Electron Backscatter Diffraction Analysis of Tilt, Twist and Strain Variations in MOVPE GaN on Sapphire

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Introduction

Although hugely important for characterizing metallics, electron backscatter diffraction (EBSD) has not, until recently, had much uptake for characterization of semiconducting materials largely as a result of the angular resolution limit of ~0.5°(~10^{-2} rads) on lattice misorientation. The introduction of cross-correlation based analysis of EBSD patterns has seen a step change in the angular resolution to ~10^{-4} rads [1] which is sufficient to enable analysis of the much smaller misorientations and even local elastic strain fields that are more typical in semiconducting materials [2]. Measurement of tilt, twist and elastic variation in GaN layers on basal plane sapphire are reported.

Methodology

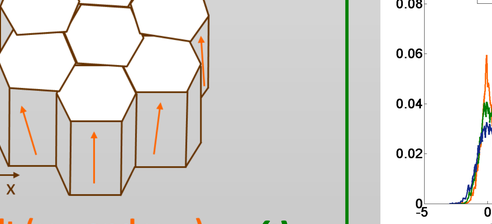

Figure 1: Schematic diagram to show the experimental set up of an EBSD system. An EBSD pattern (EBSP) image will be formed on the CCD comprising a large number of nearly straight bands termed Kikuchi bands.

EBSD mapping

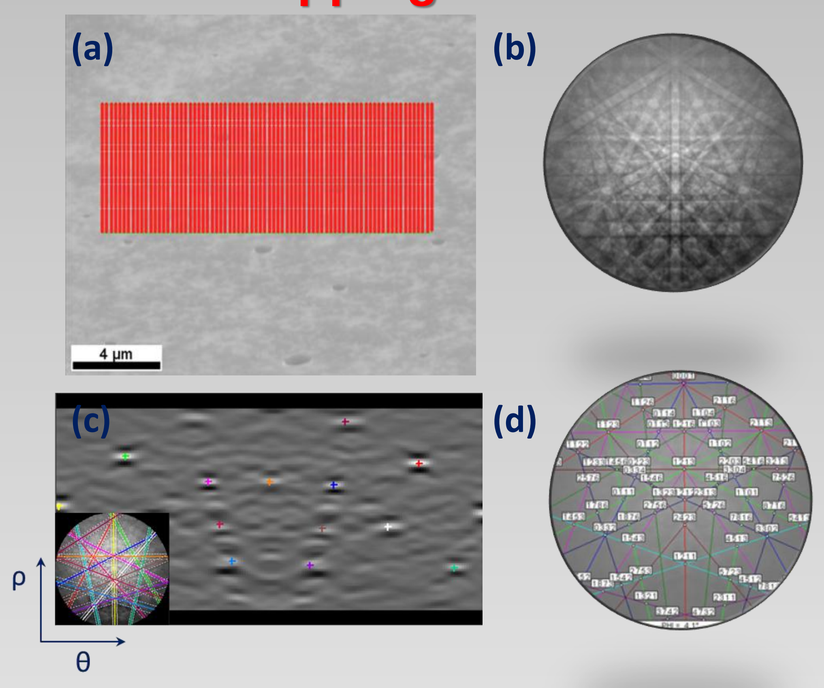

Figure 2: Overview of EBSD indexing procedure showing pattern capture through to determination of crystal orientation. (a) The beam is stepped across the sample surface in a regular grid, (b) at each point the EBSD pattern of GaN with background correction is captured, (c) Hough transform from spatial domain to Hough domain (lines are converted into peaks), (d) the pattern is indexed by looking up the reference crystallographic table [3].

Cross-correlation analysis

The shift between similar features in the EBSD pattern with respect to a reference pattern can be measured using cross-correlation based method.

