Simulation and Indexation of polycrystallites LAUE

From Data to Measurements

Towards Automation: Dream or Reality?

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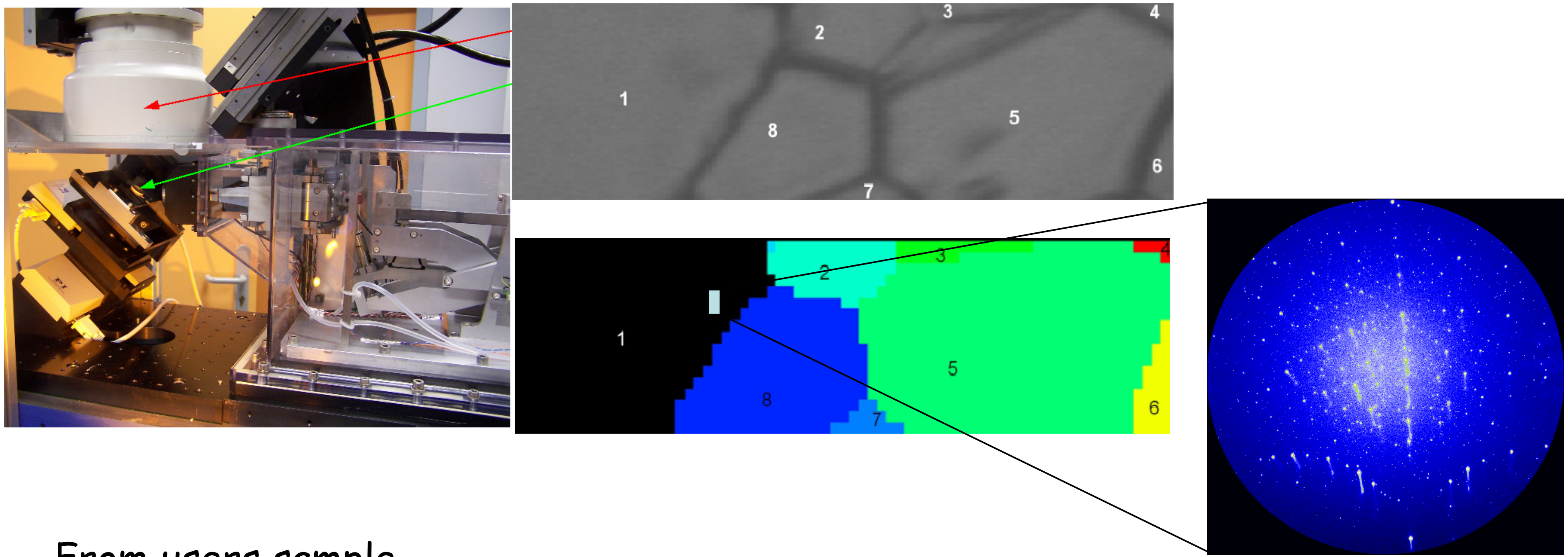
Outline

- Context
- Simulate Laue Patterns
  - *- Origin*
  - *- information-signal nature*
  - *- maths*
- Pattern indexation-recognition
  - *- Handle Experimental data*
  - *- Indexation procedures*
- ► Conclusion

Context



From users sample…

by means of microdiffraction experiments…

… and data analysis

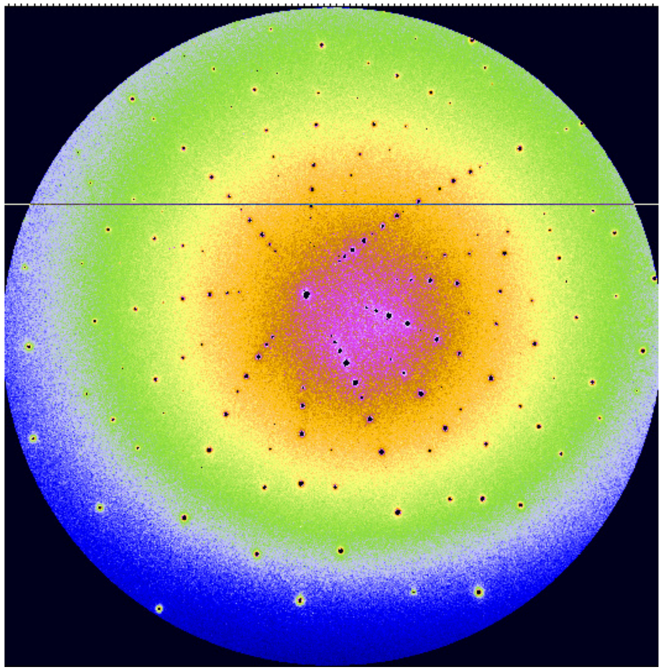
… to 2D orientation and strain mapping

Will Laue diffraction be as simple as other 2D microscopy techniques ?

Context

When use microdiffraction ?

- *Collection of a few selected image*
- *Each image = sum of Laue Pattern of a 1-3 single crystals*
- *Single crystal Laue Pattern contains less than 100 peaks*
- *Spot are round and intense*



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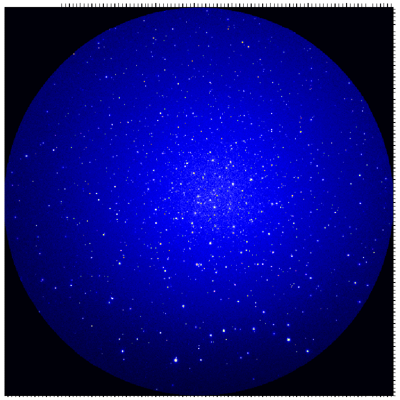
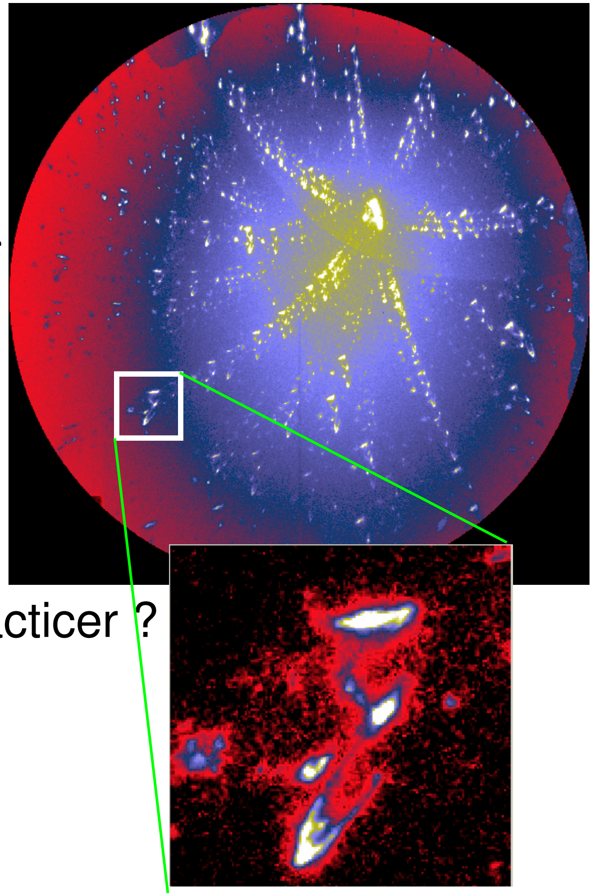
Context

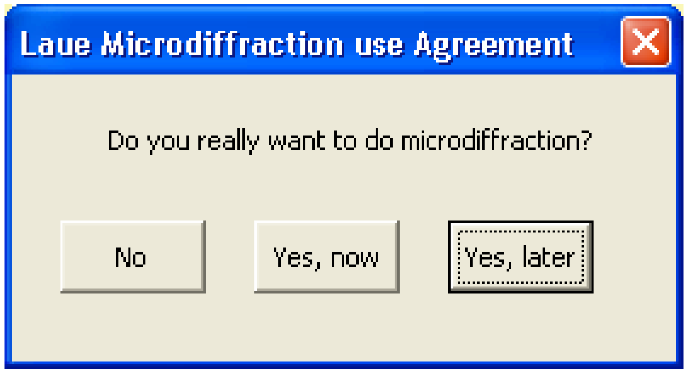
When NOT use microdiffraction ?

- *Collection of much more than thousands images*
- *Each image = sum of Laue Pattern more than a dozen images*
- *Single crystal Laue Pattern contain more than a few hundreds spots*
- *Each spot is actually ill-shaped or divided into several other spots*
  (themselves ill-shaped as well)

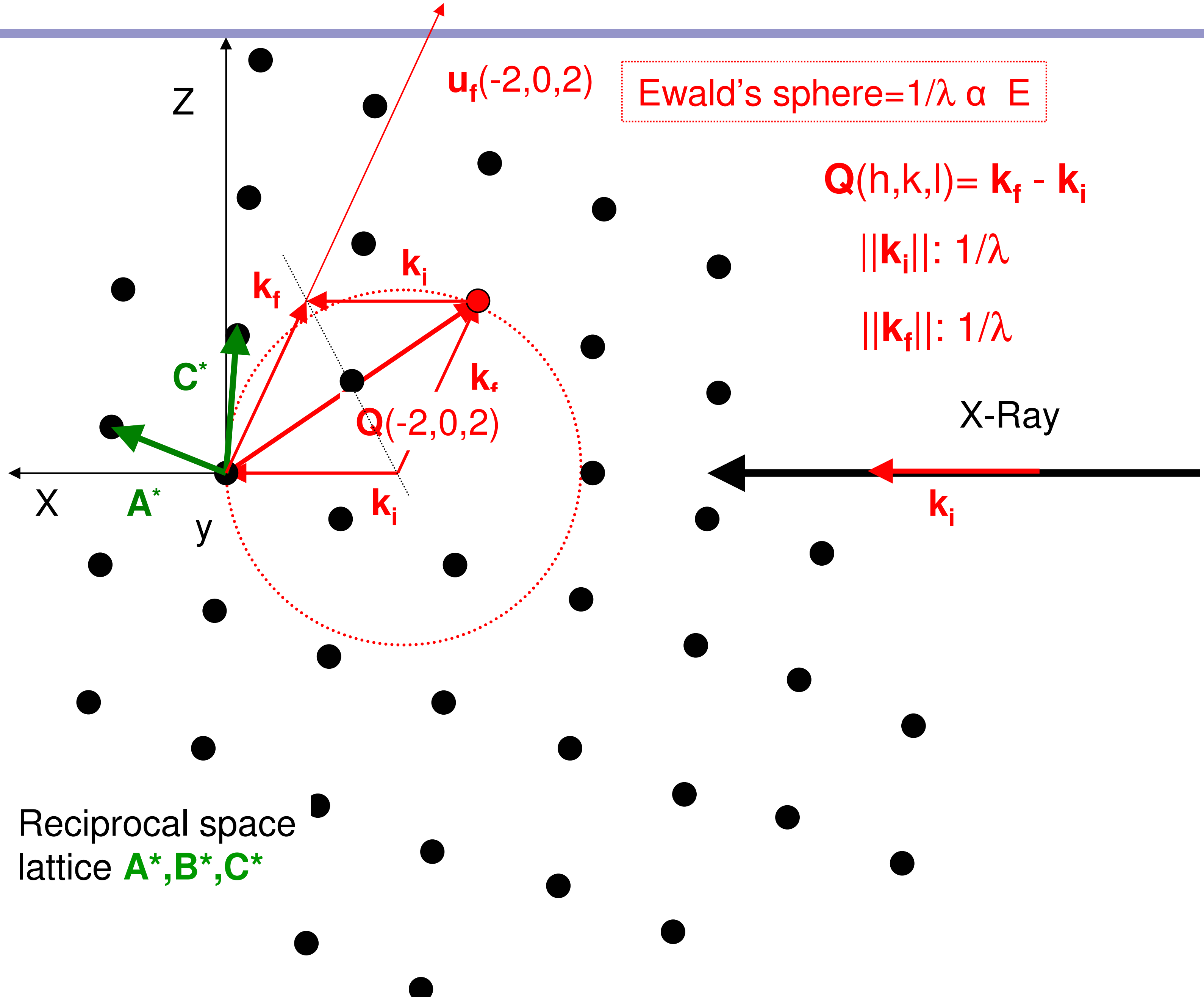




How to become a good microdiffraction practicer ?
- *Be easy with Maths/data mining/computing*
- *Be Patient*
- *Trust only yourself*



Simulate Laue Pattern: ewald's sphere



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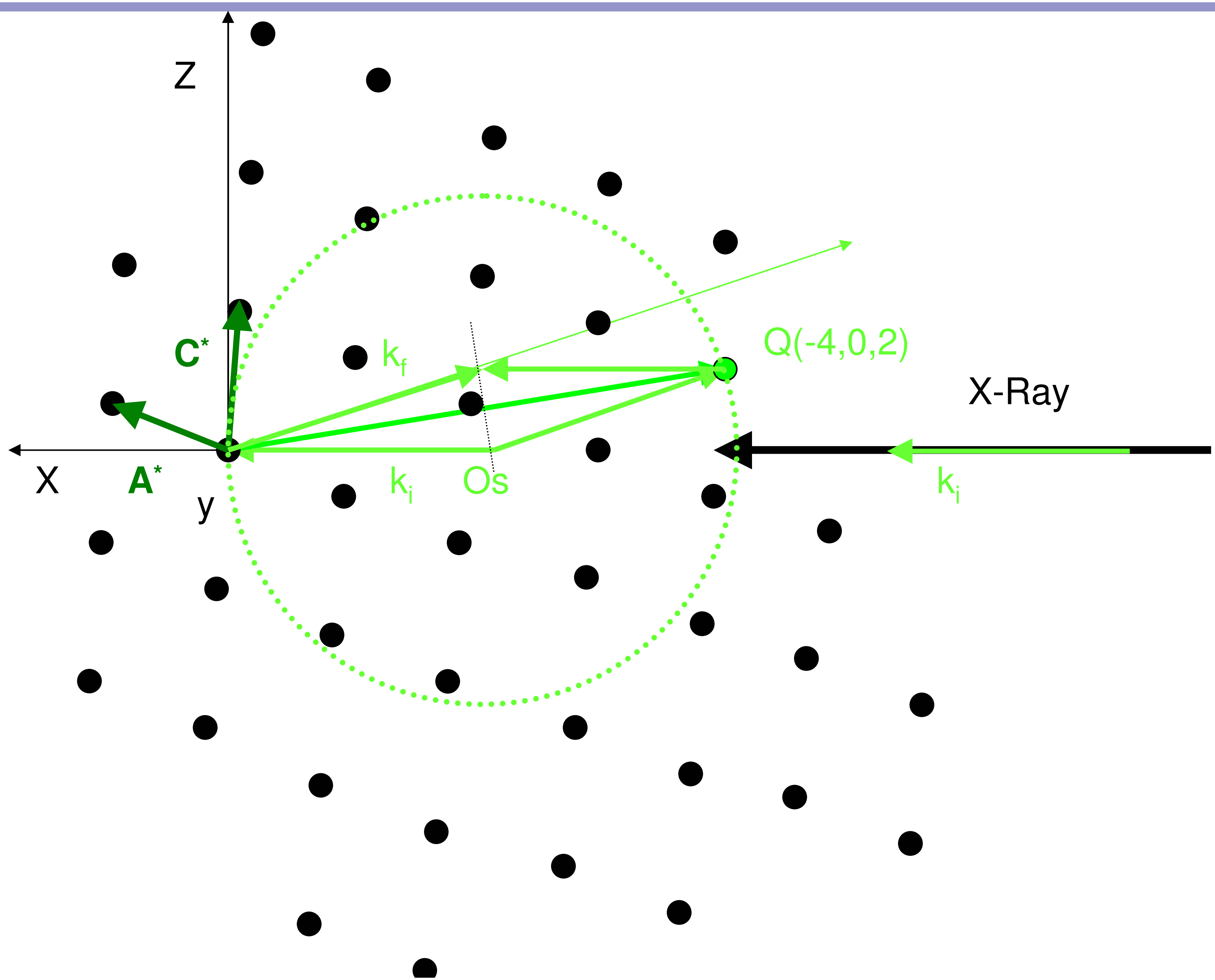

