

X-ray diffraction studies of GaN p-i-n structures for high power electronics



ENGINEERING
HONORS PROGRAM
UNIVERSITY OF MICHIGAN

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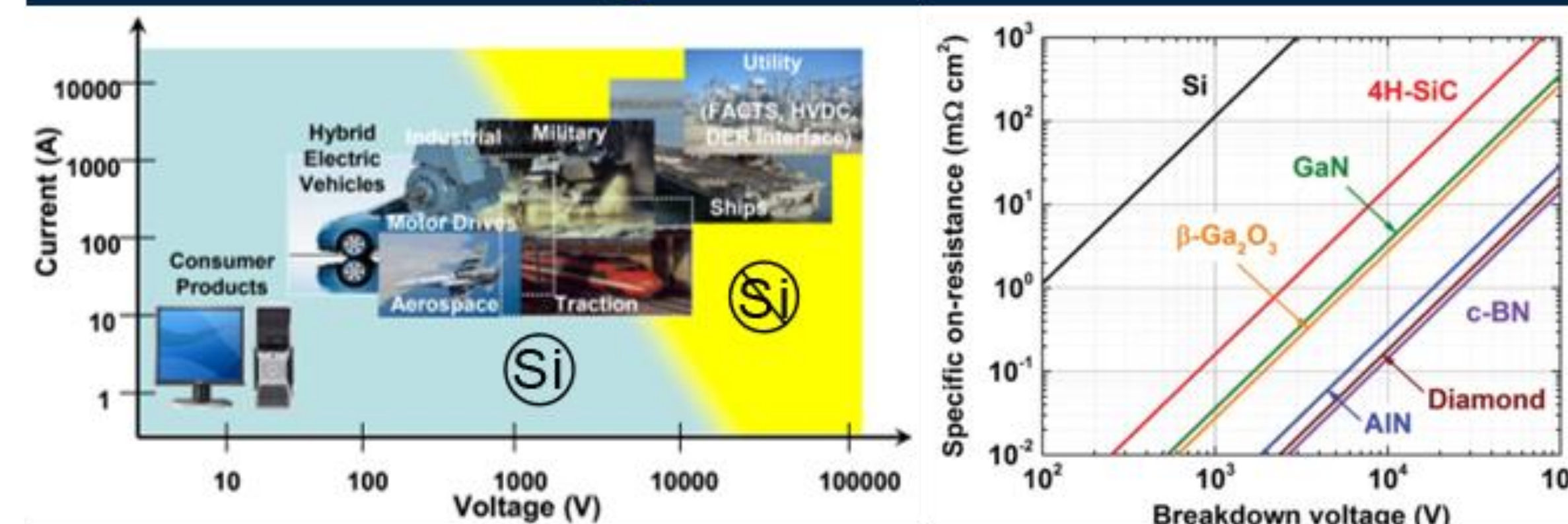
³Department of Electrical Engineering, Yale University, New Haven, CT 06520, USA



Introduction

Although Si-based electronics are used to power light-emitting diodes and electric vehicles, their utility in high power applications is limited by a low breakdown voltage. The most promising alternative power devices consist of vertical GaN devices, which often require regrown active regions. Here, we report on x-ray diffraction studies of the crystallinity of the GaN p-i-n structures prepared with and without ex-situ ambient exposure and/or chemical etching.

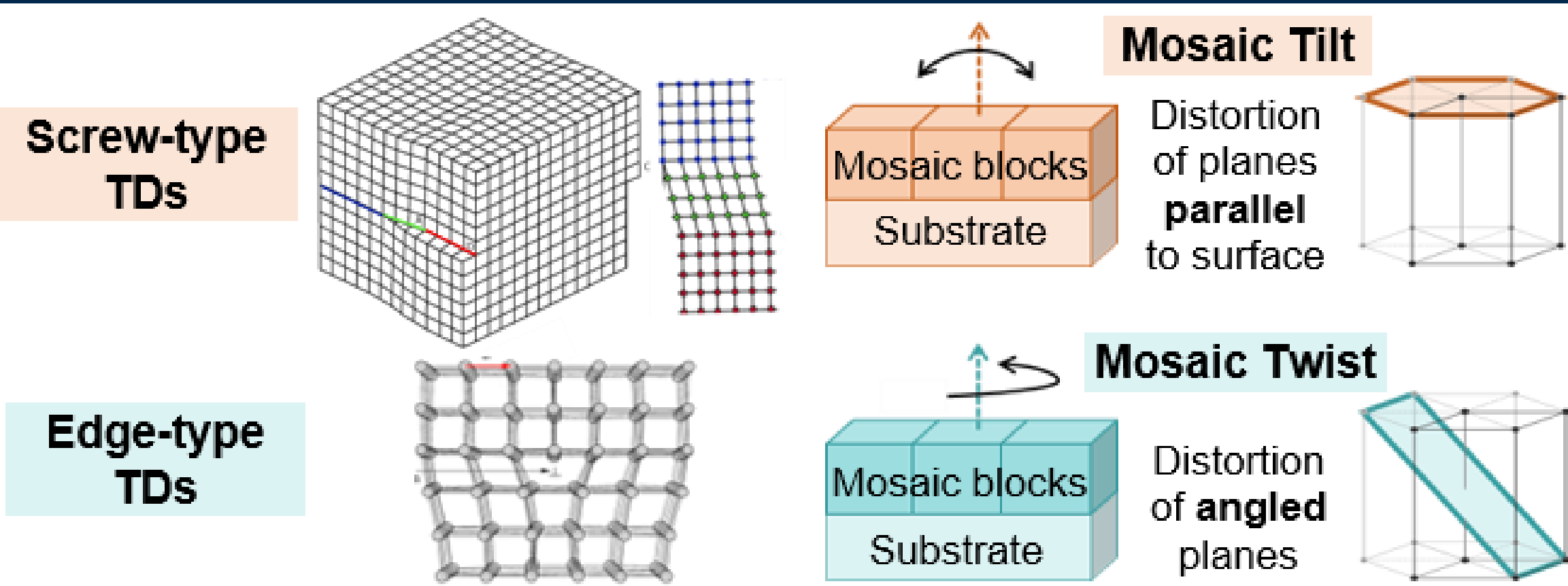
GaN for High Power Electronics



- Blue: LEDs and electric vehicles utilize silicon-based power electronics [1].
- Yellow: Power transmission and distribution require alternative approaches [1].

GaN outperforms Si, SiC with low on-resistance and high breakdown voltage [2].

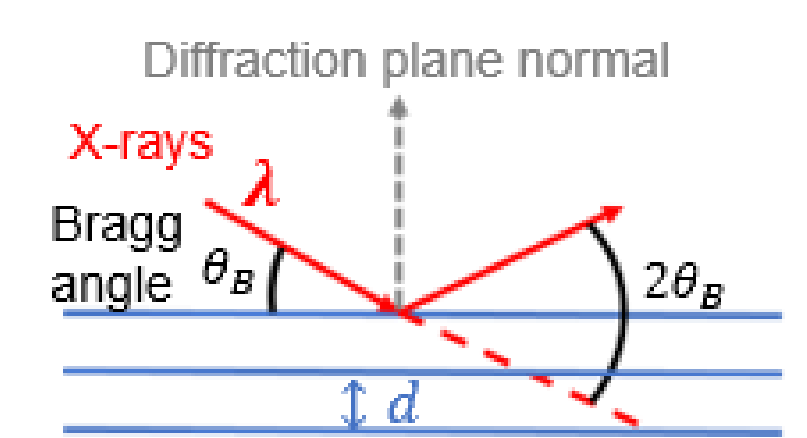
Threading Dislocations (TDs)



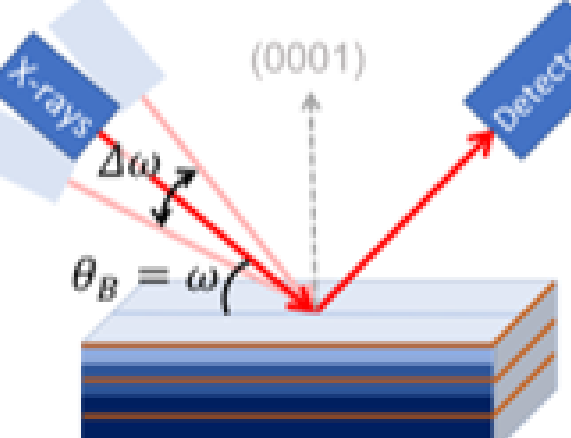
How can we quantify screw- and edge-type dislocation densities?

High Resolution X-ray Diffraction (HRXRD)

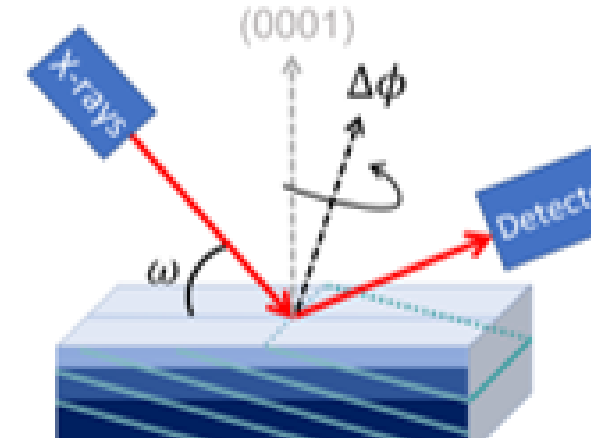
Bragg's Law: $n\lambda = 2d\sin\theta_B$



Symmetric $\Delta\omega$ RC



Asymmetric $\Delta\phi$ RC



Pseudo-Voigt Analysis of HRXRD

$$P(x) = I_0[\eta C(x) + (1 - \eta)G(x)]$$

$$L_{||} = \frac{0.9\lambda}{\beta_{\omega}(0.017475 + 1.50048\eta - 0.534156\eta^2)\sin(\theta_B)}$$

$$\alpha_{\omega} = \beta_{\omega}[0.184446 + 0.812692(1 - 0.998497\eta)^{1/2} - 0.659603\eta + 0.44554\eta^2]$$

- $P(x)$ Pseudo-Voigt function
- $C(x)$ Cauchy profile
- $G(x)$ Gaussian profile
- η Fitting parameter
- $L_{||}$ Lateral correlation length
- $\Delta\omega$ rocking curve FWHM
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- α_{ω} Mosaic tilt angle
- b_s Screw TD Burger's vector
- α_{ϕ} Mosaic twist angle
- b_e Edge TD Burger's vector