Deformation maps r to r' (r' = Ar) with a displacement vector **Q**

$$Q = q + \lambda r$$

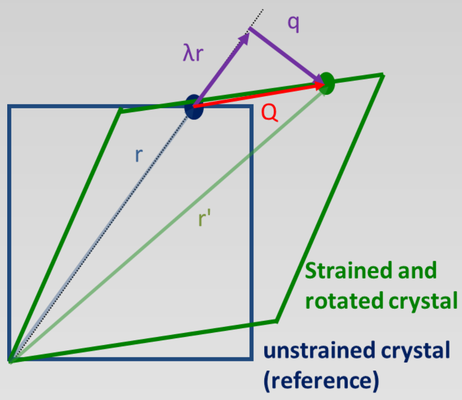

Figure 3: Schematic diagram showing how a strain and rotation (exaggerated) act to alter a zone axis direction **r** shifting across the EBSD screen by **q**.

- **q** is the perpendicular components of **Q** to r
- A is the displacement gradient tensor
- I is the identity matrix

$$\mathbf{A} - \mathbf{I} = \begin{pmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \frac{\partial u_1}{\partial x_3} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} & \frac{\partial u_2}{\partial x_3} \\ \frac{\partial u_3}{\partial x_1} & \frac{\partial u_3}{\partial x_2} & \frac{\partial u_3}{\partial x_3} \end{pmatrix}$$

- EBSD can measure components of Q that are perpendicular to r

$$q = \{A - (\lambda + 1)I\}\, r$$

measurement of q for 4 different directions, r, allows 8 of the 9 degrees of freedom in **A** to be found.

Samples

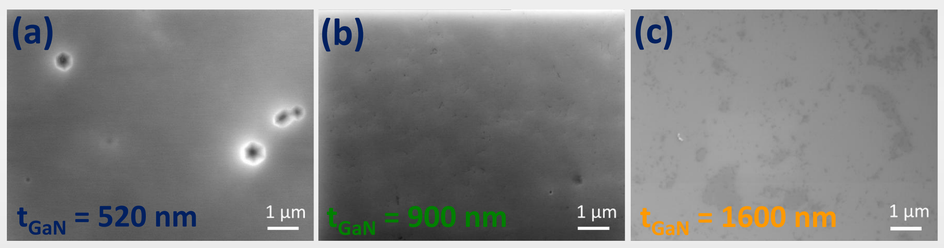

Figure 4: Top view SEM images of GaN with different thickness (t_{GaN}) grown on Al_2O_3 (a) 520 nm, (b) 900 nm and (c) 1600 nm.

Raman

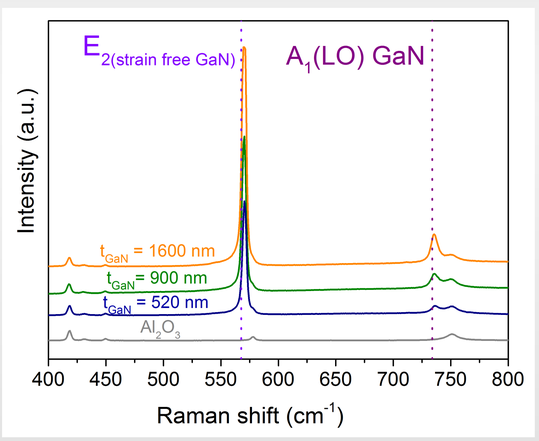

***Figure 7*:** Raman spectra for MOVPE-GaN samples. The dotted line represents the position of the strain free E_2 mode at 567.7 cm^{-1} [5]. All samples have positive Raman shift showing that they exhibit compressive in plane strain.

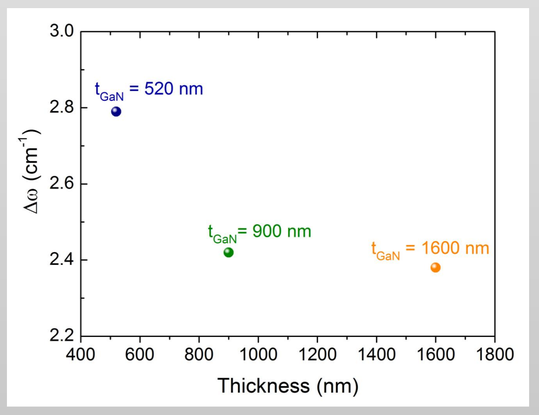

Figure 8: Raman shift evolution with the GaN layer thickness. $\Delta\omega = \omega\ E_2^{measured} - \omega\ E_2^{strain\ free}$.

