Mapping Anti-phase Domains by Polarity Sensitive Orientation Imaging using Electron Backscatter Diffraction

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Motivation and Background

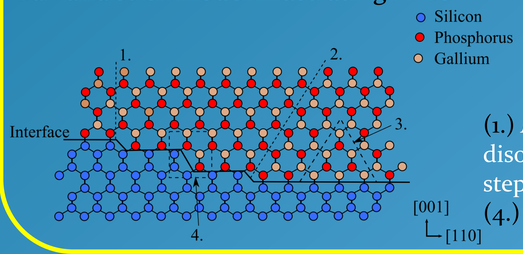
- Often extended defects such as dislocations and antiphase boundaries (APBs) are electrically active and are problematic for minority carrier devices, such as GaAs solar cells, AlGaN-based UV-LEDs, transistors and SiC power devices as well as $LaSrMnO_3$ based spintronic devices.
- Advanced structural characterisation techniques which are rapid to use, non-destructive and structurally definitive on the nanoscale are in demand, and prerequisite especially for a detailed understanding of extended-defects and their influence on the properties of materials.
- Here we demonstrate a novel application of electron backscatter diffraction (EBSD) in a field emission scanning electron microscope to image and quantify antiphase domains (APDs) on a 70 nm thick single crystalline GaP thin film grown on (001) Si substrates.

Antiphase domains in GaP.

When a non-centrosymmetric phase like zincblende GaP ($\bar{4}3m$) is epitaxially grown on a centrosymmetric phase like Si ($m\bar{3}m$), two non-equivalent and pseudo-symmetric orientations may occur although for both orientation solutions the crystal lattice shows the same ideal match.

The consequence of this is the formation of APDs and the boundary separating the pseudo-symmetric domains is called APB. In simple geometric terms, the GaP crystal appears to be rotated by 90° around [001] between the sides of the APB.

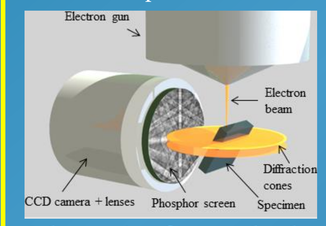
Ball and stick model illustrating APBs



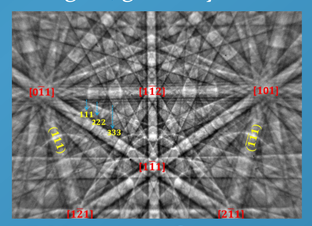
(1.) APBs parallel to (110) due to sub-lattice occupation disorder, (2.) APBs along the $\{111\}_{Si}$ due to monoatomic steps, (3.) annihilation of APBs along (111) and (110) and (4.) annihilation of APBs due to diatomic steps.

EBSD in a scanning electron microscope.

The quasi-elastically backscattered electrons produce a diffraction signal, generally referred to as a EBSD pattern [1].



Schematic of a standard EBSD detection geometry

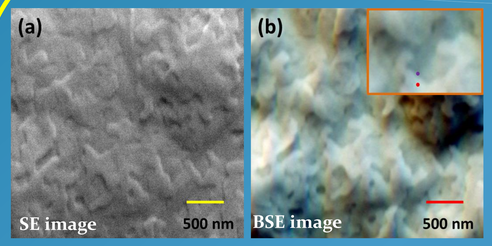


EBSD pattern from a GaP thin film.

An asymmetry in the intensity profile across a Kikuchi bands can be due to either the excess-deficiency effect or due to the breakdown of Friedel's rule for the intensity at the symmetrically located Bragg angle locations, leading to $I_{hkl} \neq I_{\overline{hkl}}$

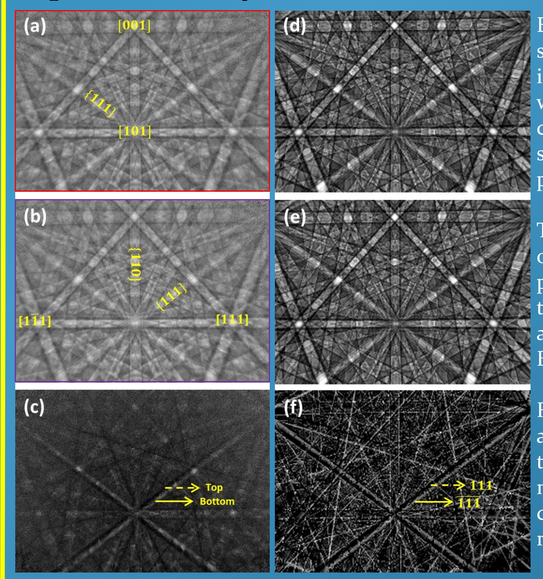
Due to asymmetric stacking sequence of Ga atoms and P atoms along ⟨111⟩ and ⟨$\bar{1}\bar{1}\bar{1}$⟩, Kikuchi bands formed from non-centrosymmetric lattice planes like {111} and {$\bar{1}\bar{1}\bar{1}$} show an asymmetry in the intensity profile (i.e. intensity maximum is marginally shifted out of the centre of the Kikuchi band which allows the observation of the inversion symmetry [2].

