Structural Analysis of InN and GaInN using XAFS and X-ray Diffraction Measurements

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Recently, it was reported that the bandgap energy of InN is not 1.95 eV [1] which had was believed by many researchers, but near 0.8 eV [2,3]. It is important for science and industry to determine the native bandgap energy of InN and to understand the structural difference of InN films with bandgap energies of 0.8 eV and 1.95 eV. We analyzed the local structures around the In atoms of MBE-grown InN which has an optical absorption- and emission-edge near 0.8 eV, using X-ray absorption fine structure (XAFS) of In *K*-edge [4]. The measurement had been difficult because there was no useful facility which could generate a bright x-ray around an energy of 28 keV such as SPring-8. The XAFS measurements were performed at BL16B2 and BL19B2 of SPring-8. From In *K*-edge XAFS oscillation, the inter-atomic distance of In-N and In-In was estimated to be $d_{\text{In-N}}$= 0.214 nm and $d_{\text{In-In}}$= 0.353 nm, respectively. $d_{\text{In-In}}$= 0.353 nm is close to the a-axis lattice constant of a=0.3536 nm measured using x-ray diffraction (XRD). The c-axis lattice constant was also estimated to be c= 0.5701 nm. Because the radial structure function was similar to that obtained in a simulation based on the ideal structure of wurtzite and zinc-blende InN, as shown in Fig.1, we conclude that the In-N atomic bond is close to an ideal sp^3-hybridization in InN film. Moreover, we found that this InN sample has a wurtzite structure because the equivalent signals of InN [1011] were observed using the pole figure of XRD. We therefore conclude that the MBE-grown InN film, which has a bandgap energy of 0.8 eV, had an ideal wurtzite structure.

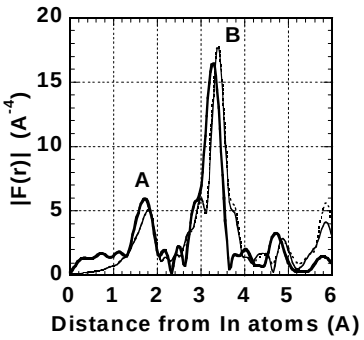

Fig.1. The radial structure function around In atoms for InN film (thick solid line). The thin solid and broken lines show the simulated data for wurtzite and zinc-blende InN., respectively.

[1] K.Osamura et al., Solid State Commun. **11** (1972) 617. [2] V.Davydov et al., phys.stat.sol. (b) **229** (2002) R1. [3] Y.Saito et al., phys.stat.sol. (b) **234** (2002) 796. [4] T.Miyajima et al., phys.stat.sol. (b) **234** (2002) 801.

