Understanding of Local Dislocation Structures in Deformed Materials Based on Microdiffraction

R. Barabash

Collaborators:

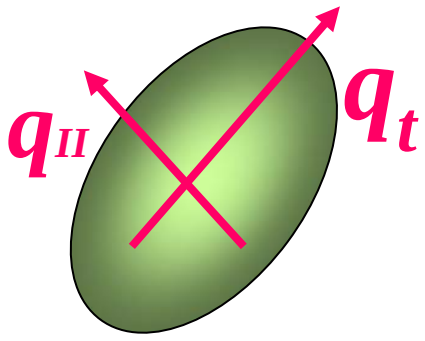
G. Ice , W. Liu, J. Pang, B. Larson, W. Yang

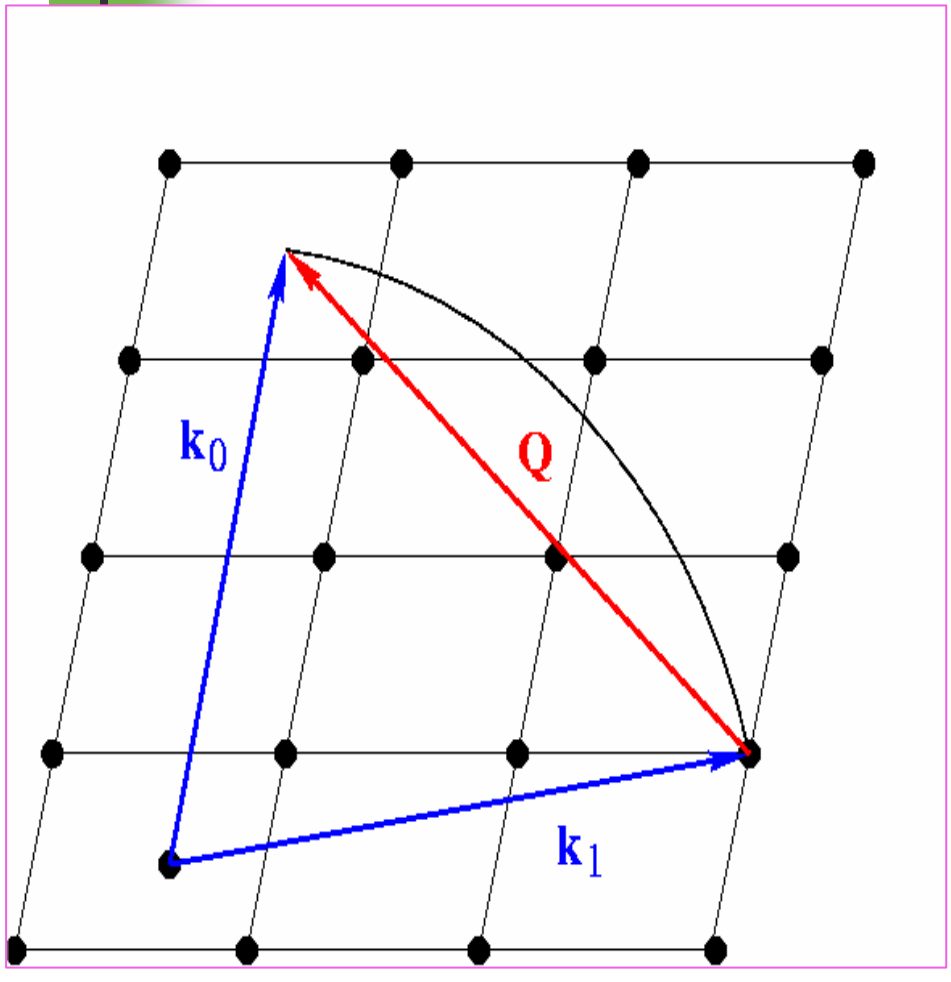
Oak Ridge National Laboratory

Workshop on Science With High Enegry X-rays,

Argonne, August 10, 2004

Two Directions of q Become Important:

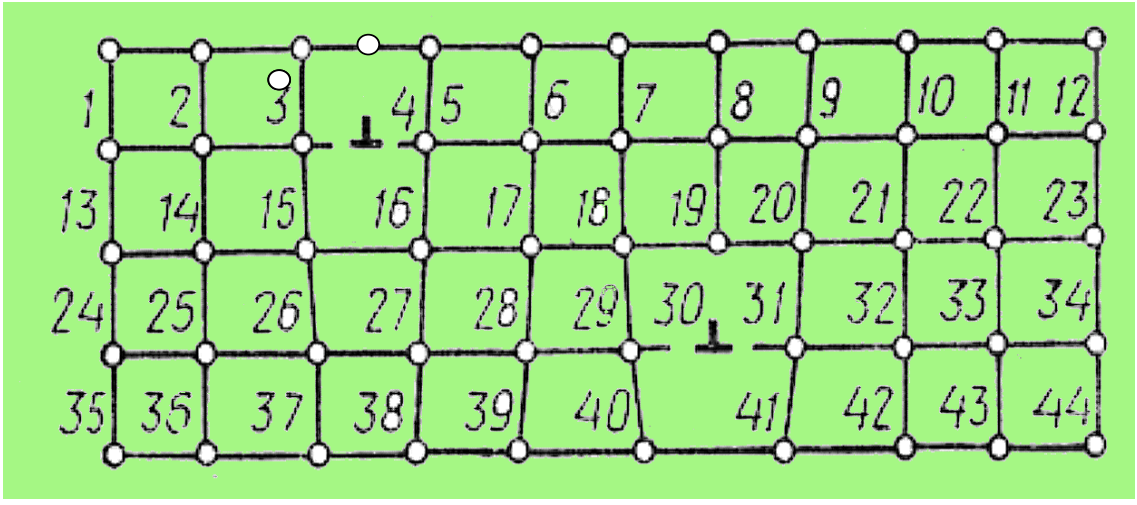




- **q_{II} parallel to Q**
  - **radial intensity $I(q_{||}) \cong I(2\theta)$**
  - **depends on the translation part of the long - range displacement fields *u(R)* caused by lattice defects**
- **q_t perpendicular to Q**
  - **transverse plane $I(q_t) \cong I(\omega)$ (rocking curves)**
  - **depends on the rotation part of the displacement fields *u(R)***

RANDOM NUMBERS DESCRIBE THE DISLOCATION DISTRIBUTION

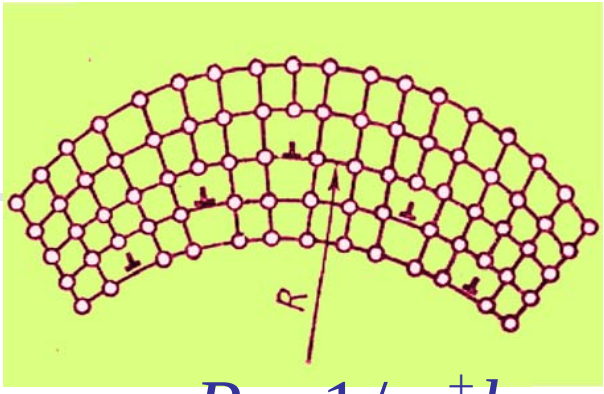
$$C_t = \begin{cases} 1, \text{(present)} \\ 0, \text{(absent)} \end{cases}$$