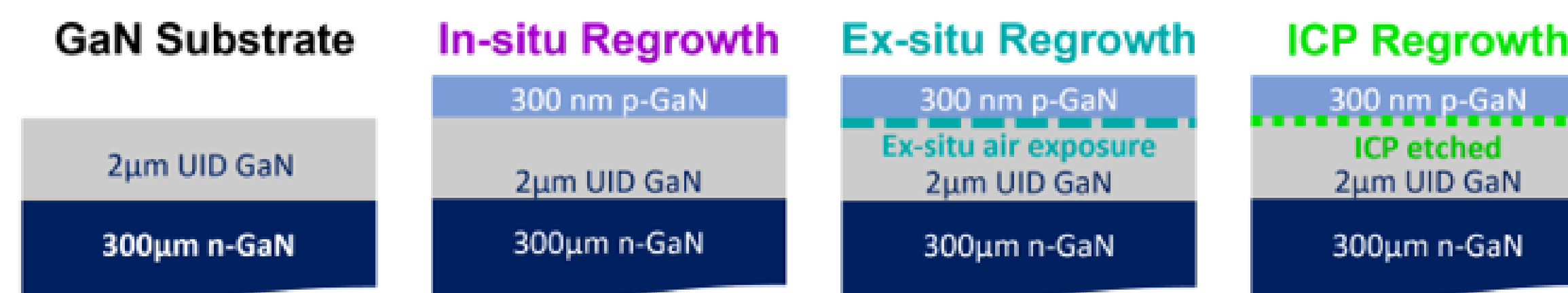
Screw TD density

$$N_s = \frac{\alpha_{\omega}^2}{2\pi b_s^2 \ln 2}$$

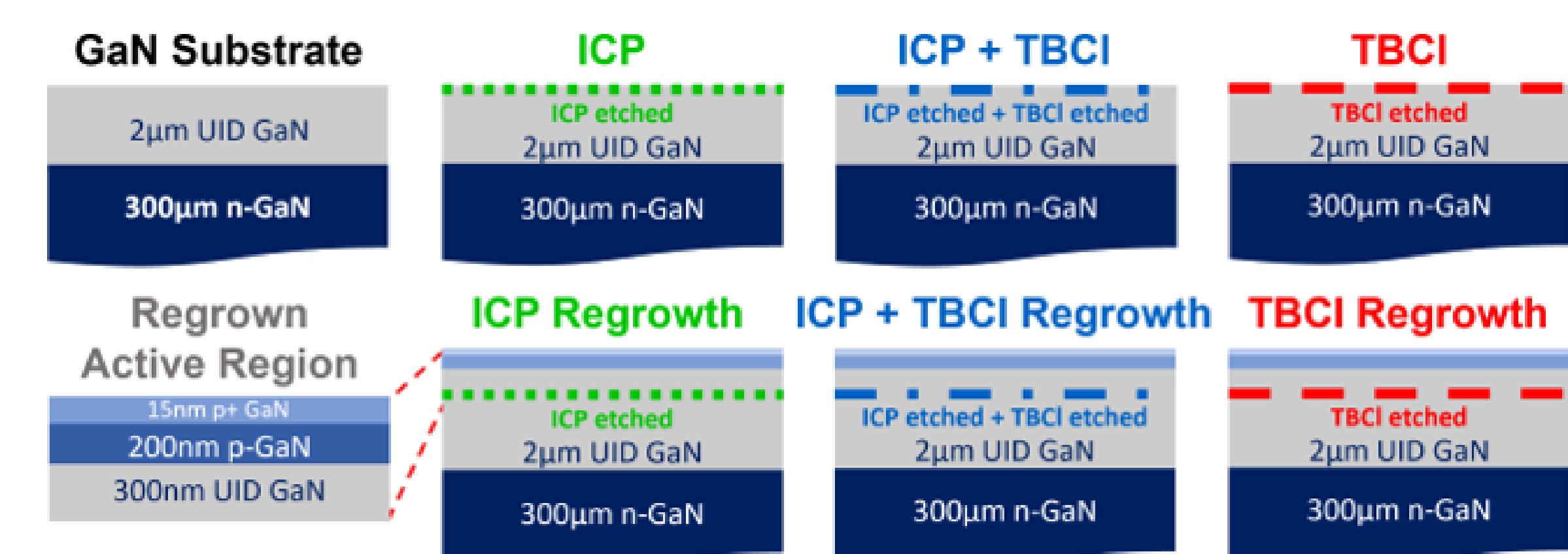
Edge TD Density

$$N_E = \frac{\alpha_{\phi}}{\sqrt{2\pi \ln 2} |b_E| L_{||}}$$

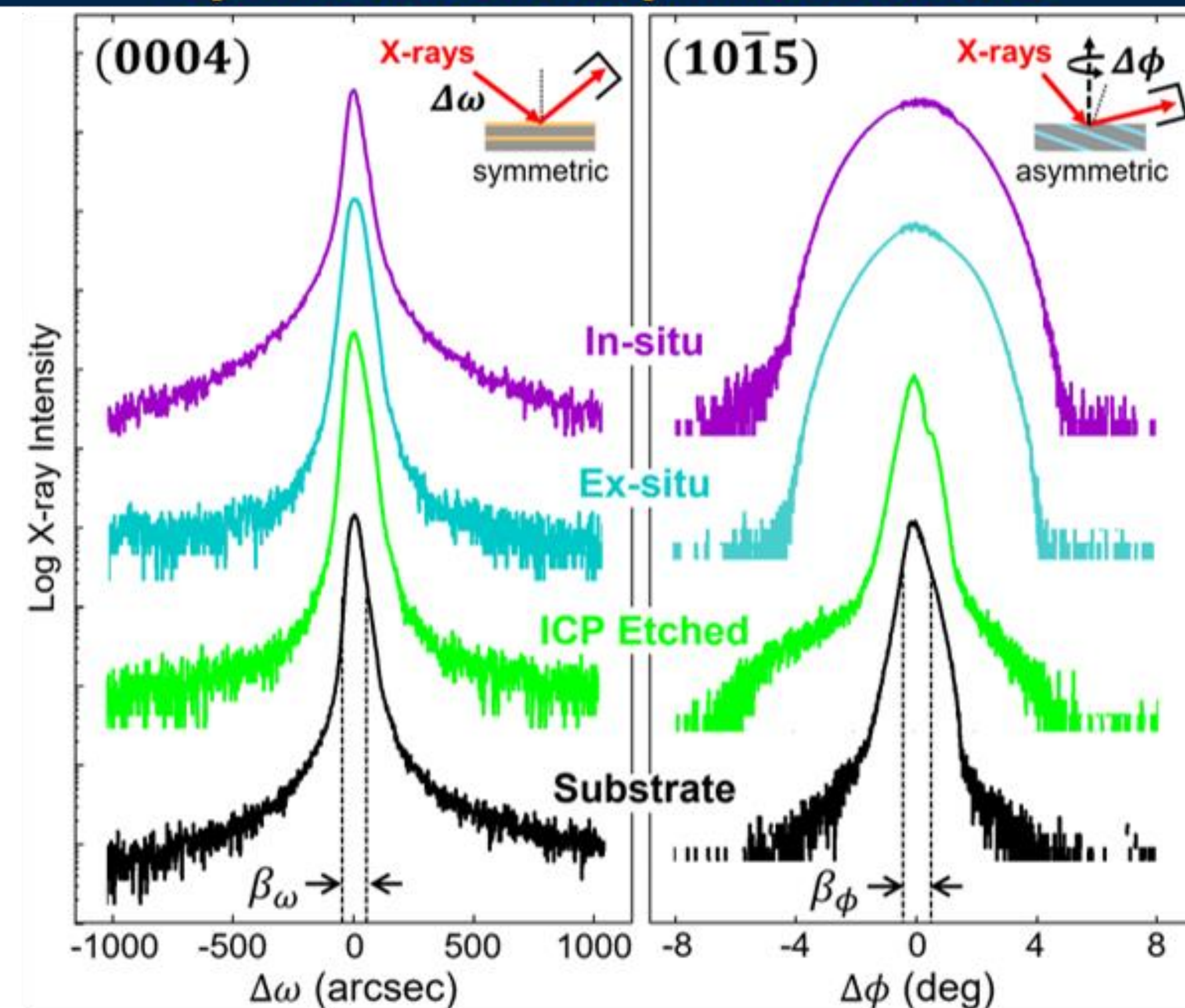
Regrowth Interface at p-n Junction



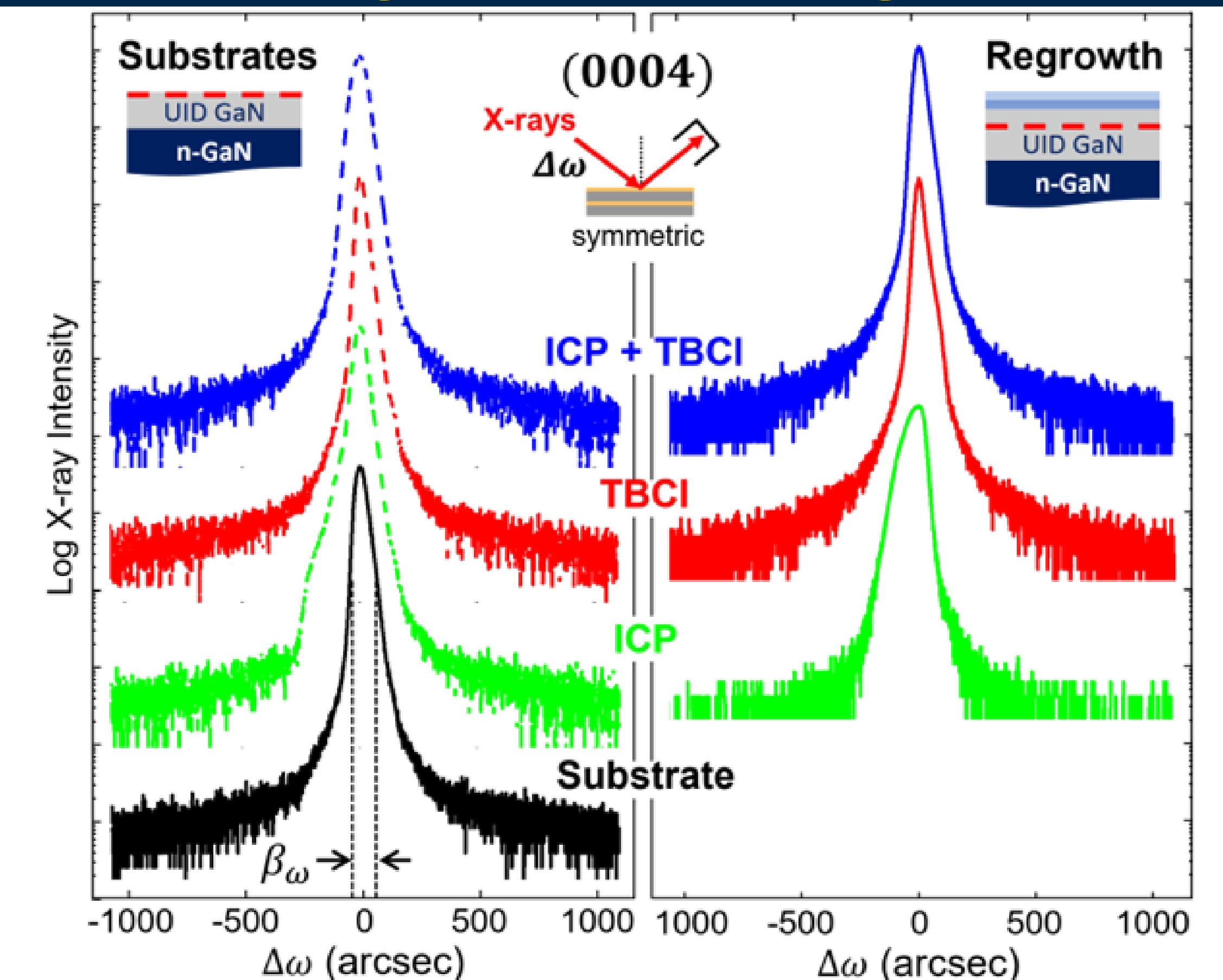
Regrowth Interface in UID Layer



Symmetric and Asymmetric Scans



Symmetric Scans Only



Structure & Electronic Properties Correlation

Sample	$\delta\omega$ (arcsec)	η (from $\Delta\omega$)	α_{ω} (10^{-4} rad)	N_s (10^8 cm $^{-2}$)	$L_{ }$ (μ m)	$\delta\phi = \alpha_{\phi}$ (10^{-4} rad)	N_E (10^8 cm $^{-2}$)
In-situ	52	0.428	1.5	1.9	1.7	528	47.5
Ex-situ	68	0.033	3.2	8.6	11	454	6.4
ICP Etched	59	0.229	2.2	4.2	2.4	102	6.2
Substrate	50	0.222	1.9	3.1	3.0	108	6.3

Probing the structure with XRD & RBS

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ICP + TBCI Regrowth	47	0.287	1.6	2.3	2.5		
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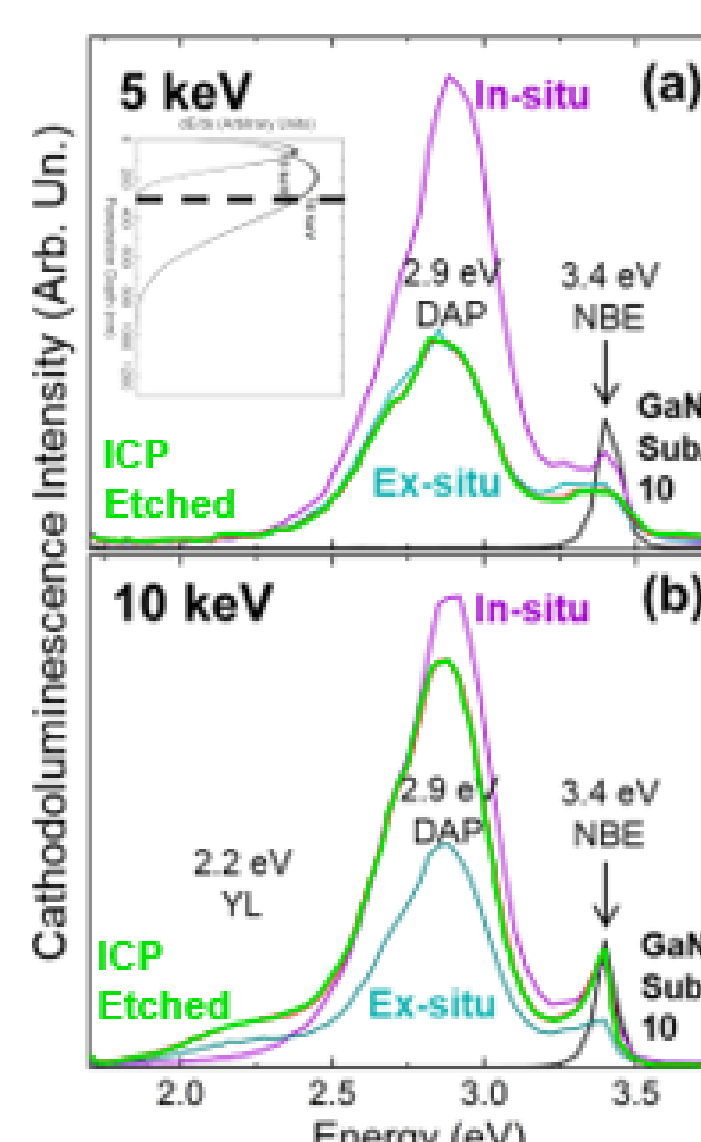
Probing the structure using XRD:

- Ex-situ and ICP Etched had the largest screw-type TD densities
- In-situ had the lowest screw-type TD density and the highest edge-type TD density

Probing electronic properties using cathodoluminescence

- Donor acceptor pair emission (DAP) near the surface is lowest for Ex-situ and ICP Etched
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Ambient air exposure worsens crystallinity and electronic properties, but ICP etching can partially restore the electronic properties.