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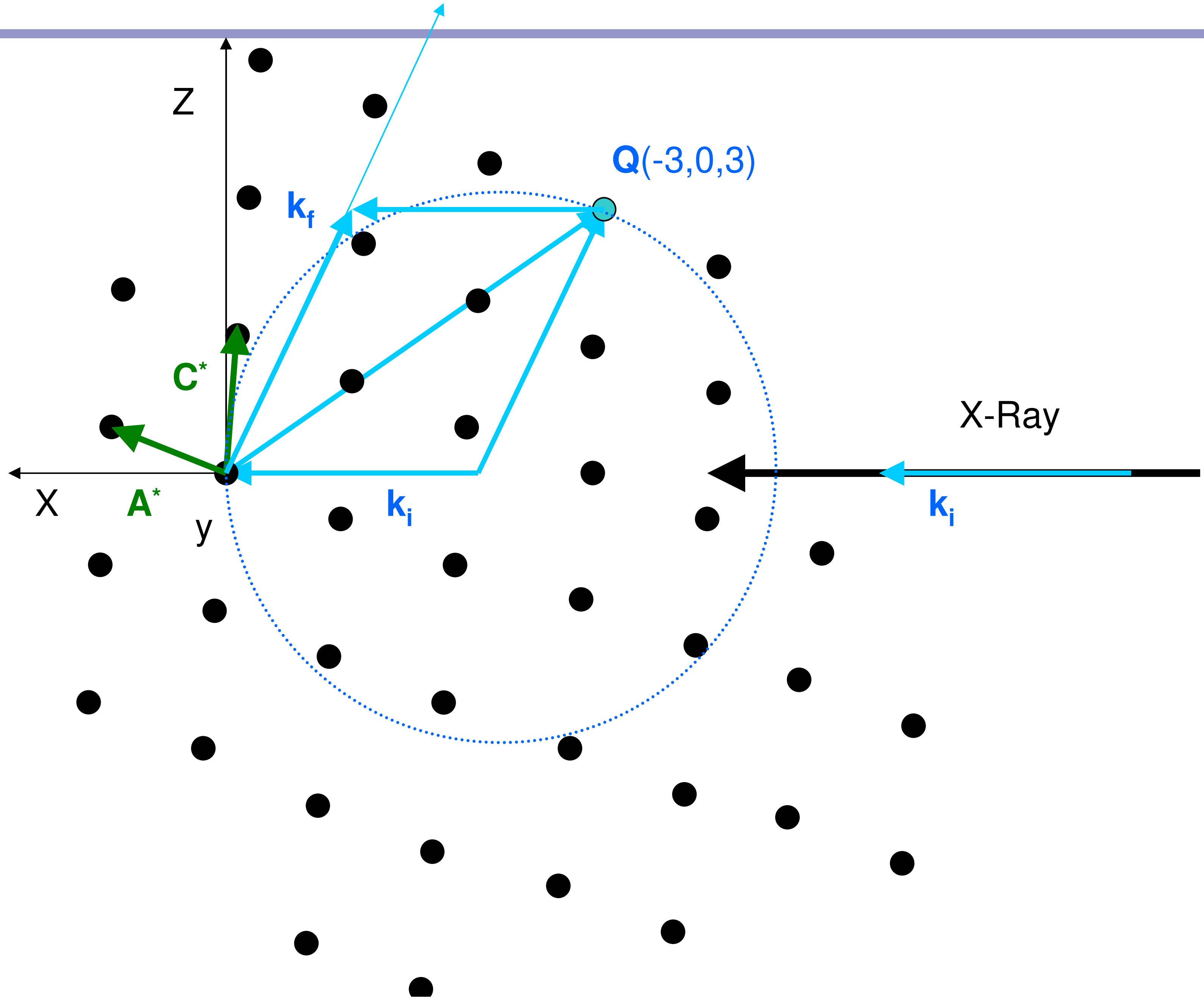

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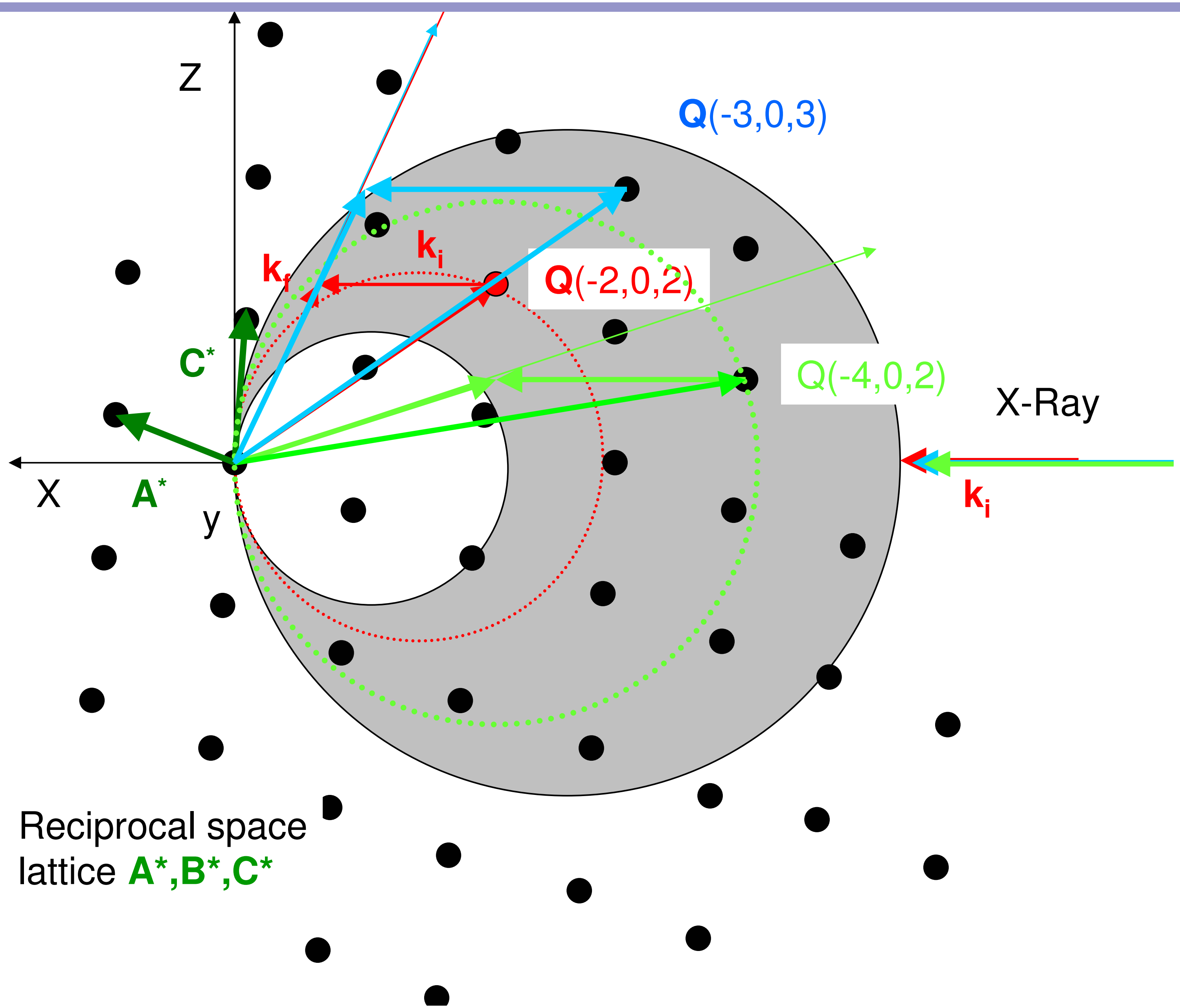
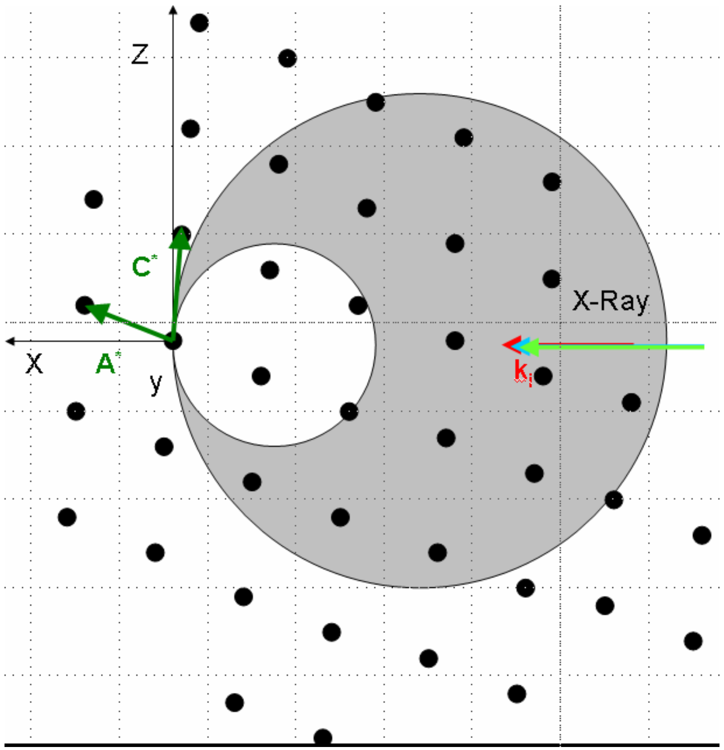
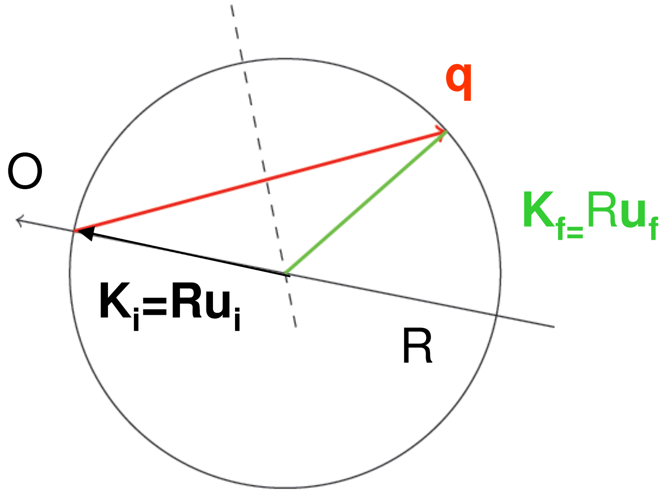


Simulate Laue Pattern: algorithm



1. Find all lattice hkl nodes in between two spheres
2. Compute **q** in lab. frame (O,X,Y,Z)
3. Compute **kf**,**uf**, E



$$R(\mathbf{q}) = \frac{\|\mathbf{q}\|^2}{2\mathbf{q}.\mathbf{u_i}}$$

$$\mathbf{k_i} = R\mathbf{u_i}$$

$$\mathbf{k_f} = \mathbf{q} + \mathbf{k_i}$$

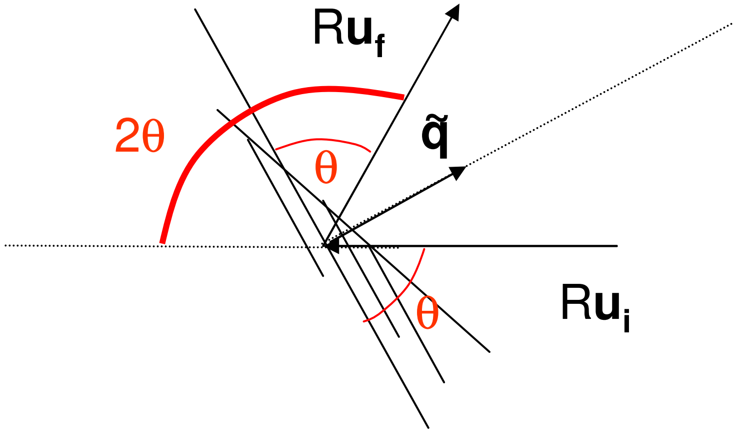
Energy=12.398 R R=1/λ

Simulate Laue Pattern: Laue pattern properties

Reflection-by-a-plane transform (normal **q**)

$$\mathbf{u_f} = [M(\mathbf{q})]\mathbf{u_i} \qquad m_{ij} = \delta_{ij} - 2\frac{q_i q_j}{\|\mathbf{q}\|^2}$$

$$\mathbf{u_f} = \mathbf{u_i} - \frac{2\mathbf{q}.\mathbf{u_i}}{\|\mathbf{q}\|^2}\mathbf{q} = \mathbf{u_i} - \frac{\mathbf{q}}{R} = \mathbf{u_i} - 2\sin\theta\tilde{\mathbf{q}}$$



