Structural and Optical Properties of Ga Auto-incorporated InAlN Epilayers

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Motivation

$In_xAl_{1-x}N$ is a wide and direct bandgap semiconductor spanning an energy range of 0.7–6.2 eV. It has an advantage over other ternary nitride alloys in that it can be lattice matched to GaN with an InN content of 17%, reducing strain induced composition inhomogeneity and defects, which improves crystalline quality and device efficiency[1,2]. This gives InAlN the potential to replace other alloys such as AlGaN and InGaN in optoelectronic and power transistor devices. Recently it has been reported that unintentional Ga incorporation can occur during MOCVD growth of InAlN layers on GaN buffers in close-coupled showerhead MOCVD reactors[3,4]. The Ga incorporation has been associated with left over trimethylgallium (TMGa) precursor and Ga deposits on the susceptor and reactor walls[3,5]. Another proposed cause is diffusion of Ga from the underlying GaN layer[4]. Unwanted Ga incorporation can change the structural, electrical and optical properties of the nominal InAlN material, giving rise to unwanted characteristics. The bandgap has a strong dependence on composition, which determines the emission wavelength and efficiency of an optoelectronic device. Ga auto-incorporation can be difficult to determine through x-ray diffraction (XRD) alone, which is often the primary measurement after growth. This is due to the interplay of composition and strain, and therefore Ga inclusion can often be missed. In this work we present a thorough analysis of the composition of Ga auto-incorporated InAlGaN layers using wavelength dispersive x-ray (WDX) spectroscopy, Rutherford backscattering spectrometry (RBS) and x-ray diffraction (XRD) techniques. The optical properties of these InAlGaN layers are also investigated using cathodoluminescence (CL) measurements and related to the composition data.

Sample Details

- Nominally ~80nm InAlN layers grown on 1µm thick GaN buffers on 0.4 degree miscut sapphire substrates.
- Grown in 3×2" AIXTRON close coupled showerhead MOCVD reactor.
- All layers non-intentionally doped.
- Parameters held constant for all samples:
  - ❖ Temperature = 790
  - ❖ Total Pressure = 70 mbar
  - ❖ V/111 Ratio = 5481

Table 1: Selected growth parameters for the nominally InAlN epilayers grown in this series.

InAlN layer growth condition	Sample A	Sample B	Sample C
NH3 (mmol/min)	56	168	56
TMIn (µmol/min)	5	16	5
TMAl (µmol/min)	5	16	5
Growth time (s)	1330	1300	2520
Reactor total flow (sccm)	8000	24000	24000

Techniques

- WDX qualitative measurement used for determination of Ga auto-incorporation on a Cameca SX100 EPMA.
- WDX quantitative measurement and layers program used for composition result of the thin InAlGaN layers.
- Confirmed composition by RBS and XRD.
- XRD providing further strain information.
- CL measurements were performed as hyperspectral mapping for optical analysis.

