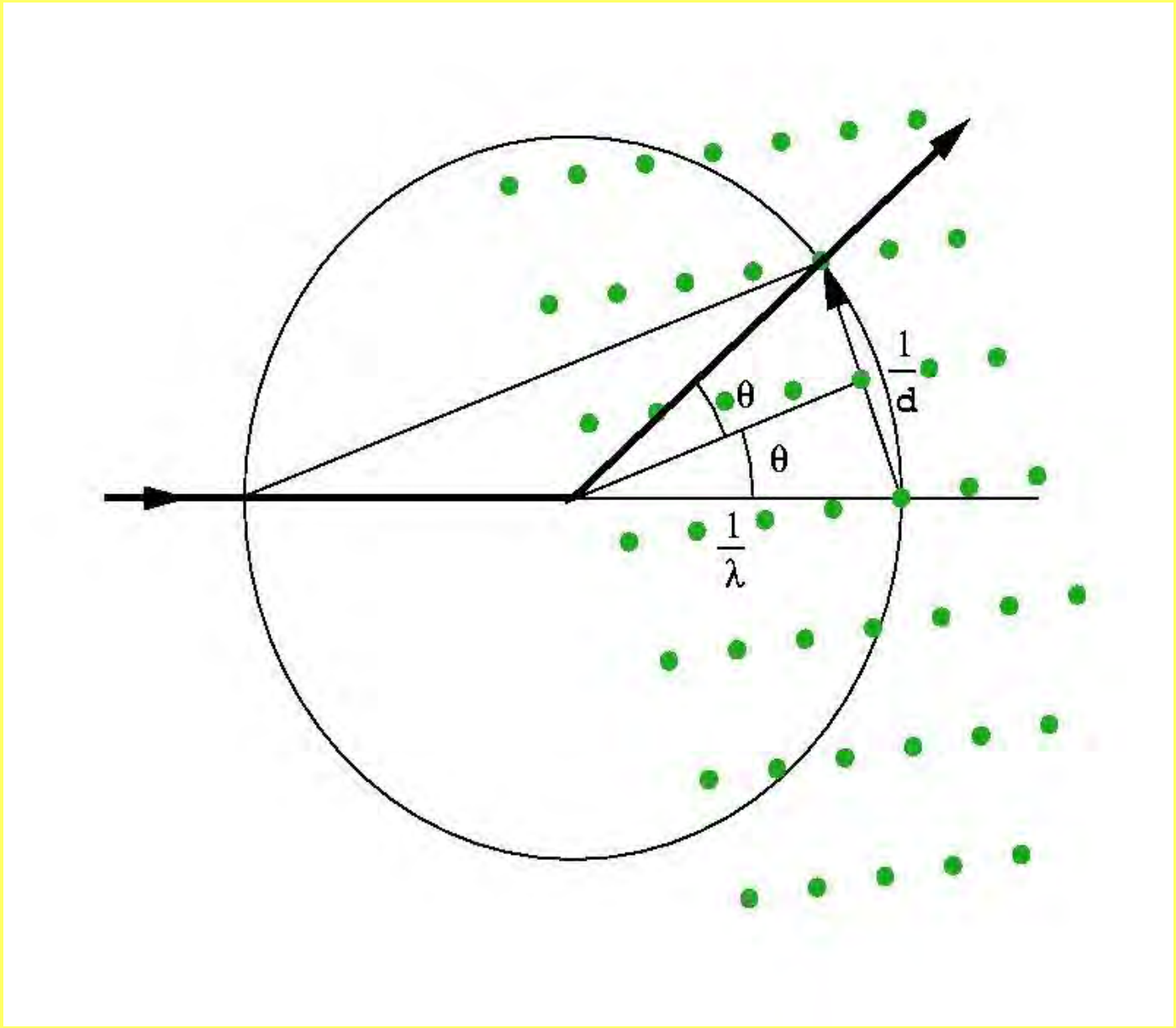
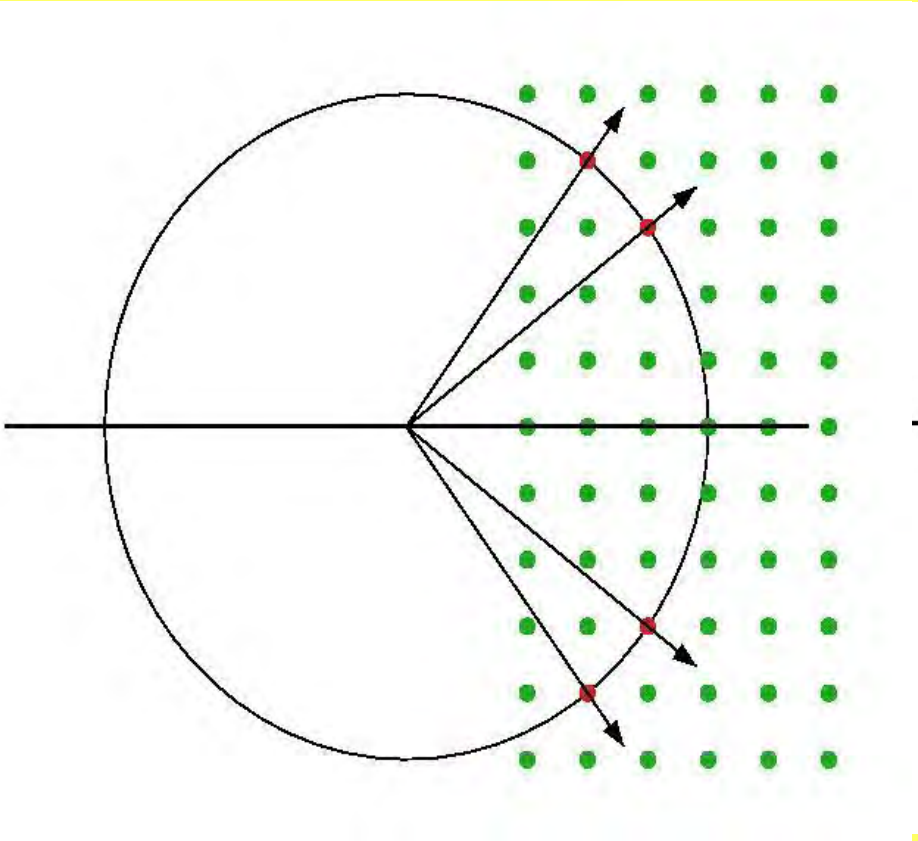