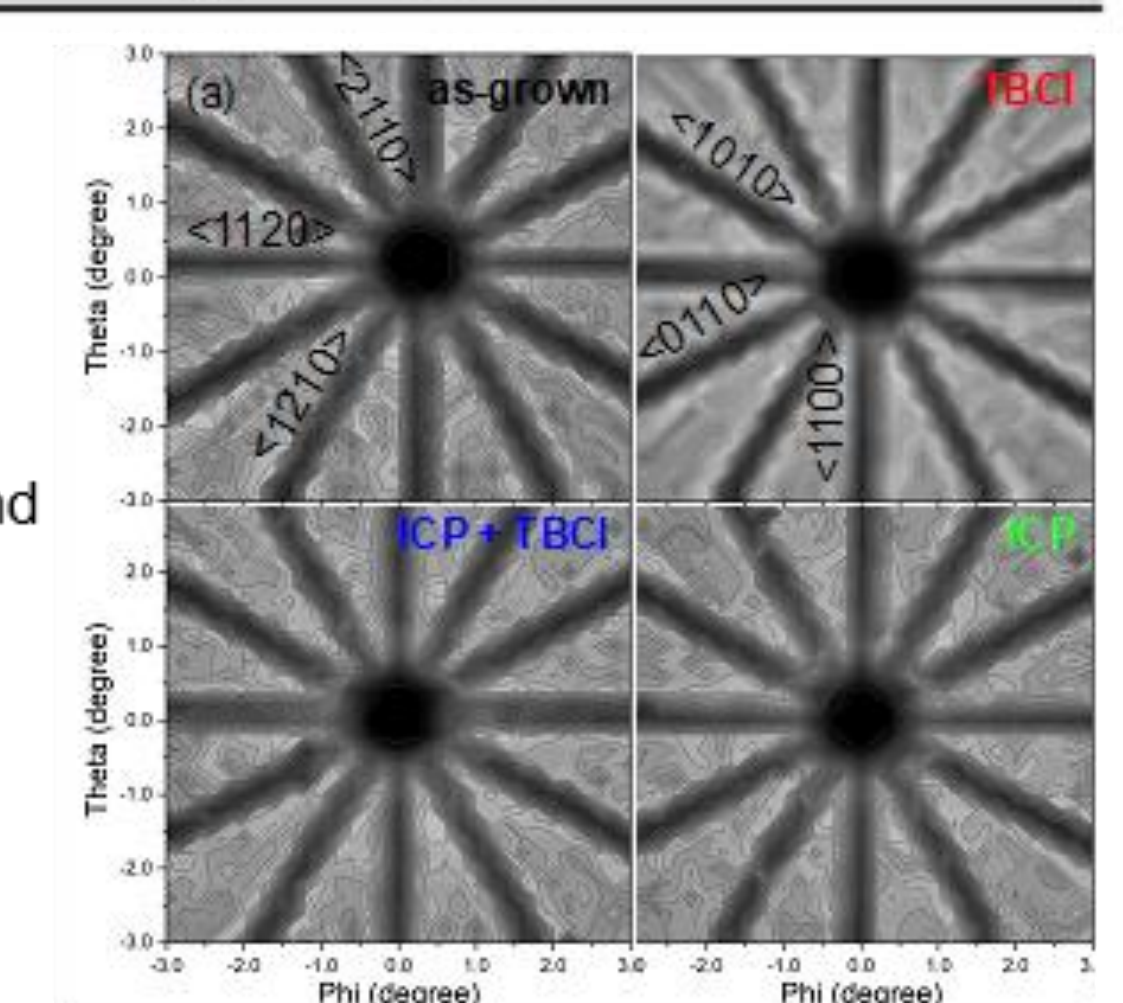
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Rutherford backscattering (RBS)

- RBS channeling maps allow us to determine the fraction of displaced Ga and N atoms
- ICP and ICP Regrowth had the largest fraction of displaced Ga and N atoms

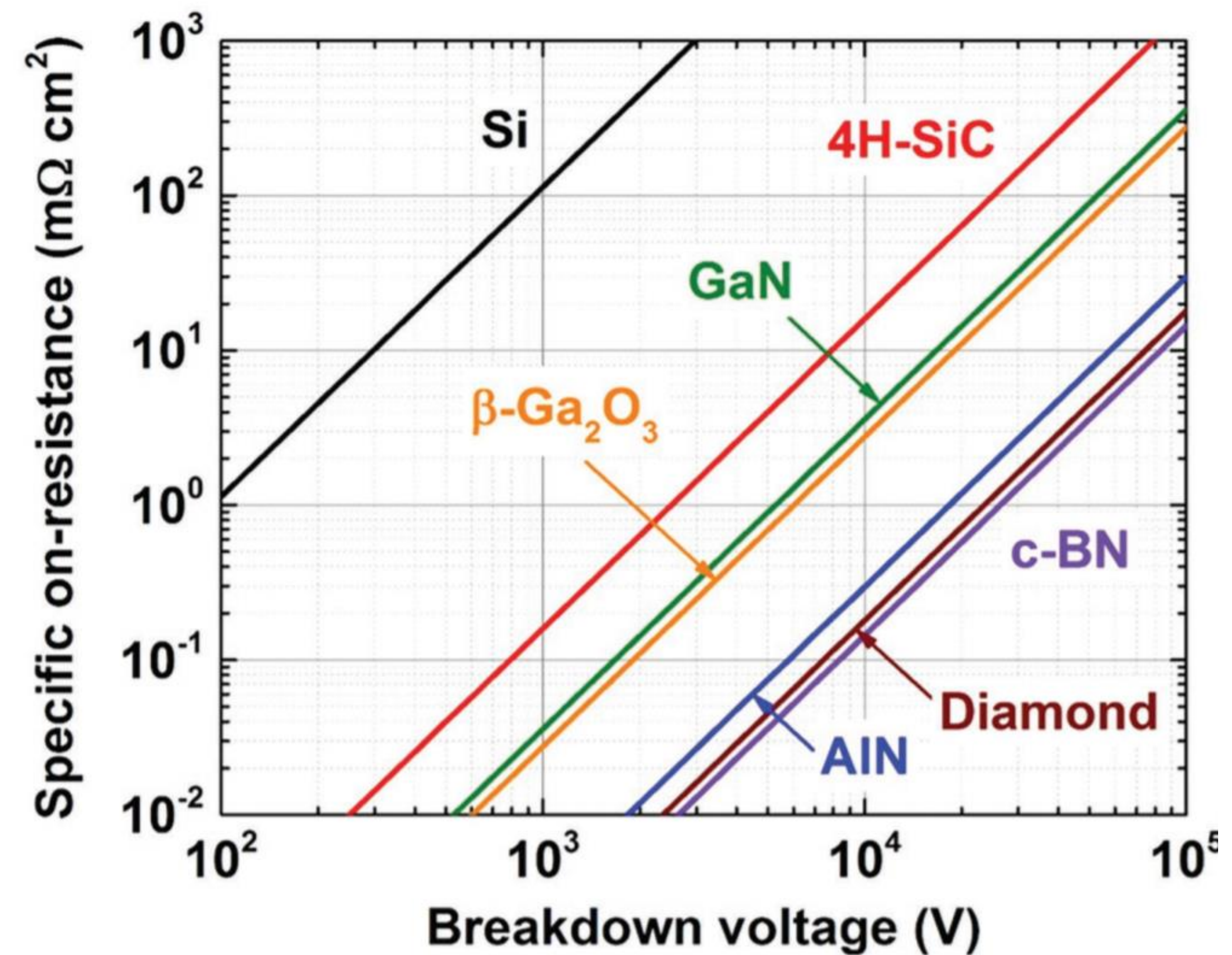
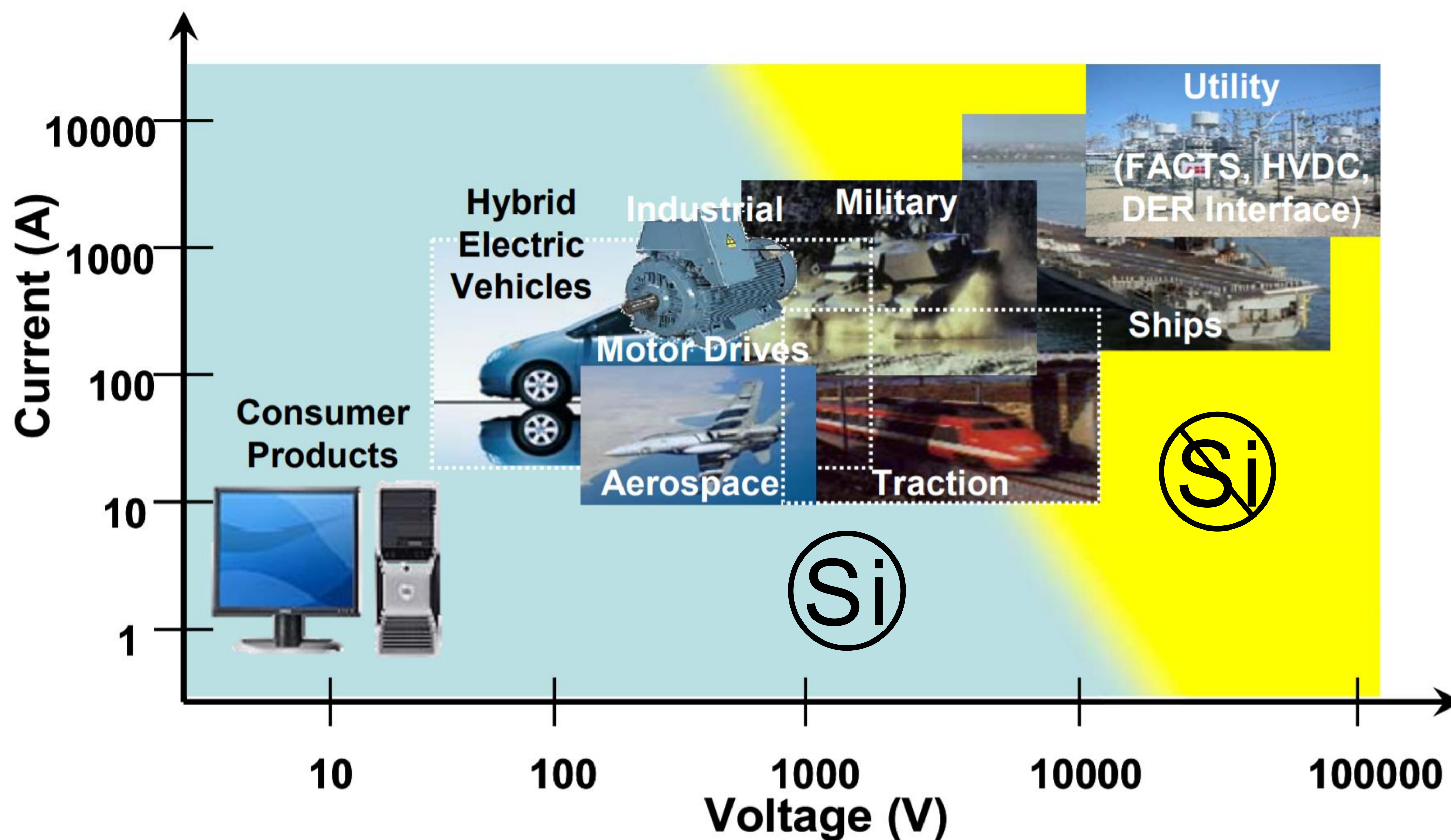
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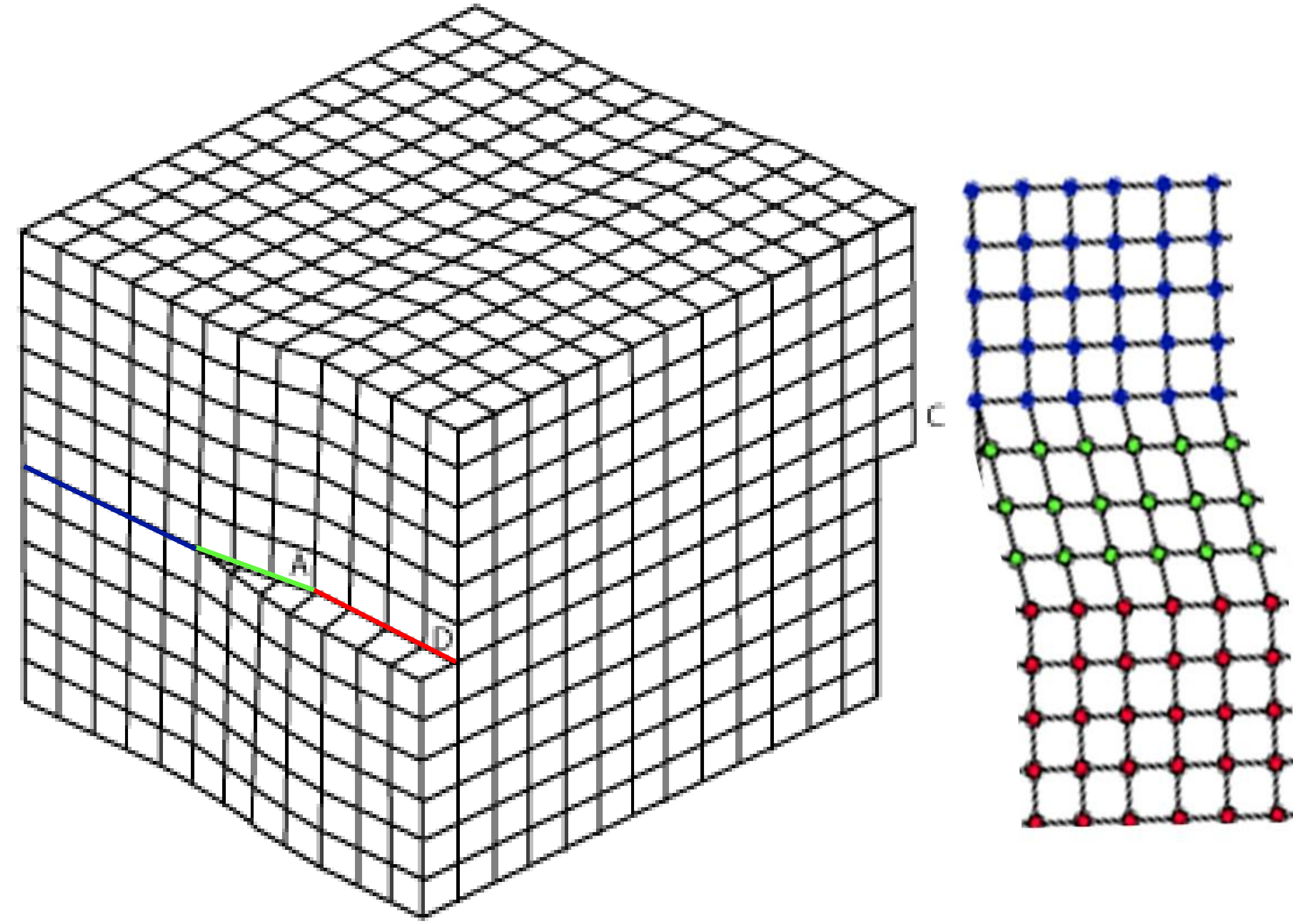