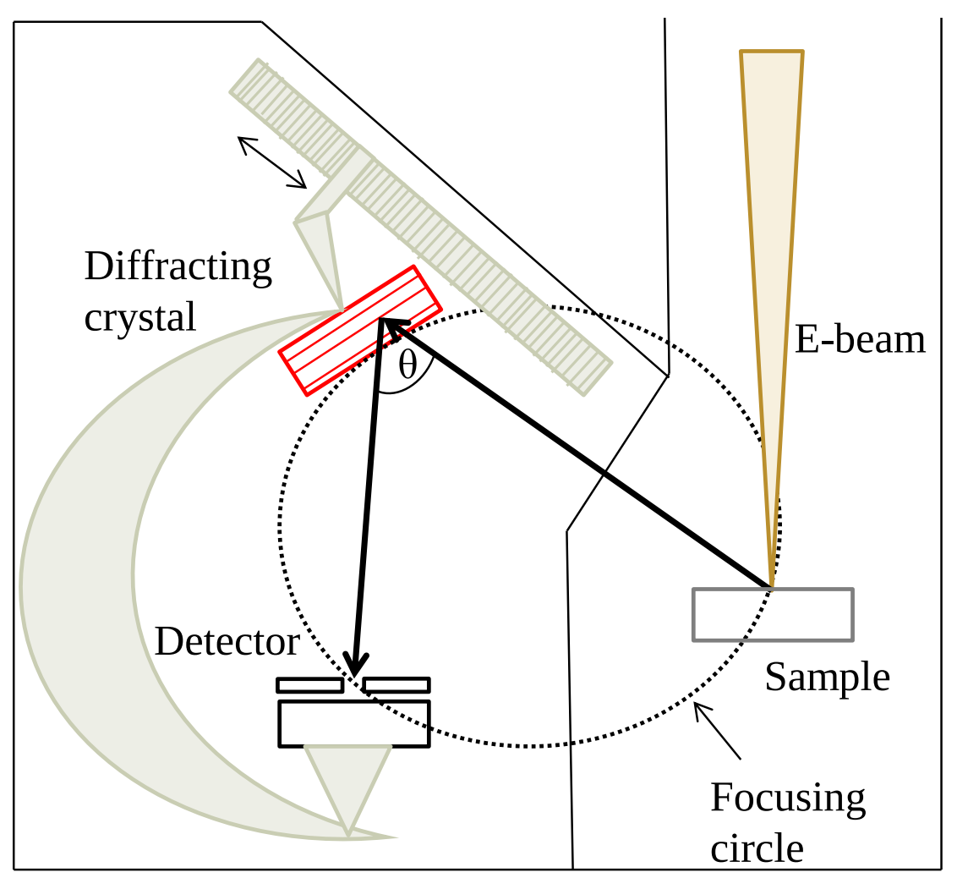

Figure 1: Schematic of WDX spectrometer

Ga Auto-incoporation

- Evidence of Ga auto-incorporation in nominal 80 nm InAlN layer by WDX 2kV qualitative measurement.
- Beam contained within top layer (Figure 2a).
- Ga Lα and Lβ lines detected (Figure 2b).