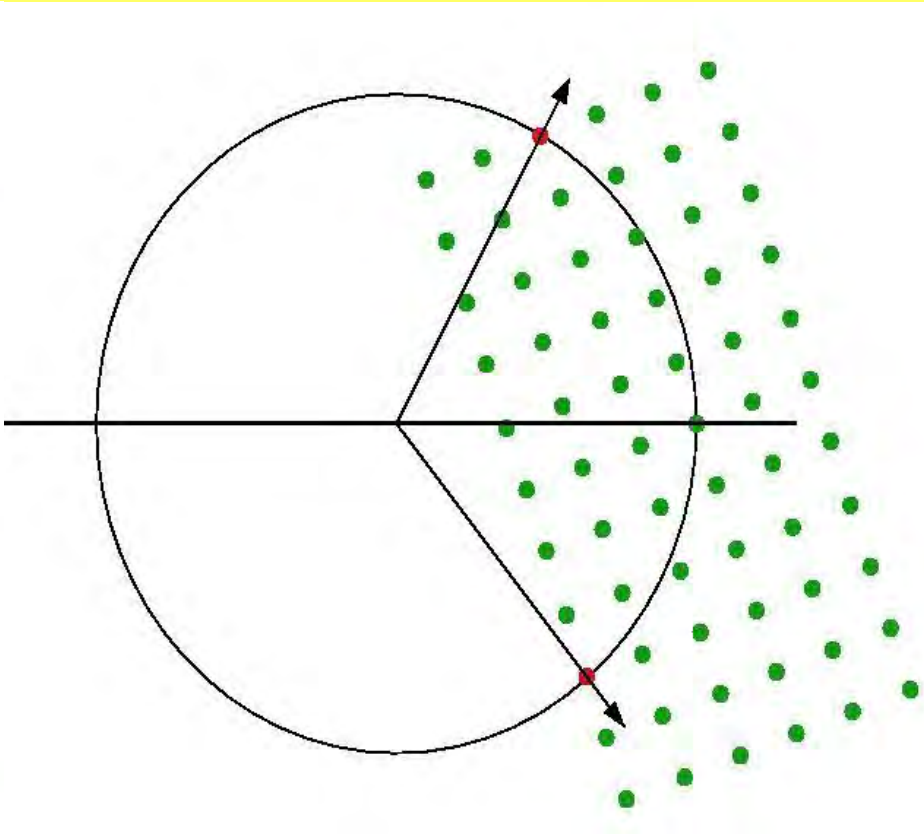
Data collection strategy