Total displacement of this *S*-th cell u_i is due to all dislocations

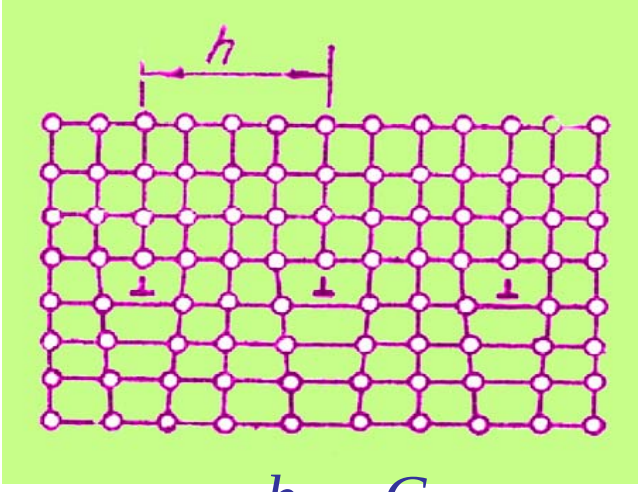
$$\vec{u}_s = \sum_t c_t \vec{u}_{st}$$

Bent Crystal



$$R = 1/n^{+}b$$

Dislocation pile up



$$\sigma = \frac{b}{h}\frac{G}{1-\mu}$$

Scattering by crystals with dislocations

$$I(\mathbf{Q}) = \left| \sum_i f_i \exp(i\mathbf{Q}(\mathbf{R}_i^0 + \mathbf{u}_i)) \right|^2$$

- $\mathbf{R}_i$ -relaxed co-ordinates
- $\mathbf{u}_i$ displacements

$$I(\mathbf{Q}) = f^2 \sum_{i,j} e^{i\mathbf{Q}\Delta} e^{-T}$$

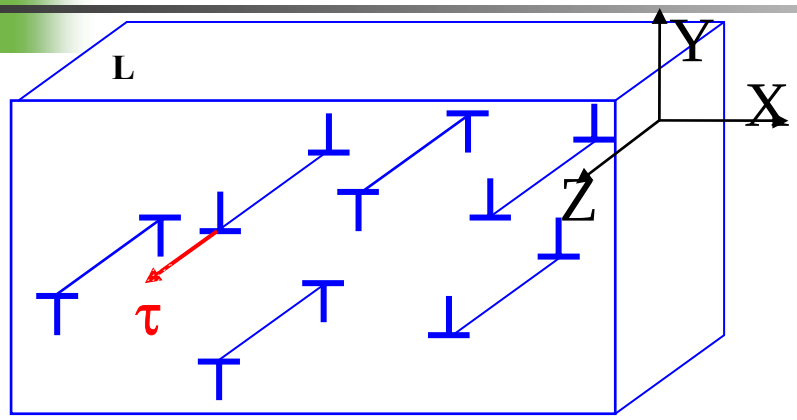
$$T = nS \sum_t 1 - e^{\left(i\mathbf{Q}(\mathbf{u}_{it} - \mathbf{u}_{jt})\right)}$$

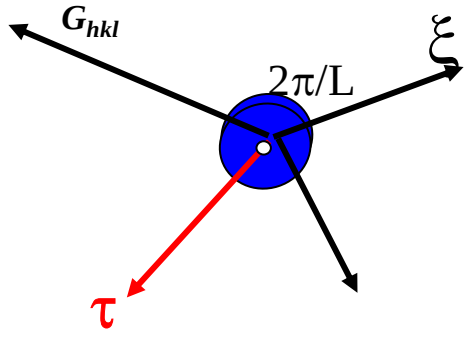
- Scattering on average lattice
- Scattering due to dislocation displacements
- Weak correlation

Dislocations Orientation Influences Streak Axes

Real Space

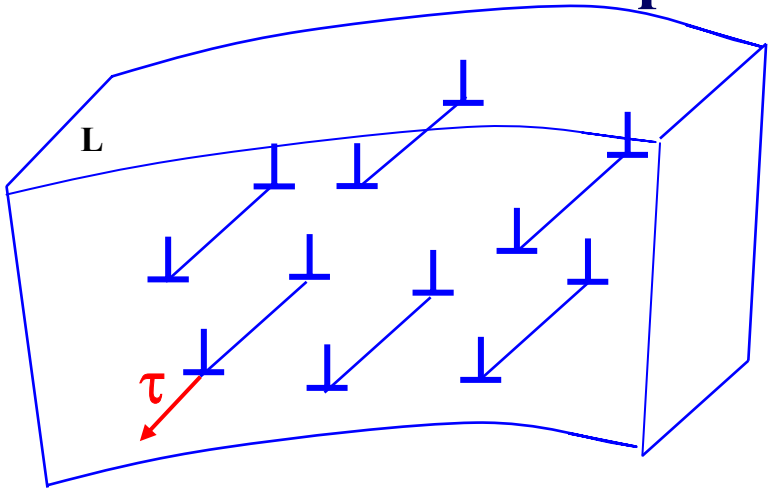
Reciprocal Space

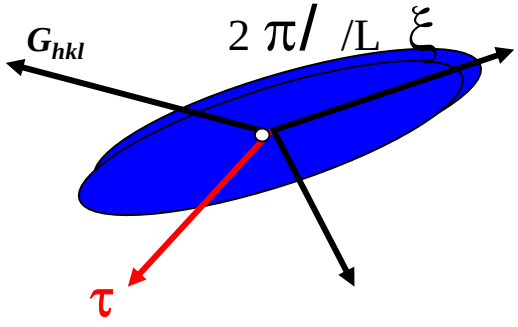




$$\xi = \frac{\tau \times g}{|\tau \times g|},$$

$n^+ = n$: No macroscopic lattice rotation





$$\nu = \frac{\xi \times g}{|\xi \times g|}$$

$n^+ >> n$: Excess of one sign leads to macroscopic lattice rotation

Predominance of One Sign Dislocations Creates both Local and Macroscopic Lattice Rotations

