Theoretical model of contrast produced by surface normal TDs as observed by ECCI

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Background

Evidence suggests that a high density of dislocations correlates with poor optoelectronic performance in semiconductor based devices.

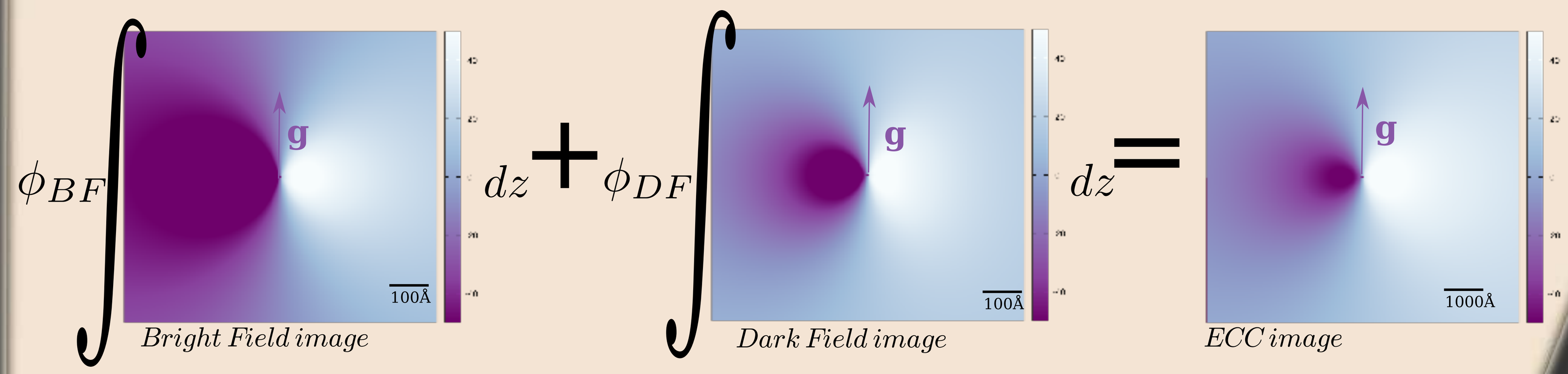
Threading dislocations (TDs) are line defects that run through the material and reach its surface. They are believed to act as non-radiative recombination centres affecting the luminescence output efficiency.

Dislocations bend the lattice of the perfect crystal introducing **local strain** providing a characteristic marker that can be observed. The electron microscope is one tool that measures this marker.

Electron channelling contrast imaging (ECCI) is a non-destructive scanning electron microscope technique that can provide material structural information by measuring the intensity of the backscattered electrons [1]. It is the purpose of this study to provide a model of the threading dislocation contrast thus observed.

ECC images

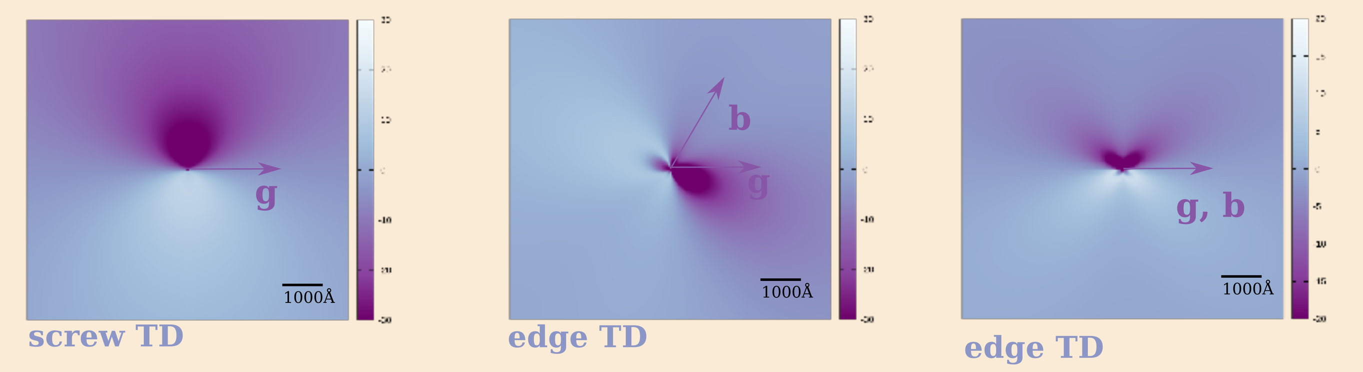
Using the assumption that the backscattered signal comes from a single inelastic scattering event (Rossouw et al.[6]), the ECC image is then calculated as the weighted sum of the integrated BF and DF signal. The weighting factor is the cross section for impact ionisation (ϕ) for the given detector angle (α).