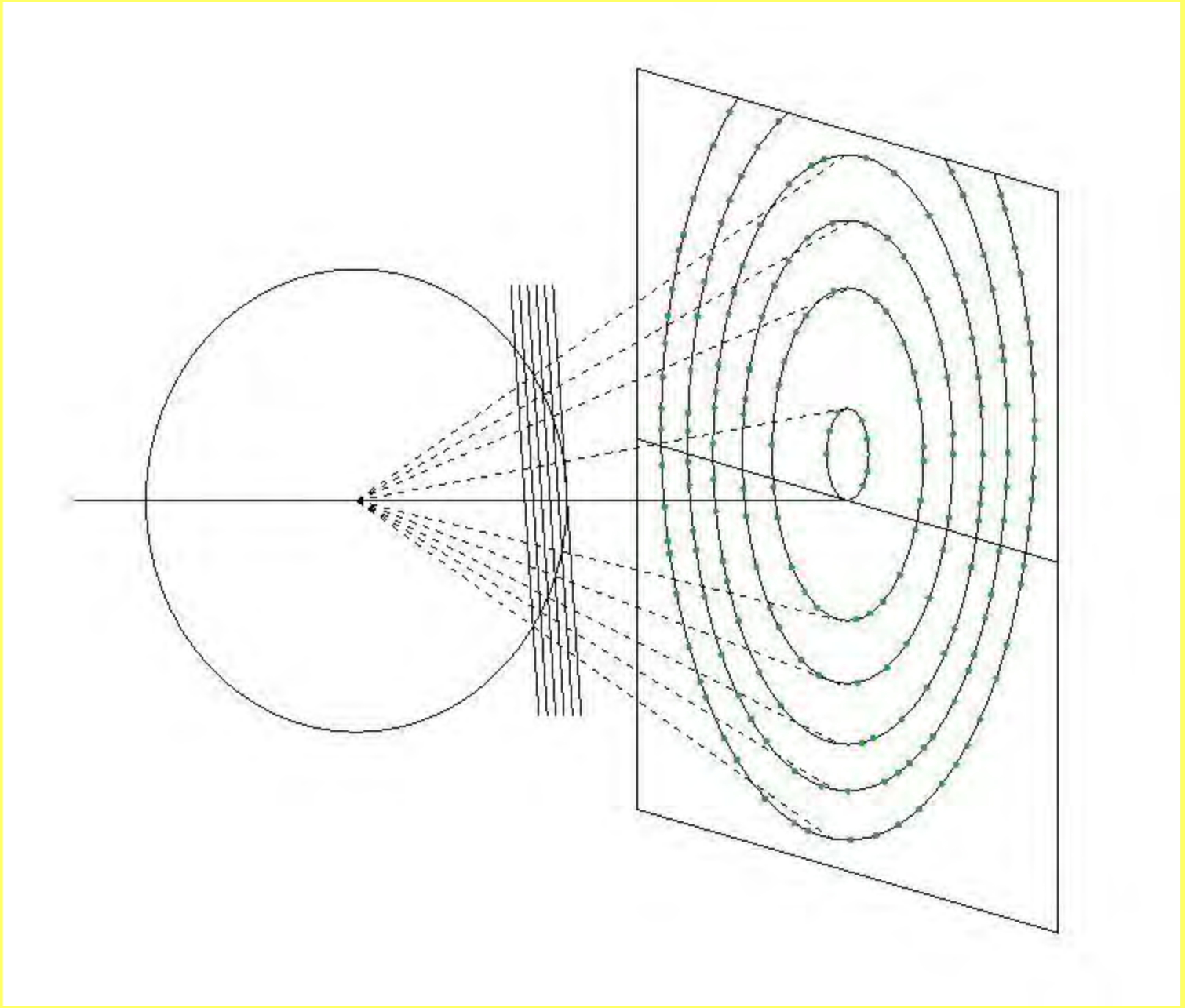
Completeness

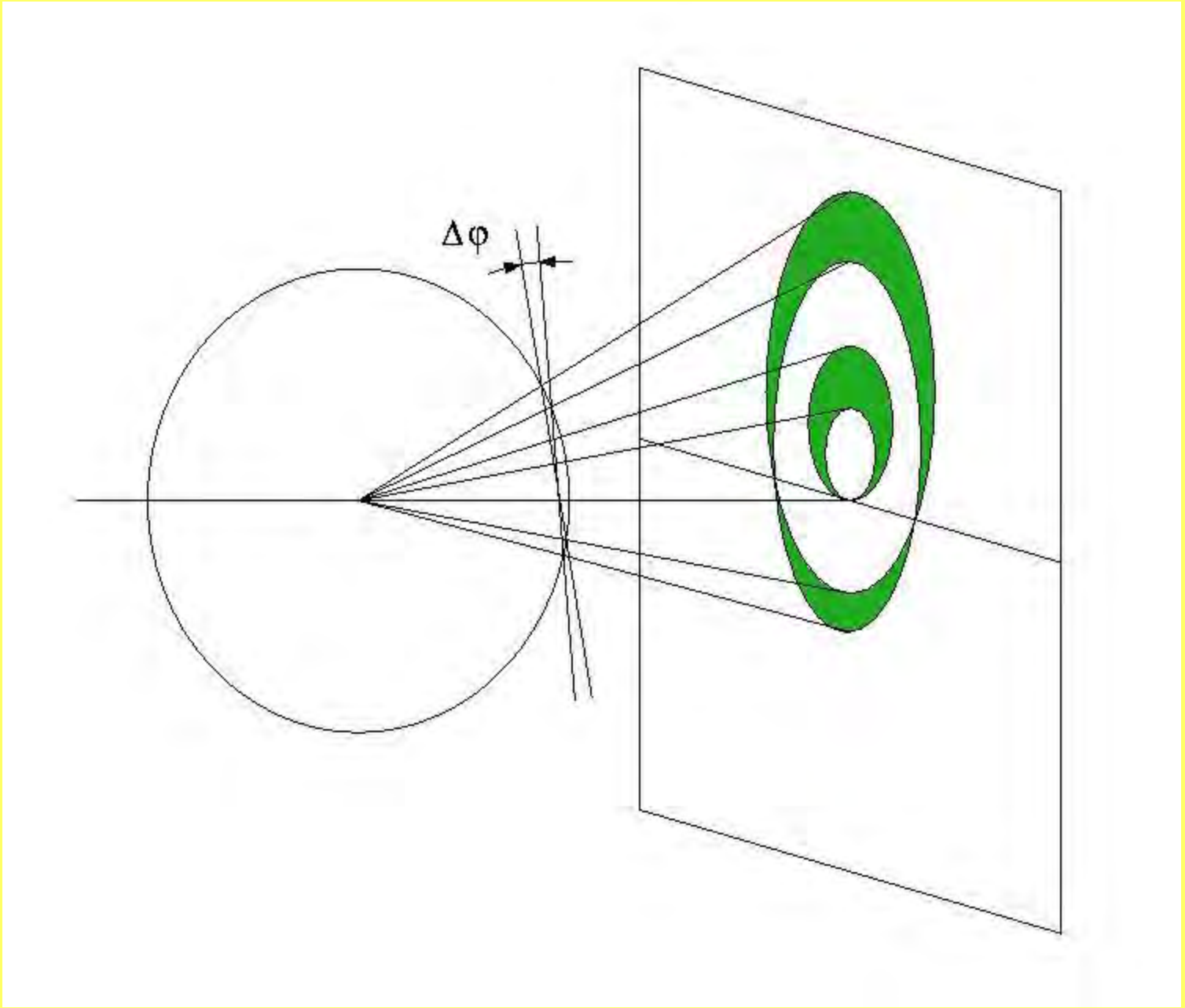
Quantitative (indices)	Qualitative (intensities)
- asymmetric unit	- overloads
- mosaicity	- multiplicity
- overlap of profiles	- Rmerge, I/sigma
- blind region	- sigma estimation
- rotation range	
- non-equiv. indexing	

