Modelling electron channeling contrast for threading dislocations in nitride semiconductors

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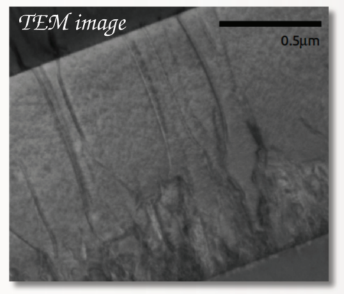
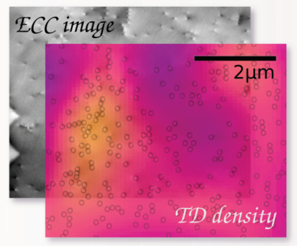
Background



Threading dislocations in AlGaN grown on sapphire. Cross-section TEM image showing TDs originating at the sapphire interface, propagating thought the nitride layer and reaching the next interface or surface. By permission of David Thomson .

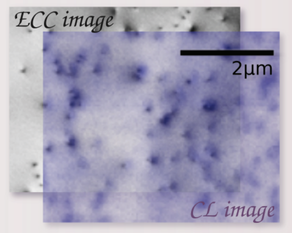


ECC images provide characterisation information for a statistically meaningful sample size of dislocations. Plan view ECC image of polar AlGaN sample grown on sapphire showing dislocation densities of $10^9/cm^2$. The large number of imaged dislocation allows for meaningful statistical tests. For instance, the image of the TD density distribution in the lower panel shows the actual clustering behaviour of dislocations when compared against a statistically random density distribution. ECCI by permission of Mohammad Nouf-Allehiani.

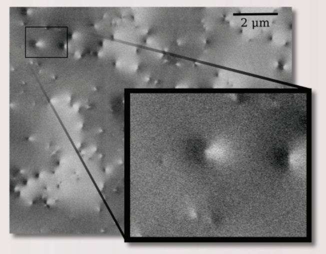
Threading dislocations (TDs) are common native defects of group III nitrides materials, introduced through bulk heteroepitexial growth on a lattice mismatched substrate. These extended dislocations propagate through the layer and can harm the optoelectronic properties of the film. For instance, high densities of TDs have been linked to luminescence output reduction and efficiency drop in GaN-based devices (1).

The SEM based electron channelling contrast imaging (ECCI) technique can be used to observe and characterise these defects (2). Unlike transmission electron microscopy (TEM) imaging, it requires no destructive sample preparation and can produce images containing a large number of defects (3) even for relatively small dislocation densities.

Nevertheless, to correctly map the contrast profile to the dislocation character a careful model of diffraction interaction with the dislocation induced strain is required. The model could then be used as in integral part of identifying TD Burgers vector orientation based on ECC images.



TDs acting as non-radiative carrier recombination centers. Plan view cathodoluminescence image (blue) overlaid on the ECC image (gray) from the same area of a Si-doped GaN sample. Such studies point towards the carrier trapping properties of these defects, at which locations carriers of opposite signs can recombine without producing photons. By permission of Dr. Jochen Bruckbauer.



TDs contrast in the SEM. The image of a single crystal surface in high magnification mode should consist of a constant backscattered electron yield as the beam is scanned over a small area. A dislocation changes the orientation of the crystal lattice locally affecting the diffraction of the electron beam. Fluctuations in the intensity of backscattered electrons show as darker-brighter contrast around the line defect. By permission of Mohammad Nouf-Allehiani.

Dynamical diffraction

Electrons interact 100 times more strongly with matter than X-rays or neutrons. They will suffer multiple diffraction even in very thin samples. With every diffraction event the information about the crystallinity of the material is reinforced. Any departure from perfect lattice is readily observed as intensity contrast.

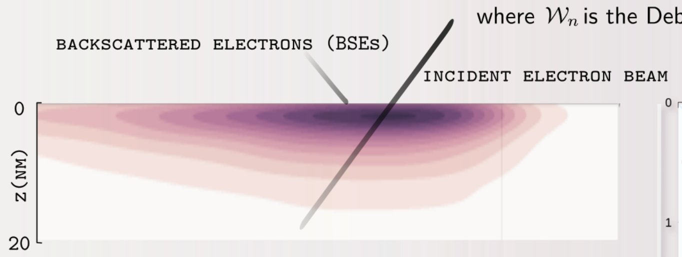
For the electron diffraction model the dynamical Howie-Whelan-Darwin two beam scattering equations (4) is used here.