screw dislocation along GaN(0001)
[11-20] reflection
t = 0.5 ξ_g
w = 0
α detector = 40°
η sample = 90°

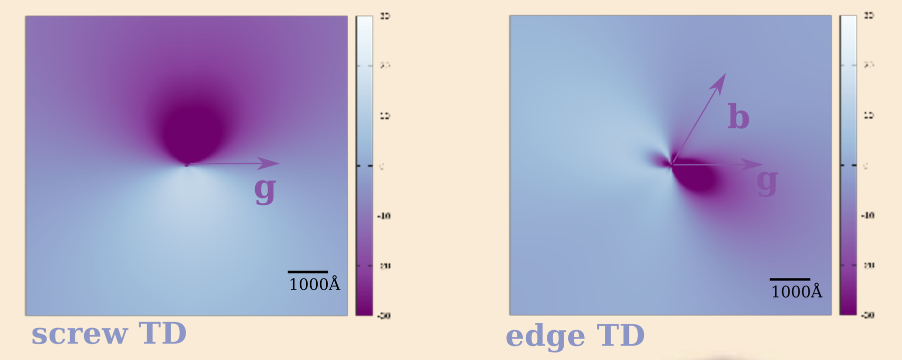
Backscatter geometry

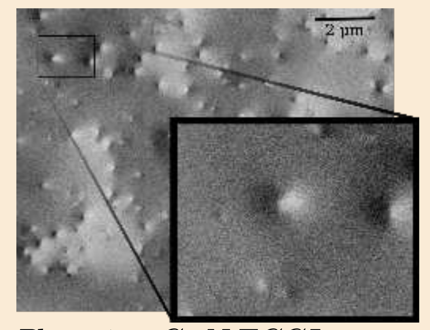
η = 90°



Forescatter geometry

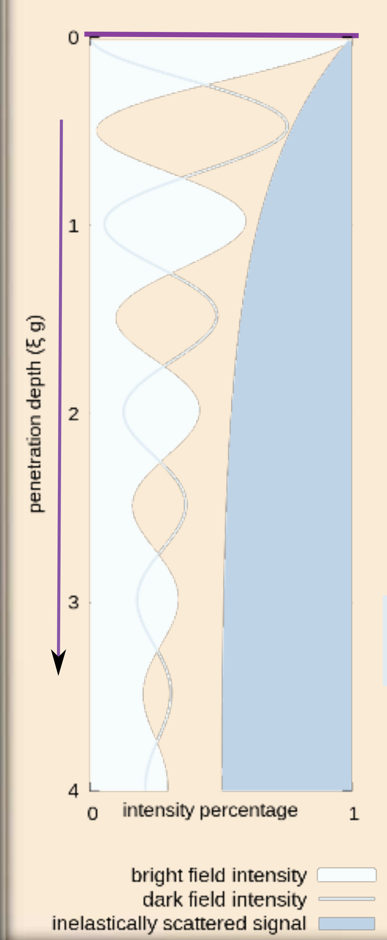
η = 20°





Plan view GaN ECCI. By permission of Allehiani Nouf Mohammad

Model



On entering the sample the electron beam is modulated by the periodicity of the lattice potential into standing waves (beams).

In addition to the directly transmitted beam (bright field signal - BF), we also consider to a first approximation one diffracted beam (dark field - DF).