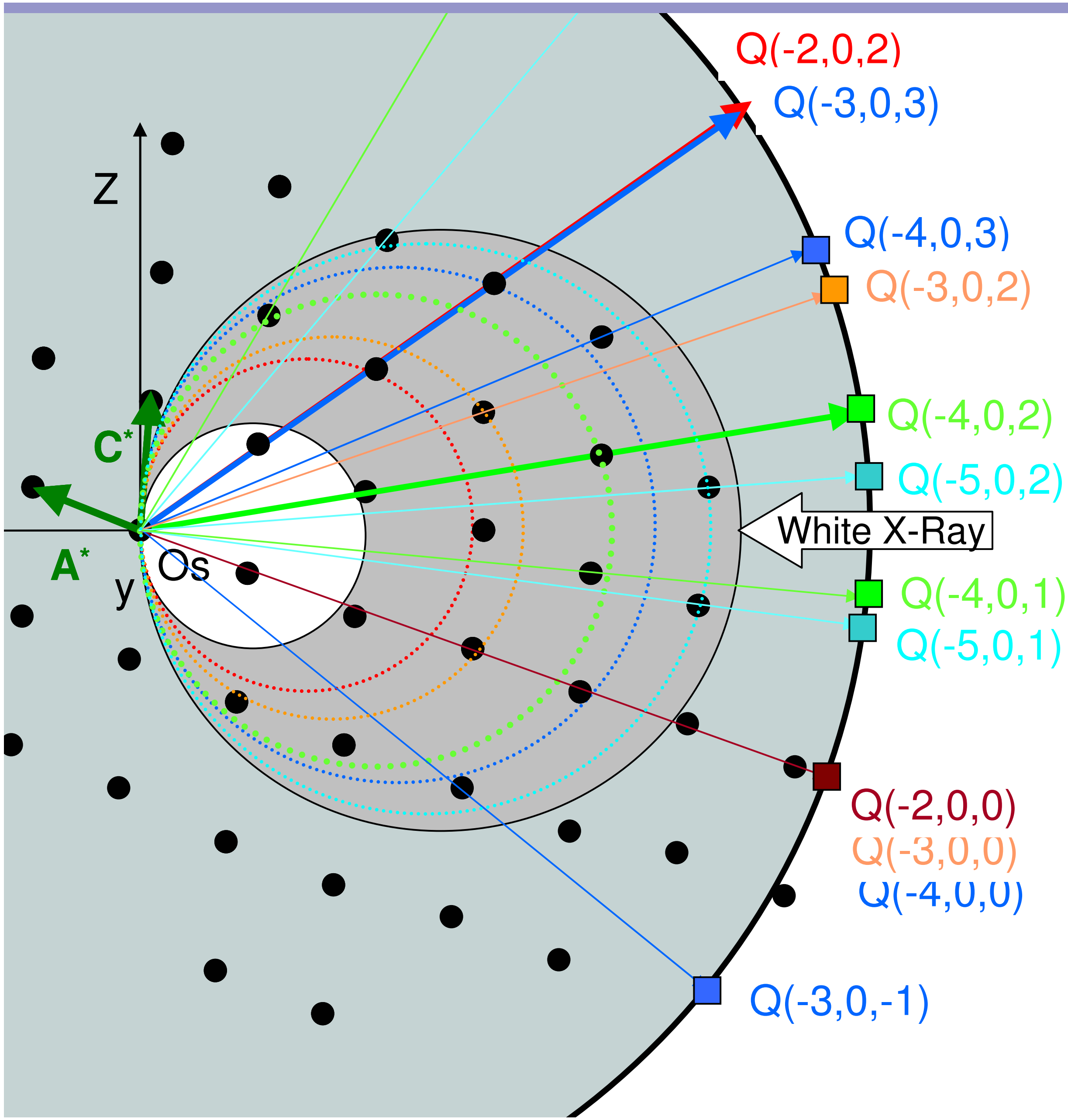
Mathematical property

$$\forall a \in \mathbb{R} \quad \begin{aligned} M(a\mathbf{q}) &= M(\mathbf{q}) \\ \mathbf{k_f}(a\mathbf{q}) &= \mathbf{k_f}(\mathbf{q}) \end{aligned}$$

- Laue pattern is invariant by homothetical transform
- $\mathbf{u_f}$ represents all RS vectors lying in the same direction
- Harmonic RS nodes have Laue superimposed spots
- Mapping:

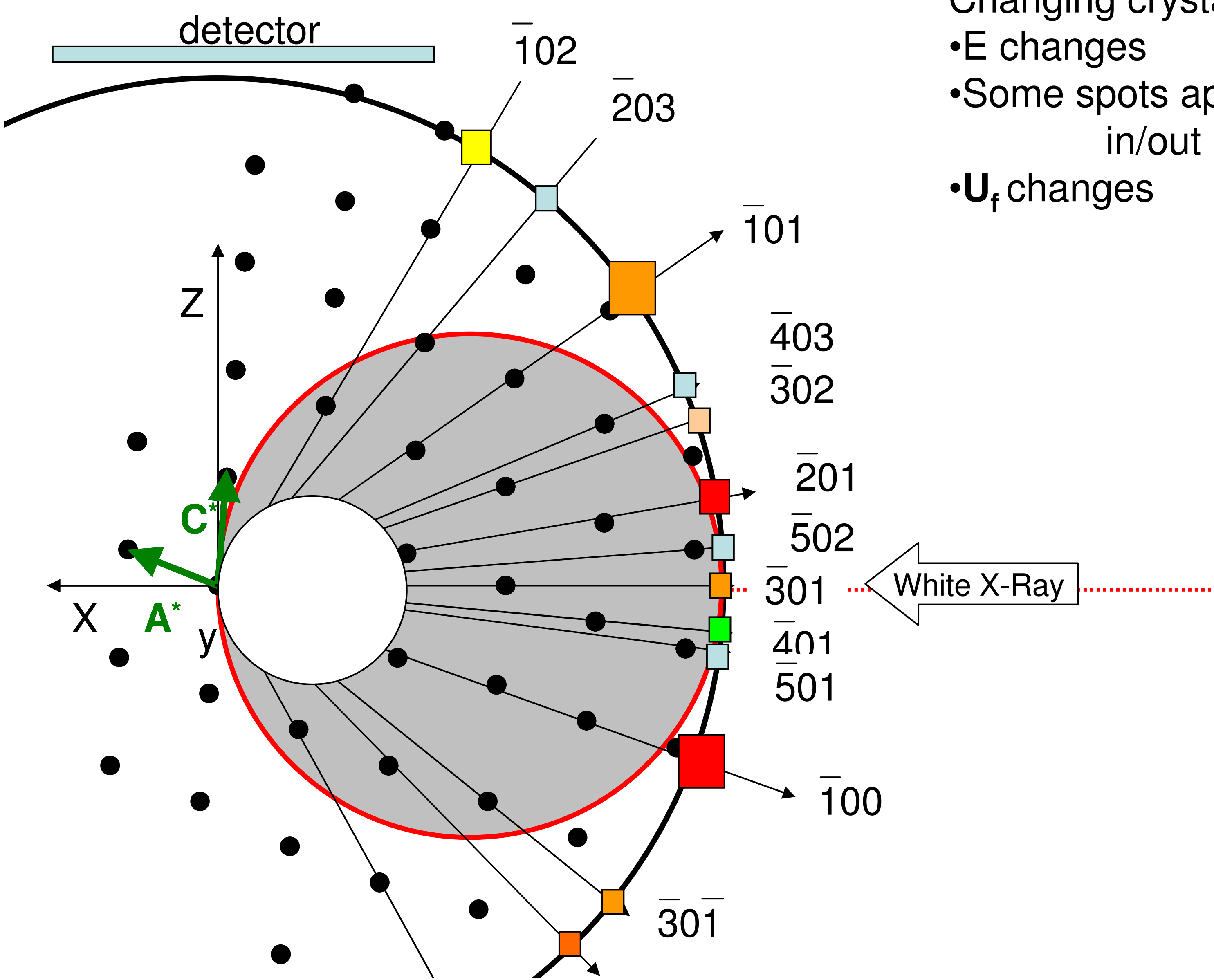
1 RS direction ⇔ 1 u_f direction ⇔ 1 single spot on CCD
Angle between u_f ⇔ angle between RS directions

Simulate Laue Pattern: directions sphere Σ_d



An Other Mapping:
3D direction unit vector $\tilde{\mathbf{q}}$
⇔
unit vector $\mathbf{u_f}$
⇔
point on unit sphere (Σ_d) surface

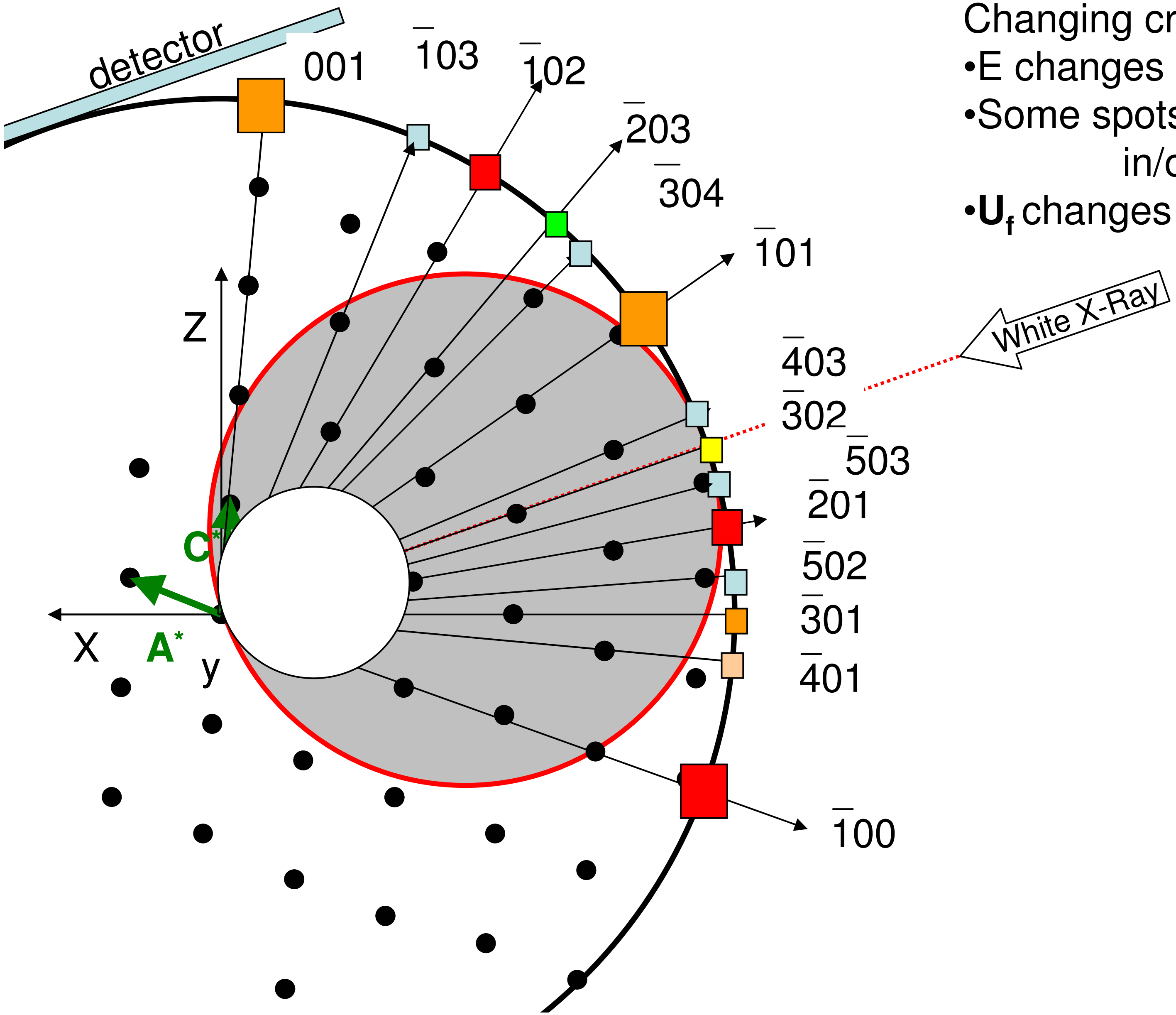
Simulate Laue Pattern: directions sphere Σ_d



Changing crystal orientation:

- E changes
- Some spots appear/disappear in/out ([Emin,Emax])
- $\mathbf{U_f}$ changes

Simulate Laue Pattern: directions sphere Σ_d



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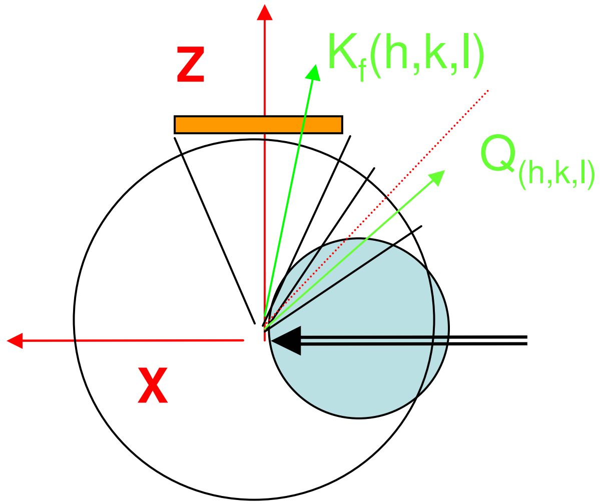
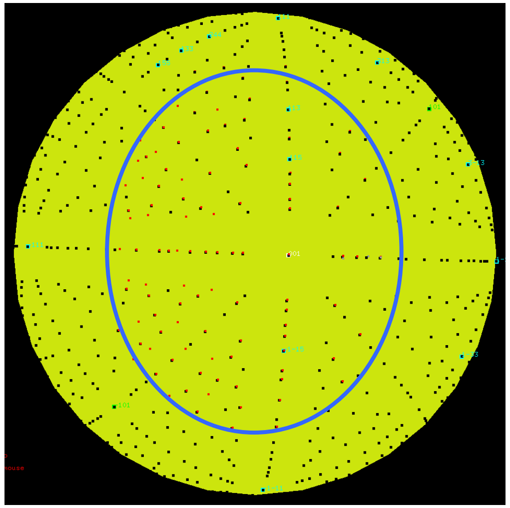
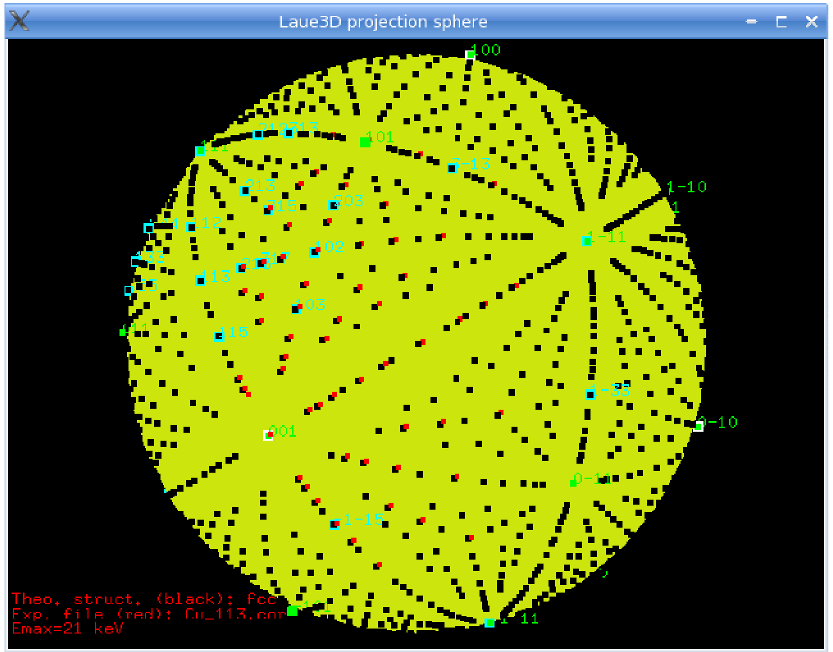
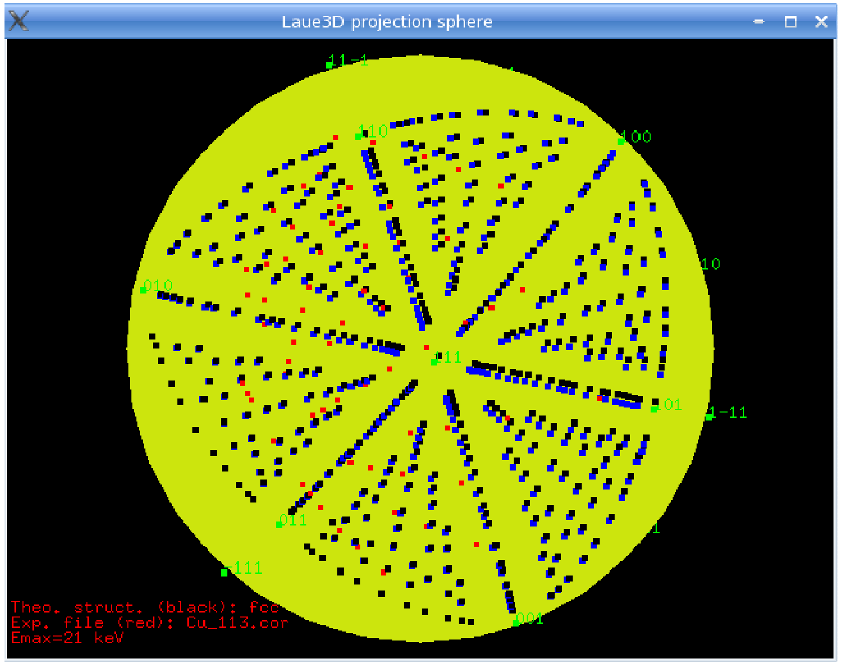
Simulate Laue Pattern: directions sphere Σ_d