On their way in, electrons suffer, to a first approximation, one large angle incoherent event which sends them directly to the detector.

The probability for an electron to reach the detector after the incoherent event is given by:

$$P(z) = \int_0^z (\eta_T|T| + \eta_D|D|)\, dz \quad where \quad \eta \propto \sum_n Z_n^2\, \mathcal{W}_n\, \Omega_{detector}$$

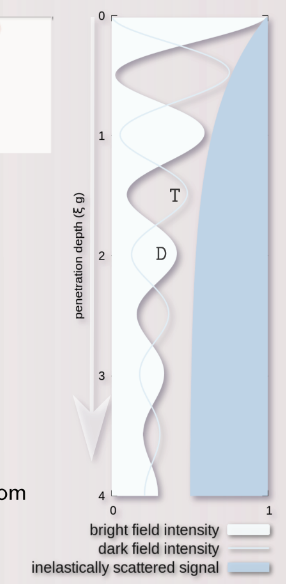
where $\mathcal{W}_n$ is the Debye-Waller factor.



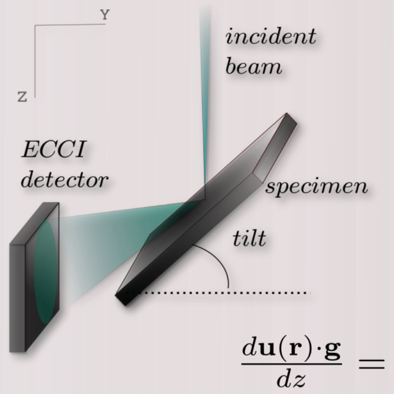
$$\frac{dD}{dz} = (i - \mathscr{A})T + (-\mathscr{N} + 2iw + 2i\beta')D$$

$\mathscr{N}$ is the inelastic scattering coefficient
$\mathscr{A}$ is the dynamical scattering coefficient
w is the local deviation from the Bragg condition
β' is the sampled dislocation strain

Coefficients A and N can be calculated numerically from the Fourier coefficient of the electrostatic potential.



Strain...



The variation in the displacement field, **u**(r), as sampled by the ECC micrograph around a dislocation is given by the change in the local lattice curvature. The correction to the variation from the local Bragg condition, s_g, is given by Tunstall (5):

$$\beta' = \frac{\partial \mathbf{u}\cdot\mathbf{g}}{\partial z} + \theta_B \frac{\partial \mathbf{u}\cdot\mathbf{g}}{\partial \hat{g}}$$

where θ_B is the Bragg angle.

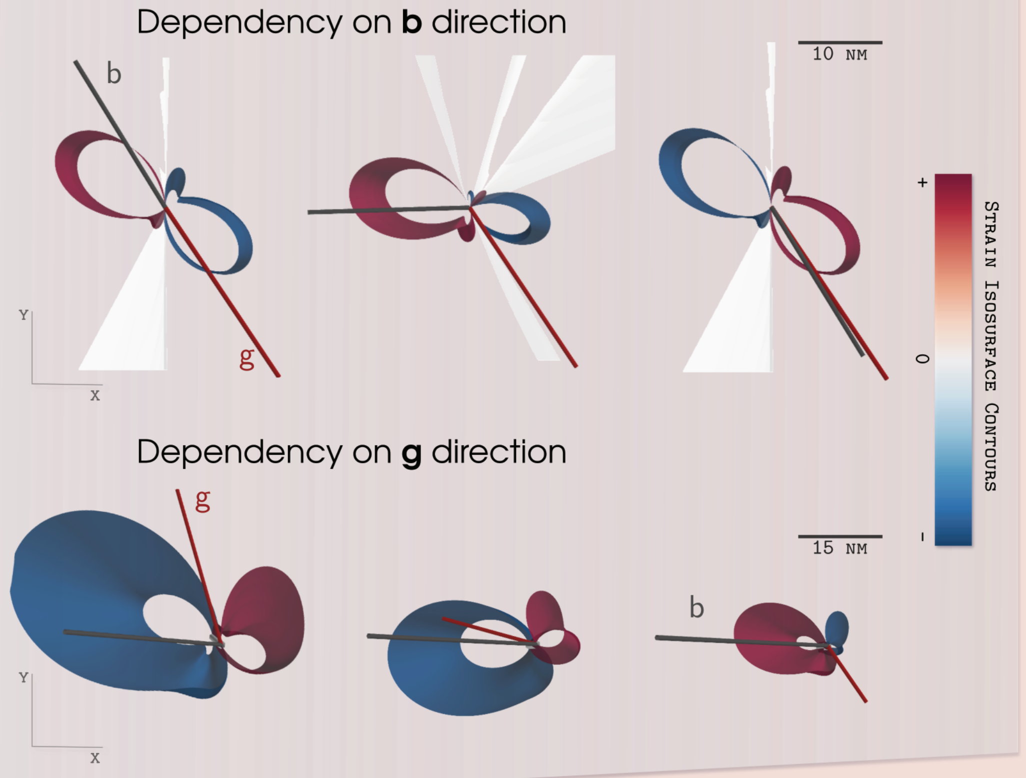
$$\frac{d\mathbf{u}(\mathbf{r})\cdot\mathbf{g}}{dz} = (r_{inc})_i^d \frac{\partial u_j^d}{\partial x_i}\bigg|_{\mathbf{r}} \mathcal{T}_{jl}^{ds} B_{lm} g_m$$