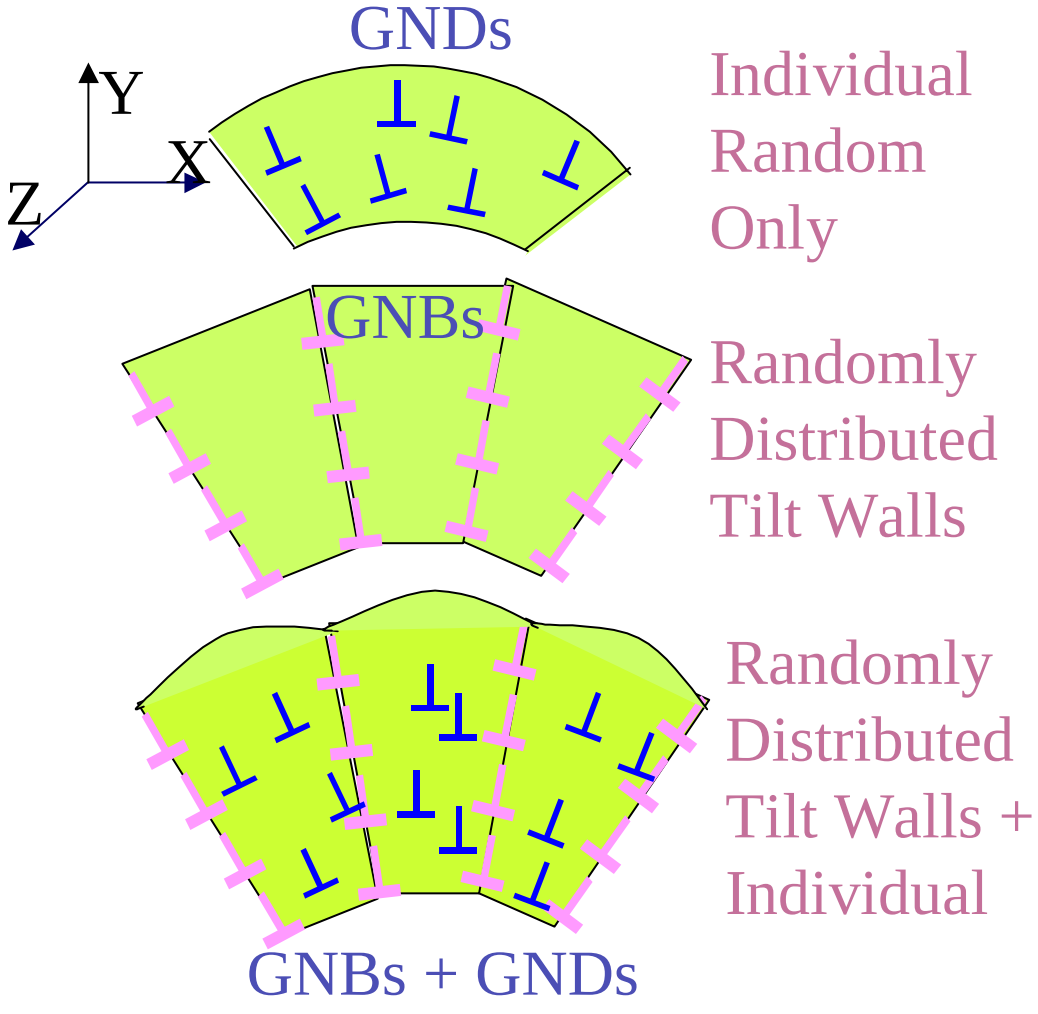
Distortion Tensor

- Mean tensor of dislocation density: $\rho_{zx} = \boldsymbol{n^+ b}$

$$\varepsilon_{klm} \frac{\partial \omega_{mn}}{\partial x_l} = -\rho_{kn}$$

- Nonzero components:
- $\omega_{xy} = -\omega_{yx} = \boldsymbol{n^+ bx}$
- **Macroscopic Rotations** around the *Z* axis

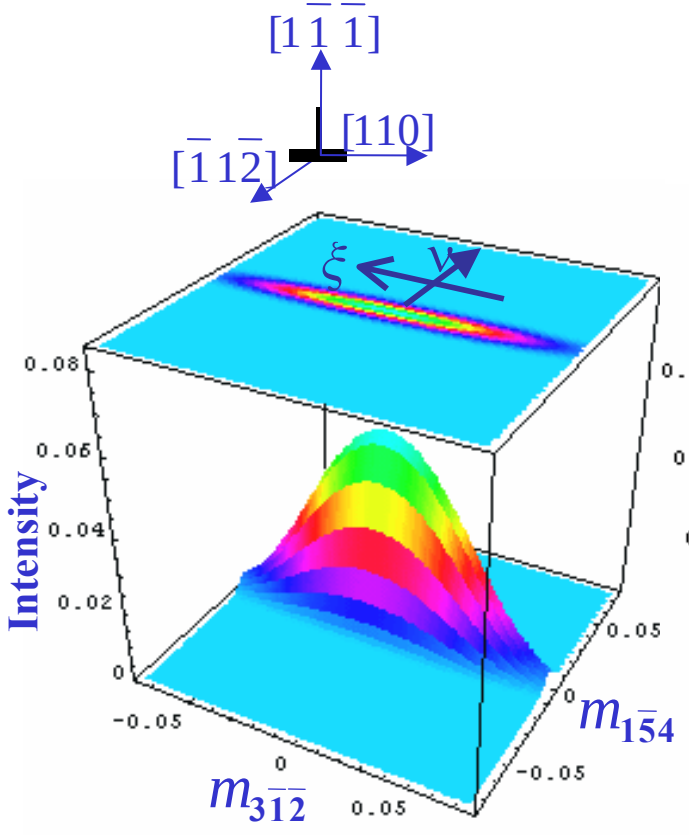
Dislocation Arrangements



Orientation of Unpaired Dislocations Influences Character of White Beam Reflection

Reflection (222); Plane (111); Crystal size L=2500

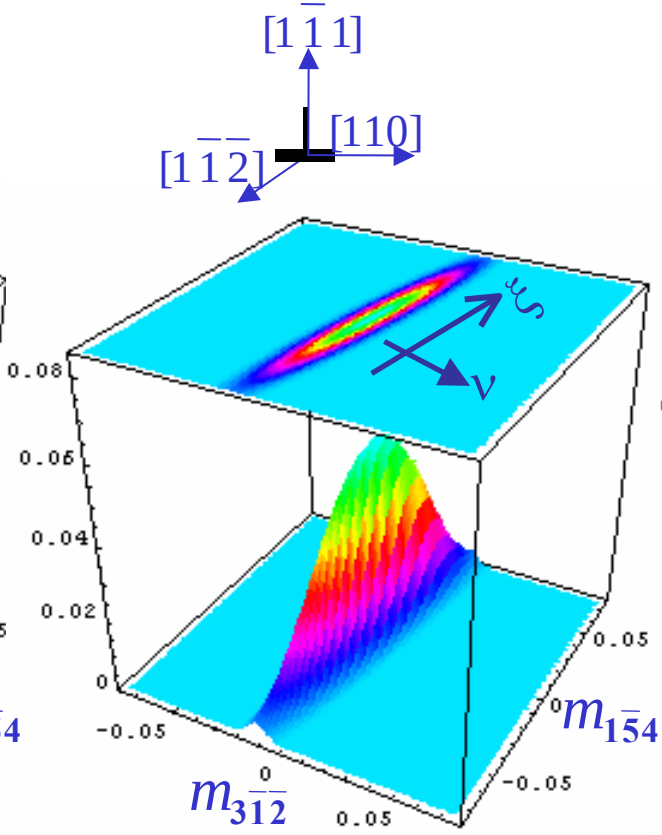
$n=10^{11}cm^{-2}$ $n^{+}=2.5*10^{10}cm^{-2}$