Strain, twist and tilt measurements

Mosaic Model

A mosaic model is widely used to describe the epilayer microstructure in which the in-plane and out-of-plane rotations of grains are quantified by the mosaic twist and tilt, respectively [4].

Figure 5: Variation in (a) twist and (b) and (c) tilt around $[10\bar{1}0]$ and $[11\bar{2}0]$ respectively, in GaN thin films of various thickness.

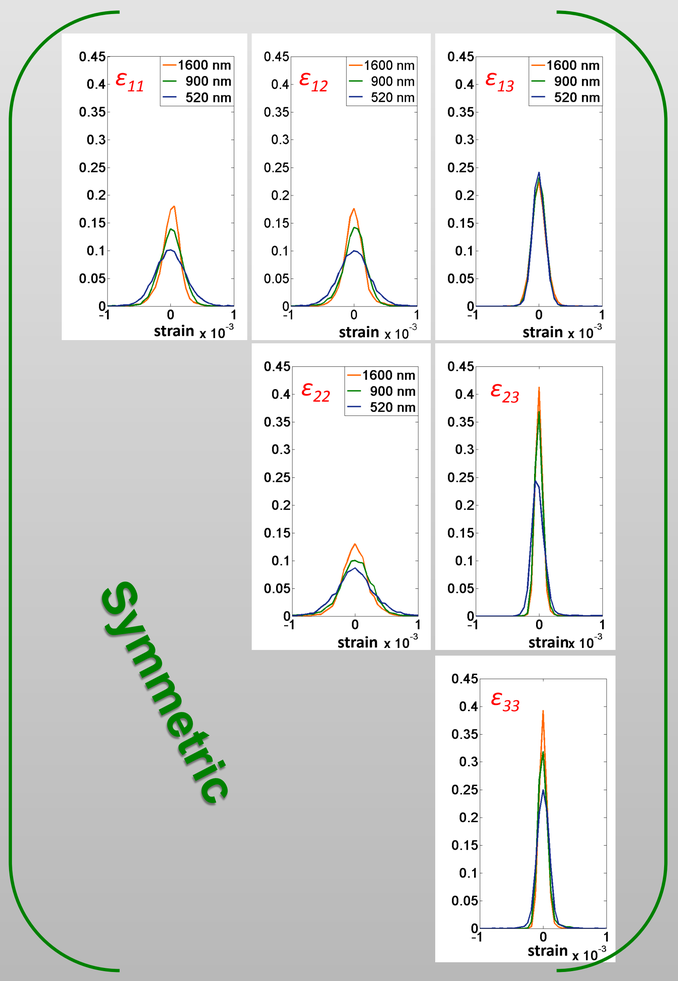

Figure 6: Variation in strain measured in GaN thin films of various thickness (520 nm, 900 nm and 1600 nm).

Results

- Maps histograms were constructed of the rotations about the surface normal (twist mosaic) and two orthogonal axes in the surface plane (tilt mosaics).
- The width of the twist mosaic was larger than the tilt mosaic and both reduced in magnitude for larger layer thickness.
- The strain variations were somewhat smaller than those for the rotations and again decreased at larger layer thickness.
- Raman indicates that the three GaN layers deposited on Al_2O_3 exhibit compressive average strain. Non-linear behavior with the thickness is exhibited for the MOVPE-GaN samples.

Reference

[1] Wilkinson AJ, Meaden G and Dingley DJ (2006) *Ultramicroscopy,* **106**, 307-313.
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[4] Chierchia R, Böttcher T, Heinke H, Einfeldt S, Figge S, and Hommel. D (2003) *J. Appl. Phys.* **93**, 8918-8925.
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Acknowledgments

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