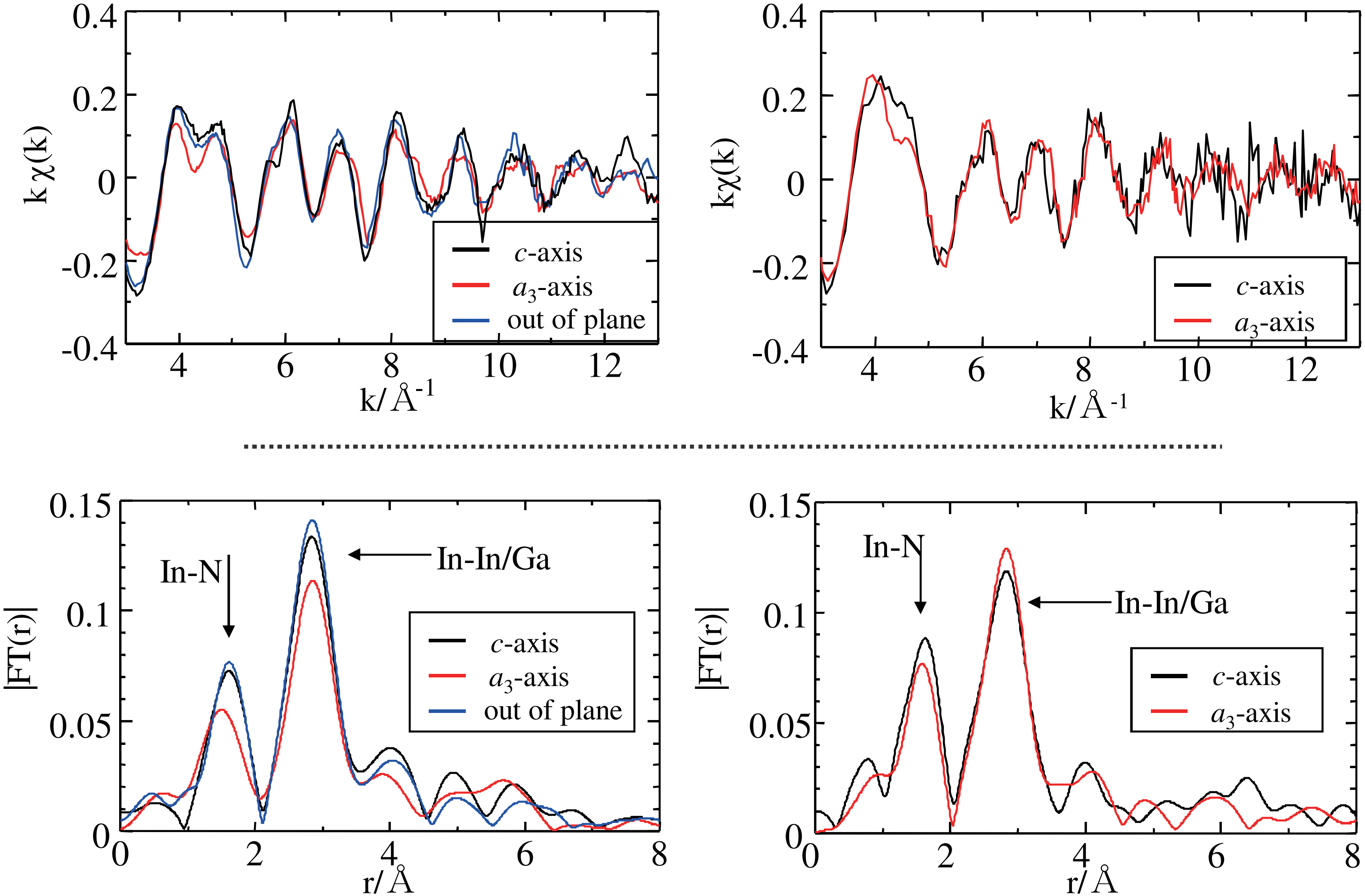
XANES



m-plane $In_{0.06}Ga_{0.94}N$

SQW $In_{0.145}Ga_{0.855}N$

EXAFS $k\chi(k)$ and FT

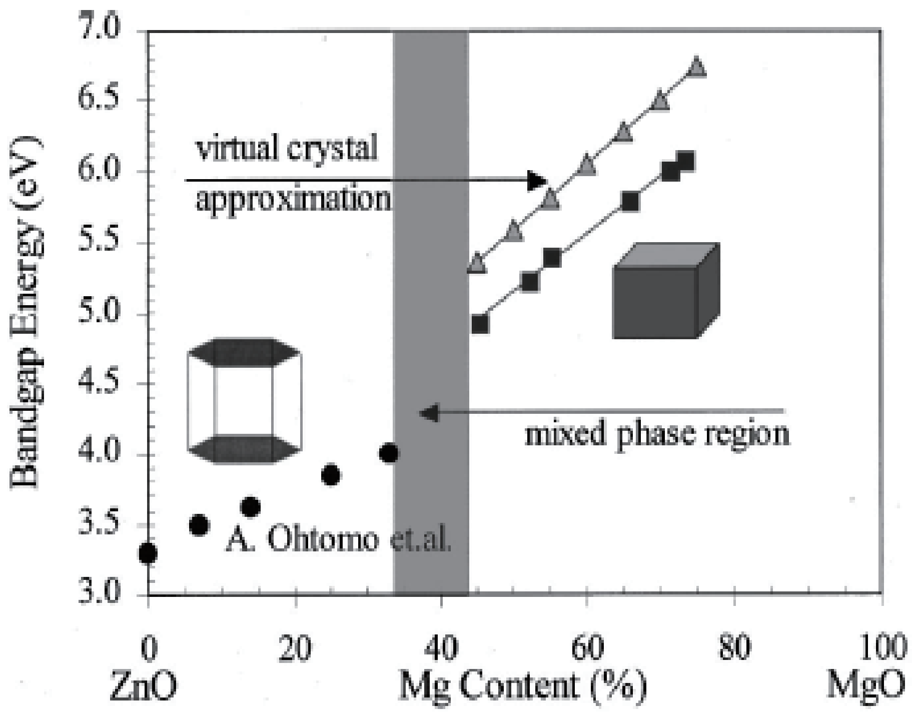


m-plane $In_{0.06}Ga_{0.94}N$ SQW $In_{0.145}Ga_{0.855}N$

$Mg_xZn_{1-x}O$

In $Mg_xZn_{1-x}O$, the band gap can be controlled by Mg composition. This is expected to be a new LED and/or LD material in place of InGaN.