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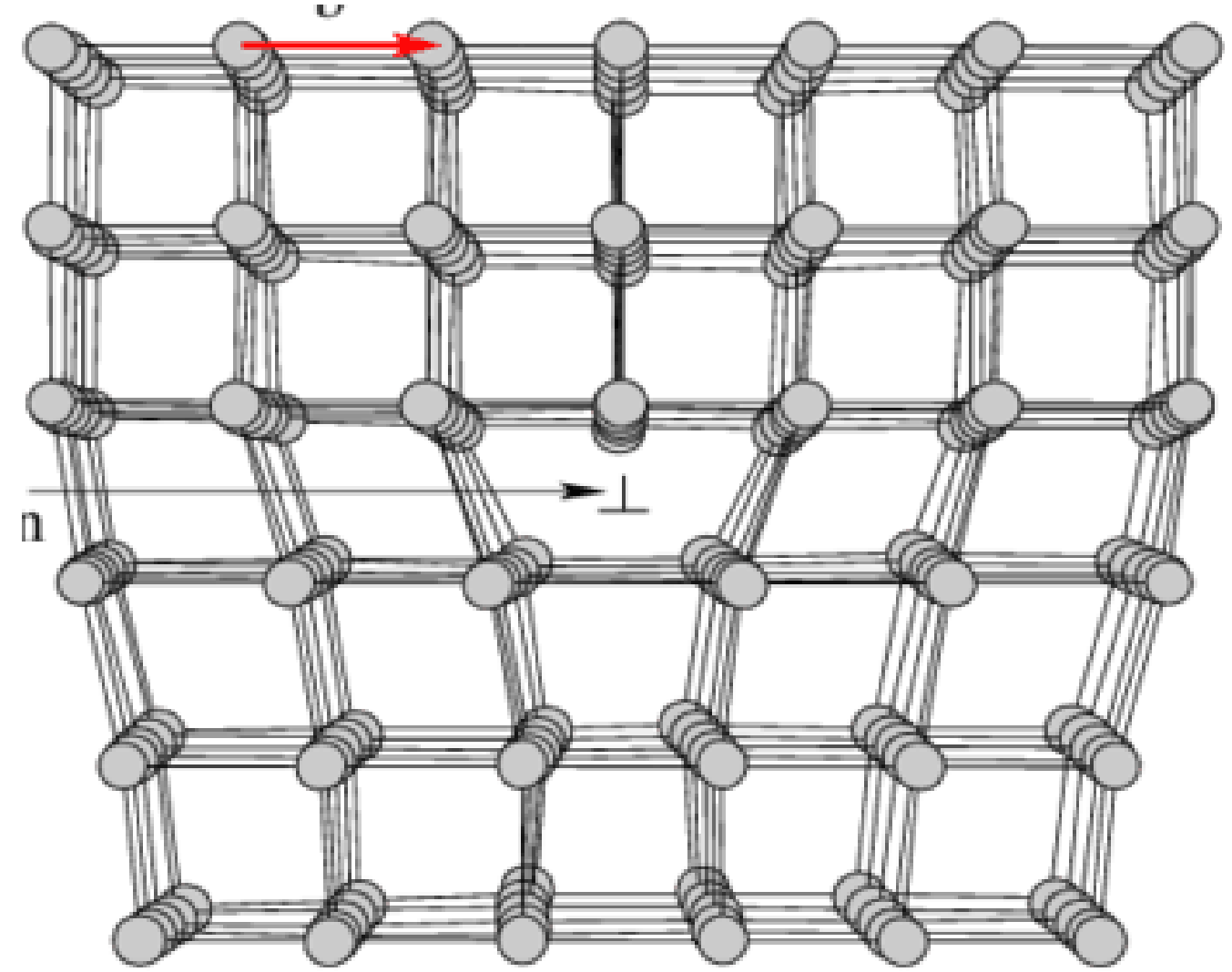
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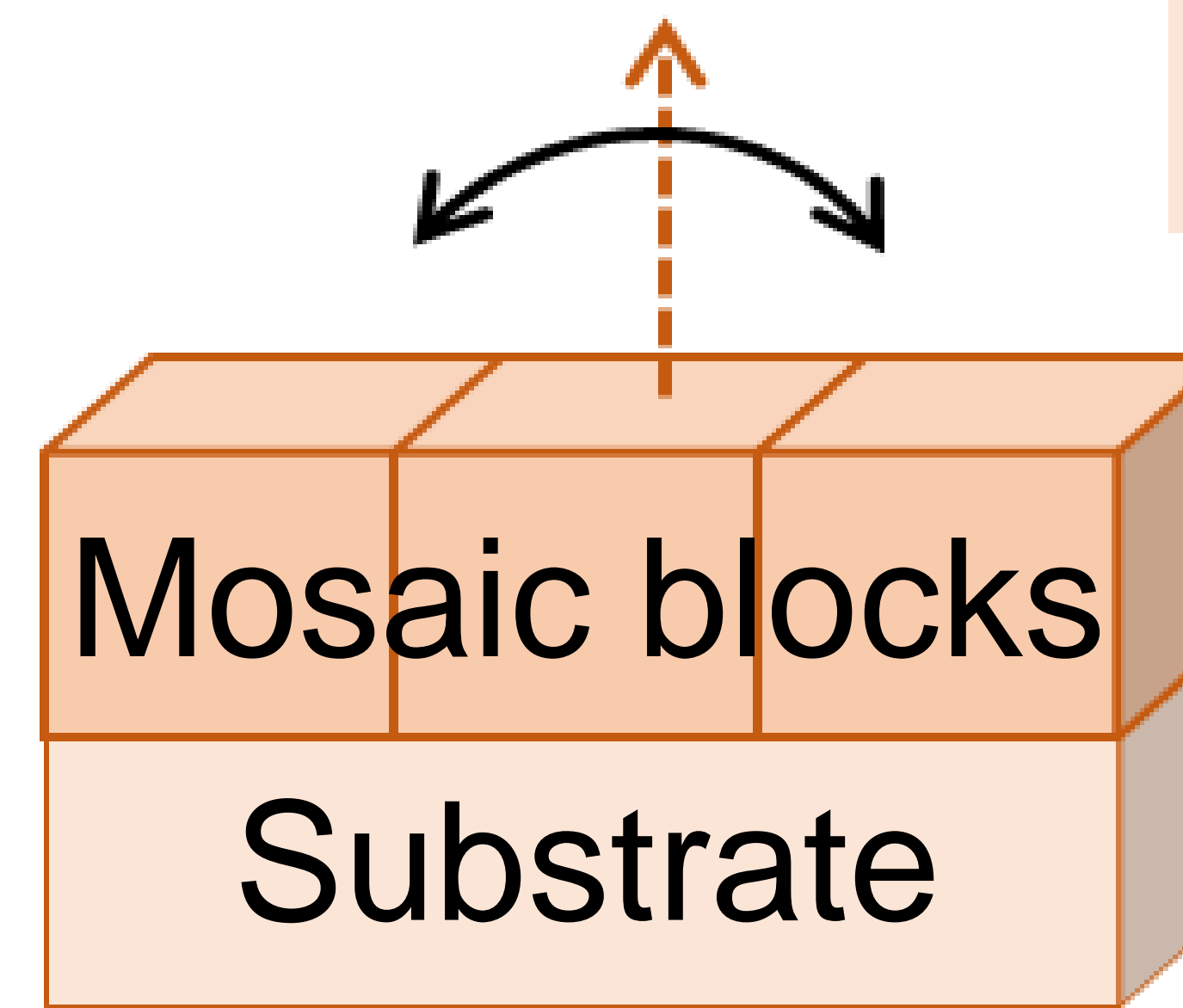
Screw-type TDs