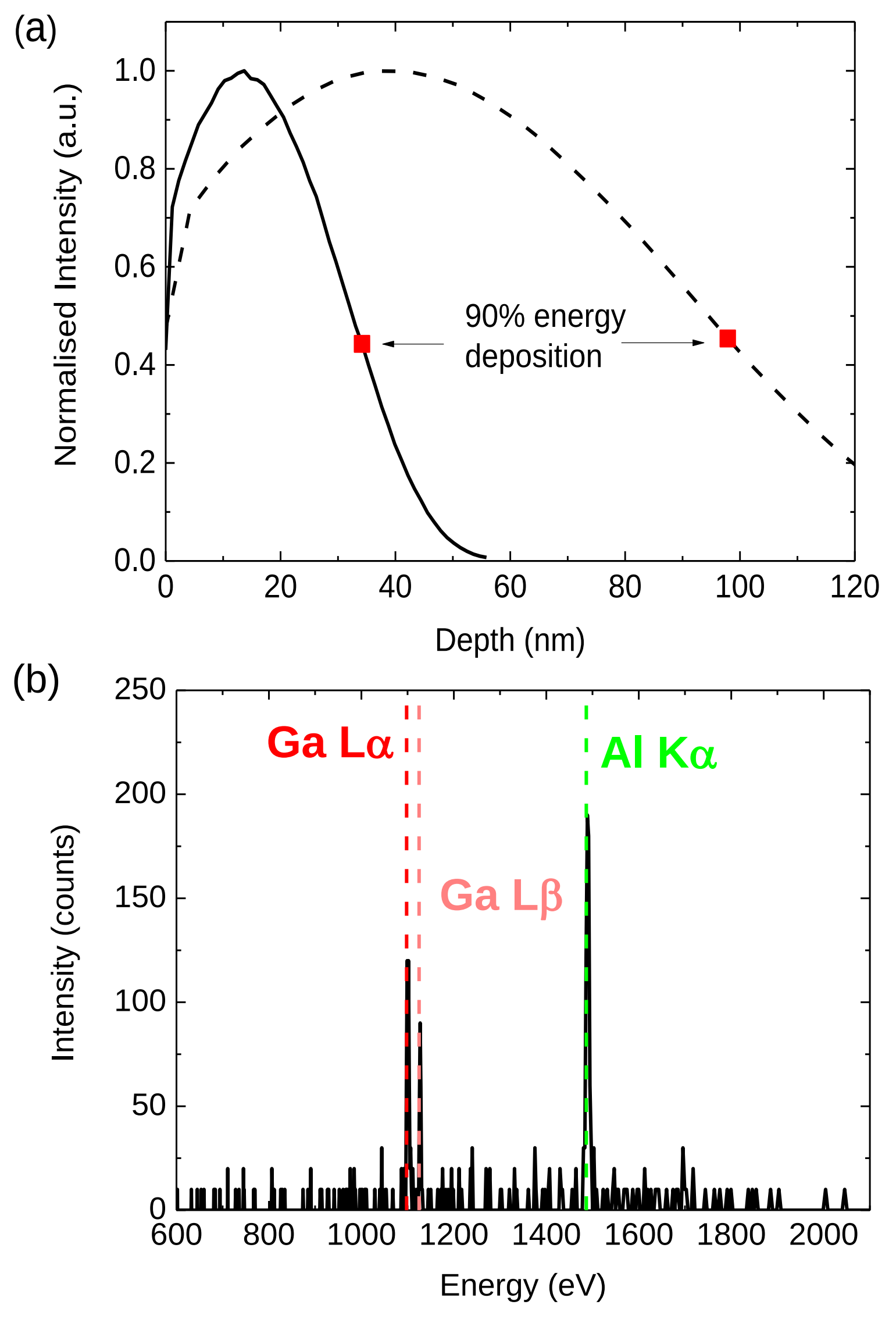

Figure 2: (a) Beam energy deposition from Monte Carlo electron trajectory simulations of 2 kV (solid line) and 4 kV (dashed line) beam energies. (b) Example WDX spectrum from the TAP crystal using a 2 kV beam showing the presence of Ga.