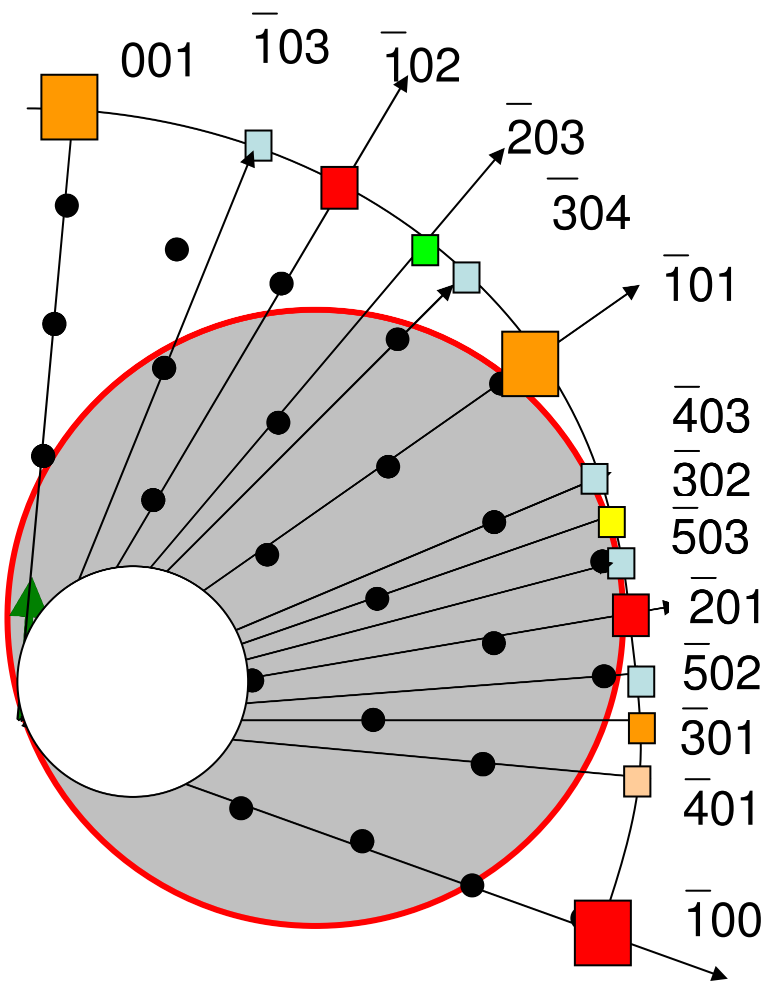


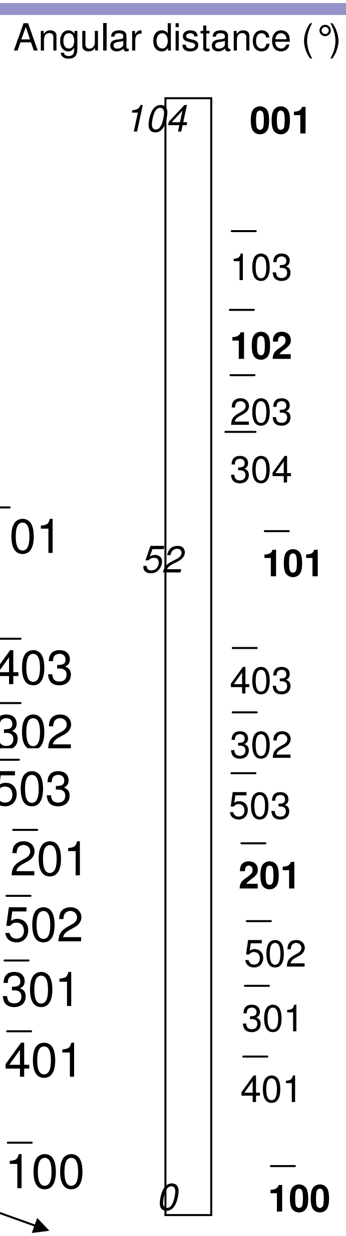




Simulate Laue Pattern: zone axis

Zone axis example: [010]





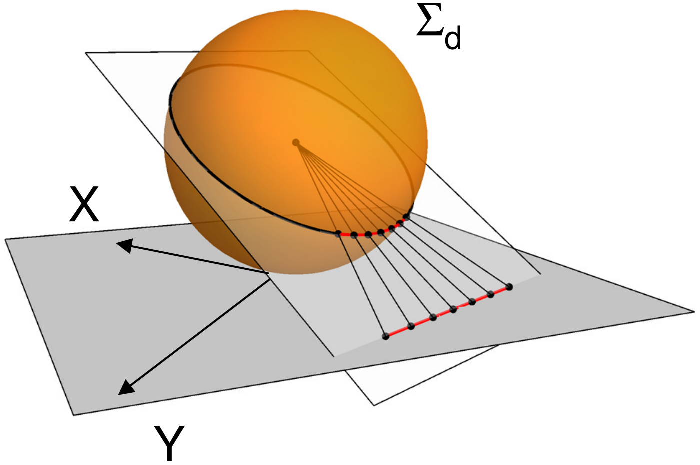
Zone axes [uvw]: hu+kv+lw=0

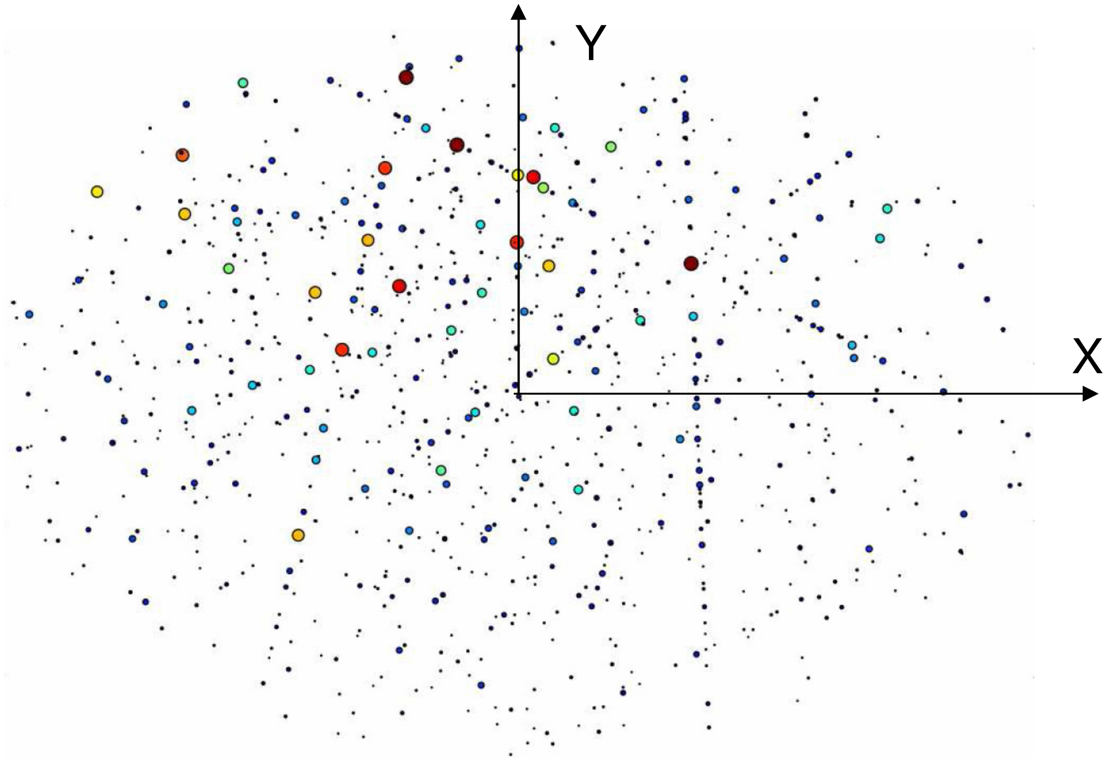
If (h_1,k_1,l_1) and (h_2,k_2,l_2) belong to [uvw]
$\Rightarrow (h_1+h_2,k_1+k_2,l_1+l_2)$
1- belongs to [uvw]
2- in between (h_1,k_1,l_1) and (h_2,k_2,l_2)

- Spot sequence of [uvw] in q direction space is in $\mathbf{u}_f$ space:
  - unchanged in order
  - rescaled in angular distance
- Spot is sequence of [uvw] in q direction space is conserved in $\mathbf{u}_f$ space
- Low u,v,w zone axis is dense (numerous spots)
- Low h,k,l spot have desert neighbourhood
- Low h,k,l spot is at intersection of dense zone axes

Simulate Laue Pattern: *gnomonic projection*

Zone axis great circle is a straigth line on gnomonic plane!





$$X = \frac{\cos\phi \sin(\lambda - \lambda_0)}{\cos c}$$

$$Y = \frac{\cos\phi_1 \sin\phi - \sin\phi_1 \cos\phi \cos(\lambda - \lambda_0)}{\cos c},$$

$$\cos c = \sin\phi_1 \sin\phi + \cos\phi_1 \cos\phi \cos(\lambda - \lambda_0).$$

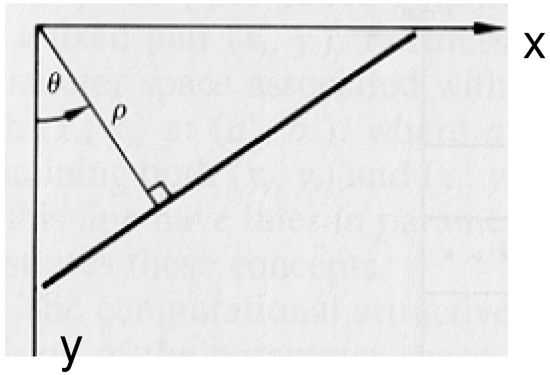
Nice space where information is more readable
(see zone & spot recognition)

Simulate Laue Pattern: Hough transform

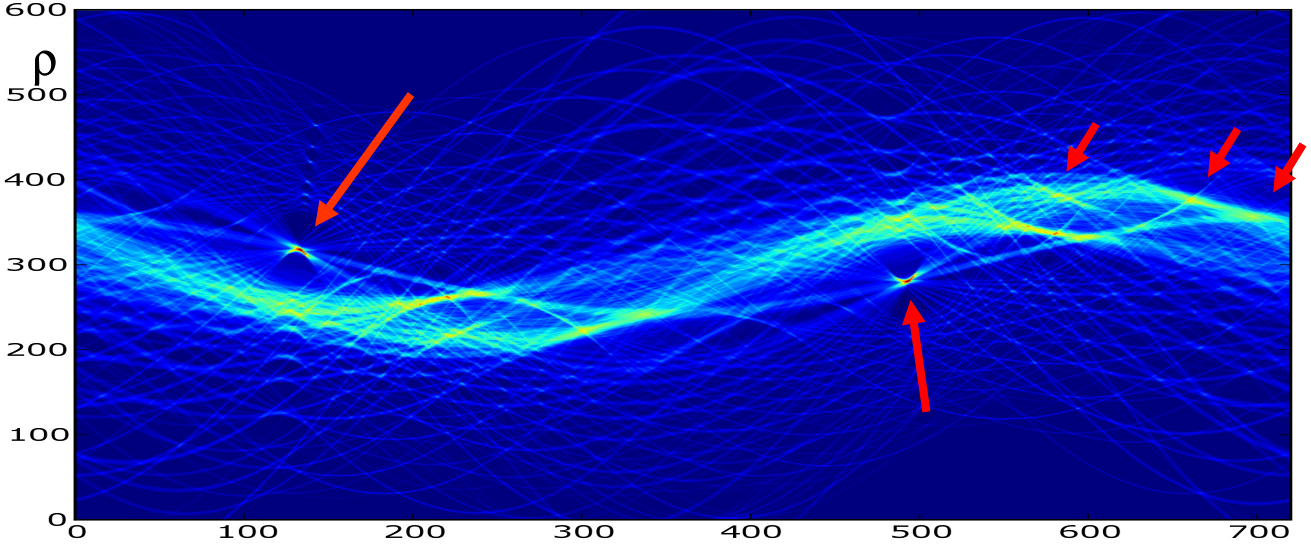
Hough transform reveals lines in digital image

$\rho = x\sin\theta - y\cos\theta$

(x,y) -> HT -> sinusoidal curve in (ρ,θ)



- Build an accumulator array of sinusoides
- Locate intense sinusoides intersection



Hough transform 27000 most intense pixels

→ Corresponding spots are likely to belong to the same crystal !!