Band gap and In concentration x for $Mg_xZn_{1-x}O$



S. Choopun, R. D. Vispute, W. Yang, R. P. Sharma, T. Venkatesan, H. Shen, Appl. Phys. Lett. **80** 1529 (2002)

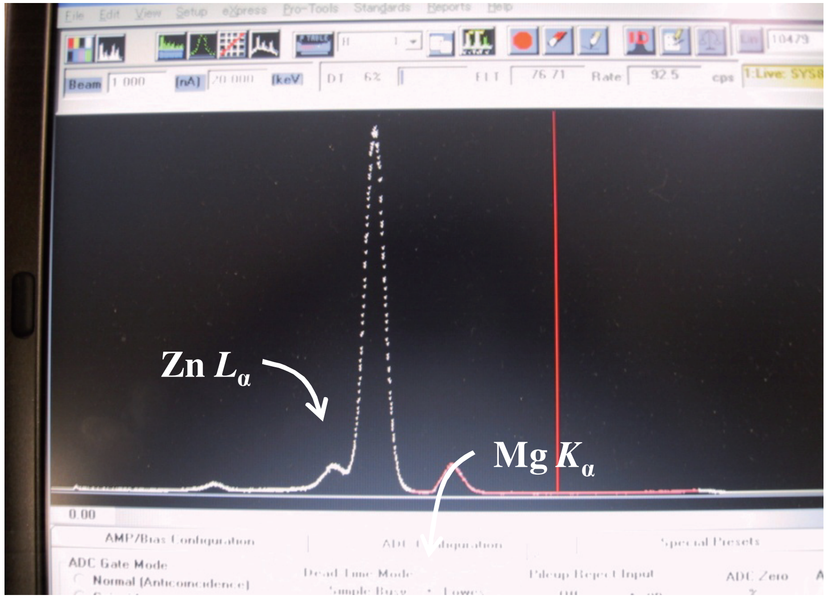
Local structure around Mg atom

$Mg_{0.06}Zn_{0.94}O$

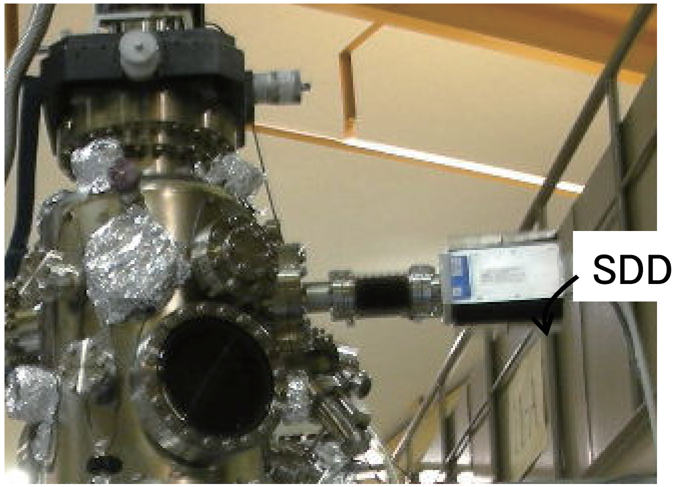
Mg *K*-edge (1306eV)

KEK-PF11A

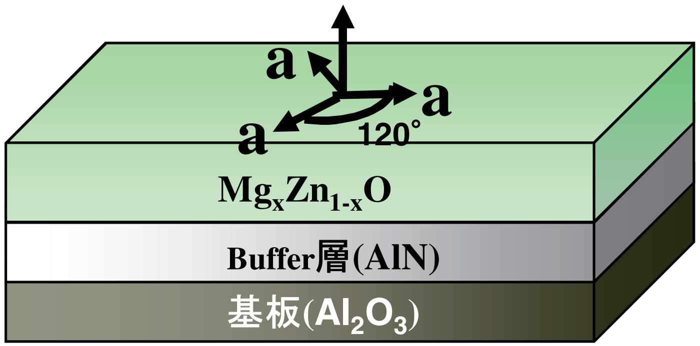
Silicon Drift Detector(SDD)