where Einstein summation is applied to subscripts. The superscripts '*d*' and '*s*' indicate the dislocation frame and sample frame, respectively, in which the vectors were defined.
The coordinate transformation matrix $\mathcal{T}_{ij}^{ds}$ translates vectors from the sample to the dislocation frame.
B is the reciprocal structure matrix.

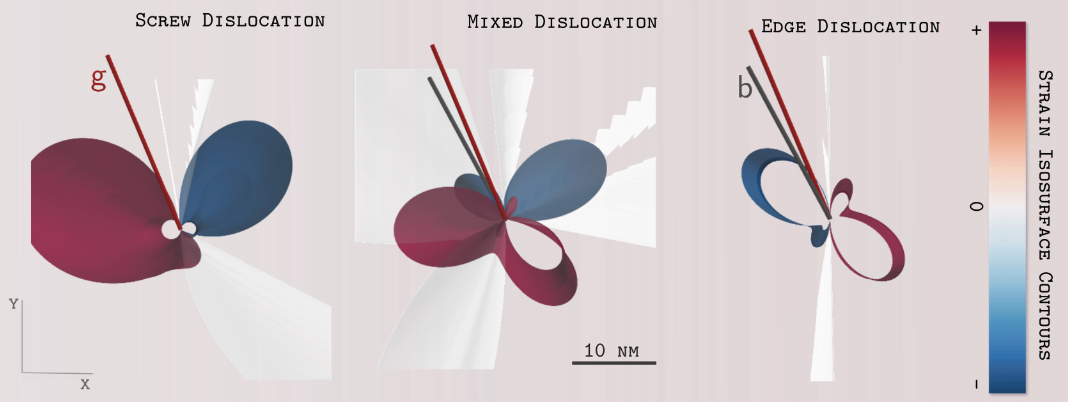
The displacement field is derived by Yoffe (6) from elasticity theory for dislocations intersecting a surface at an angle and takes into account the surface relaxation.

For the same diffraction condition the strain profile around a TD follows the edge component Burgers' vector. This has been proposed previously from experimental observation by Naresh-Kumar er al (7).

For the same dislocation, the diffraction condition will not change the symmetry of the observed strain.



...in hexagonal crystals



MATERIAL	GaN
GROWTH DIRECTION	[001]
CRYSTAL ROTATION	58.4
SAMPLE TILT	-49.6
TD LINE	[001]
DIFFRACTION CONDITION	[75-3]

Note that the surface relaxation affects the first few nanometers of material.