Compositional Results

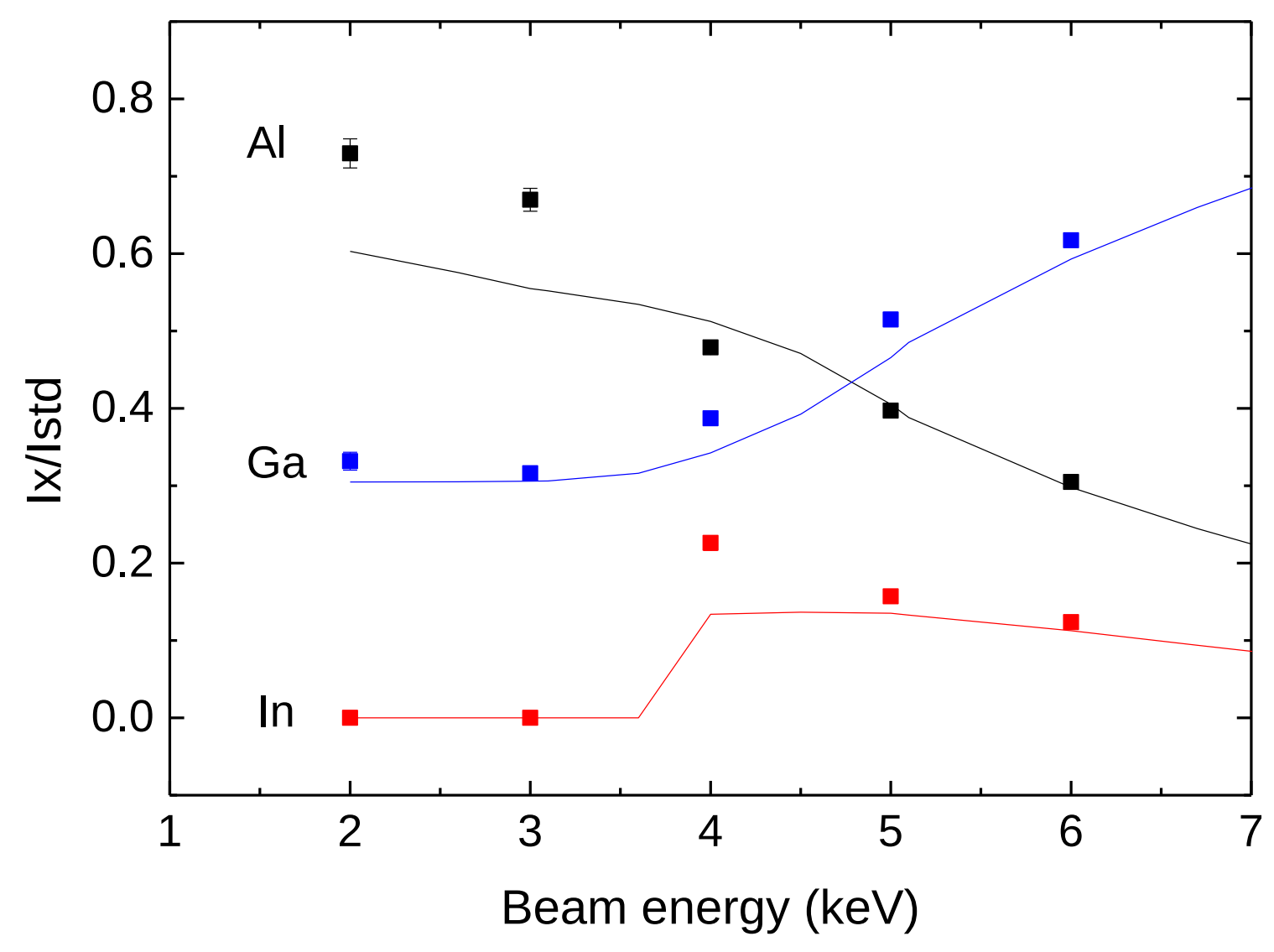

Figure 3: WDX measurement (points) and simulation (lines) of InAlGaN-GaN bilayer for sample A.