$\xi=[3\bar{1}\bar{2}]; \nu=[1\bar{5}4]$

$h_{\xi}/h_{\nu}=8.6$

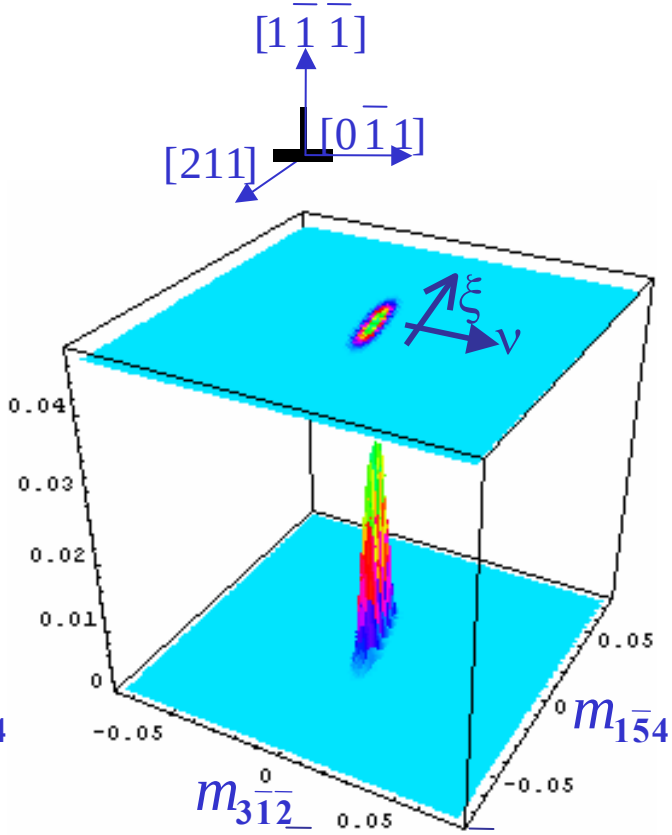
$|\tau G_{hkl}|=0.47$



$\xi=[1\bar{3}2]; \nu=[\bar{5}14]$

$h_{\xi}/h_{\nu}=8.6$

$|\tau G_{hkl}|=0.47$

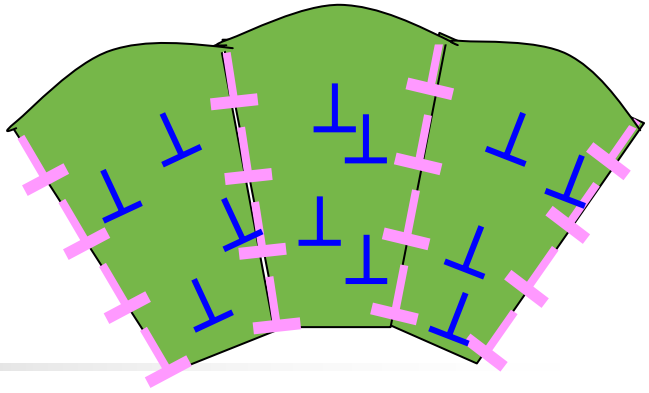


$\xi=[0\bar{1}1]; \nu=[211]$

$h_{\xi}/h_{\nu}=6.8$

$|\tau G_{hkl}|=0.94$

Individual and Boundary Dislocations Have Different Influence on Scattering



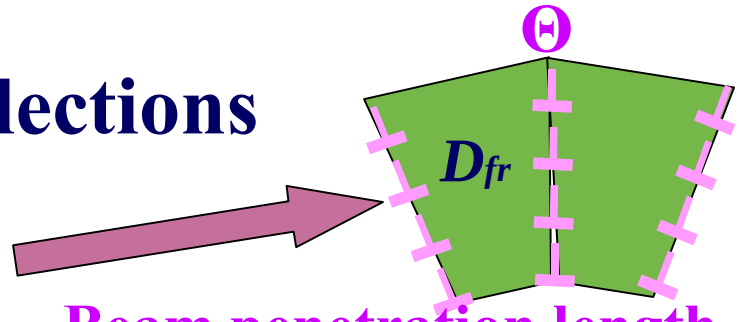
- *Grouping of dislocations into a "thin" tilt wall:*
  - *Changes the shape*
  - *decreases FWHM*
  - *Factor (h/D_{fr}):*

  if $h << D_{fr}$

- *Due to local strains, individual GNDs influence the length of the streak more than the same number of dislocations in a boundary*

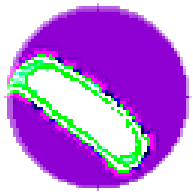
- *The $FWHM_{fr}$ depends on the density of GNDs and on the experimental resolution function.*
- *As the resolution function improves, a larger number of separate spots can be detected within a streak as observed experimentally*

Splitting of White Beam Reflections

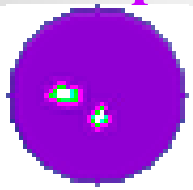


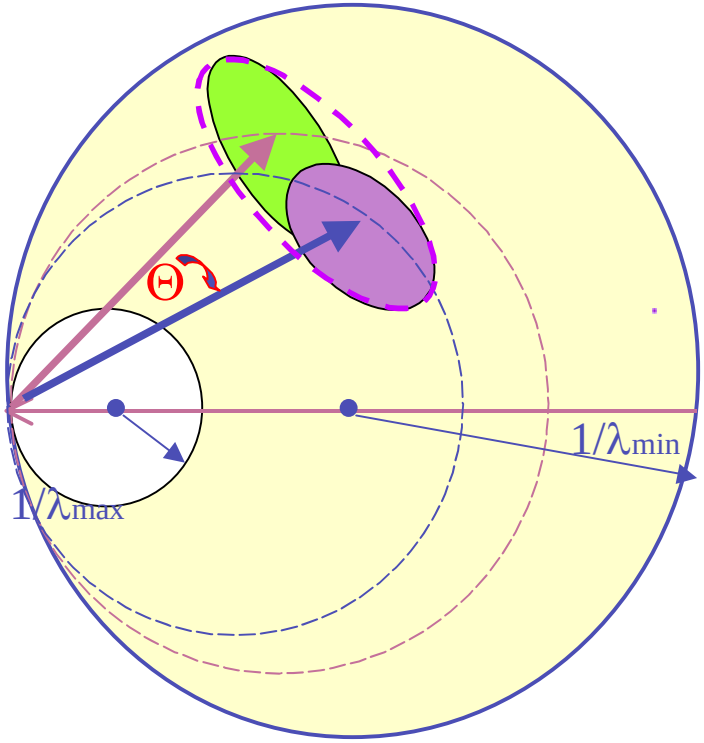
Beam penetration length *L*

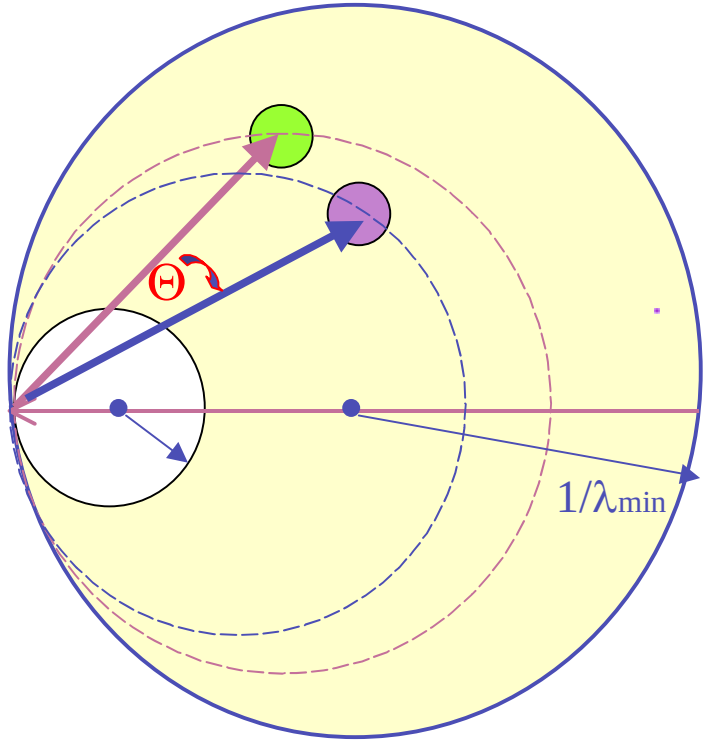
Criterion:

$K \ll 1$ 

$$K = \left(\frac{\Theta G_{hkl}}{FWHM_{fr}} \right)^2 \frac{D_{fr}}{L}$$

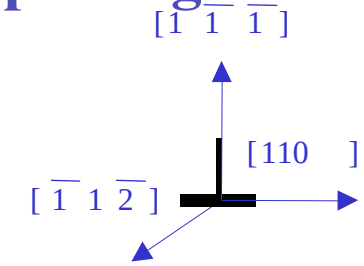
 $K \geq 1$



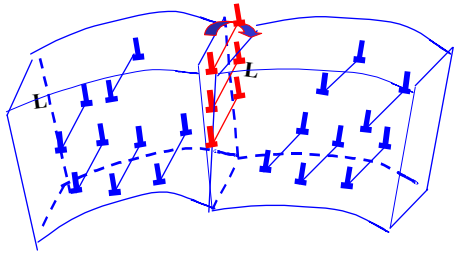


Energy Spread in the Incident Radiation Causes a Change in Evald's Spheres Cutting the Reciprocal Lattice

Splitting of Laue Spots due to Grouping of Dislocations into GNB

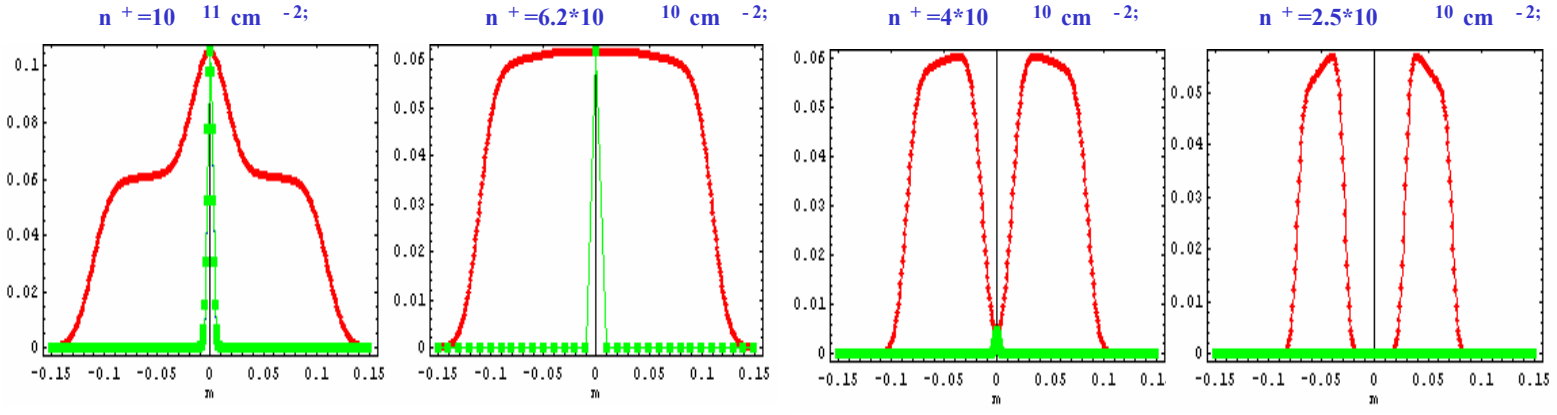


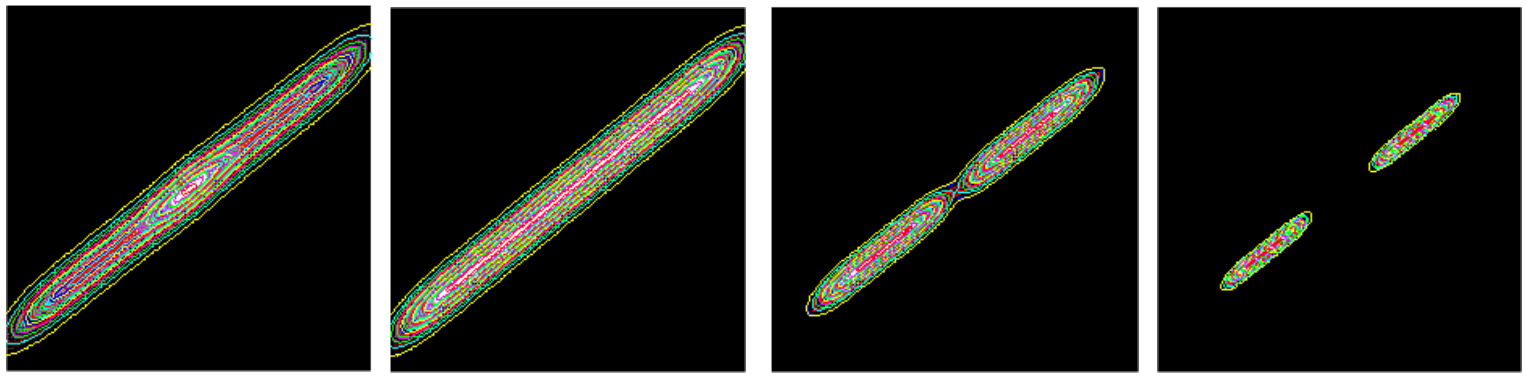
Primary dislocation set



Θ = 2 ^{0} Θ = 2.07 ^{0} Θ = 2.12 ^{0} Θ = 2.14 ^{0}

n $^{+}$=10 ^{11} cm $^{-2}$; n $^{+}$=6.2*10 ^{10} cm $^{-2}$; n $^{+}$=4*10 ^{10} cm $^{-2}$; n $^{+}$=2.5*10 ^{10} cm $^{-2}$;