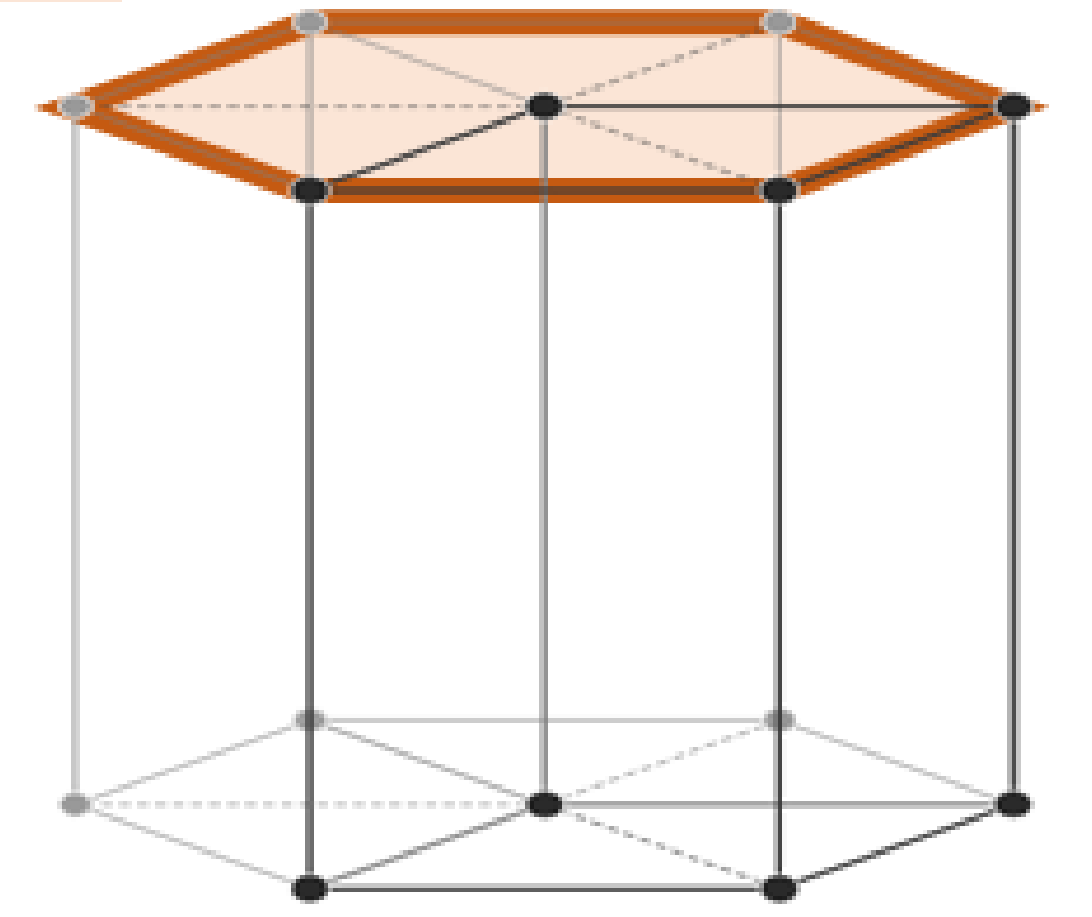
Edge-type TDs



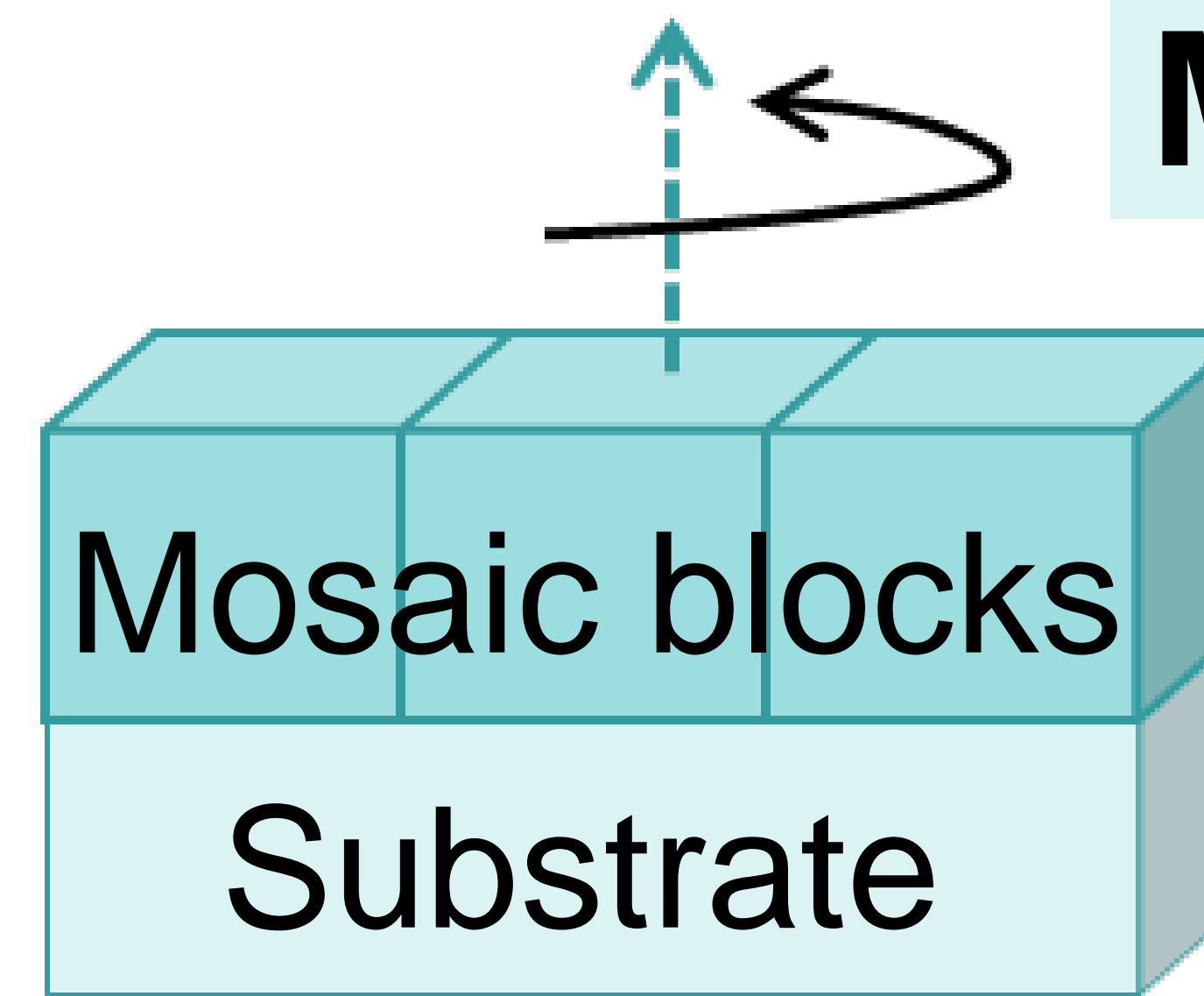
Mosaic Tilt



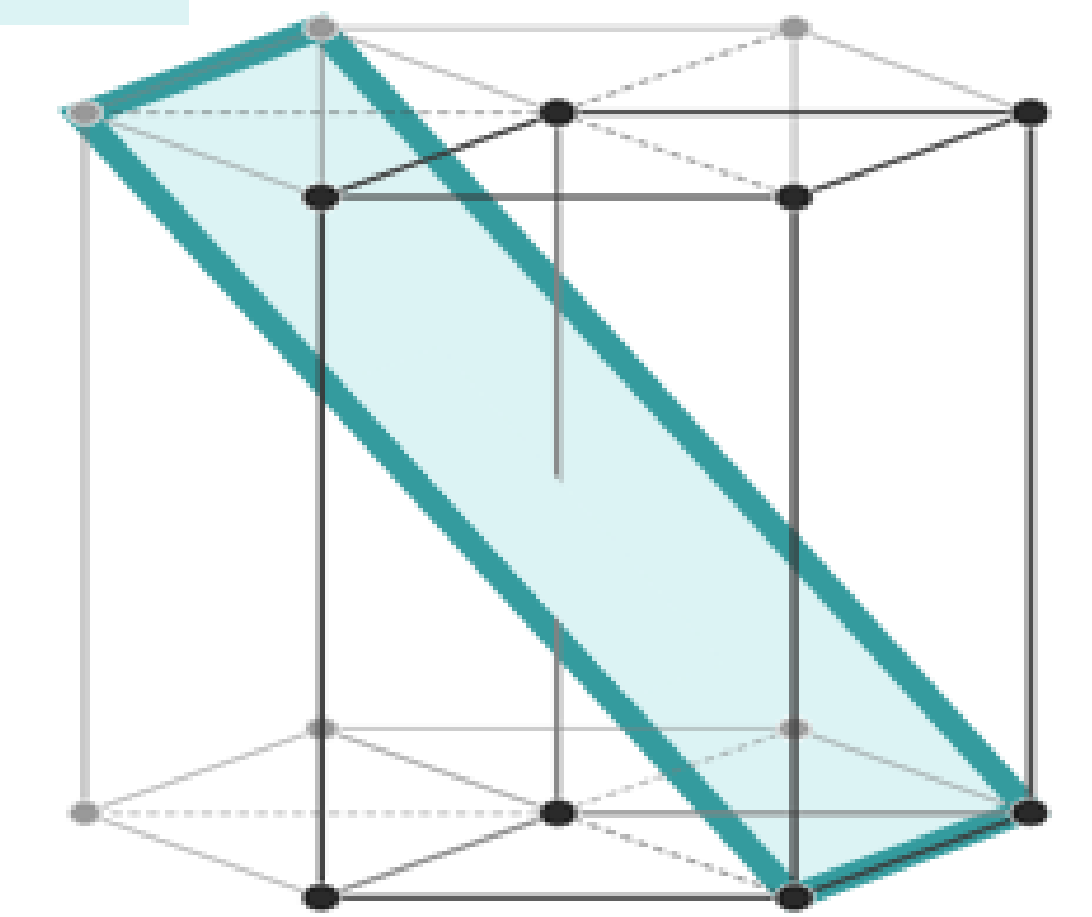
Distortion of planes **parallel** to surface