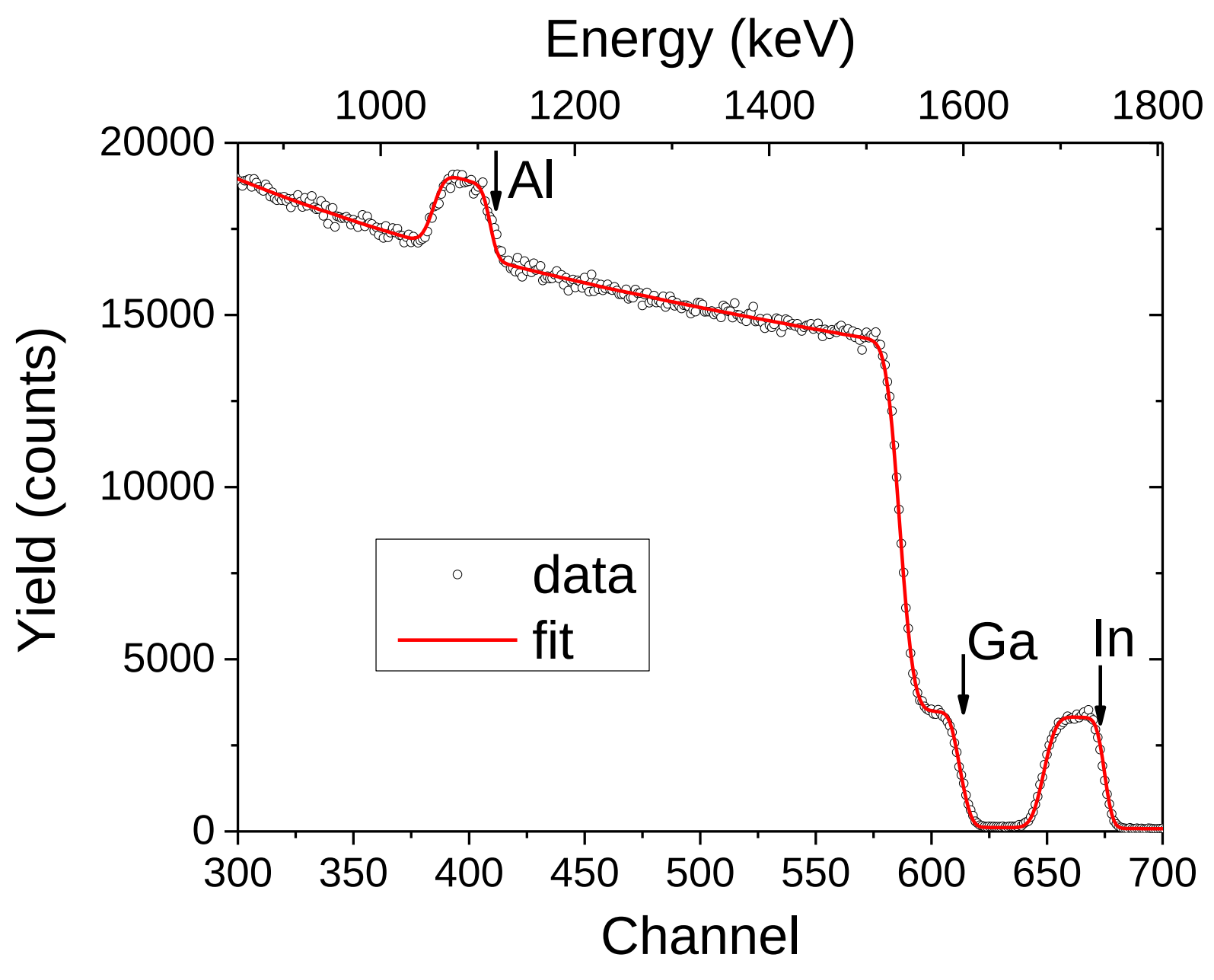

Figure 4: RBS plot of the InAlGaN layer on GaN of sample A, showing the aluminium, gallium and indium signal. Arrows indicate elements at the surface.