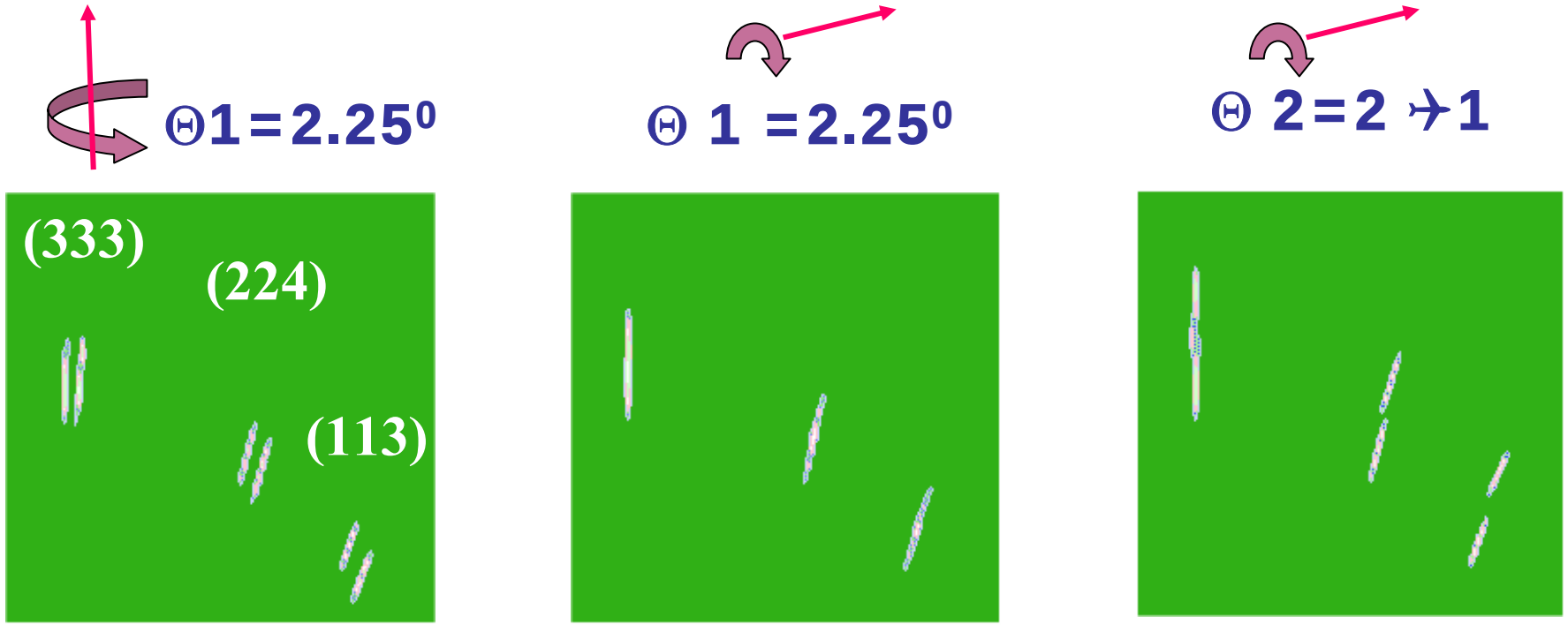




Plane (001)

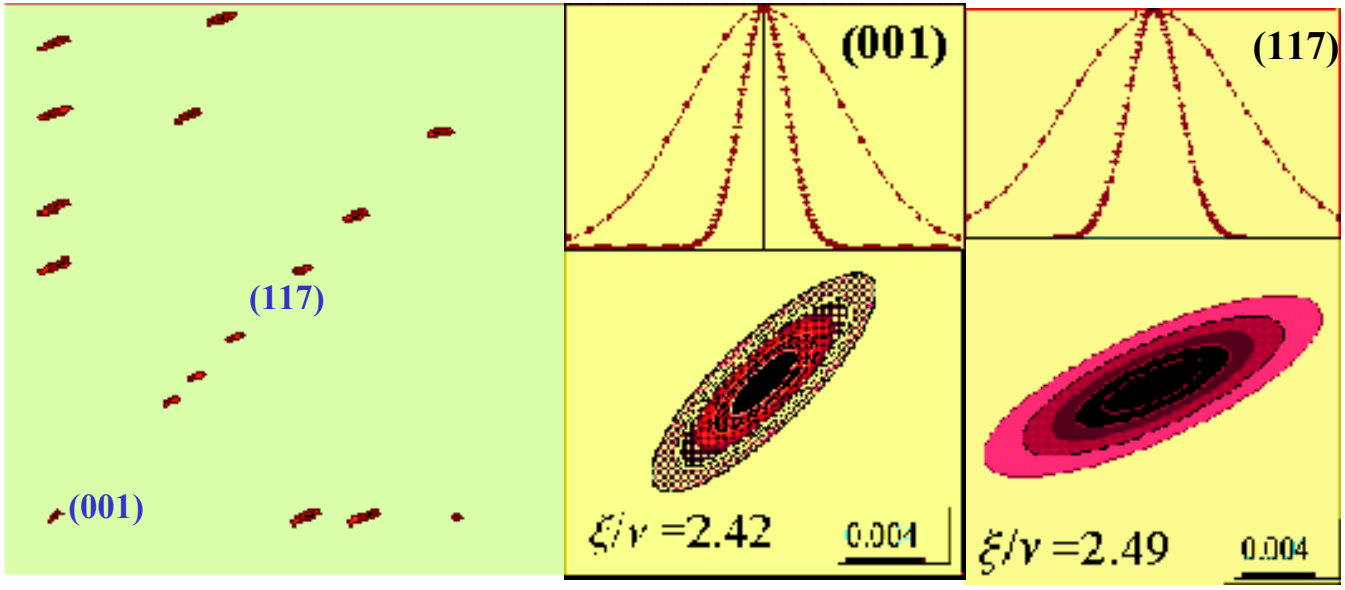
Laue image allows to determine orientation and angle of geometrically necessary boundary and density of unpaired dislocations within each domain

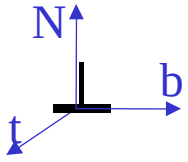
- Orientation of the boundary differs 90^0
- Misorientation angle of the boundary twice bigger



Surface normal= [111], $n+=4*10^{11}cm^{-2}$

A single orientation of GNDs explains the orientation of all Laue Spots





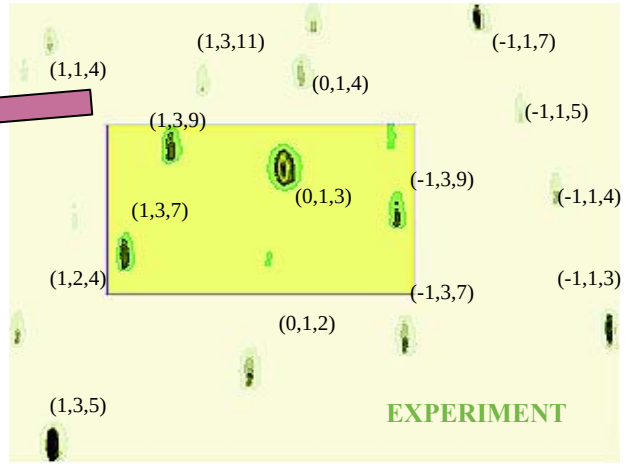
b=[110]; t=[-11-2]; N=[1-1-1]

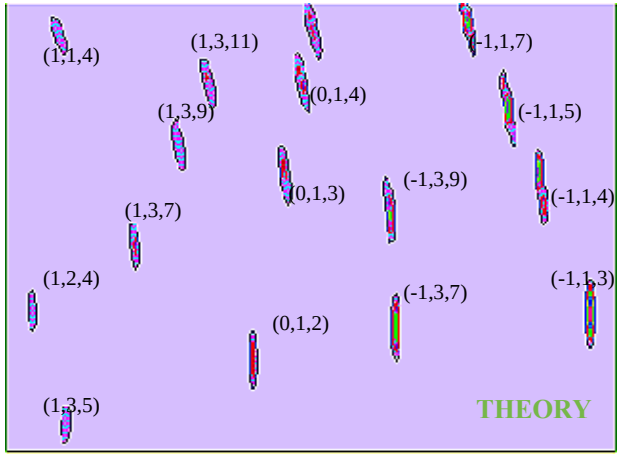
Laue Images From *Ir Weld* Reveal Plastic Deformation in the Heat Affected Zone

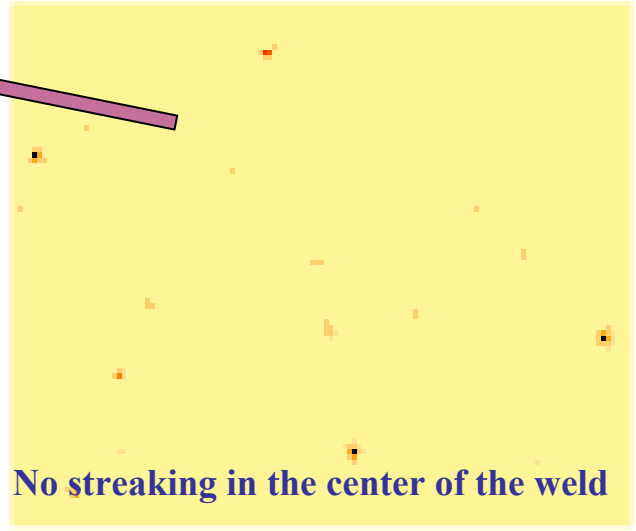
***Irradiated volume:*0.7*0.7*2μm**

Heat Effected Zone

Weld







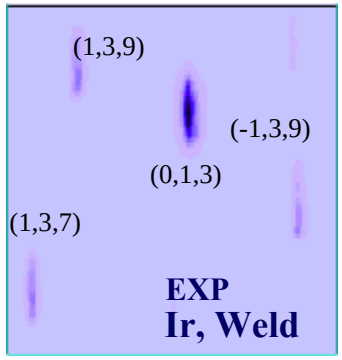
b=[0,1,-1];