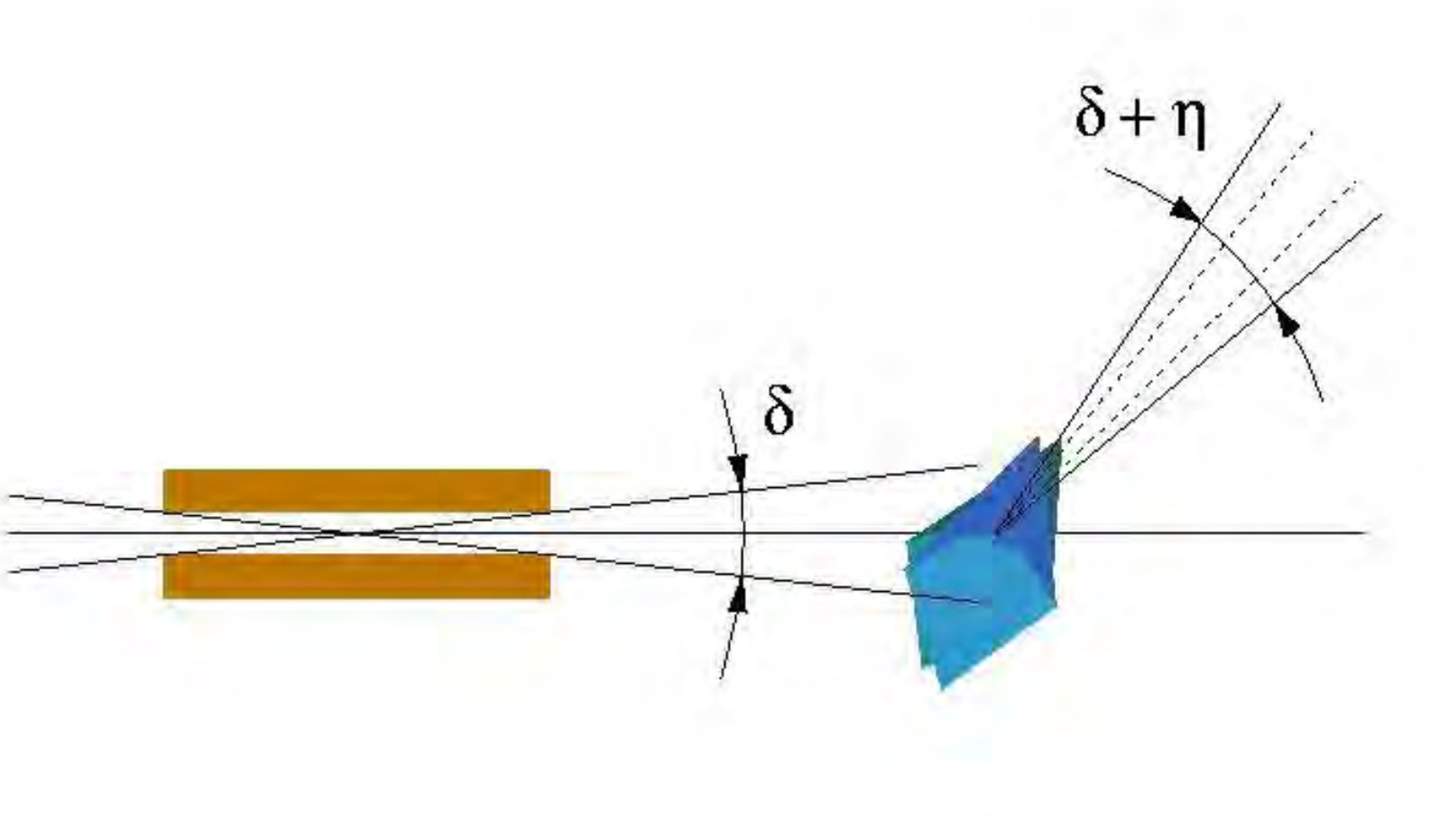

θ
θ
1/d
1/λ

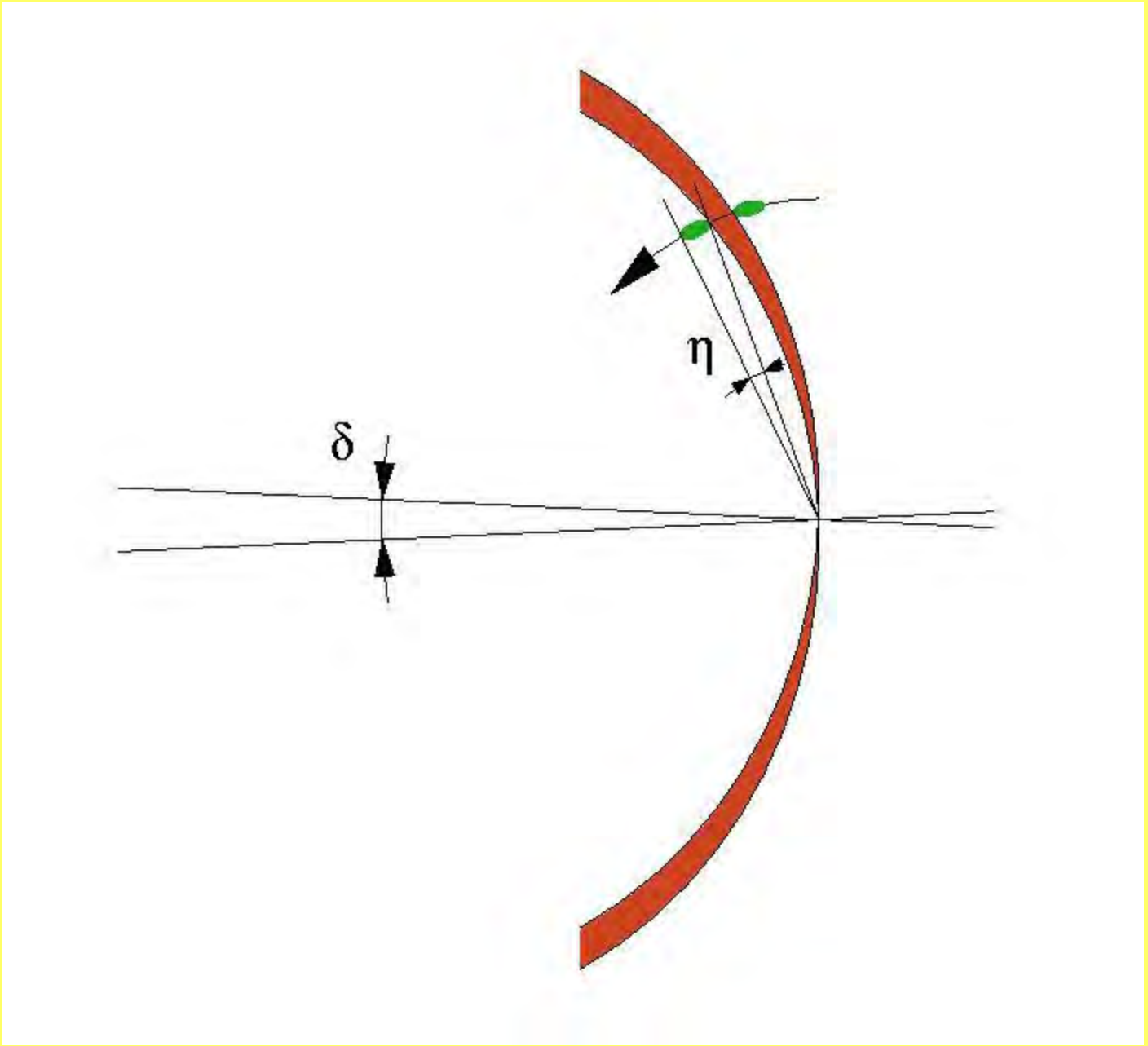