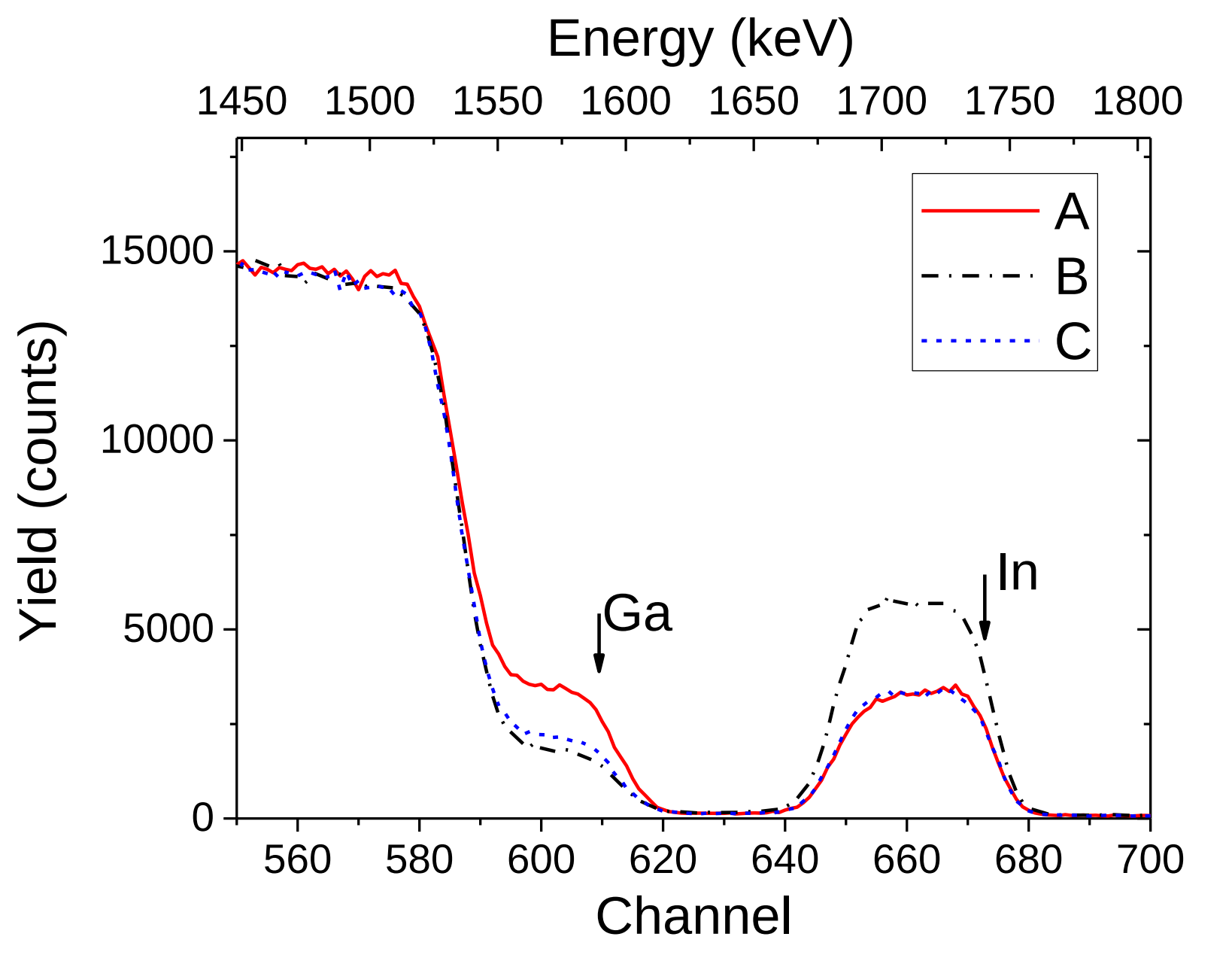

Figure 5: Measured RBS spectra of all samples highlighting the small shoulder at 1600 keV due to Ga in the top layer. Arrows indicate elements at the surface.

- WDX layers program used to determine InAlGaN layer composition by fitting simulated k-ratios (I_x/I_{std}) to measured data over a range of beam energies (Figure 3). I_x and I_{std} are the x-ray intensities of the measured sample and standard, respectively.
- RBS confirms the presence of Ga at the surface by the Ga peak around 1600 keV in Figure 4.
- All samples show the presence of Ga in the top layer with sample A having the higher Ga yield and sample B having the higher In yield (Figure 5).
- RBS composition and thickness was determined through "NDF" code fitting of the measured spectra. RBS thickness is approx 10% less than thickness determined by XRD.
- Both WDX and RBS composition results are in good agreement (Table 2).

Table 2: Composition fraction results from WDX and RBS measurements, checked for consistency by XRD. Thickness results determined by XRD and RBS.

	Sample A		Sample B		Sample C	
	WDX	RBS	WDX	RBS	WDX	RBS
AlN%	69.0	72.2	73.0	74.9	79.0	79.7
InN%	7.0	7.9	15.0	14.4	7.0	8.0
GaN%	24.0	19.9	12.0	10.7	14.0	12.3
XRD thickness (nm)	87.5		82		88	
RBS thickness (nm)	79		79		81	

Structural Results

- Reciprocal space maps (RSMs) were performed to gain further information on strain.
- All samples were found to be fully strained to the underlying GaN layer, having the same a lattice parameter as shown in Figure 6.
- The InAlGaN c lattice parameter varied across the sample set:
  - ❖ Sample A = 5.072 Å
  - ❖ Sample B = 5.116 Å
  - ❖ Sample C = 5.046 Å
- Vegards law calculation in good agreement with the RSM lattice parameter values.