Mosaic Twist



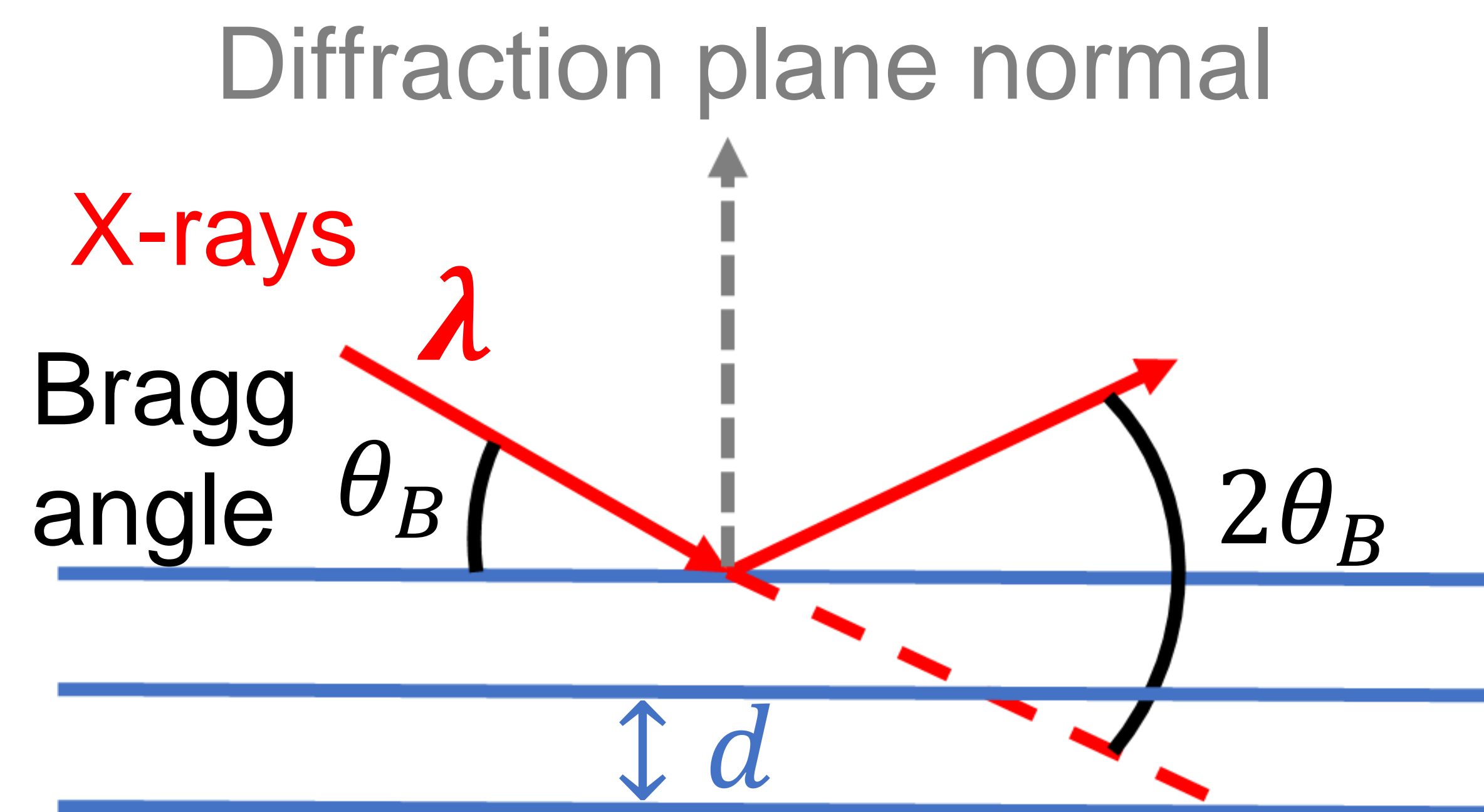
Distortion of **angled** planes



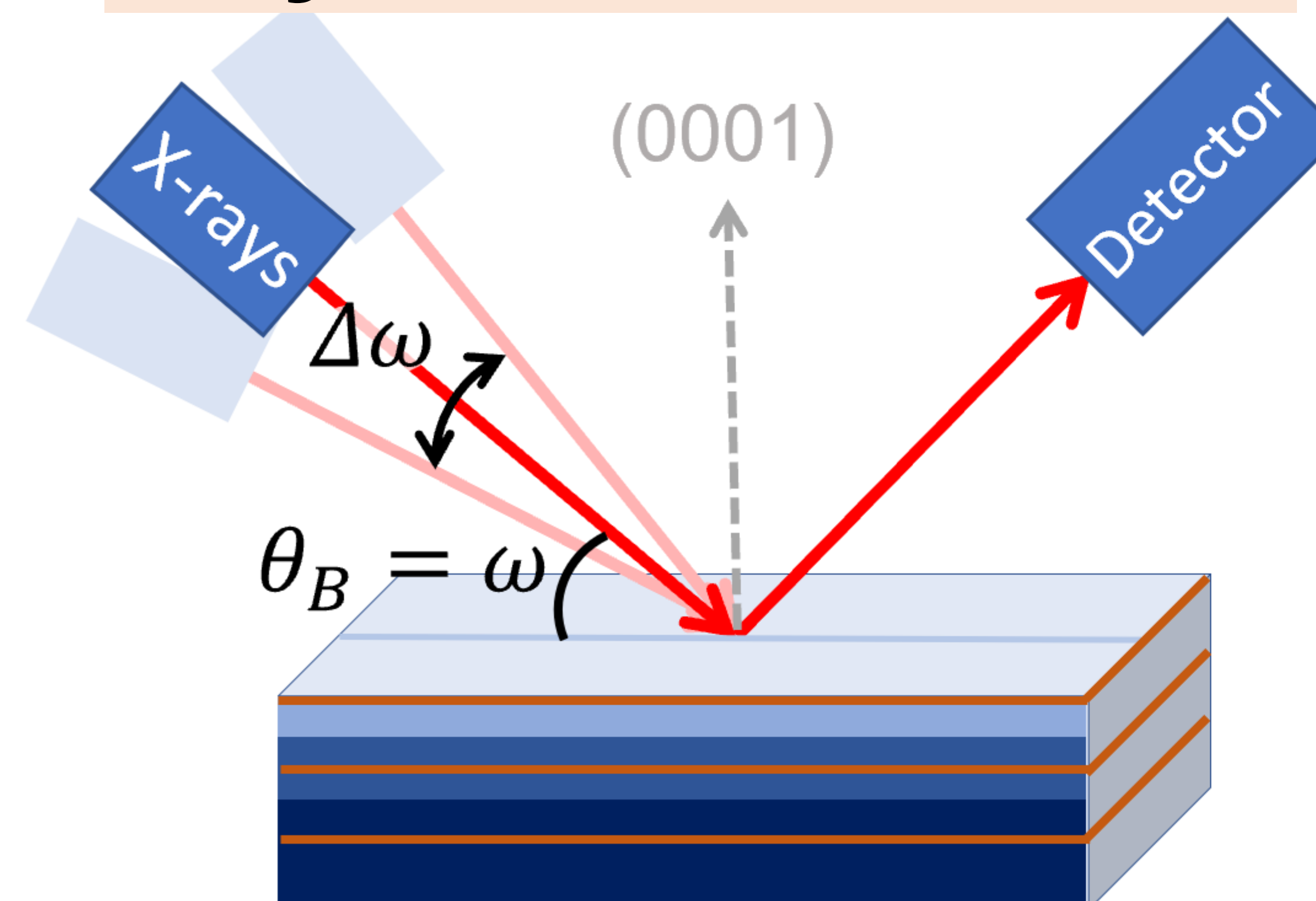
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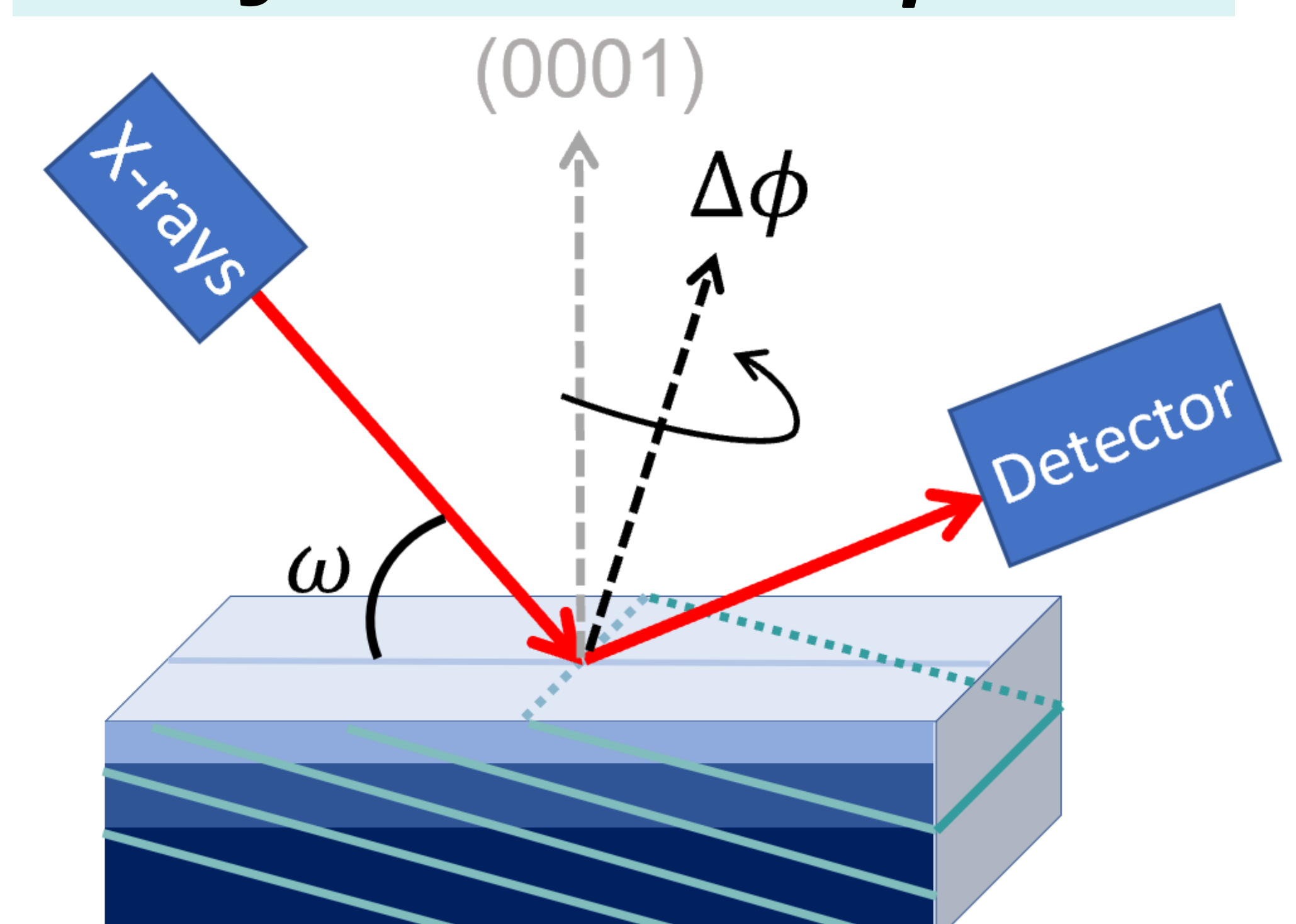
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$$0.9\lambda$$

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Screw TD density

$$N_S = \frac{\alpha_{\omega}^2}{2\pi b_S^2 \ln 2}$$

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Regrowth Interface at p-n Junction