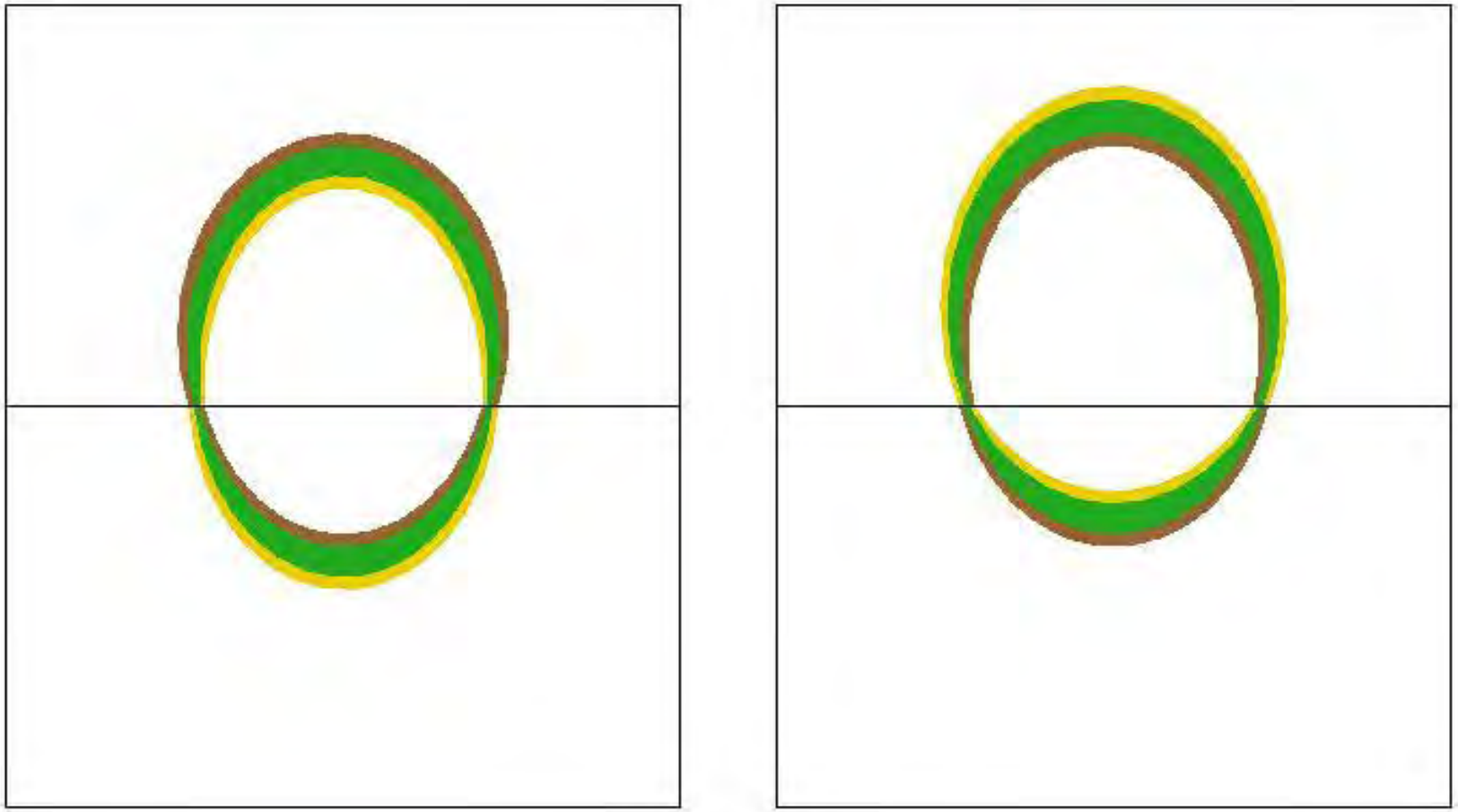


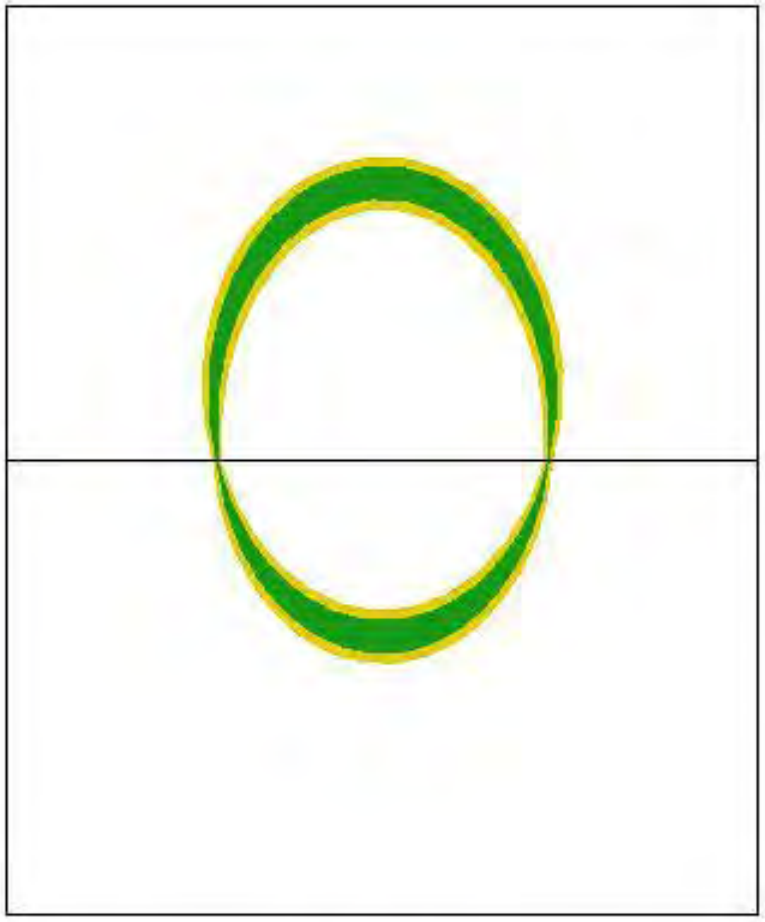



Δφ

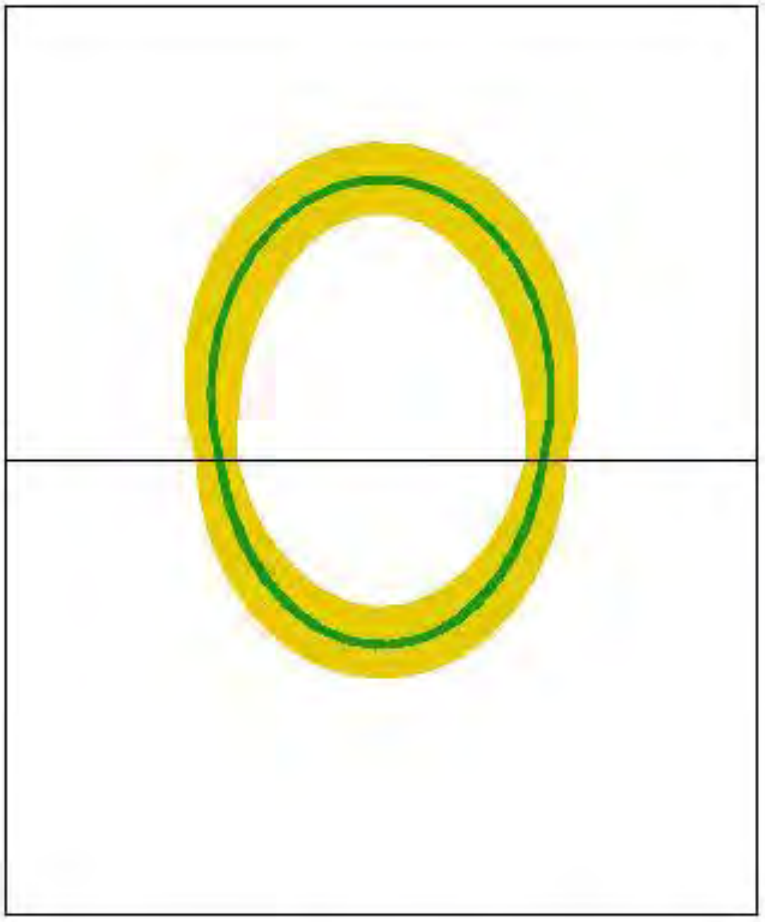