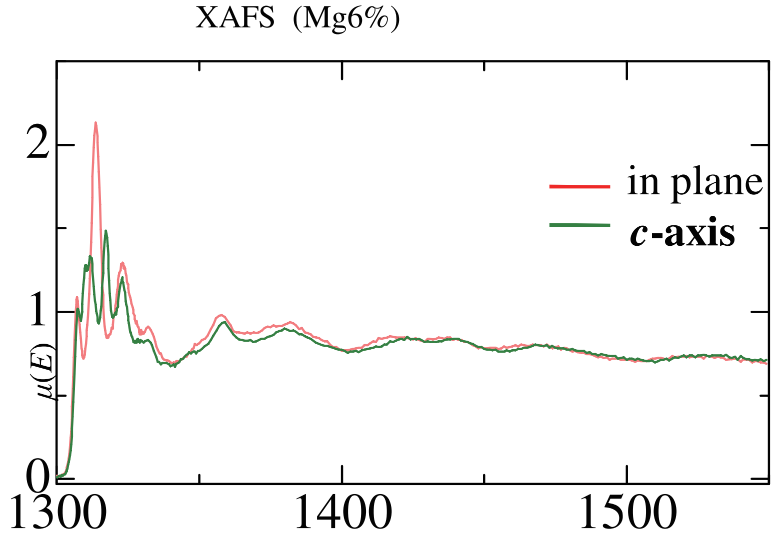
Fluorescence profile

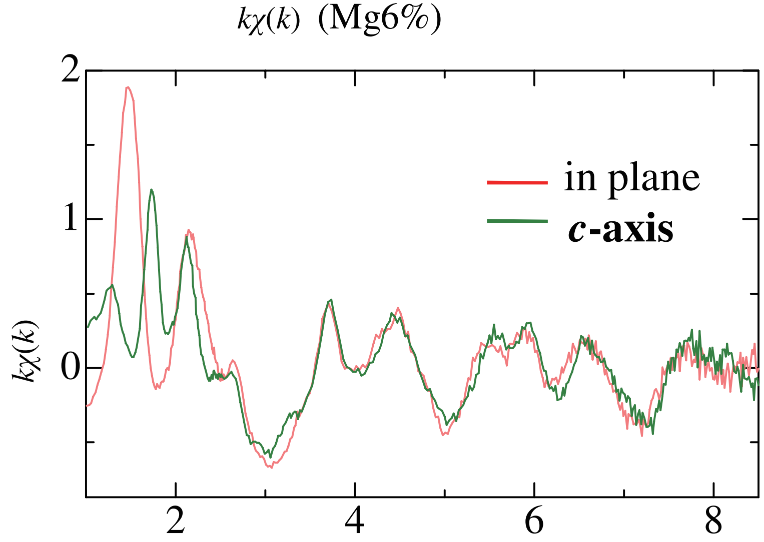


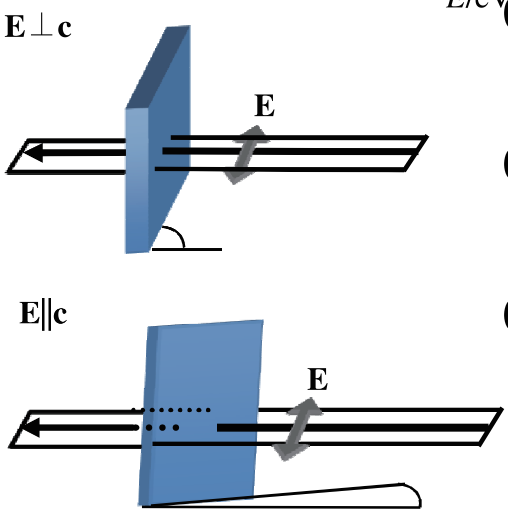
Chamber and SDD at BL11A

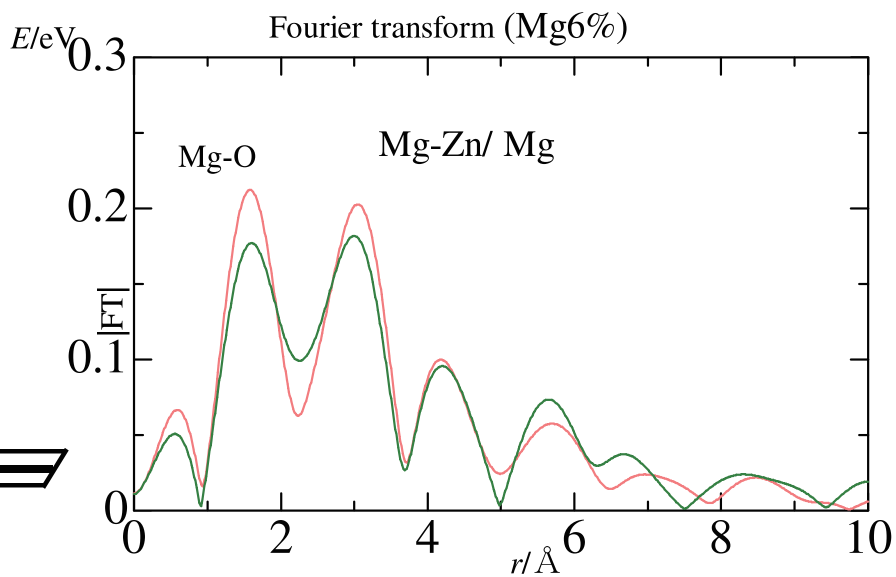


Mg *K*-edge *c*-plane and *c*-axis



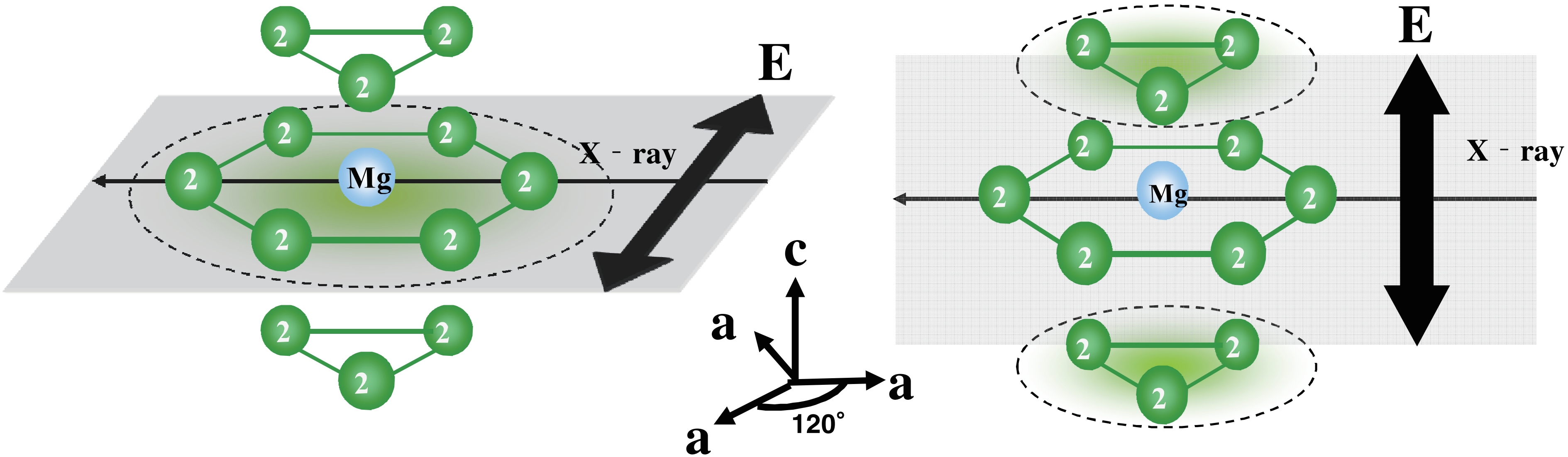






Simulation calculation by FEFF8.10

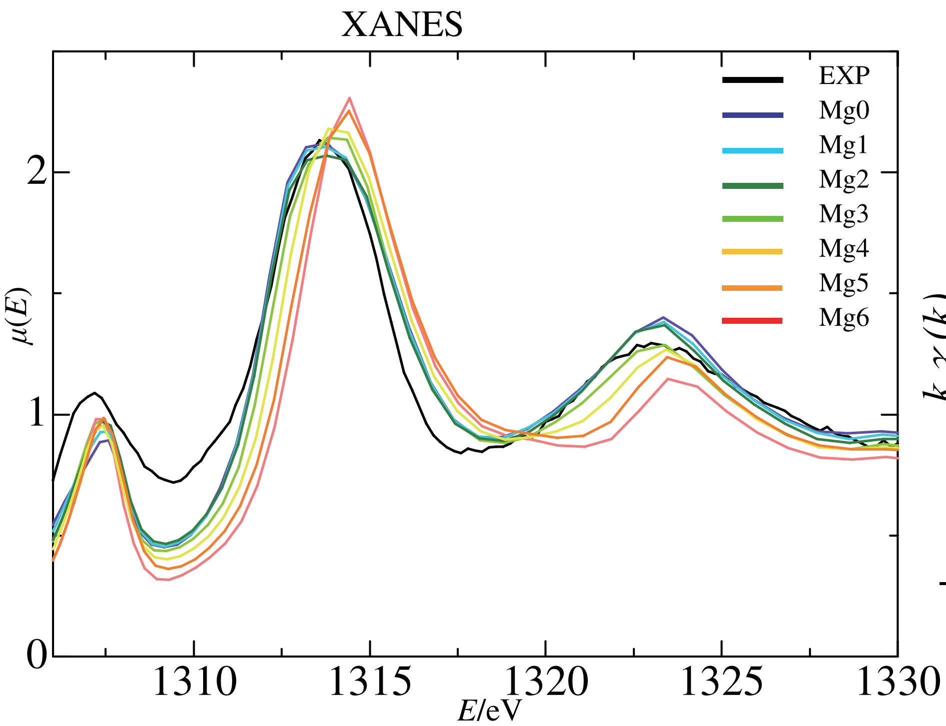