XAFS及びX線回折法による InN系半導体の構造解析

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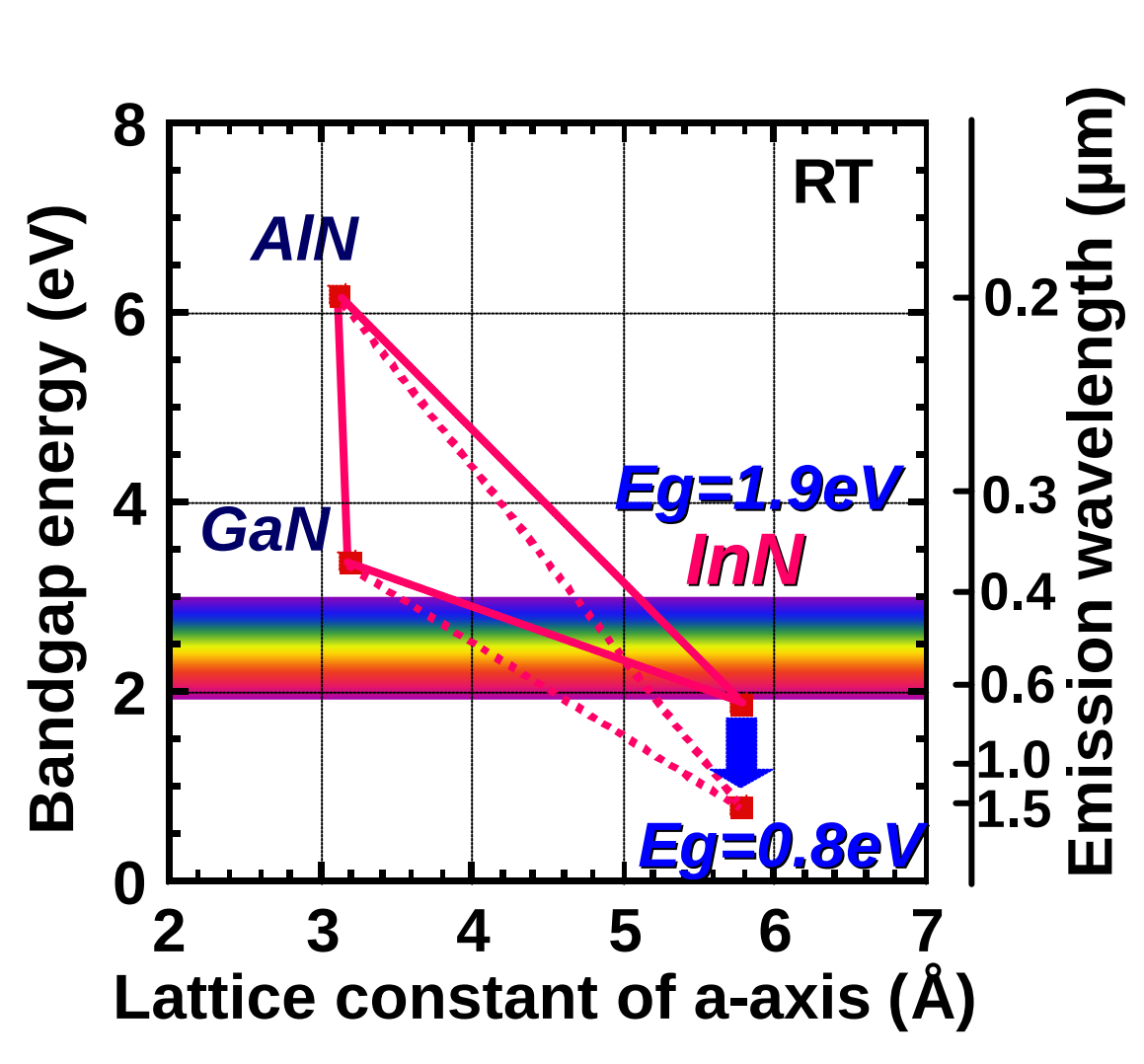
Bandgap Energy of InN



Previous reports
Eg=1.9 eV

K.Osamura et al.(1972)
T.L.Tansley et al. (1986)

Recent reports
Eg=0.8 eV

T.Inushima et al. (2001)
V.Y.Davydov et al.(2001)
J.Wu et al. (2002)
Y.Saito et al. (2002)
T.Matsuoka et al. (2002)

$Ga_{1-x}In_xN$-based optical device
λ = 360nm～1.55μm ?

Sample structure

LT-InN

InN (d=1.5μm)
(0001) sapphire

MBE growth

Source: In metal

Nitrogen plasma (RF)

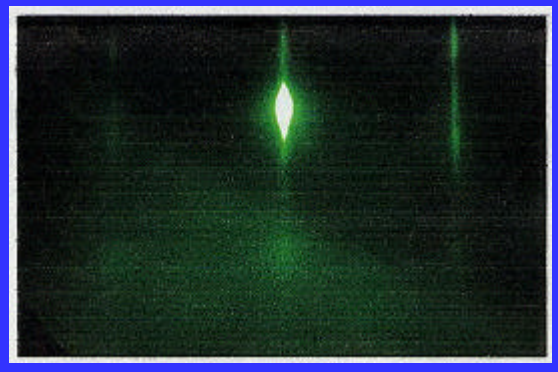
Tg= 530 ° C

LT-InN: Tg=300 ° C, 30 nm

Y.Saito et al., Jpn. J. Appl. Phys. 40 (2001) L91.