Part of the signal is progresivelly lost to inelastic events. The rest of the beam amplitude is transfered dynamically between the two beams.

$$\frac{dD}{dz} = (i - \mathscr{A})T + (-\mathscr{N} + 2iw + 2i\beta')D \qquad (1)$$

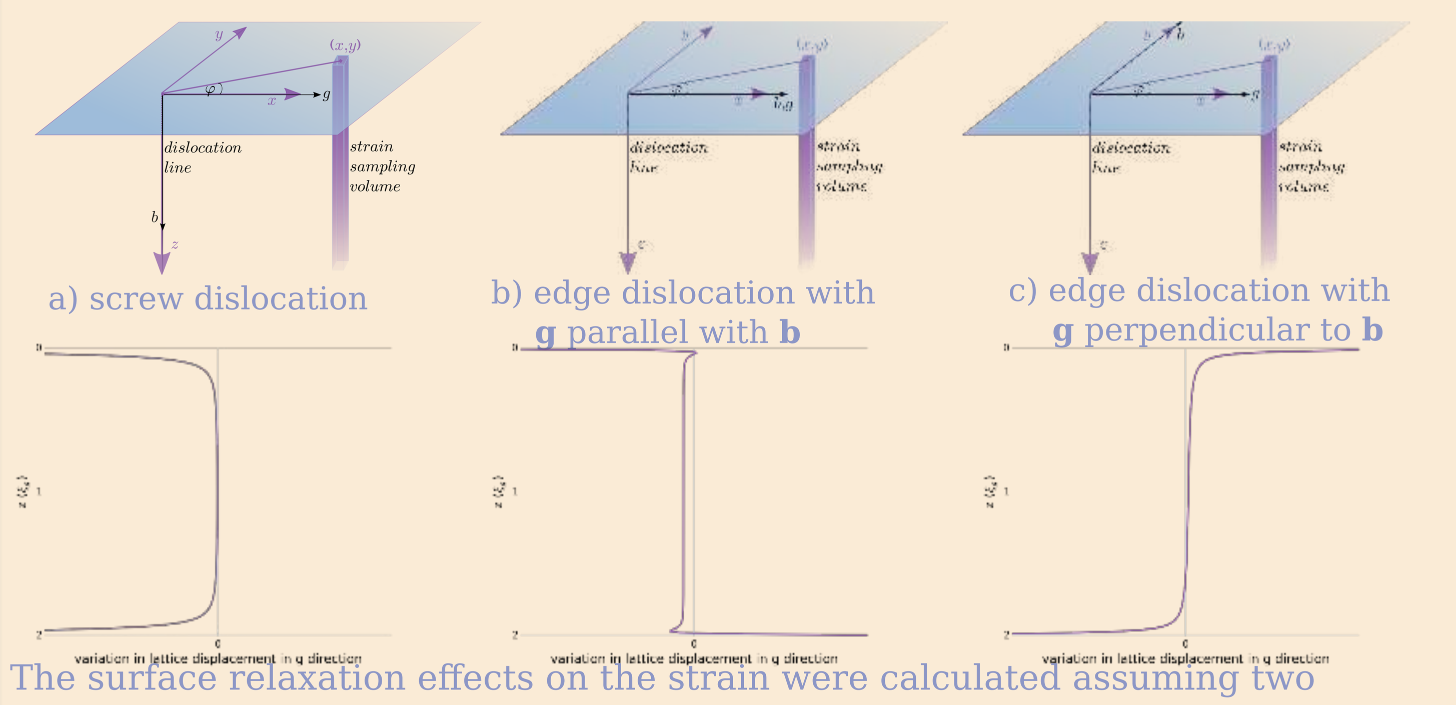
change in diffracted beam amplitude with penetration depth = *signal transferred from the transmitted beam* - *electrons lost to inelastic scattering* + *change in beam amplitude due to change in strain*

$$\mathscr{N} = \frac{\xi_g}{\xi_0'} \qquad \mathscr{A} = \frac{\xi_g}{\xi_g'} \qquad w = \xi_g s_g$$

ξ_0' *is related to the linear absorbtion coefficient*
ξ_g *is the extinction distance for reciprocal lattice vector g*
ξ_g' *is the coresponding anomalous absorbtion distance*
s_g *is the deviation from the Bragg condition*
β' *is the change in strain to which the specific g direction is sensitive*

(1) Howie -Whelan eq. in the column approximation [2]