GaN Substrate



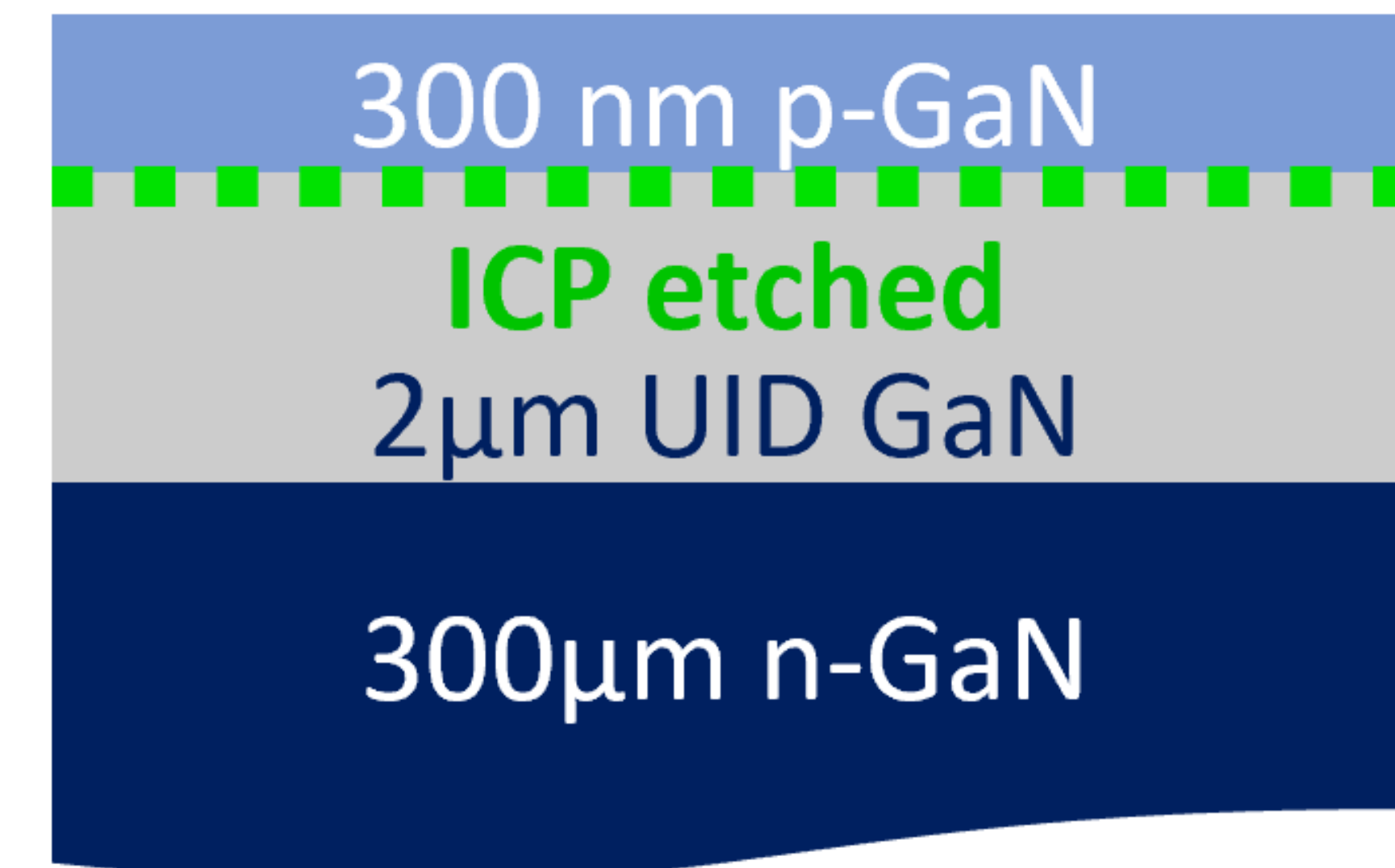
In-situ Regrowth



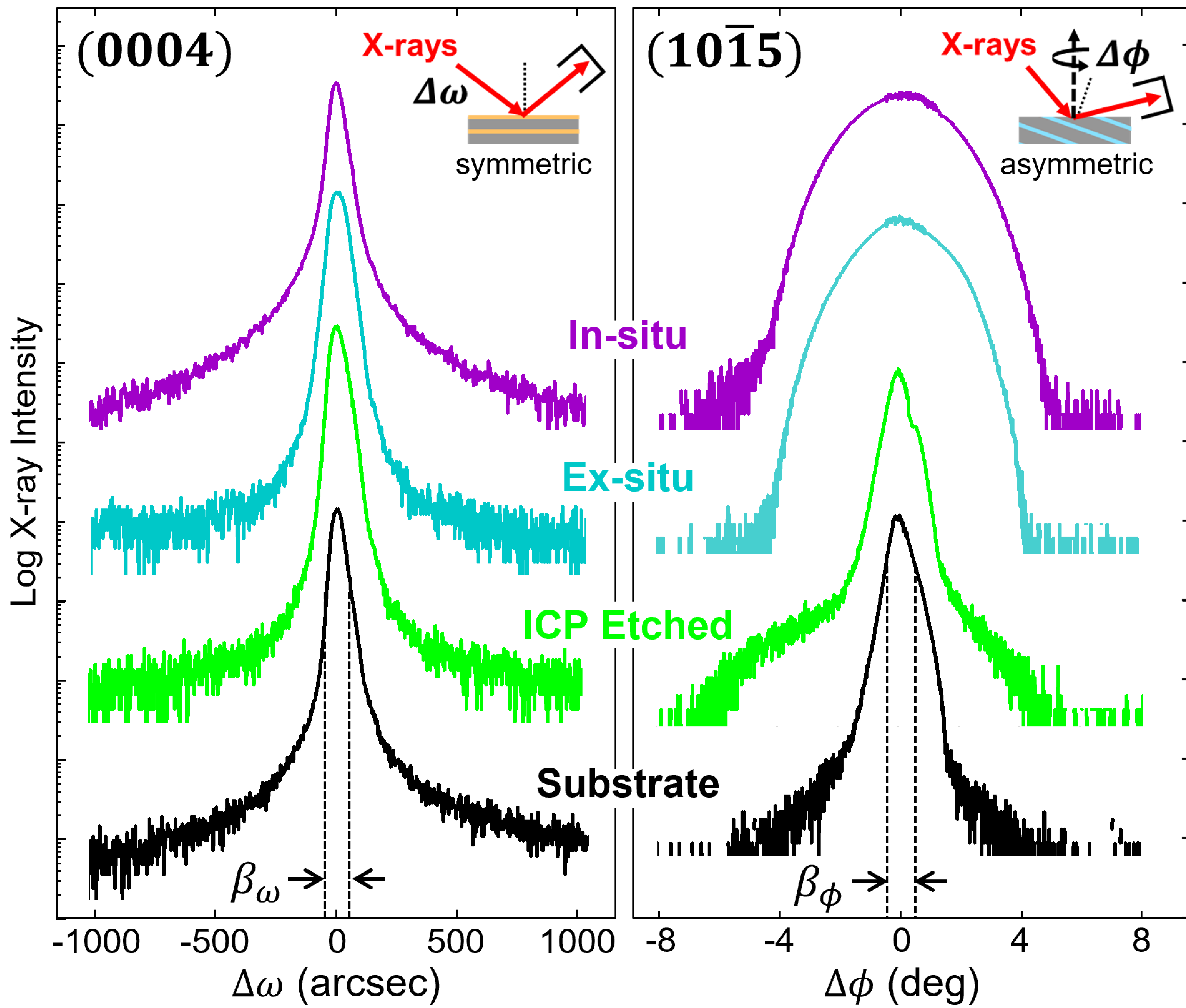
Ex-situ Regrowth



ICP Regrowth

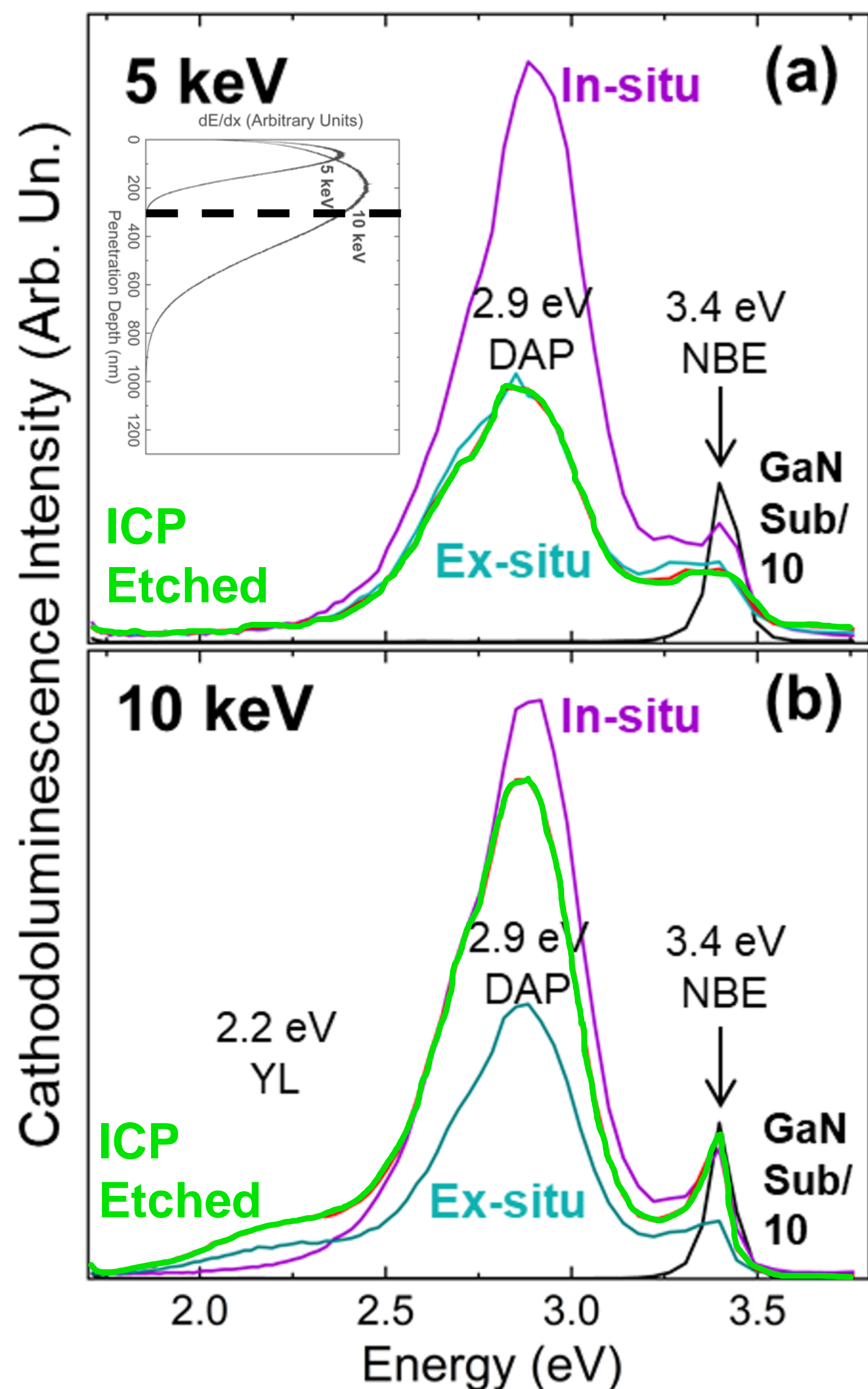


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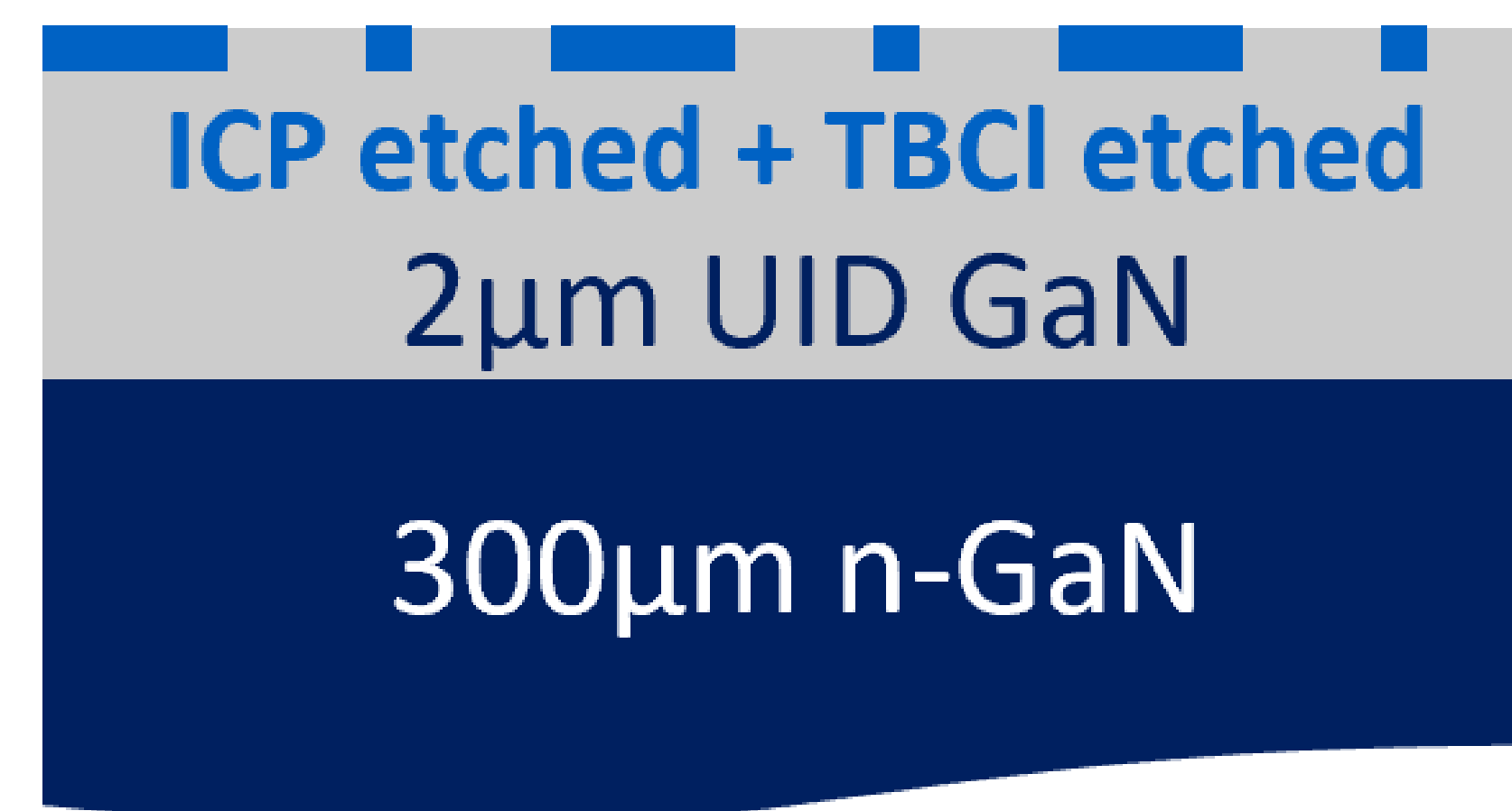
GaN Substrate