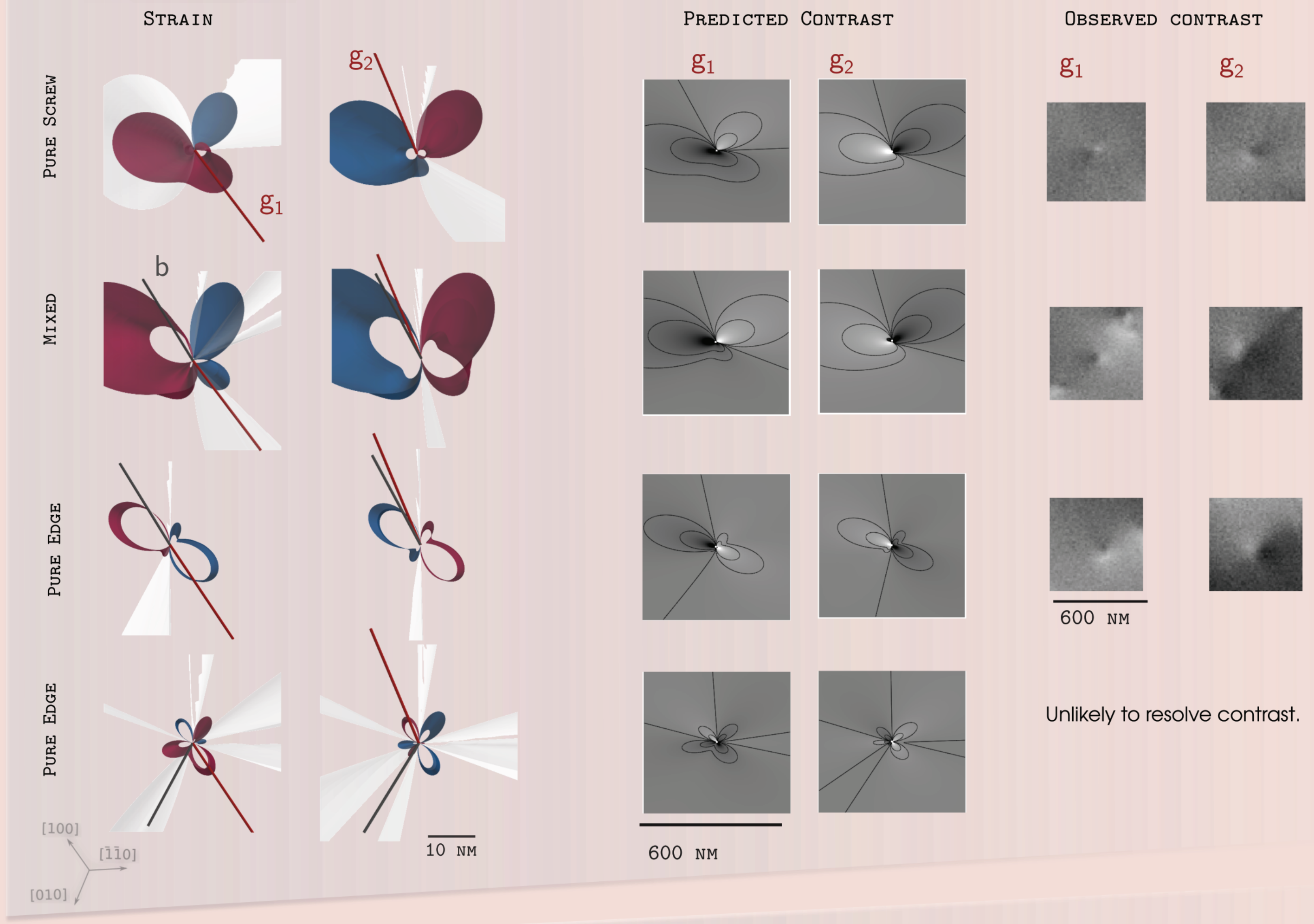
Contrast

The contrast, as the effect of variation from diffraction condition caused, in turn, by the strain of the dislocation, holds the same symmetry as the strain profile (8). Quantitatively, it is calculated as the integration over the penetration depth of the diffraction beams affected by dislocation strain. For the resolution of the SEM, contrast associated to dislocation occurs more likely when the strain profile displays only two zero planes.

DIFFRACTION CONDITION

g_1	[-7-5-3]
g_2	[75-3]

ECC maps supplied by Dr. G. Naresh-Kumar as published in ref [7].



Conclusions

The SEM based ECCI technique can be used as an identification and characterisation tool of threading dislocations over relatively large areas in nitrades semiconductors.

While the charactersation is more involved then in TEM, which benefits from the applicability of the 'invisibility criteria', simulations of ECCI dislocation strain profile can predict the observed dislocation contrast.

We propose that the ECCI dislocation contrast is uniquely predicted by the ECCI strain profile. The equivalence between ECCI strain and ECCI contrast can aid not only the physical understanding of the observed images but can predict the behaviour of the contrast.

For instance, we can predict that the contrast profile will always follow the edge component of the Burgers vector and that the diffraction condition will not affect its symmetry.

This work could form the basis of automated threading dislocation characterisation in nitrades materials, by using the possible predicted dislocation contrast profiles as a data base for machine learning.

Acknowledgments

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References

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