Simulate Laue Pattern: from q to detector

$$\mathbf{q} = UB\mathbf{G}$$

transfer vector
in lab. Frame (O,x,y,z)

Unitary rotation matrix
Orientation matrix

$$\mathbf{G} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \qquad \mathbf{G} = \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

RS node vector in unit cell frame

U definition:

9 non independent elements

3 angles

U decomposition:

- 3 rotations / lab. Frame axes
- 3 Euler rotations
- Rodrigues expression
- Quaternion

$$R_x(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix} R_y(\theta) = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix} R_z(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

$$U = R_x(\theta_x)R_y(\theta_y)R_z(\theta_z)$$

$$\begin{bmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$R(\phi\mathbf{u}) = \cos\phi Id_3 + (1-\cos\phi)\begin{pmatrix} u_x^2 & u_x u_y & u_x u_z \\ u_y u_x & u_y^2 & u_y u_z \\ u_z u_x & u_z u_y & u_z^2 \end{pmatrix} + \sin\phi \begin{pmatrix} 0 & -u_z & u_y \\ u_z & 0 & -u_x \\ -u_y & u_x & 0 \end{pmatrix}$$

$$e_0 \equiv \cos\left(\frac{\phi}{2}\right) \qquad \mathbf{e} \equiv \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix} = \hat{\mathbf{n}} \sin\left(\frac{\phi}{2}\right)$$

$$\mathbf{Q} = [e_0, \mathbf{e}] = [w, x, y, z] \quad Q = \begin{pmatrix} 1-2(y^2+z^2) & 2(xy-zw) & 2(xz+yw) \\ 2(xy+zw) & 1-2(x^2+z^2) & 2(yz-xw) \\ 2(xz-yw) & 2(yz+xw) & 1-2(x^2+y^2) \end{pmatrix}$$

Simulate Laue Pattern: from q to detector

$$\mathbf{q} = UB\mathbf{G}$$

transfer vector
in lab. Frame (O,x,y,z)

$$\mathbf{G} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \qquad \mathbf{G} = \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

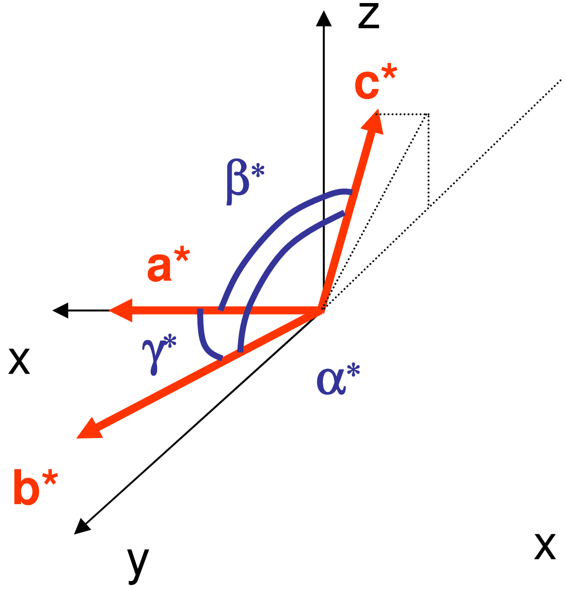
RS node vector in unit cell frame

$$B = \begin{pmatrix} a_x^* & b_x^* & c_x^* \\ a_y^* & b_y^* & c_y^* \\ a_z^* & b_z^* & c_z^* \end{pmatrix}$$

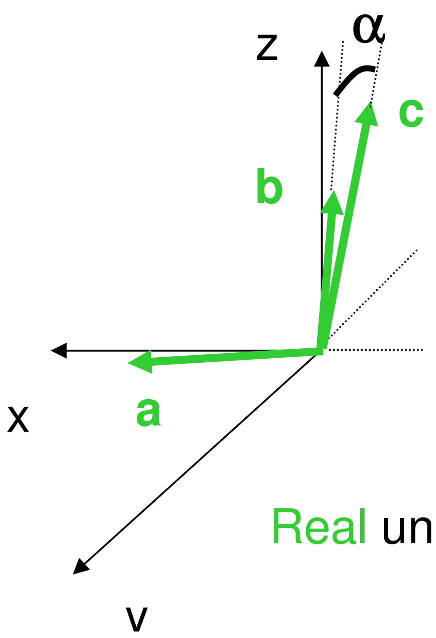
Unit cell / strain matrix

$$\begin{pmatrix} a^* & b^* \cos\gamma^* & c^* \cos\beta^* \\ 0 & b^* \sin\gamma^* & -c^* \sin\beta^* \cos\alpha \\ 0 & 0 & c^* \sin\beta^* \sin\alpha \end{pmatrix}$$

$$\cos\alpha = \frac{\cos\beta^* \cos\gamma^* - \cos\alpha^*}{\sin\alpha^* \sin\beta^*}$$



Reciprocal unit cell



Real unit cell

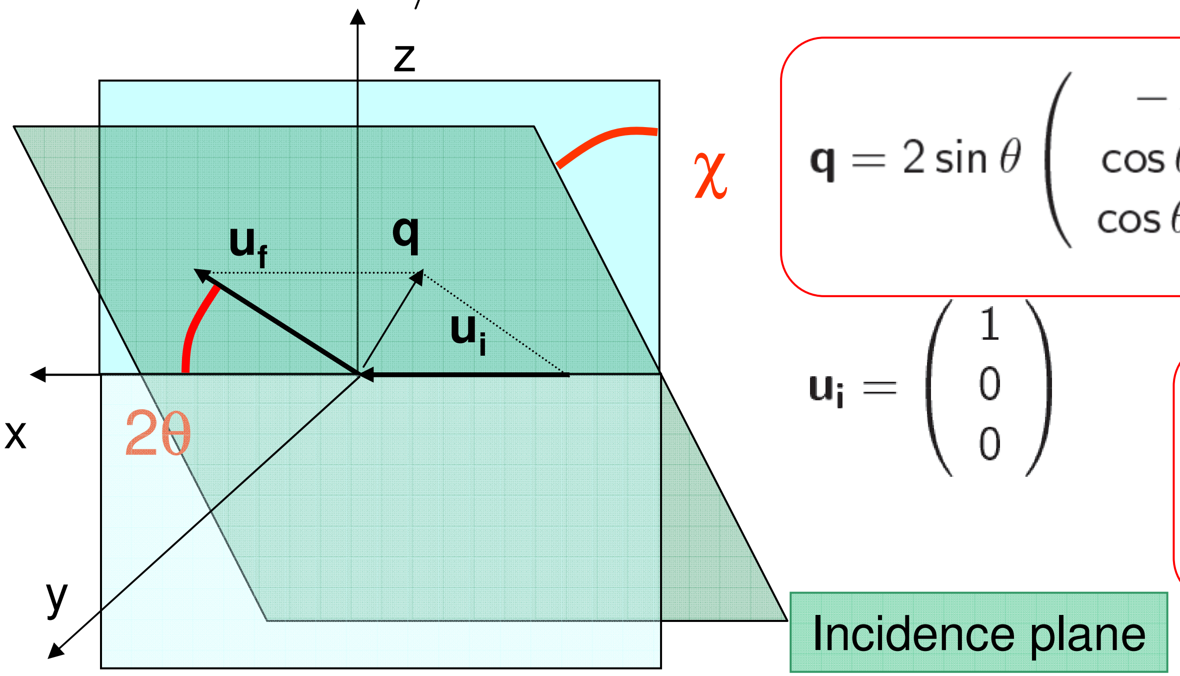
Simulate Laue Pattern: from q to detector

$$\mathbf{q} = UB\mathbf{G}$$

transfer vector
in lab. Frame (O,x,y,z)

$$\mathbf{G} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \qquad \mathbf{G} = \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

RS node vector in unit cell frame

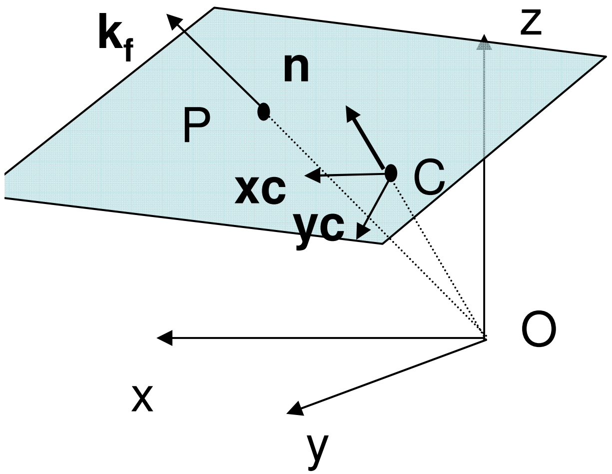


$$\mathbf{q} = 2\sin\theta \begin{pmatrix} -\sin\theta \\ \cos\theta\sin\chi \\ \cos\theta\cos\chi \end{pmatrix} = 2\sin\theta\tilde{\mathbf{q}}$$

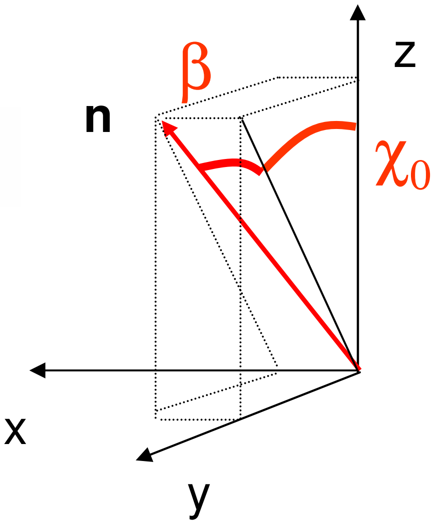
$$\mathbf{u_i} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\mathbf{u_f} = \begin{pmatrix} \cos 2\theta \\ \sin 2\theta\sin\chi \\ \sin 2\theta\cos\chi \end{pmatrix}$$

Simulate Laue Pattern: detector geometry



$$\mathbf{OC} = d\mathbf{n}$$



$$\mathbf{n} = \begin{pmatrix} \sin\beta \\ \cos\beta\sin\chi_0 \\ \cos\beta\cos\chi_0 \end{pmatrix}$$

Detector plane equation (lab. frame)

$$x\sin\beta + y\cos\beta\sin\chi_0 + z\cos\beta\cos\chi_0 = d$$

$\mathbf{u_f}$ intersects CCD plane at P

$$\mathbf{OP} = d_p \begin{pmatrix} \cos 2\theta \\ \sin 2\theta \sin\chi \\ \sin 2\theta\cos\chi \end{pmatrix} \qquad d_p = \frac{d}{\cos 2\theta\sin\beta + \sin 2\theta\cos\beta\cos(\chi-\chi_0)}$$

Build a direct frame Rc=(O,$\mathbf{x_c}$,$\mathbf{y_c}$=$\mathbf{n}$^$\mathbf{x_c}$,$\mathbf{n}$) and express CP in it

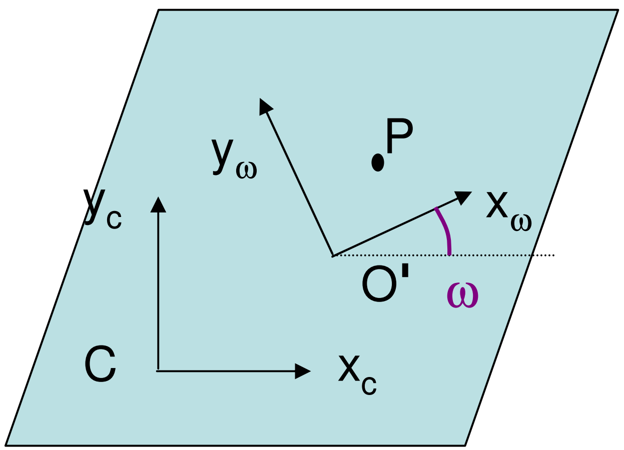
$$\mathbf{x_c} = \frac{1}{\sqrt{\cos^2\beta\cos^2\chi_0 + \sin^2\beta}} \begin{pmatrix} \cos\beta\cos\chi_0 \\ 0 \\ -\sin\beta \end{pmatrix}$$

$$\mathbf{y_c} = \frac{1}{\sqrt{\cos^2\beta\cos^2\chi_0 + \sin^2\beta}} \begin{pmatrix} -\cos\beta\sin\chi_0 \\ \cos^2\beta\cos^2\chi_0 + \sin^2\beta \\ -\cos^2\beta\sin\chi_0\cos\chi_0 \end{pmatrix}$$

Matrix from R to Rc:

$$D(\beta,\chi_0) = (\mathbf{x_c}, \mathbf{y_c}, \mathbf{n})$$

Simulate Laue Pattern: detector geometry



$$\mathbf{CP} = \frac{165}{2048}\left(\begin{pmatrix} x_0 \\ y_0 \\ 0 \end{pmatrix}_{\text{pixel}} - \begin{pmatrix} \cos\omega & -\sin\omega & 0 \\ \sin\omega & \cos\omega & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_P \\ y_P \\ 0 \end{pmatrix}_{\text{pixel}}\right)$$

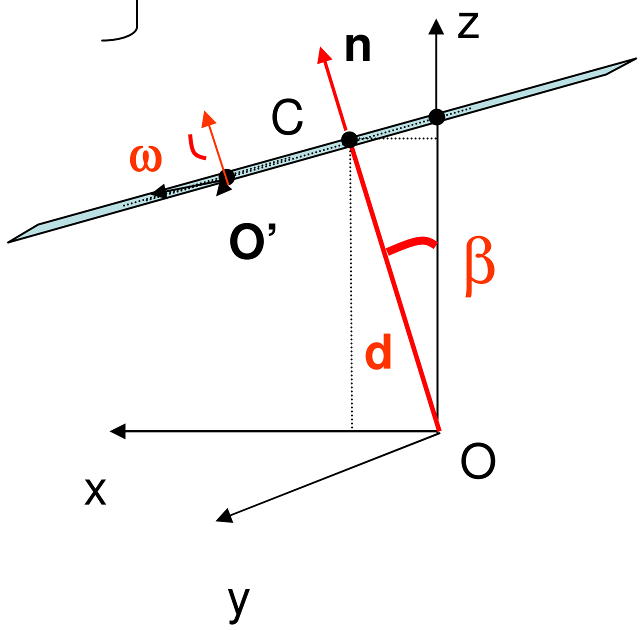
$$\mathbf{CP} = \mathbf{CO} + \mathbf{OP} = D(\beta,\chi_0)\left(\begin{pmatrix} 0 \\ 0 \\ -d \end{pmatrix} + d_p \begin{pmatrix} \cos 2\theta \\ \sin 2\theta \sin\chi \\ \sin 2\theta \cos\chi \end{pmatrix}\right)$$

General detector parameters:
$d,\beta,\chi_0,x_0,y_0,\omega$

Patterns on CCD with { $\chi_0 = 0$; $\chi_0 = \alpha$ and sample rotated/x-axis by α } are identical

Detector parameters:
d,β,x_0,y_0,ω

Arbitrary value of χ_0 (then set to 0)
=>
OP(2θ=cst,χ) is the shortest for χ=0



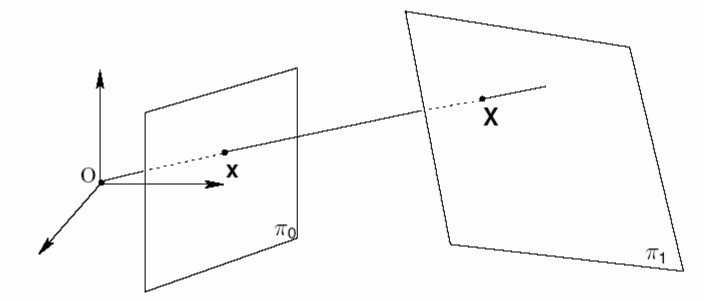
Simulate Laue Pattern: detector geometry

Determination of these parameters = **detector calibration** procedure

Non-linear equations => non linear fitting

Alternative method?