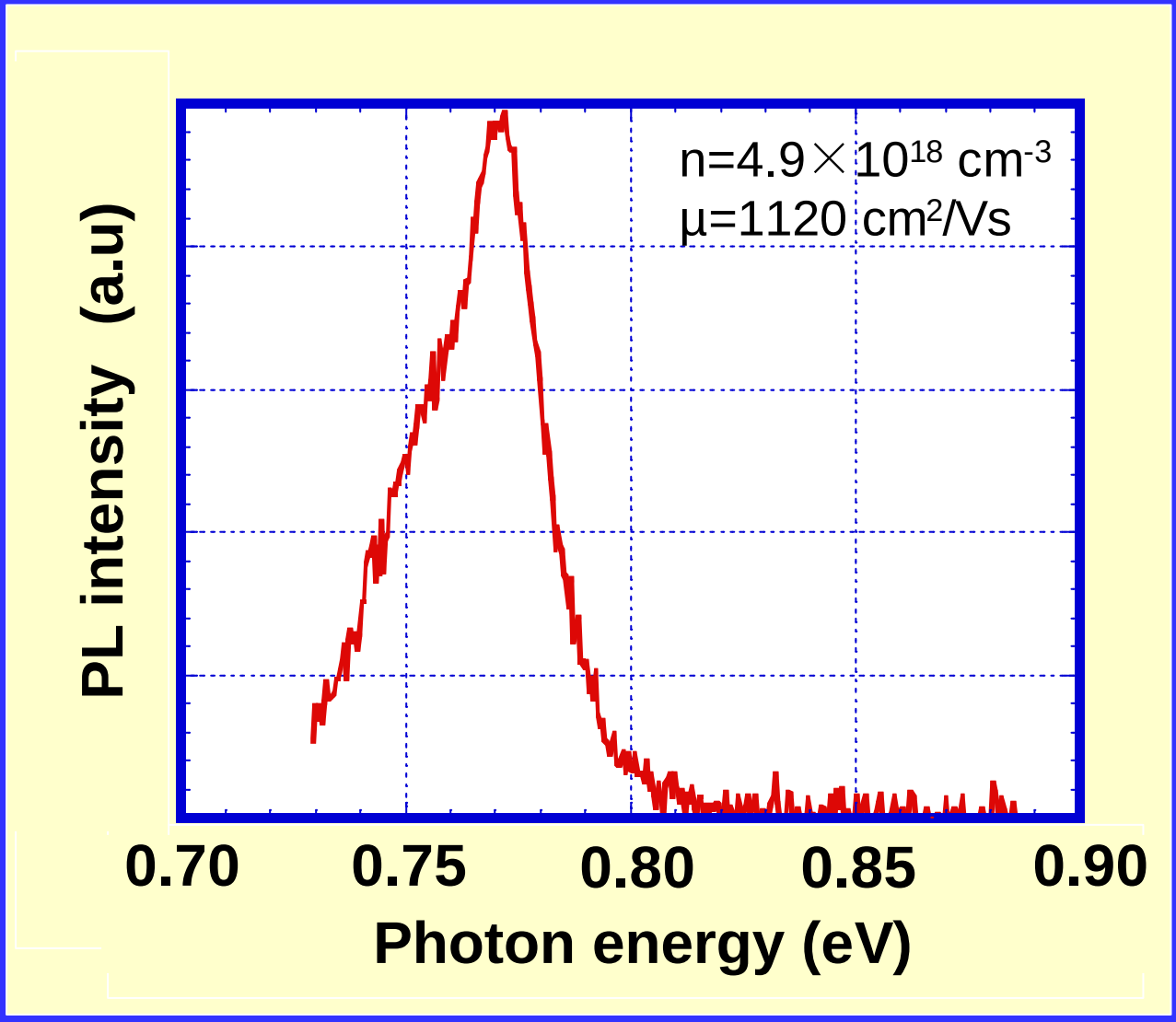
RHEED

e-beam//<11-20>



e-beam//<10-10>

Photoluminescence spectrum