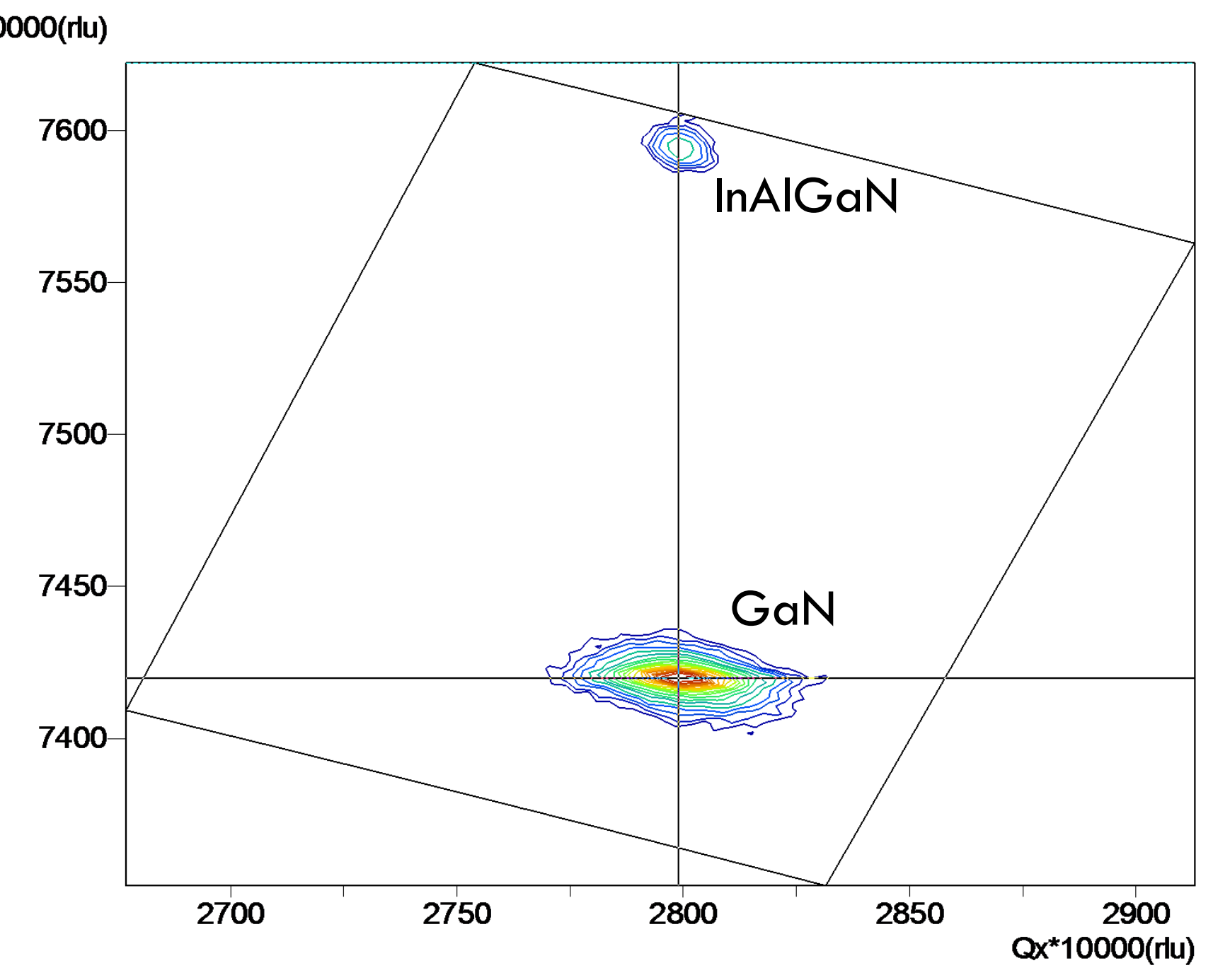

Figure 6: [105] RSM of sample A illustrating fully strained layer.