From 3D computer graphics and camera vision



With homogeneous coordinates (central projection is linearised)

$$\underbrace{\begin{pmatrix} x_P \\ y_P \\ 0 \\ 1 - z_P/z_0 \end{pmatrix}}_{P} = \underbrace{\begin{pmatrix} A & D & G & x_T \\ B & E & H & y_T \\ 0 & 0 & 0 & 0 \\ -Cz/z_0 & -Fz/z_0 & -Iz/z_0 & 1 - z_T/z_0 \end{pmatrix}}_{\mathbf{M}} \underbrace{\begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}}_{\mathbf{u_f}}$$

M includes CCD plane rotation and offset + central projection
Calibration Matrix

=> linear fitting: Minimize ($\Sigma_i \; ||M\mathbf{u_{fi}} - P_{expi}||$) by varying $d, \beta, x_0, y_0, \omega$

=> linear algebra: simply find M and use it as it is!

Indexation of Laue Pattern: Handle Experimental data

Prior to indexation, data reduction & image processing

On a single image or all images

- **Background removal**
  - *- local or **global***
  - *- image substraction*
  - *- user-defined*
- Intensity thresholding
  - *- local or global*
  - *- user-defined*
  - *- most intense pixel*
- Image rebinning (digital processing much faster)
- Filtering: median, morphological, (non)linear, …
- Geometric operation
  - *- all or selected pixels*
  - *- reflection-transform ($\mathbf{u_f}$->$\mathbf{q}$), gnomonic projection, Hough transform*
- Features detection
  - *- local or global*
  - *- **peak search**, most intense peak*
  - *- blob, streak, or exploded spots detection-recognition*
- …

Handle Experimental data: image processing

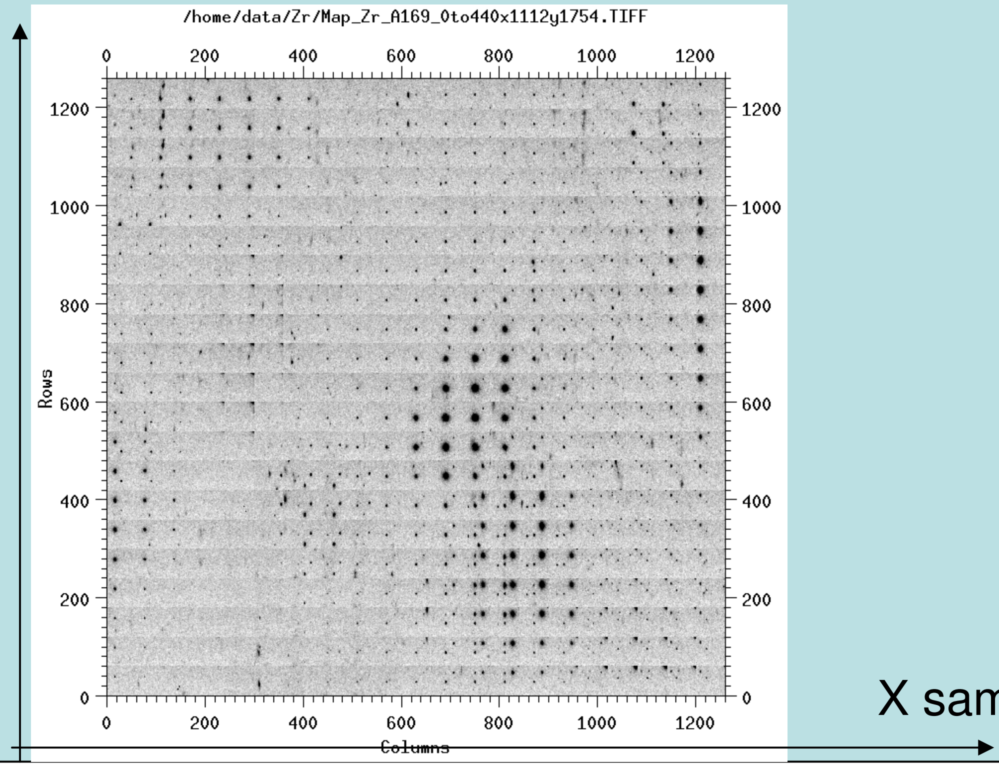
Prior to indexation, data reduction & image processing

2D map

- **Mosaic**
  - select a small pixels array in each image
  - layout a mosaic according to the sample scan procedures

  => *grain topography via scattering intensity of a selected bragg reflection*

Y sample



X sample

Handle Experimental data: image processing

Prior to indexation, data reduction & image processing

2D map

- Mosaic
- **Use featuring most intense peaks**
  - build sorted list $L_i(1\ldots n)$ of n most intense peaks in each image i
  - find for each i where $L_i(1)$ belongs to $L_j(1\ldots n)$

Handle Experimental data: image processing

Prior to indexation, data reduction & image processing

2D map

- Remove in image *i* previous indexed peaks from image *j*
- Pixel position images cross correlation

Locate spatial location of grain
Early determination of grain origin of major spots in images (but hkl still unknown)

- **Peak description**

- Peak position: estimation by lorentzian,gaussian fitting, centroid computation
- Shape estimation: ellipsa, numerical moments, angle of major axis
- Pixel values array centered on peak

Future errors in structure refinement may arise from:
- Ill-shaped peaks
- very sharp peak/pixel size,
- reduced intensity array to a single pixel position

Indexation of Laue Pattern

Objective

Determine (hkl) of all/some spots and their grain origin

Knowing the closest crystallographic grain structure is highly recommended
= Reference structure

1. Non-distorted or perfectly known structure
   > *grain orientation + absolute lattice parameter* — Very rare

2. (slightly) Distorted structure / Reference
   > *grain orientation + strain* — Usual

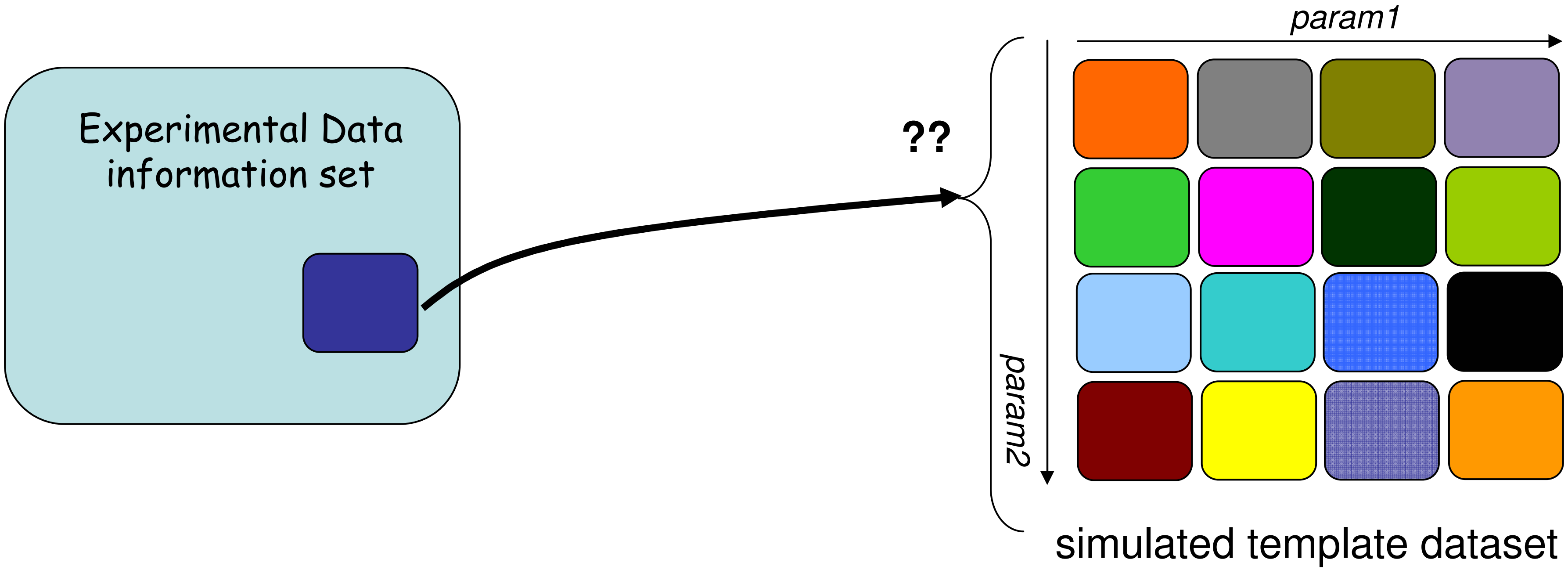
3. Distorted structure / Reference
   > *grain orientation + new phase structure* — Tedious! Try to be in case 2

Indexation	= ~ orientation of the Reference
Structure solving	= orientation and strain refinement

Indexation of Laue Pattern

Matching Principles

Try and evaluate matching between experimental and reference features



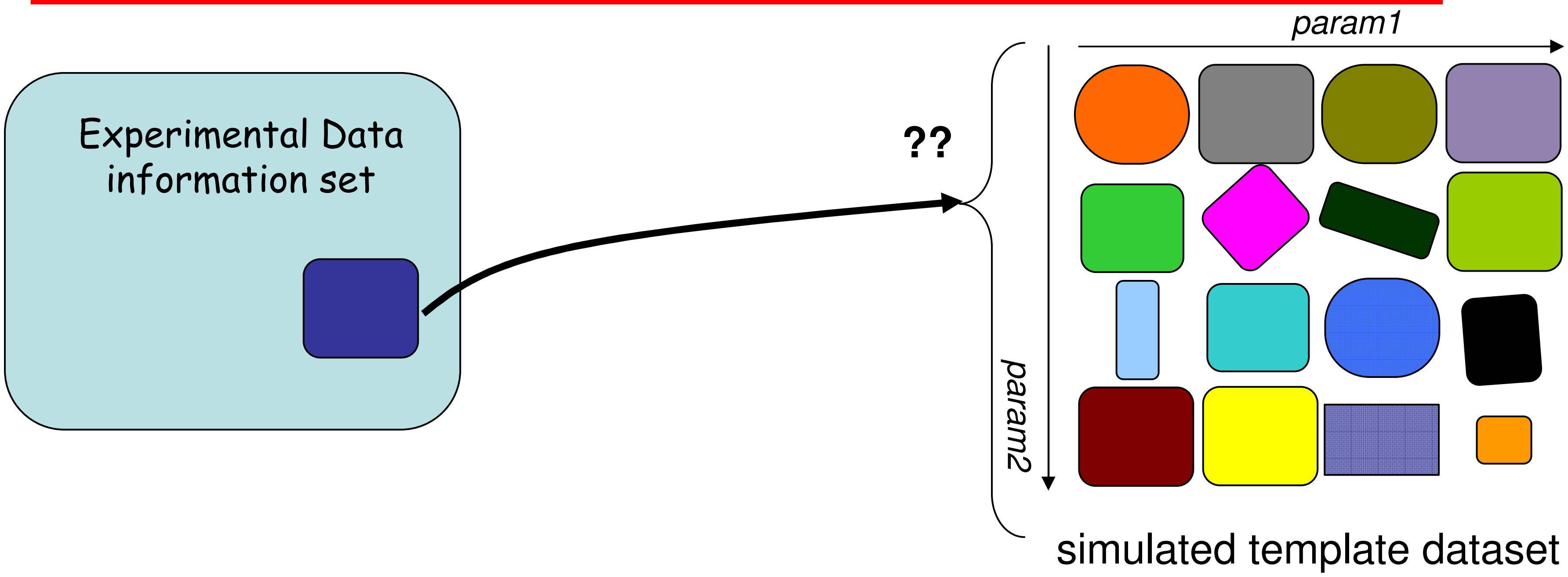
Which template matches best ?

=> Closest values of (param1,param2) ?

Indexation of Laue Pattern

Matching Principles

Try and evaluate matching between experimental and reference features



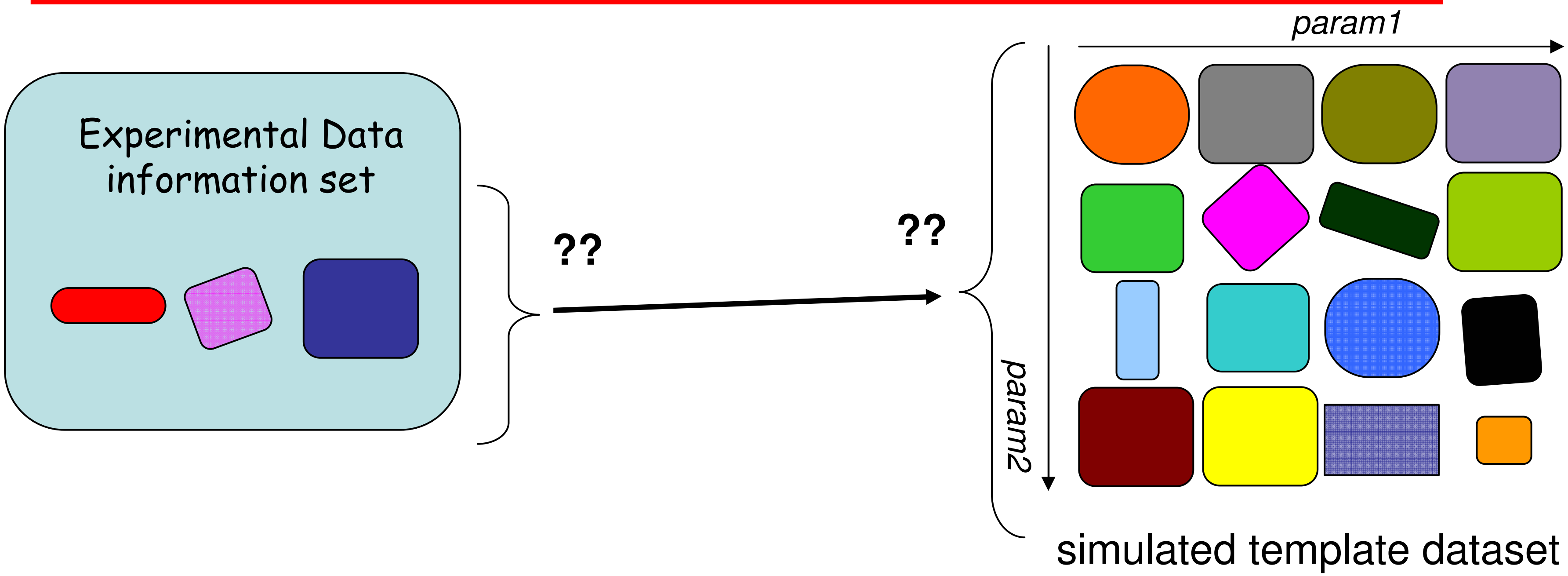
Which template matches best ?

=> Closest values of (param1,param2) ?

Indexation of Laue Pattern

Principles

Try and evaluate matching between experimental and reference features



What is the best matching ?

=> Closest values of (param1,param2) ?