Results and Discussion



The red and purple dots which may well be regions with two orientations corresponding to a difference in the location of cation atoms (eg. Ga) and anion atoms (P) in the two sub-lattices.

Experiment vs Dynamical electron diffraction theory.



ESPRIT DynamicS software is used which implements the Bloch wave approach for calculating the simulated EBSD patterns.

The crystal orientations were parameterised using the ZXZ-type Euler angles (ψ_1, ϕ, ψ_2) in the Bunge convention.

For quantifying the agreement between two EBSD patterns, the normalised cross-correlation coefficient, r [2] is used.

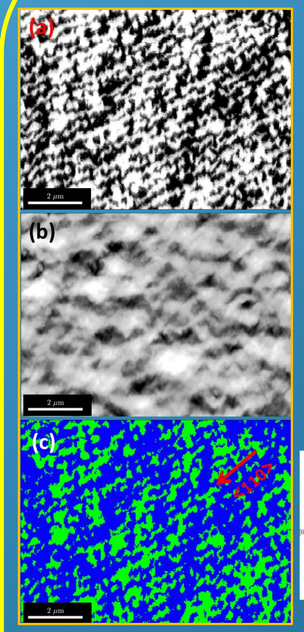
(a) Experimental EBSD pattern from the red dotted area, (for e.g.; the location of cation (Ga) atoms), with r = 0.627 and ϕ_2 = 180.9 ° and **(b)** from the purple dotted area (for e.g.: P site with r = 0.627 and ϕ_2 = 270.9 °) and **(d & e)** the corresponding dynamical simulations. **(c)** Normalised difference intensity image $(I_a\text{-}I_b)/(I_a\text{+}I_b)$ of the two experimental patterns and **(f)** normalised difference intensity image of the two simulated patterns.

Values of r > 0.6 like those observed in this study indicate convincing fits between the experimental and simulated EBSD patterns.

The strong asymmetric intensity difference between the {111} and {$\bar{1}\bar{1}\bar{1}$} in the normalised difference intensity images clearly indicates the crystal structure rotation by 90° confirming the presence of APDs in the GaP thin film.

Please note the reliable discrimination of the Kikuchi bands intensity asymmetry is only possible when the intensity shift due to the breakdown of Friedel's rule is considerably larger than the excess-deficiency effect [3].

Imaging antiphase domains.



(a) Region of interest asymmetry imaging from the {111} bands produced from the background corrected EBSD patterns. The bright and dark regions indicate the two different pseudo-symmetric domains.

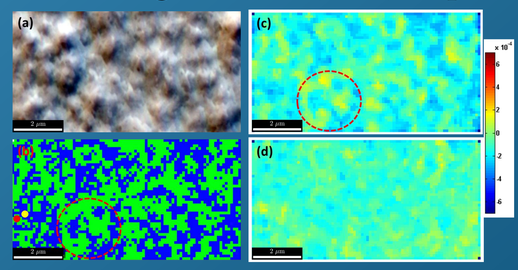
(b) Corresponding total intensity image of the raw EBSD patterns

(c) The EBSD inverse pole figure (IPF) map for the sample reference direction [1,1,1] revealing the APDs. Regions with APDs are coloured green and blue according to the IPF colour key, which indicates the expected 90° misorientation between the two possible domains.

The percentage of APDs from a scanned area of ≈ 75 μm², accounts for ≈ 50 %.

The density of the APBs is estimated to be ≈ 2.6 μm⁻¹.

Comparison of IPF maps with cross correlation based Mean Angular Error (MAE) maps.



(a) Forescatter image, **(b)** IPF map, **(c)** MAE (in radians) map plotted with green area in the IPF as a reference pattern, see red dot and **(d)** MAE map with blue area as the reference pattern, see yellow dot.

Summary and Conclusion

- We have used automatic pattern matching approach to quantify and image APDs by using the asymmetrical intensity associated with the EBSD patterns .
- We have also tested our approach on GaP samples grown on different Si substrates with and without APDs to show the reliability of our method on imaging APDs.
- The proposed analysis may well be generally applied for a wider range of other materials possessing non-centrosymmetric point groups (e.g.. GaN, SiC and ZnO).

References.

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