Optical Results

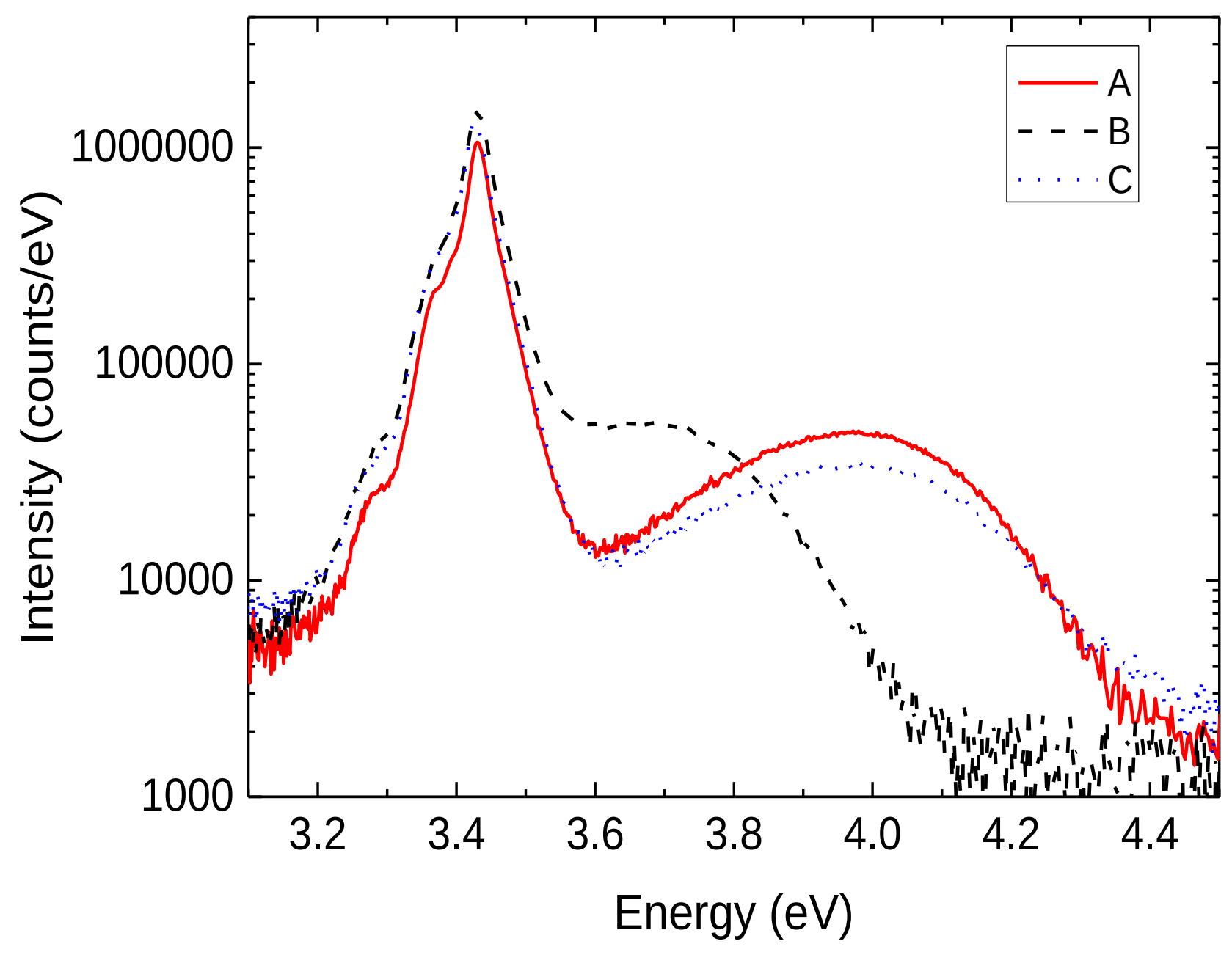

Figure 7: Mean spectra of CL maps show the InAlGaN luminescence peak.

- Optical properties were studied using CL hyperspectral mapping.
- The spectra in Figure 7 are the mean of 10^4 spectra from the mapped area.
- Strong GaN peak is evident at around 3.4 eV, which is from the underlying GaN layer.
- Broad InAlGaN luminescence peaking at around 3.7 and 3.95 eV. This luminescence is fairly uniform over the mapped area.
- Sample B is red shifted due to the higher InN content.
- GaN content has had no effect on luminescence peak energy with sample A have 10% more than sample C.

Summary

- Composition measurements confirm presence of Ga within epilayer.
- Likely cause of Ga auto-incorporation is residual Ga coming from reactor walls and delivery pipes.
- Increasing total flow rate from 8000 to 24000 sccm is seen to suppress Ga incorporation from 24 to 12 %.
- Broad luminescence peak whose peak energy varies with InN content but not GaN.

References

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