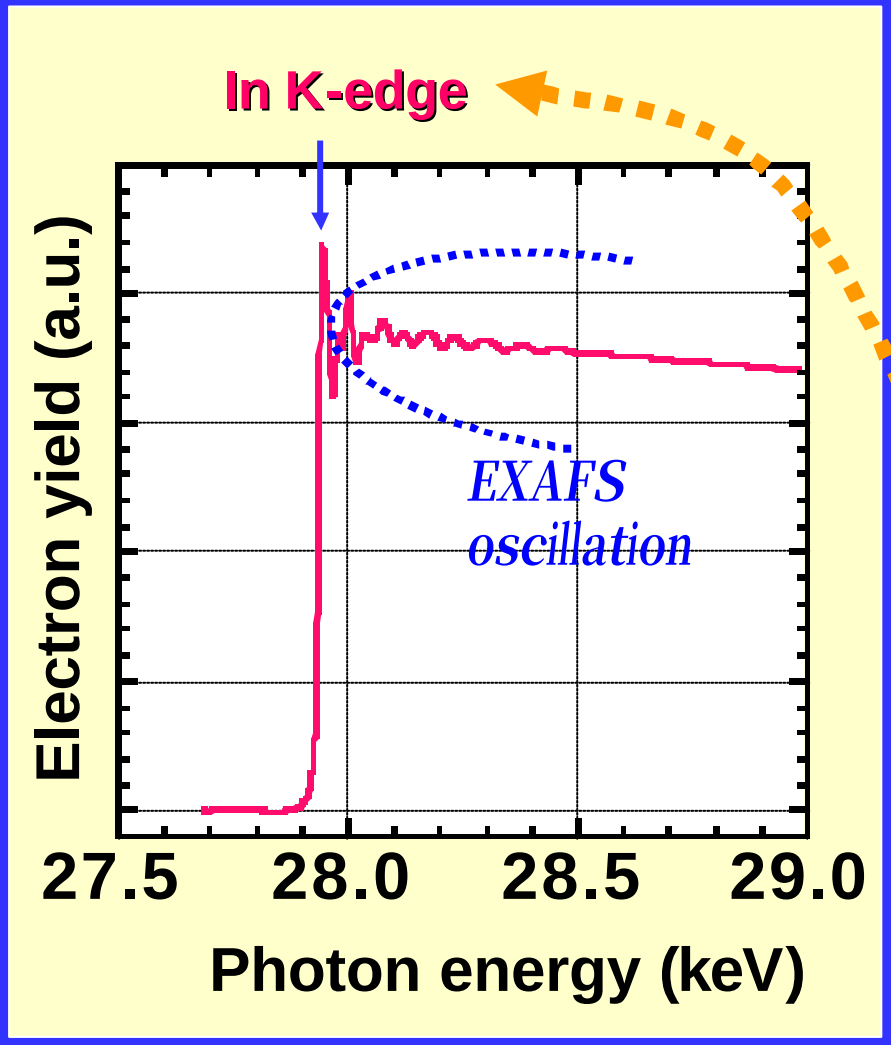
Excitation：
Ar ion laser
（λ=514.5nm）
Power：
P=2.2 W/cm²