ICP



ICP + TBCl



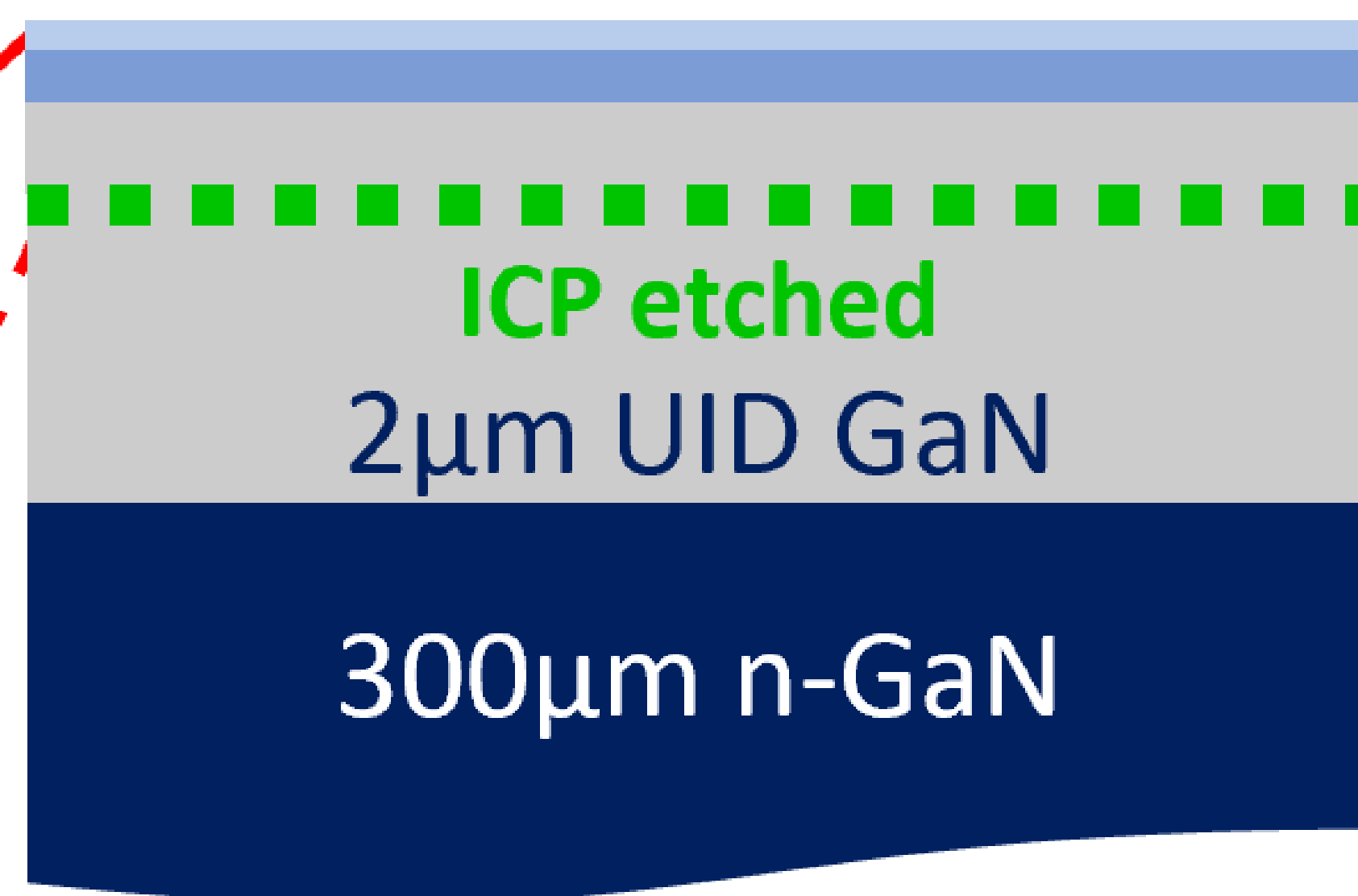
TBCl



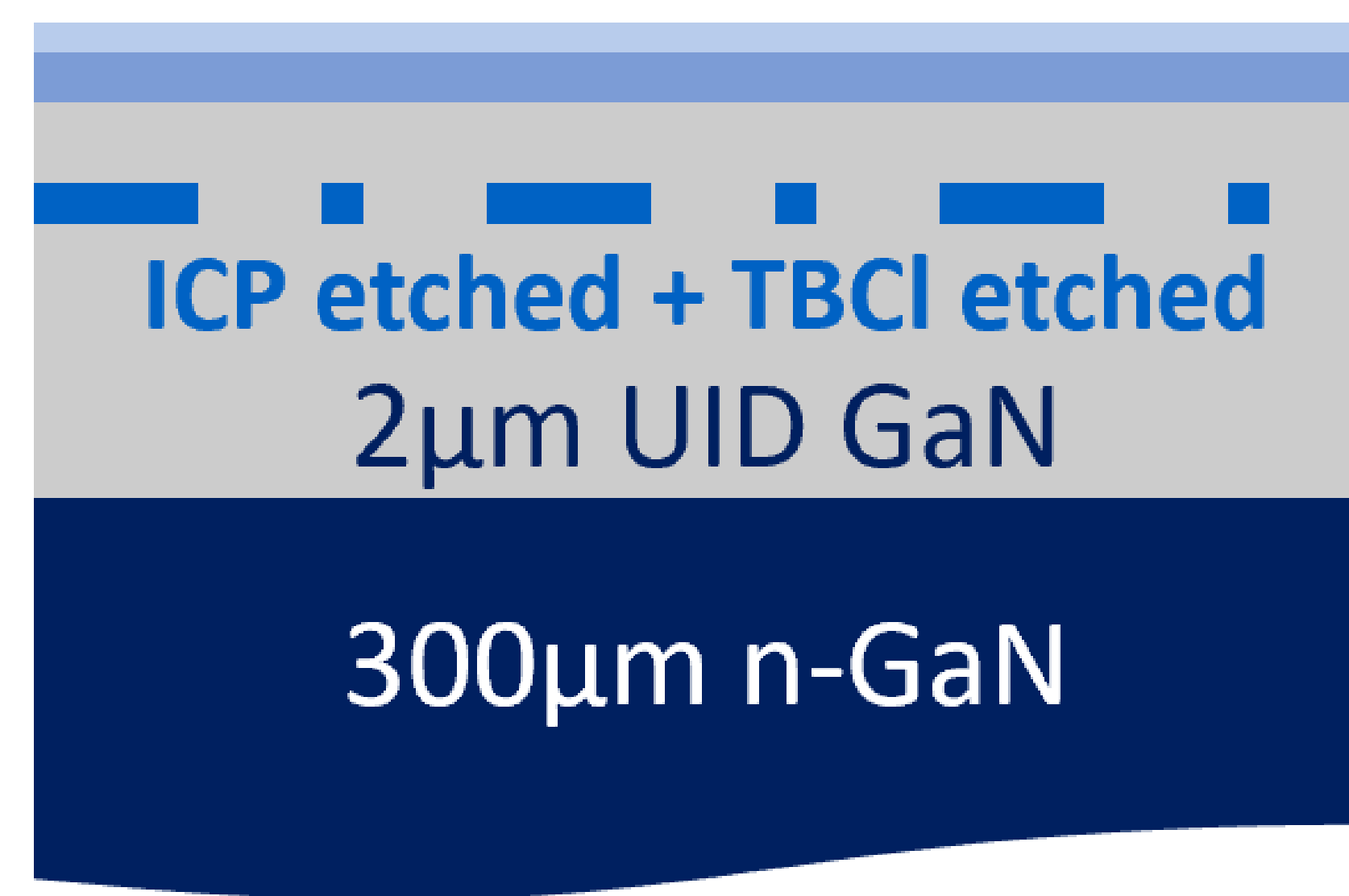
Regrown Active Region



ICP Regrowth



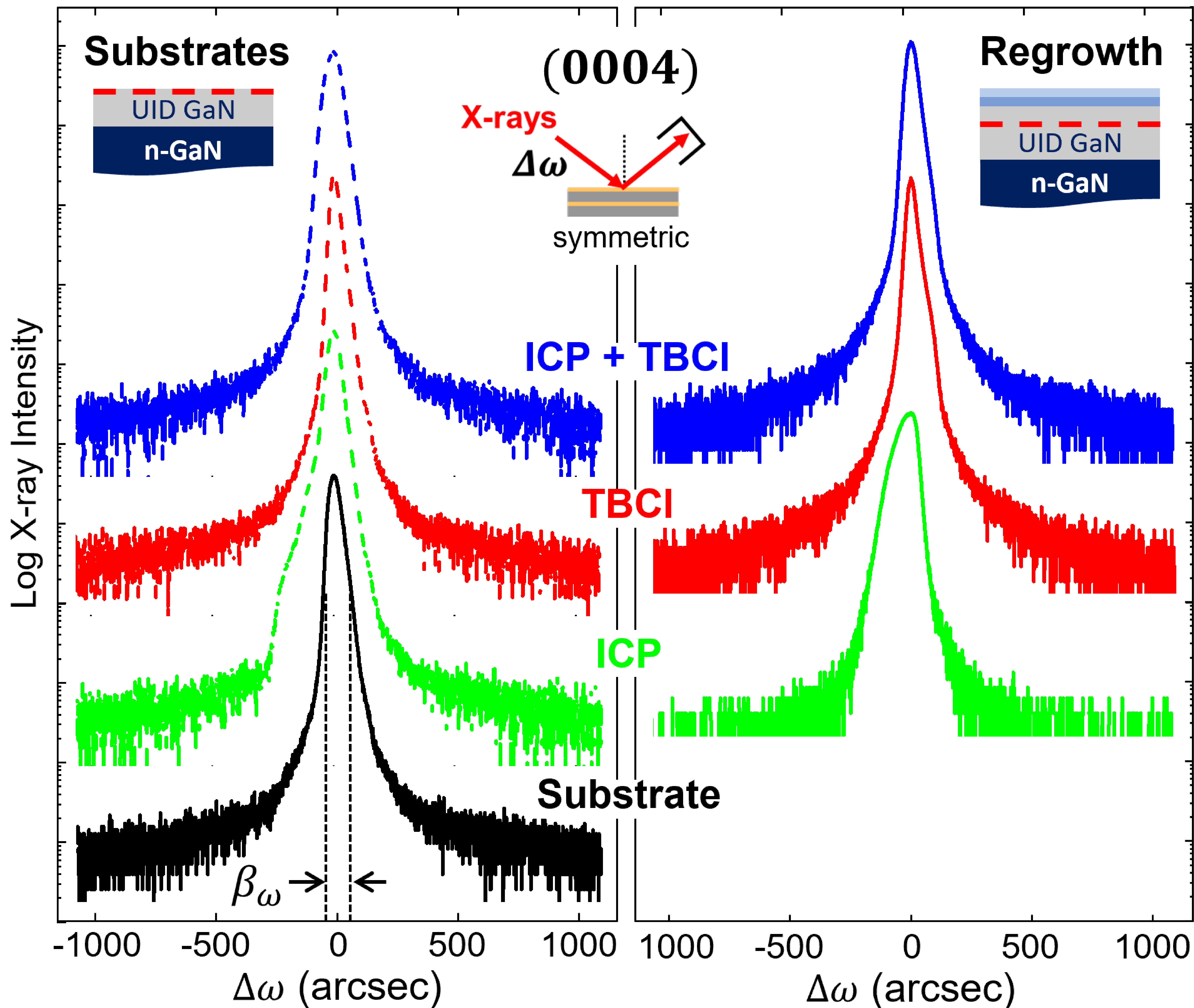
ICP + TBCl Regrowth



TBCl Regrowth



Symmetric Scans Only



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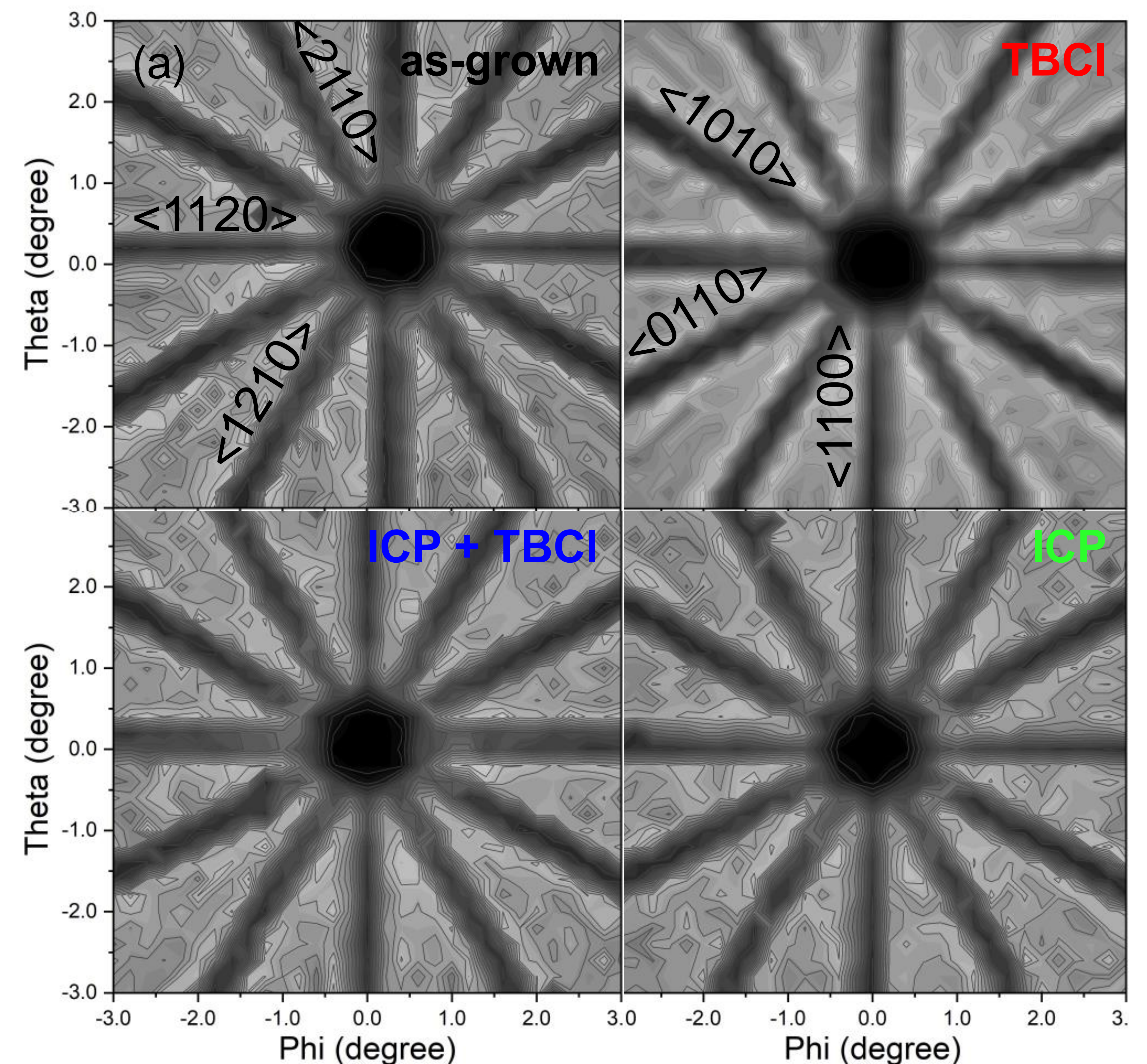
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XRD and RBS reveal **ICP Etching** lowers crystal quality overall.



References

1. L.M. Tolbert, et al., "Power Electronics for Distributed Energy Systems & Transmission & Distribution Applications: Assessing the Technical Needs for Utility Applications." (Oak Ridge National Laboratory, 2005)
2. J.Y. Tsao et al., "Ultrawide-Bandgap Semiconductors: Research Opportunities and Challenges". Adv. Electronic Mat. 4, [1600501](#) (2018).
4. De Keijser, T. , Mittemeijer, E. J. and Rozendaal, H. C., "The determination of crystallite-size and lattice-strain parameters in conjunction with the profile-refinement method for the determination of crystal structures." J. Appl. Cryst., 16: 309-316 (1983)
5. "Linear Defects - Dislocations." NDT Resource Center, National Science Foundation
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7. González-Viñas, Wenceslao & Mancini, Hector. (2003). Science of Materials: An Introduction (Pre-print).

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The Pseudo-Voigt function, $P(x)$, approximates the convolution of Cauchy, $C(x)$, and Gaussian, $G(x)$, profiles and is given by equations (1):

$$P(x) = I_0[\eta C(x) + (1 - \eta)G(x)]$$

and $0 \leq \eta \leq 1$, where η is a fitting parameter [6]. The lateral correlation length, L_{\parallel} , and tilt angle, α_{ω} , can then be calculated using equations (2) and (3), respectively:

$$L_{\parallel} = \frac{0.9\lambda}{\beta_{\omega}(0.017475 + 1.50048\eta - 0.534156\eta^2)\sin(\theta_B)}$$

$$\alpha_{\omega} = \delta\omega[0.184446 + 0.812692(1 - 0.998497\eta)^{1/2} - 0.659603\eta + 0.44554\eta^2]$$

where λ is the x-ray wavelength, $\delta\omega$ is the FWHM of the $\Delta\omega$ rocking curve, and θ_B is the Bragg angle [6].

$$N_S = \frac{\alpha_{\omega}^2}{2\pi \mathbf{b}_S^2 \ln 2}$$

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