δ + η
δ


η
δ

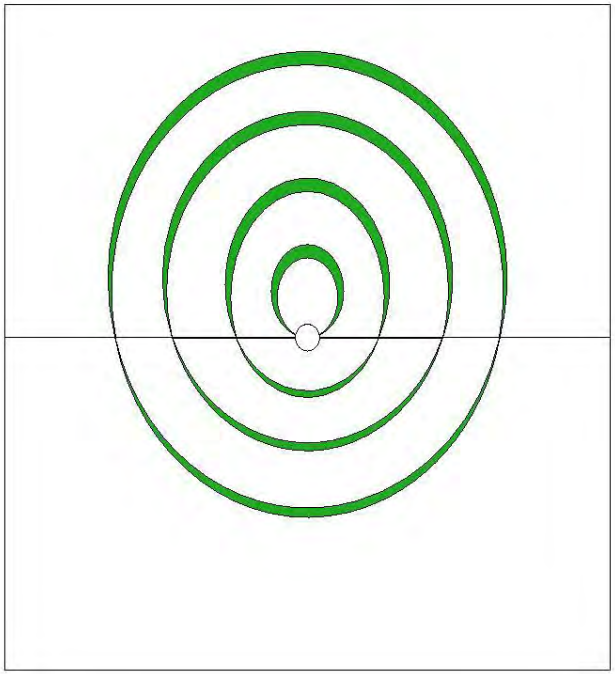


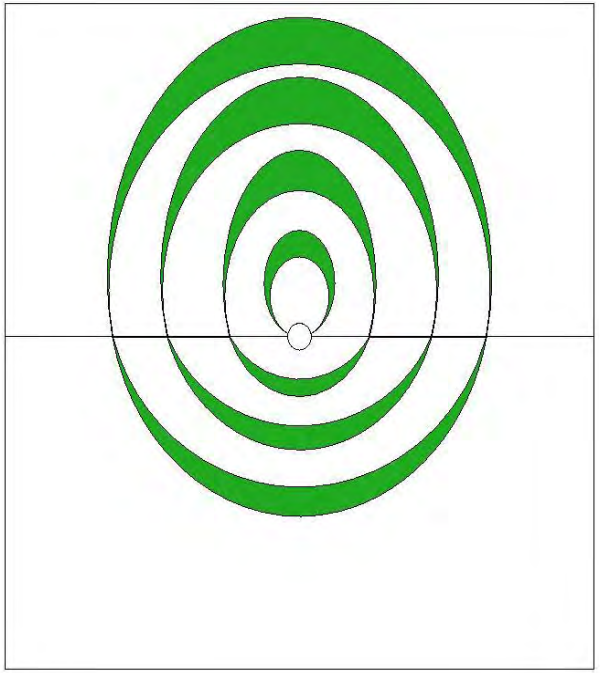