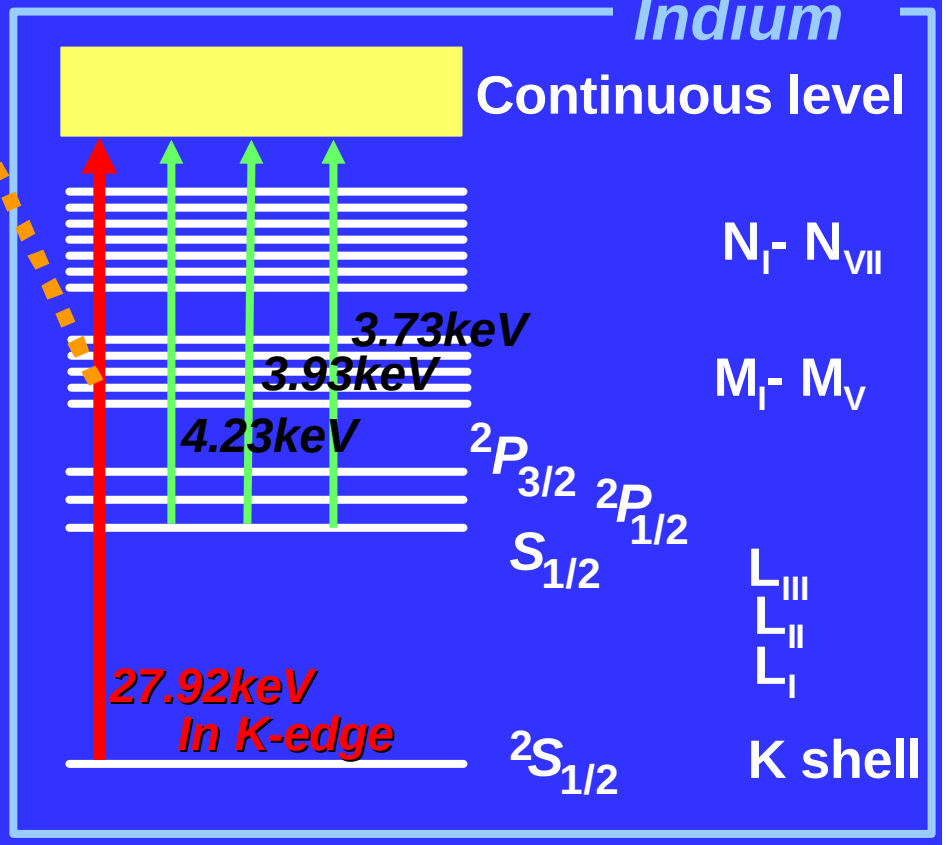
Temparature：
T=77K

Detector:
Photo multiplier tube
(InP/InGaAs)