τ=[2,1,1];

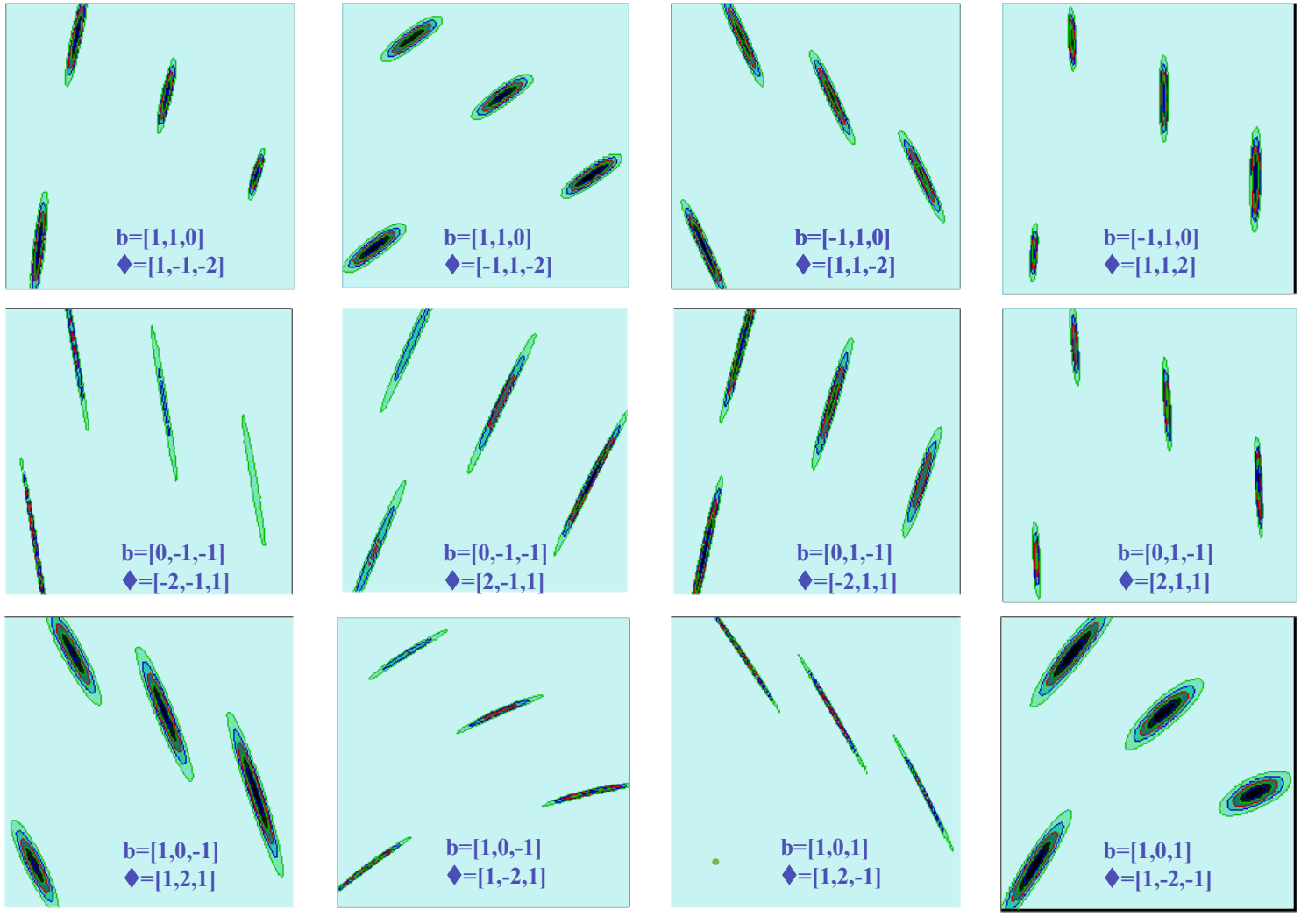
n^{+}=0.1n

How Do 12 Slip Systems Affect the Laue Pattern?

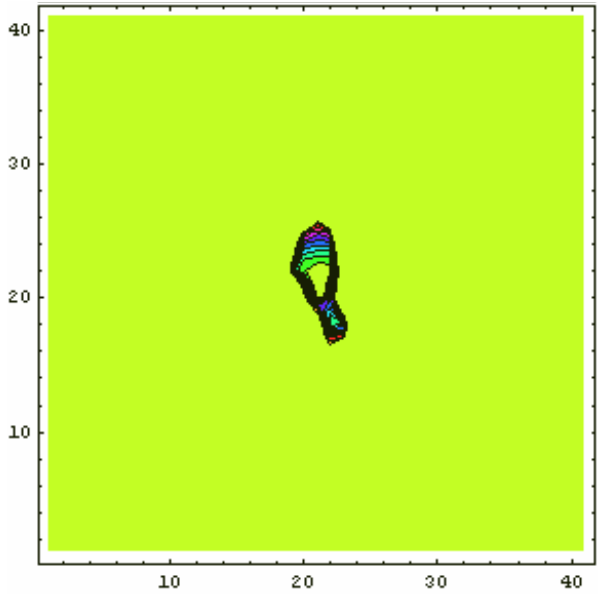
Surface normal (013), n^+=0.1n, L=500b

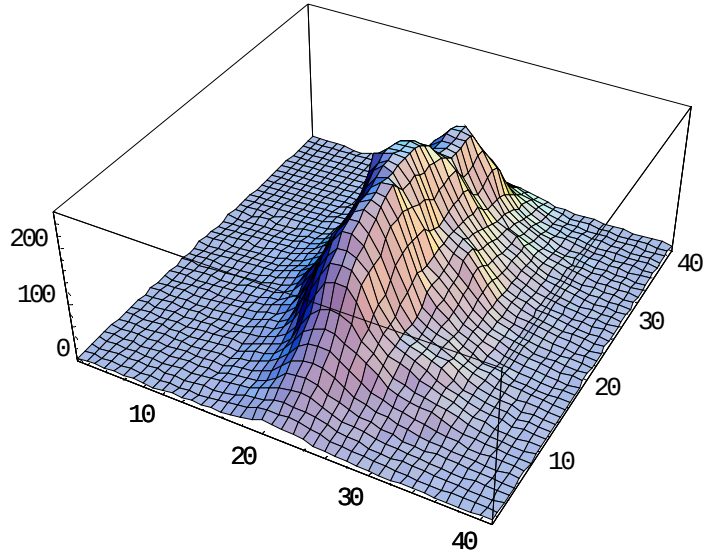


- *Slip System Changes the Direction of Streaking*
- *Contrast factor changes the length of the streak*
- *No Streaks for Some Reflections*



Slices of the 3D image at different intensity levels reveal heterogeneous dislocation structure in the heat affected zone