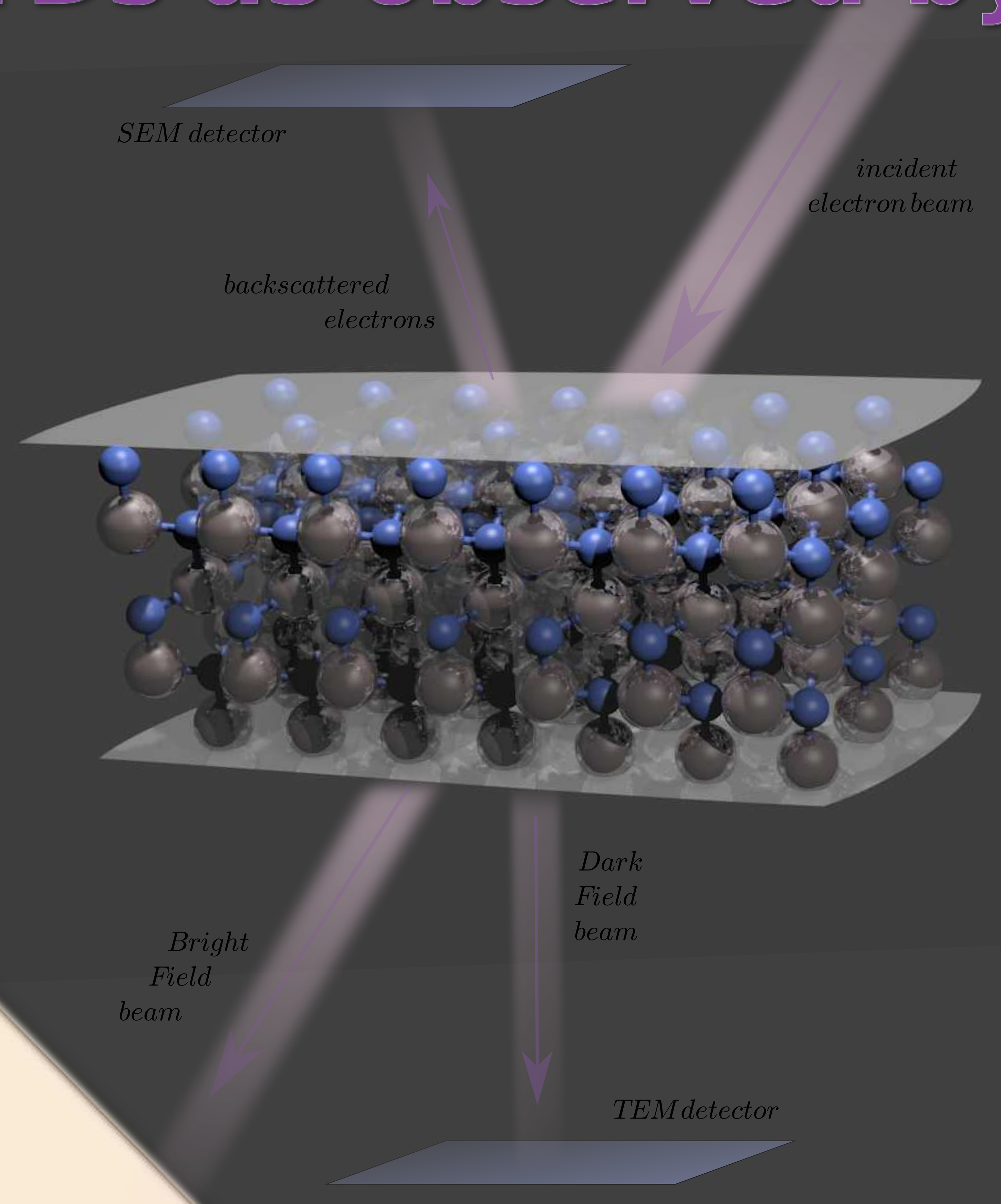
Strain variation through cubic crystal thin sample



$$\beta' = g\left(\frac{\partial u_g}{\partial z}\right)_{x,y} + \theta_B g\left(\frac{\partial u_g}{\partial r_g}\right)_z$$

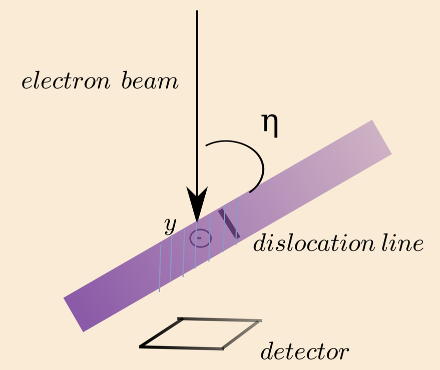
where Θ_B is the Bragg angle
u_g is the lattice displacement parallel to g
r_g is the coordinate in xy plane parallel to g

The surface relaxation effects on the strain were calculated assuming two superposed semi-infinite solids each with image displacements as derived by Yoffe [3].