Indexation of Laue Pattern

Principles

Try and evaluate matching between experimental and reference features

Matching implies (in view of automation)

- *approximated template dataset*
- *approximated matching estimation (tolerance)*
- *often lot of trial-errors:*
  - *large set of candidates*
  - *large set of template*
- *Decision threshold*
- *What are basically the features of data ?*
- *Reduction of data information with the least loss a. p.*

Indexation of Laue Pattern: methods

- *choose or select a discrete solution parameter*
- *build template dataset (TDS) or lookuptable (LUT)*
- *need to define a quantitative matching quality (MQ)*
- *choose relevant informations featuring data*

spot distance matching

Candidates = 1 to n couple(s) of spots

Reference = distance (LUT)

Matching quality = ~ distance residues (with U)

Matching result = 2 labeled spots, U matrix

Image matching

Candidate = image (**only one**)

Reference = image template dataset (TDS)

Matching quality =
~ images cross-correlation factor

Matching result = 3 orientation angles

Computation and refinement of U
Label experimental spots /all predicted spots
(Missing reflections management)

Indexation of Laue Pattern: distance matching

Candidates

Couple of Spots

(0,1) (0,2) (0,3) (0,4) (0,n)

(1,2) (1,3) (1,4) (1,n)

(2,3) (2,4) (1,n)

(3,4) (3,n)

(…)

Corresponding distance

25.2 16.3 48.3 65.4 22.3

26.6 45.0 56.2 18.6

52.1 19.5 36.7

71.7 44.1

39.1

?? ⟷ ??

LUT

hkl candidates

INTERPLANAR … PL. … STALS BETWEEN … $k_2l_2\}$

$\{h_2k_2l_2\}$	$\{h_1k_1l_1\}$ 100	110	111	210	211	221	310
100	0 90						
110	45 90	0 60 90					
111	54.7	35.3 90	0 70.5 109.5				
210	26.6 63.4 90	18.4 50.8 71.6	39.2 75.0	0 36.9 53.1			
211	35.3 65.9	30 54.7 73.2 90	19.5 61.9 90	24.1 43.1 56.8	0 33.6 48.2		
221	48.2 70.5	19.5 45 76.4 90	15.8 54.7 78.9	26.6 41.8 53.4	17.7 35.3 47.1	0 27.3 39.0	
310	18.4 71.6 90	26.6 47.9 63.4 77.1	43.1 68.6	8.1 58.1 45	25.4 49.8 58.9	32.5 42.5 58.2	0 25.9 36.9
311	25.2 72.5	31.5 64.8 90	29.5 58.5 80.0	19.3 47.6 66.1	10.0 42.4 60.5	25.2 45.3 59.8	17.6 40.3 55.1
320	33.7 56.3 90	11.3 54.0 66.9	61.3 71.3	7.1 29.8 41.9	25.2 37.6 55.6	22.4 42.3 49.7	15.3 37.9 52.1
321	36.7 57.7 74.5	19.1 40.9 55.5	22.2 51.9 72.0 90	17.0 33.2 53.3	10.9 29.2 40.2	11.5 27.0 36.7	21.6 32.3 40.5
331	46.5	13.1	22.0				
510	11.4						
511	15.6						
711	11.3						

Indexation of Laue Pattern: distance matching

Candidates

Couple of Spots

(0,1) (0,2) (0,3) (0,4) (0,n)

(1,2) (1,3) (1,4) (1,n)

(2,3) (2,4) (1,n)

(3,4) (3,n)

(…)

Corresponding distance

25.2 16.3 48.3 65.4 22.3

26.6 45.0 56.2 18.6

52.1 19.5 36.6

71.7 44.1

39.1

?? ??

E

LUT

INTERPLANAR ANGLES (I hkl candidates LS BETWEEN PLANES OF T

$\{h_2k_2l_2\}$	$\{h_1k_1l_1\}$						
	100	110	111	210	211	221	310
100	0 90						
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111	54.7	35.3 90	0 70.5 109.5				
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310	18.4 71.6 90	26.6 47.9 63.4 77.1	43.1 68.6	8.1 58.1 45	25.4 49.8 58.9	32.5 42.5 58.2	0 25.9 36.9
311	25.2 72.5	31.5 64.8 90	29.5 58.5 80.0	19.3 47.6 66.1	10.0 42.4 60.5	25.2 45.3 59.8	17.6 40.3 55.1
320	33.7 56.3 90	11.3 54.0 66.9	61.3 71.3	7.1 29.8 41.9	25.2 37.6 55.6	22.4 42.3 49.7	15.3 37.9 52.1
321	36.7 57.7 74.5	19.1 40.9 55.5	22.2 51.9 72.0 90	17.0 33.2 53.3	10.9 29.2 40.2	11.5 27.0 36.7	21.6 32.3 40.5
331	46.5	13.1	22.0				
510	11.4						
511	15.6						
711	11.3						

E

Indexation of Laue Pattern: distance matching

number of U depends on:
- LUT size (user's choice, high E_{max})
- Distance candidates list size (user's choice or not)
- Angular tolerance

Find **best U**:
- Simulate Laue Pattern for each U
- Calculate the angular residues list

- Define numerical criterion or a priority-ordered list of criteria
  depends on spots position estimation and calibration
- And sort solutions according to it

Practical strategy:

Large number of grains

Reduce the size of LUT (lower Emax)
Reduce angular tolerance
Large distance candidates list
Improve calibration
Select the roundest spots

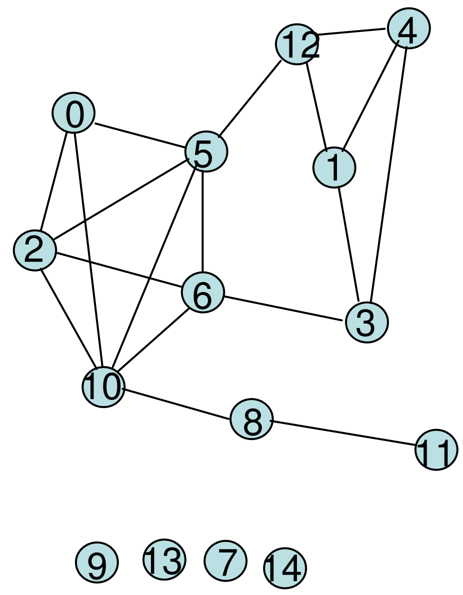
Indexation of Laue Pattern: image matching

Improvements:

Make a candidates list of:
1- spots that are likely to originate from the same grain
2- spots that have been labelled by other means

1- Clique finding (Graph theory algorithm)

-Select n peaks
-Compute all angular distance
-Compare distances with LUT
-Construct an undirected graph:
    node=peak
    edge=distance between two peaks found in LUT
-Find clique = complete subgraph
=> **highly intimate peaks**



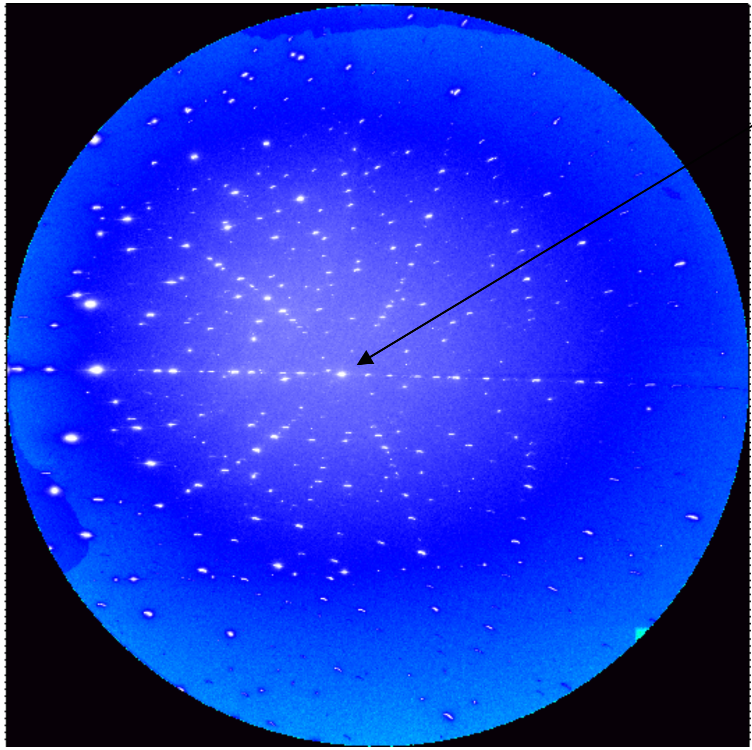
Indexation of Laue Pattern: image matching

2- peak or zone axis recognition

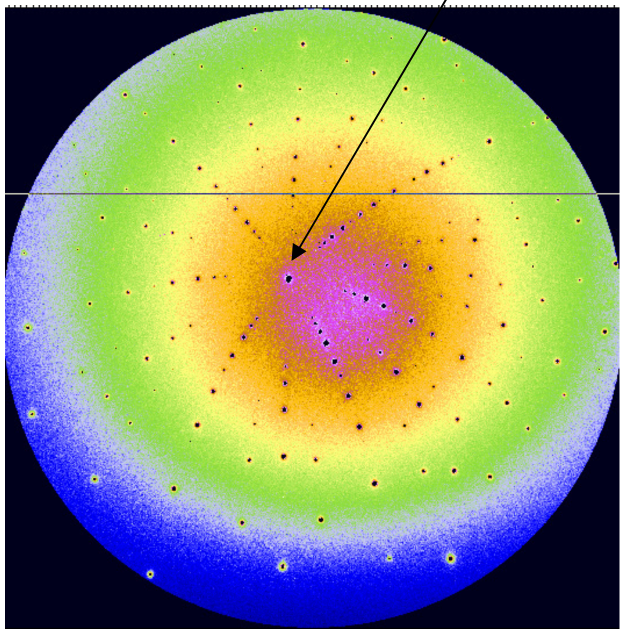
Inspired by human brains computing

Cubic (111)

CdTe



Cubic (100)



UO_2

Indexation of Laue Pattern: image matching

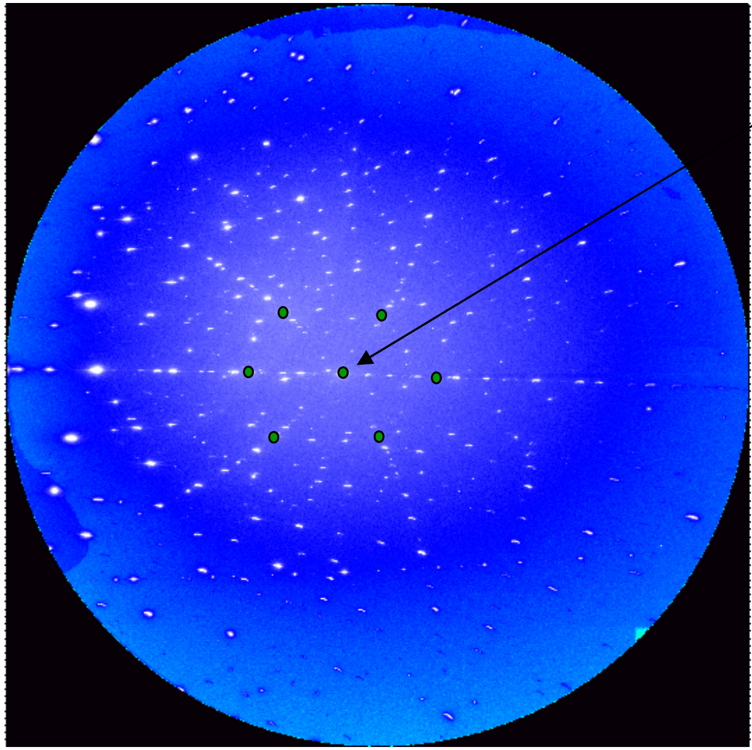
2- peak or zone axis recognition

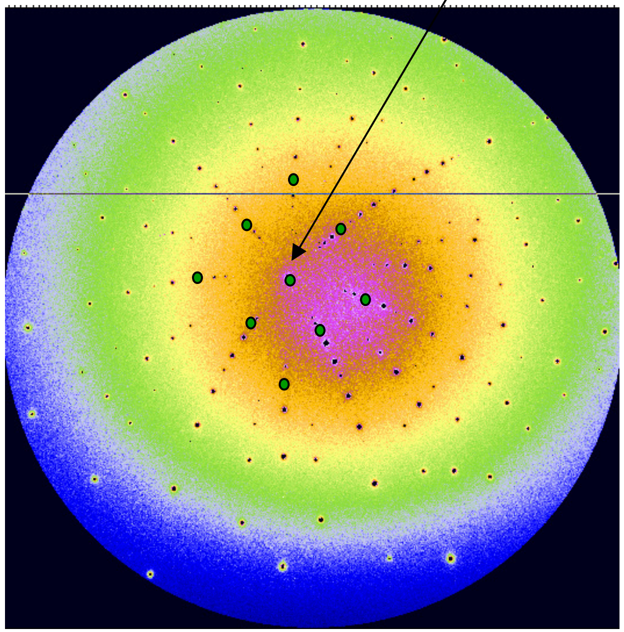
Inspired by human brains computing

Cubic (111)

Cubic (100)

CdTe





Radial environment recognition

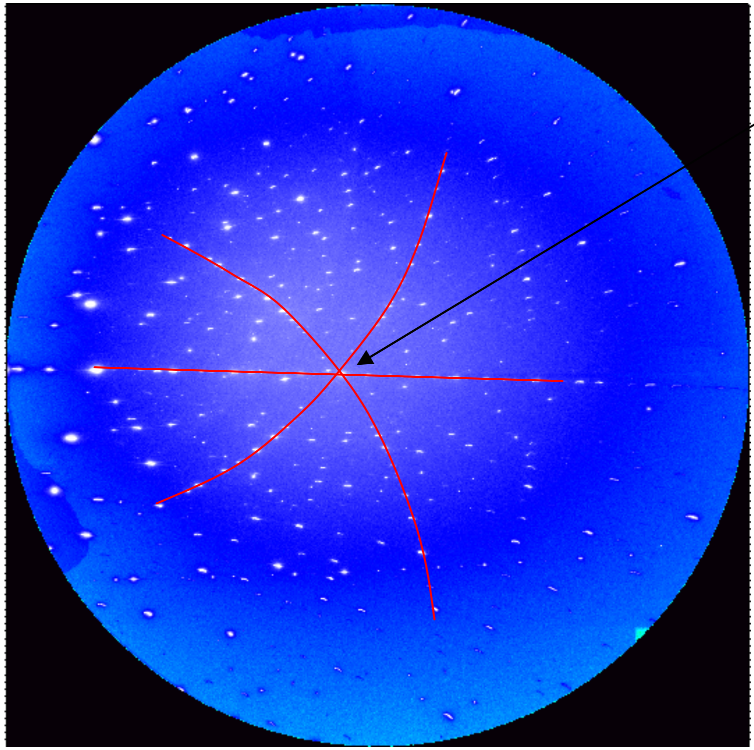
UO_2

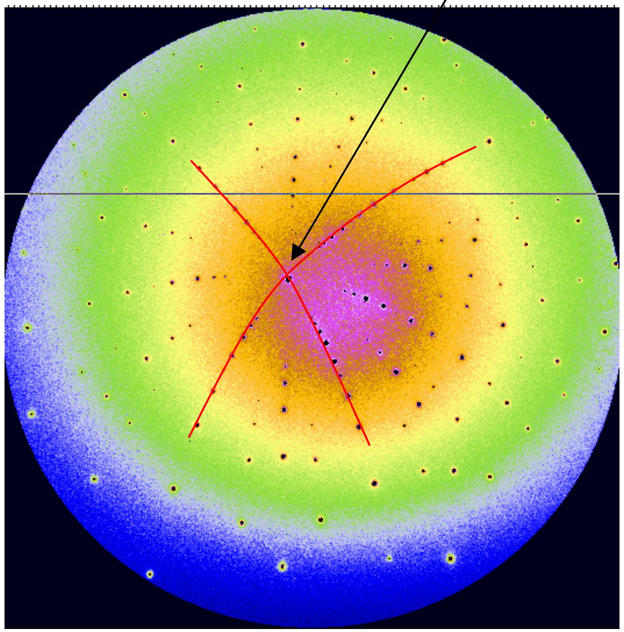
Indexation of Laue Pattern: image matching