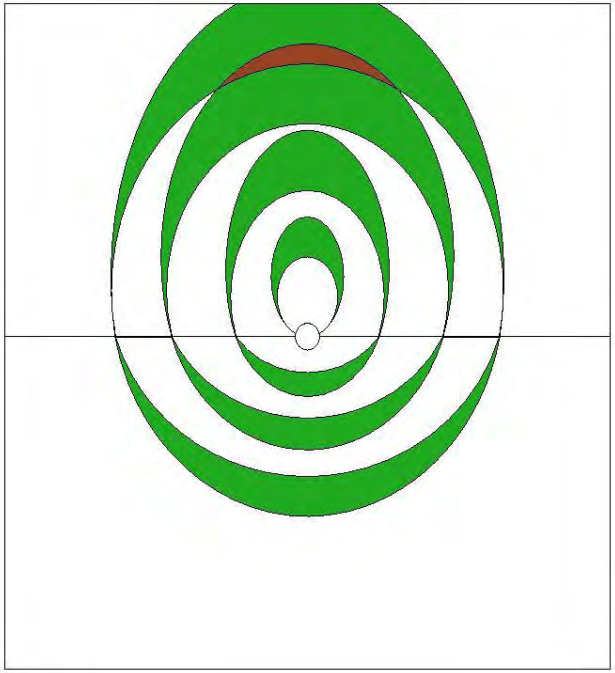
$\eta < \Delta\varphi$

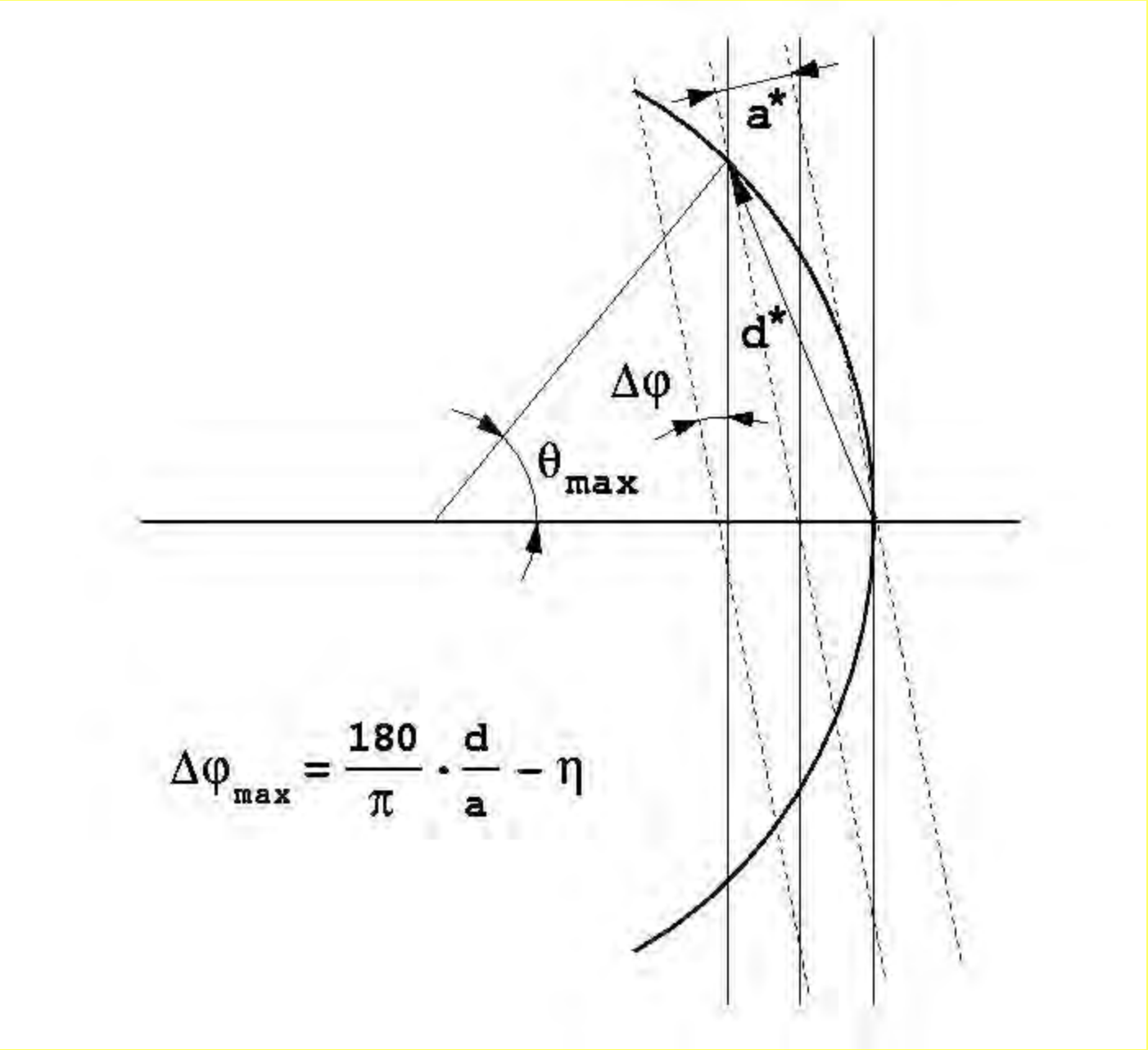