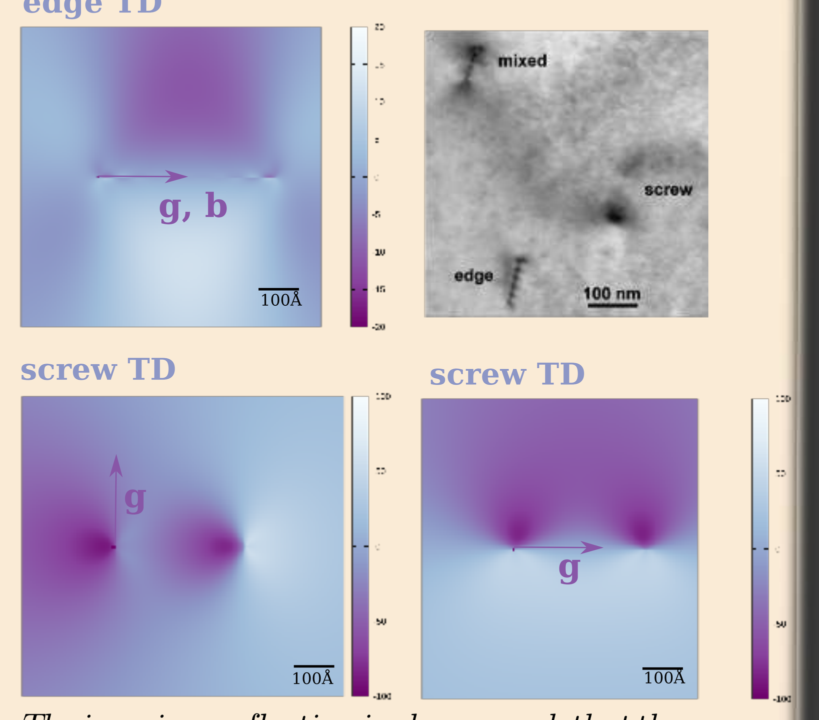


Tilting the sample

[0001] orientation
η = 78°
y = (11-20)
t = 5 ξ_g
w = 0.2

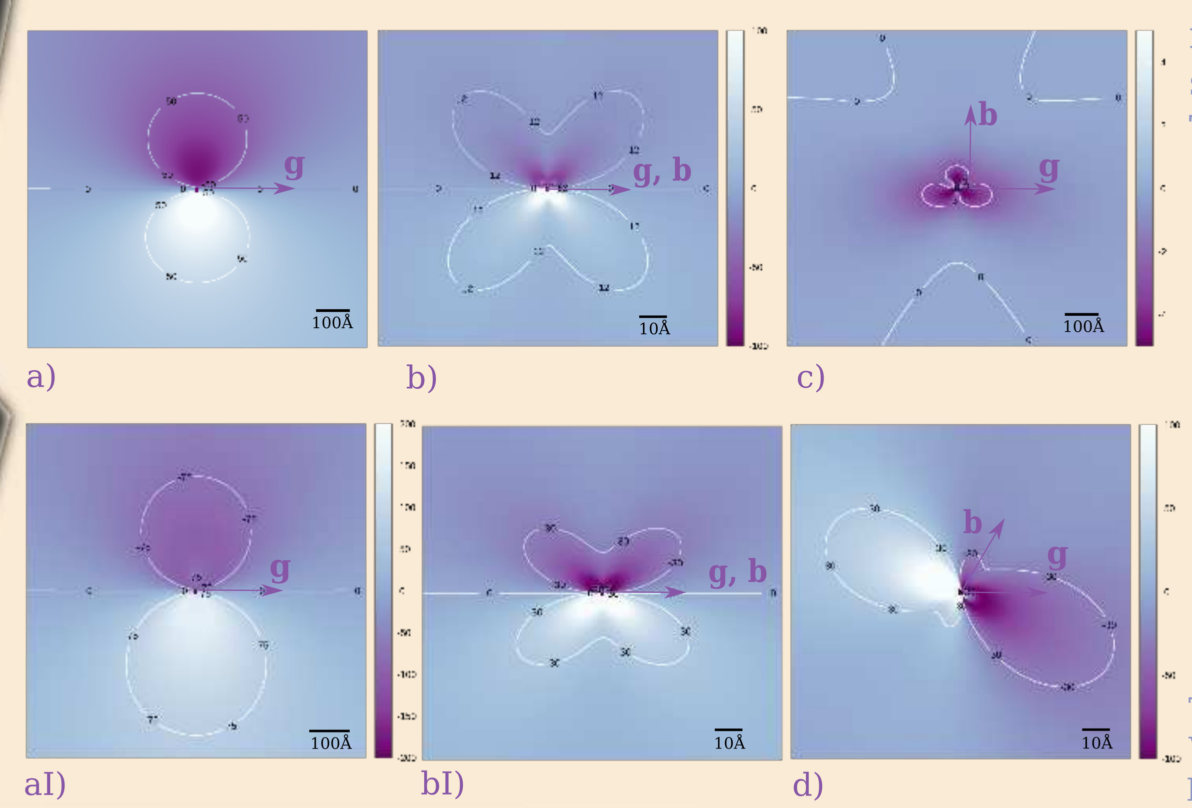


Can be easily modelled by rotating the coordinate system of the strain field by an angle η with respect to the y-axis. The integrating columns will remain along the direction of the incident beam. The simulated images show good qualitative resemblance to the experimental work of Follstaedt et al. [5].



The imaging reflection is chosen such that the invisibility criterion is achieved for the screw dislocation in the bulk of the sample

TEM bright field images



cubic Cu system

The contrast plots obtained by numerical integration of the dynamical equations show good agreement with the work of Tunstall et al.[4].

$\mathscr{A}$ = 1 $\mathscr{N}$ = 10 θ_B = 0.015 ν = 0.30

a) (311) reflection	**b) (202) reflection**	**c) (111) reflection**
$\lvert \mathbf{g}.\mathbf{b}\rvert$ = 2.3	$\lvert \mathbf{g}.\mathbf{b}\rvert$ = 2	$\lvert \mathbf{g}.\mathbf{b}\rvert$ = 1.2