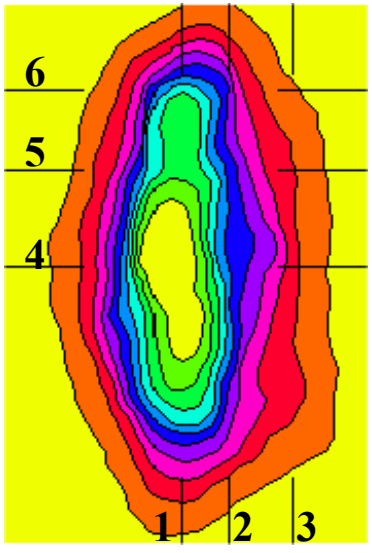


- Splitting into three scattering domains are found within the scattering region

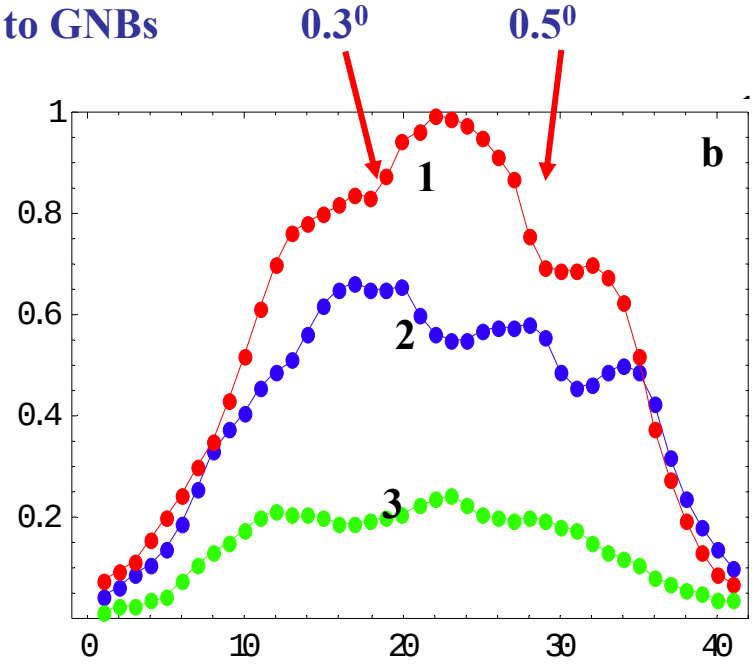
Several spikes are detected in along ξ for a grain near *Ir* weld: they indicate formation of geometrically necessary boundaries

- **Analysis of the streak profile determines misorientation of the GND**

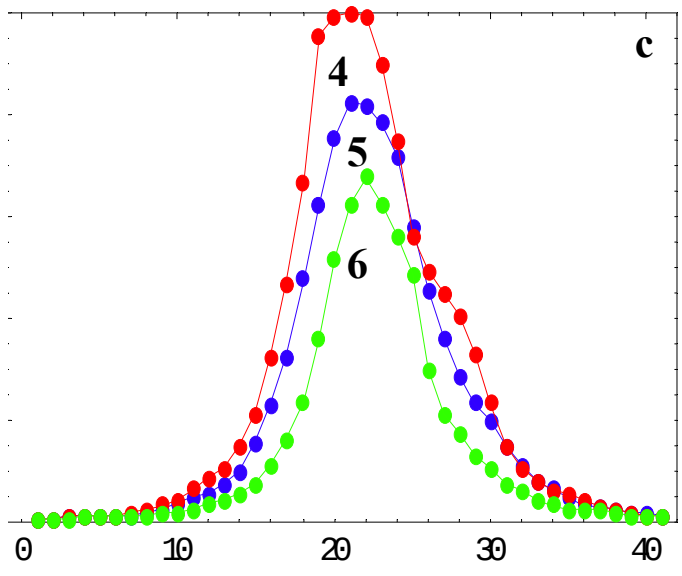
Misorientation due to GNBs



Contourmap of (135) Laue spot, showing location of intensity slices.



Slices along ξ direction show splitting of the reflection



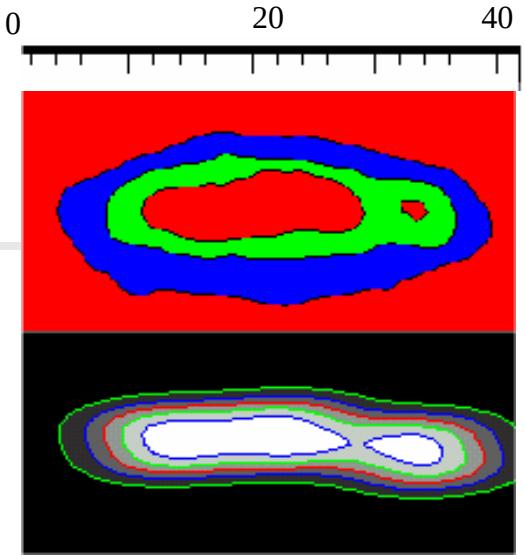
Slices along ν direction show complicated elastic-plastic state

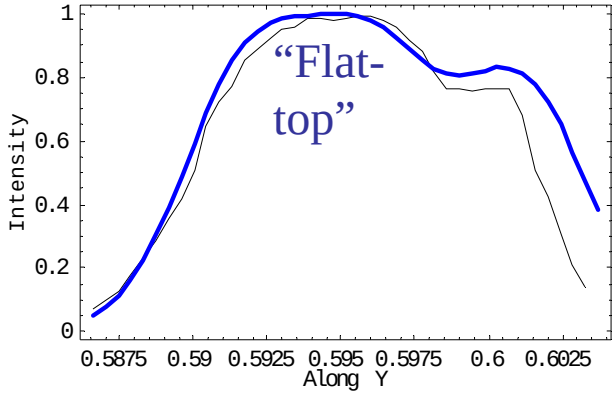
The intensity distribution of Laue diffraction is analyzed as a function of local misorientation

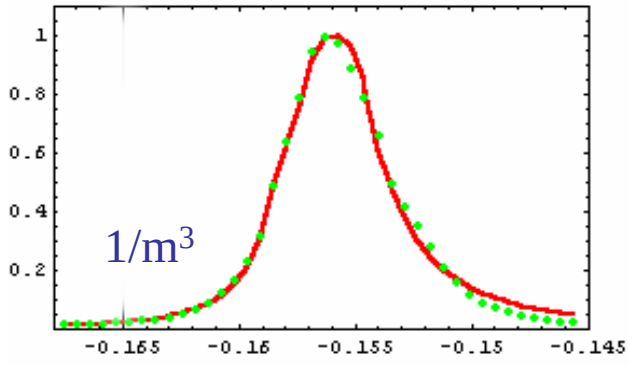
- *The best fitting parameters for dislocation density, orientation of the slip system, exact positions and misorientation angles through GNBs between scattering fragments were determined*

$$FWHM_{\xi} \propto n^{+}\sqrt{1-(\mathbf{g}\boldsymbol{\tau})^{2}}$$

$$FWHM_{\upsilon} \propto \sqrt{nbQ}$$







CONCLUSIONS

- Excess dislocations result in elongated shape of Laue images for different reflections
- Orientation of the excess dislocation set can be determined from the Laue image.
- The density of the excess dislocation set as well as the total dislocation density can be determined from FWHM of the long and short axis of the streak
- Maze of dislocation network can be understood from Laue pattern