E ⊥ c **E∥c**

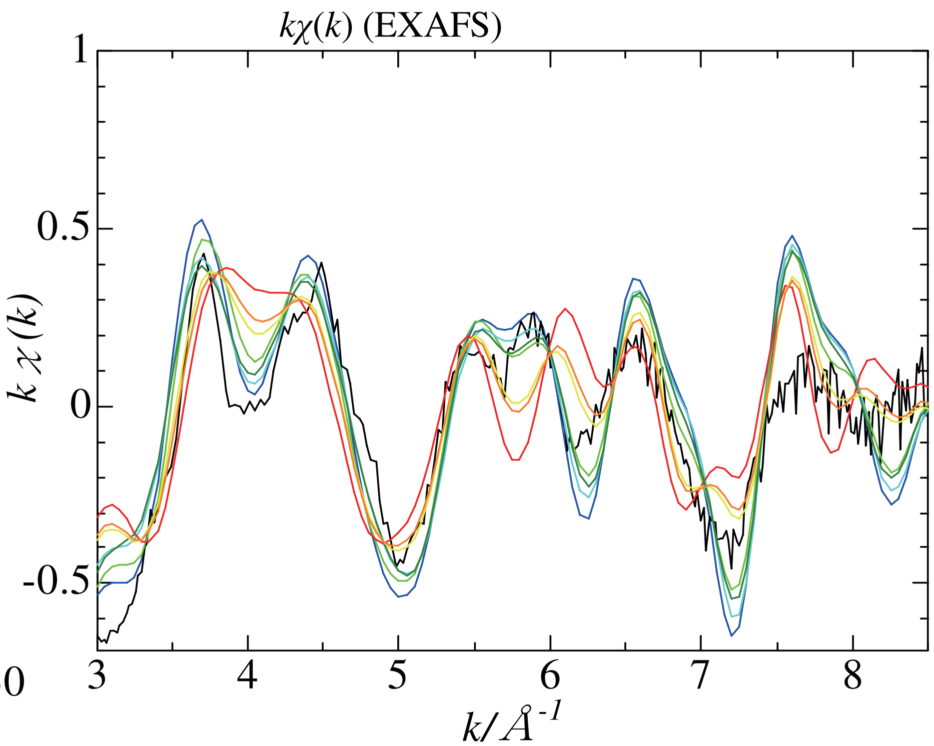


Six Zn atoms in plane **Six Zn atoms out of plane**

Zn atoms in 2ndNN are replaced by Mg

Simulation result for in plane E⊥c

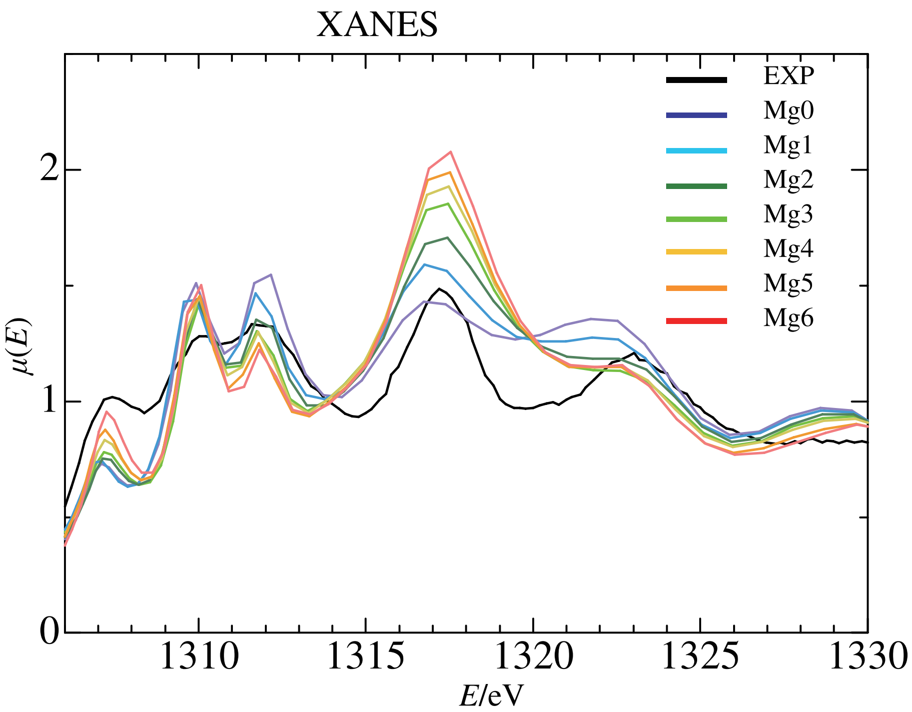


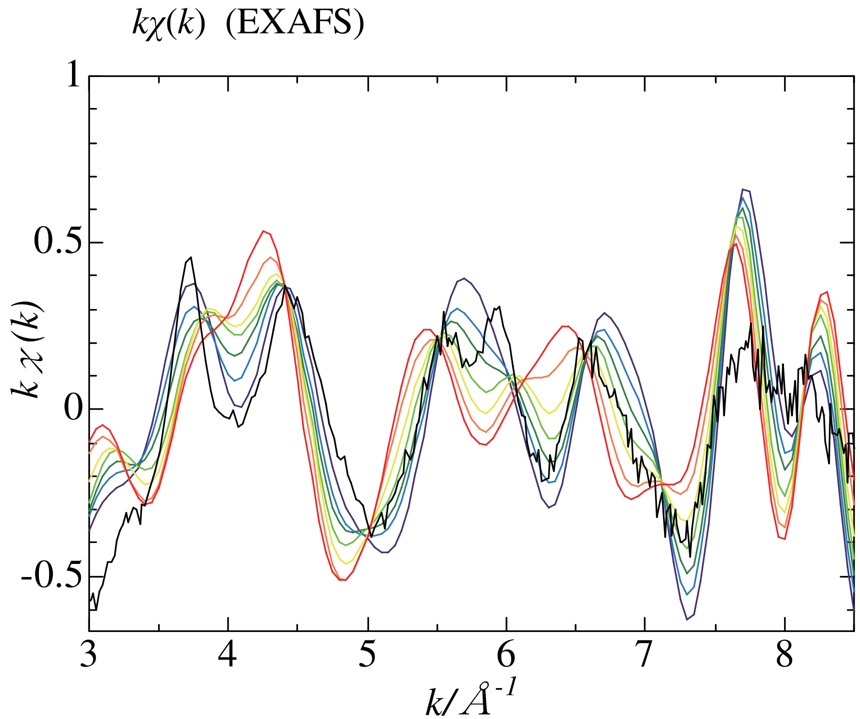


R(%)

	Mg0	Mg1	Mg2	Mg3	Mg4	Mg5	Mg6
XANES	13.0	12.5	12.0	14.0	17.6	23.0	27.5
EXAFS Fitting	28.8	31.6	37.7	47.1	55.3	41.5	73.1

Simulation result for out of plane **E||c**





R(%)

	Mg0	Mg1	Mg2	Mg3	Mg4	Mg5	Mg6
XANES	17.2	17.0	18.0	20.1	20.8	21.8	22.7
EXAFS fitting	28.4	33.8	44.9	67.9	80.9	93.0	92.2

Results for $Mg_{0.06}Zn_{0.94}O$

- XANES and EXAFS simulation calculation was applied.
- Mg atom is randomly distributed for both of in plane and *c*-axis direction in $Mg_{0.06}Zn_{0.94}O$.
- More accurate least-square fitting is desired.

Summary

- Polarization XAFS technique by fluorescence detection is valuable tool to study the local structure in the film and the quantum wells of semiconductors.

- Interatomic distance and distribution probability of the guest elements are important information for the performance of the light emitting mechanism.

The End