w = 0.16	w = 0.12	w = 0.03
t = 5.5 ξ_g	t = 2.5 ξ_g	t = 5.5 ξ_g
ξ_g =300 Å	ξ_g = 470 Å	ξ_g = 270 Å

wurtzite GaN system

$\mathscr{A}$ = 1 $\mathscr{N}$ = 2 θ_B = 0.006 ν = 0.26

aI) (11-20) reflection	**bI) (2-1-10) reflection**	**d) (11-20) reflection**
$\lvert \mathbf{g}.\mathbf{b}\rvert$ = 3.25	$\lvert \mathbf{g}.\mathbf{b}\rvert$ = 2	$\lvert \mathbf{g}.\mathbf{b}\rvert$ = 2
w = 0.2	w = 0.0	w = 0.0
t = 0.5 ξ_g	t = 0.5 ξ_g	t = 0.5 ξ_g

The extinction distances were calculated using Weickenmeier-Kohl scattering factors.
Elastic constants were derived using Voigt average.

References:

[1] Kumar, N. G., et al. , 2012, *Phys. Rev. Lett.*, **108**, 13
[2] Howie, A., and Whelan, M. J., 1961, *Proc. Roy. Soc. A*, **263**, 217
[3] Yoffe, E. H., 1961, *Phil. Mag.*, **6**, 1147
[4] Tunstall, W. J. and Hirsch, P. B., 1964 *Phil. Mag.* , **9**, 97
[5] Follstaedt, D. M., et al. , 2003, *Appl. Phys. Lett.* **83**, 4797
[6] Rossouw, P. R., et al., 1994, *Phil. Mag. A*, **70**, 985