Electron yield spectrum

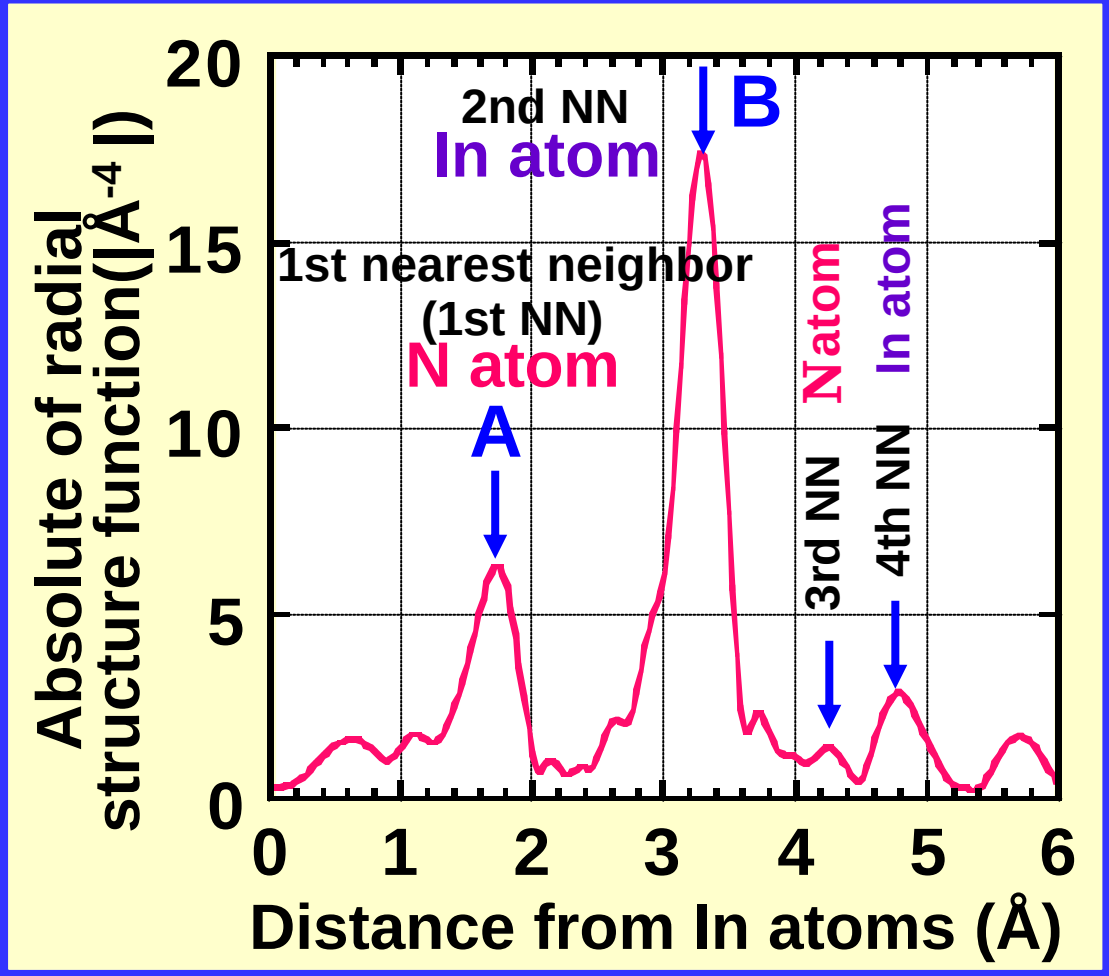
EXAFS oscillation is clearly observed above E=27.92 keV of In K-edge.