2- peak or zone axis recognition

Inspired by human brains computing

CdTe



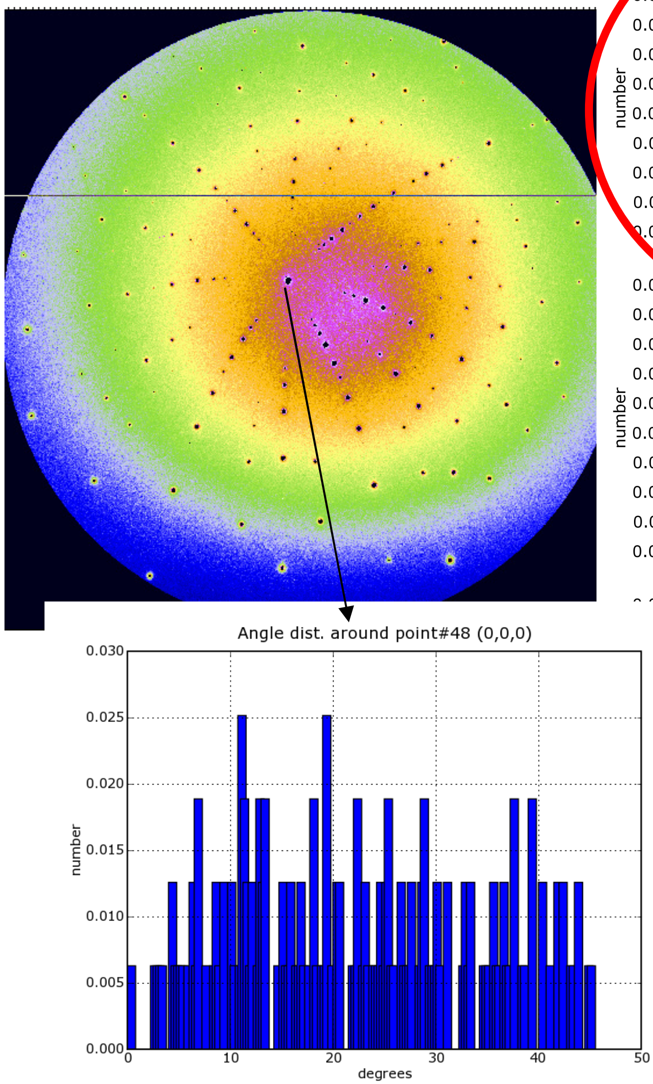


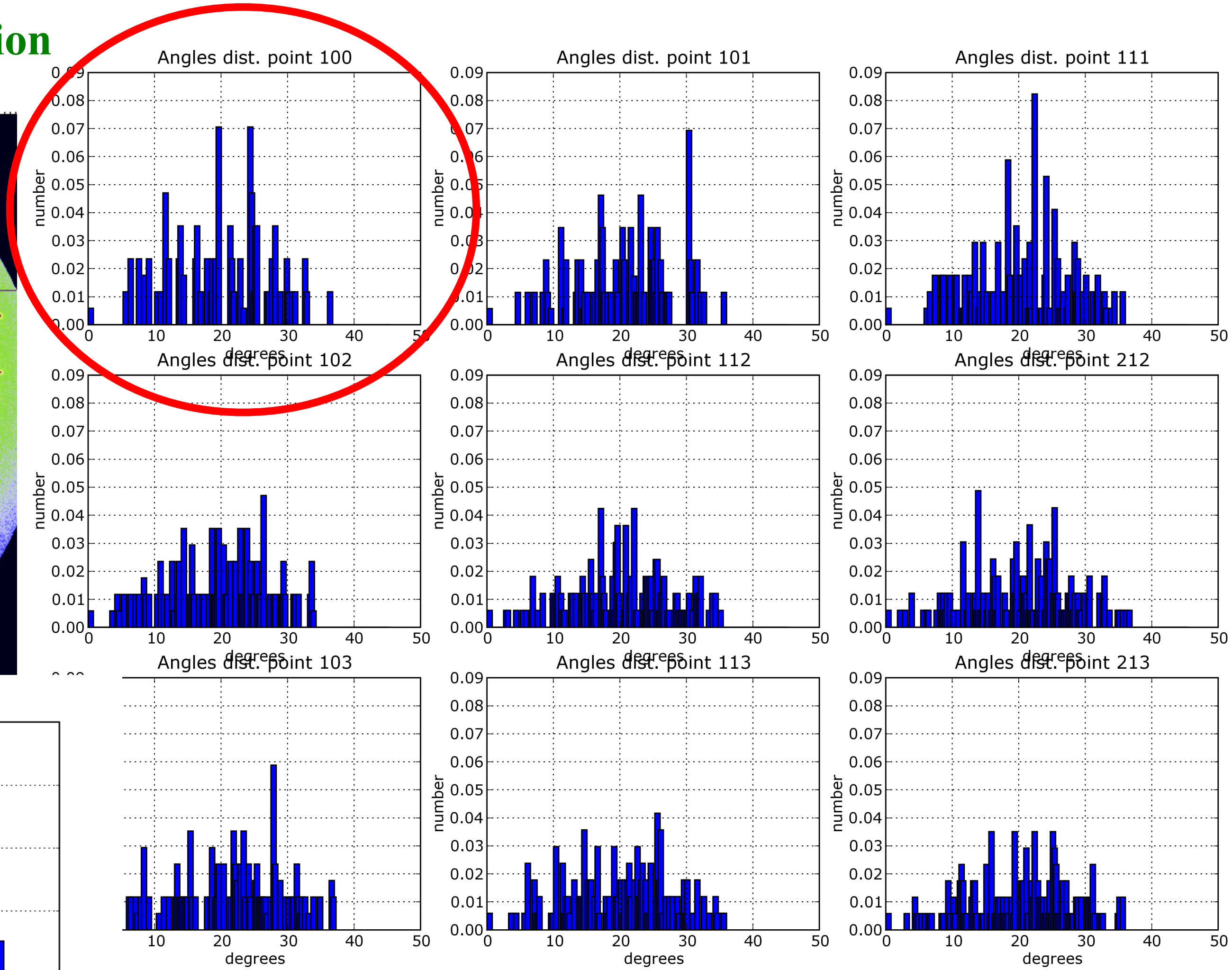
Zone axis recognition

UO_2

Indexation of Laue Pattern: peak recognition

Radial environment recognition

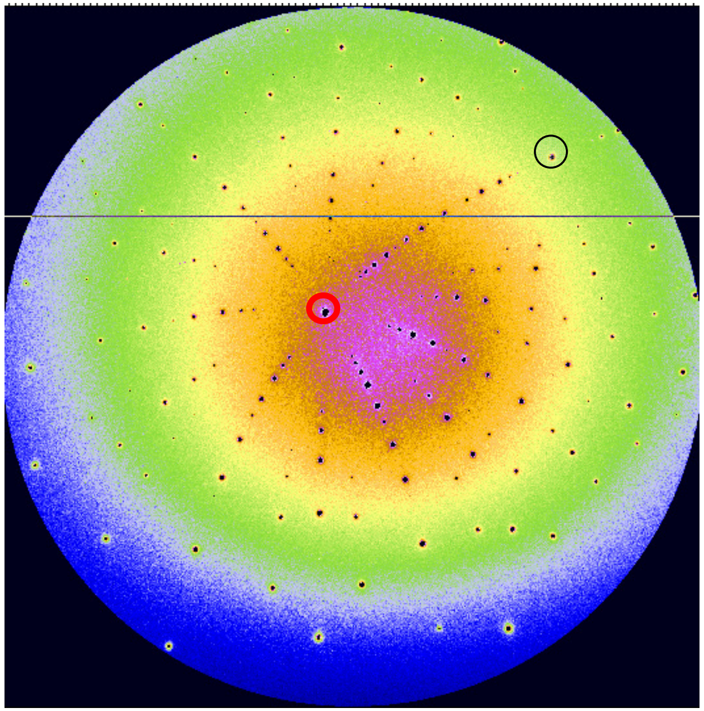


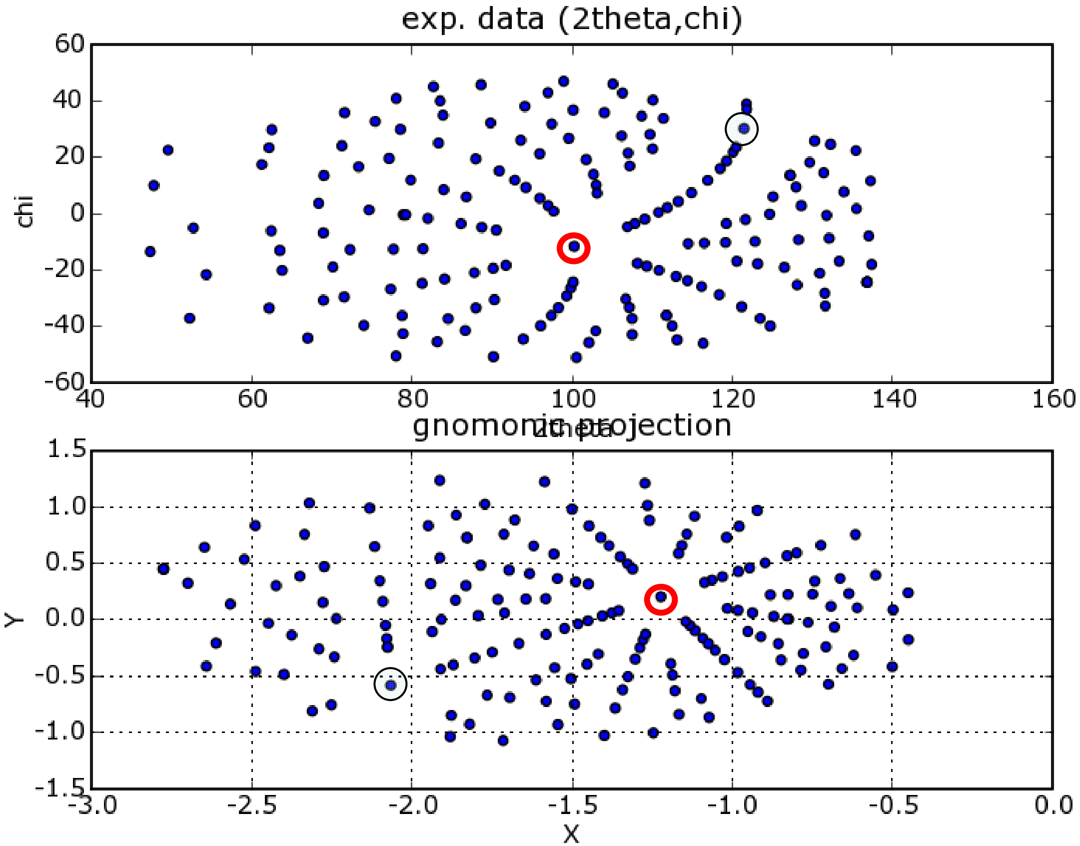


Pearson linear correlation

Indexation of Laue Pattern: zone axis recognition

Zone axis recognition





1- Locate alignements of spots (gnomonic projection + Hough transform)
2- Determine low hkl peak at zones intersection

Indexation of Laue Pattern: image matching

Objectives:
Use an assembly of peaks better than two: matching
Principles:

- Create Images database : orientation sampling (no structure strain sampling)
- Find best match between experimental data and one simulated image

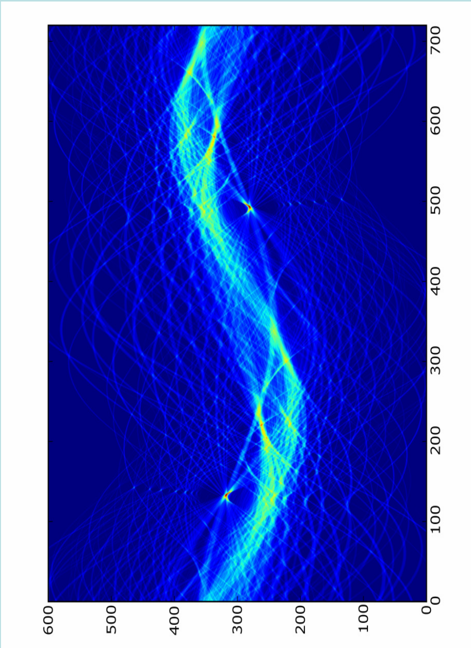
Improvements:

Intensity threshold Select most significant pixels in experimental image

Pixel position transform Matching in suitable space

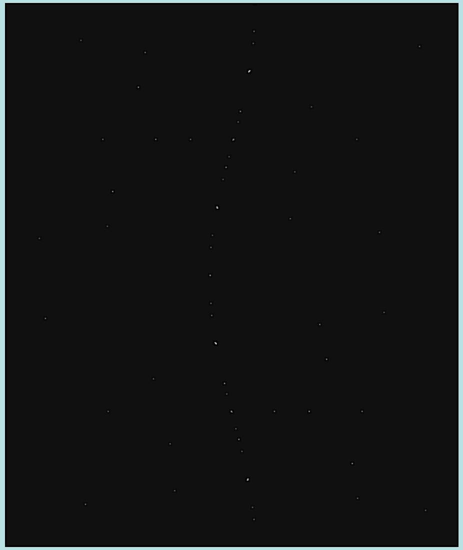
Indexation of Laue Pattern: image matching

one candidate



??

Image templates dataset



Fingerprint of one crystal orientation:
$\phi 1, \phi 2, \phi 3$

Rauch et al (2005) smart image correlation algorithm…

… adapted in Hough space of gnomonic projected data

Conclusion

Various kinds of materials/data/signals/information:

Nb grains,nb of phase,nb of spots/grains, total nb of spots …

Peaks from substrate/unwanted phase

Peak shape…

Provided that **Calibration is correctly performed**
(accurate conversion (x,y) - ($2\theta,\chi$))

Automatic data analysis is possible iff

- user gets used of his data to set up criteria for
  - *image handling*
  - *indexation*
  - *refinement*

- panel of strategies and expert system:
  - *easily user-defined*
  - *serial/parallel processing*
  - *performance test*

→ lauetools