Radial structure function around In atoms

$$\Phi(R) = (2\pi)^{-1/2} \int_{k_{min}}^{k_{max}} C(k) k^3 \exp(-2ikR)\,dk$$



Peak A→N atom

$d_{In\text{-}N}$ = 2.14 Å

Peak B→In atom

$d_{In\text{-}In}$ = 3.53 Å

X-ray diffraction
(θ-2θ) measurement

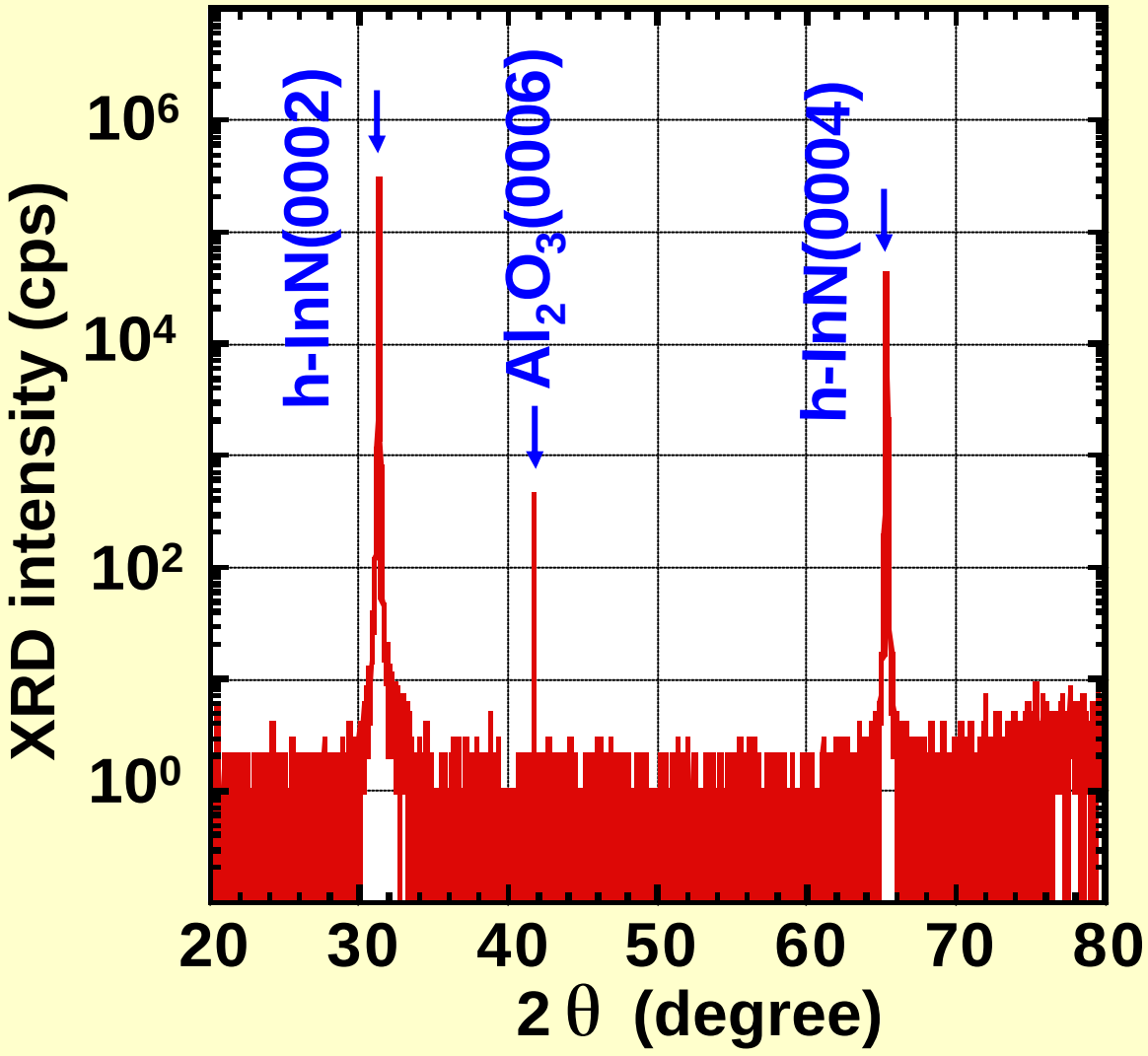
a = 3.536 Å

c = 5.701 Å

$d_{In\text{-}In} \gg a$

T. Miyajima et al., phys. stat. sol. (b) 234 (2002) 801.

X-ray Diffraction (θ-2θ scan)



Hexagonal InN
→ main phase

Cubic InN
In metal
→ no detect

XRD(θ-2θ) meas.
a= 3.536 Å
c= 5.701 Å

Conclusion I

(1) InN with 0.8 eV-PL peak

In-N bond→sp^3 hybridation

Local structure around In atom

→ideal structure of hexagonal InN

(2) Inter-atomic length

$d_{In\text{-}N}$(InN) = 2.14 Å, $d_{In\text{-}In}$(InN) = 3.53 Å

XRD meas. : a = 3.536 Å, c = 5.701 Å

$d_{In\text{-}In}$(InN) ~ a(XRD)

(3) Main phase → hexagonal InN

Cubic InN and In metal was observed in some sample.

hexagonal InN (0001) // cubic InN (111) // In (101)

Conclusion II

(1) Bandgap energy of hexagonal InN

$\rightarrow$ Eg$\leqq$0.8 eV

(2) What is the origin of Eg=1.9 eV ?

(a) High background carrier density

- Burstein-Moss shift –

T.L. Tansley et al., J.Appl.Phys. 59 (1986) 324.

D.Y.Davydove et al., phys. stat. Sol. (b) 230 (2002) R4.

(b) Crystal structure (hexagonal & cubic)

(c) $In_{2-x}O_{3-y}$ (Eg(In_2O_3)=3.1eV)

D.Y.Davydove et al., phys. stat. Sol. (b) 229 (2002) R1.