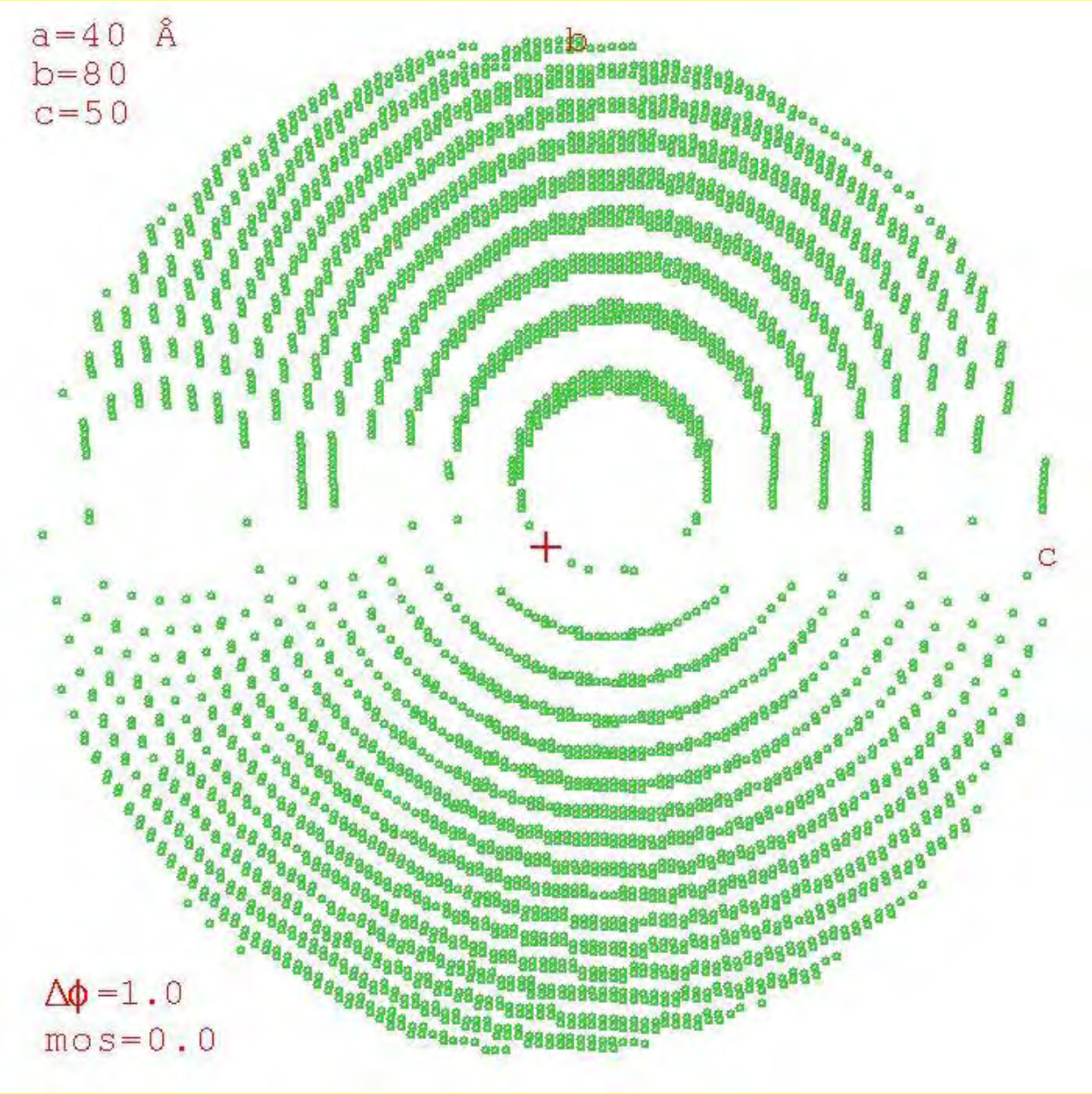
$\eta \sim \Delta\varphi$

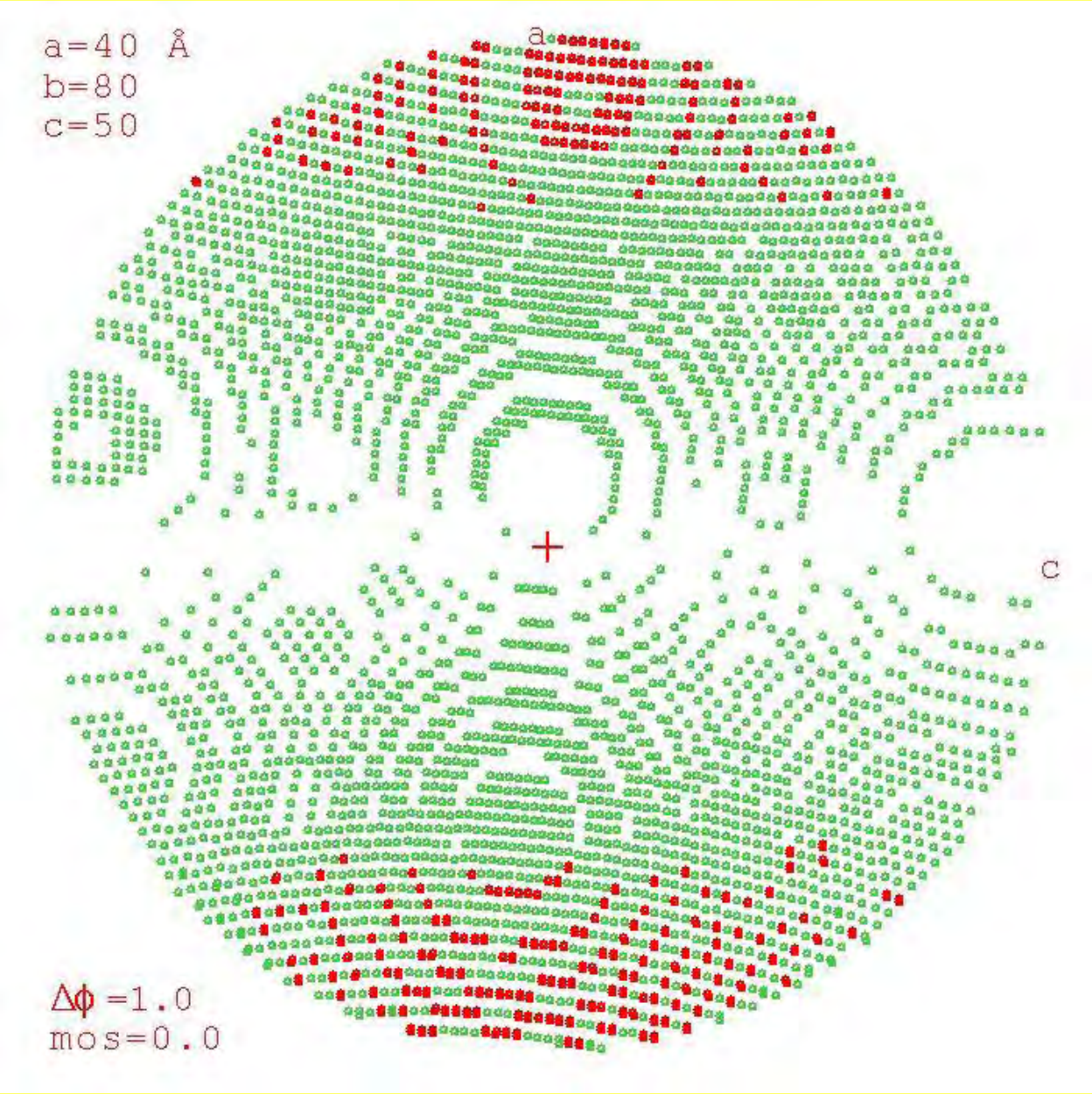


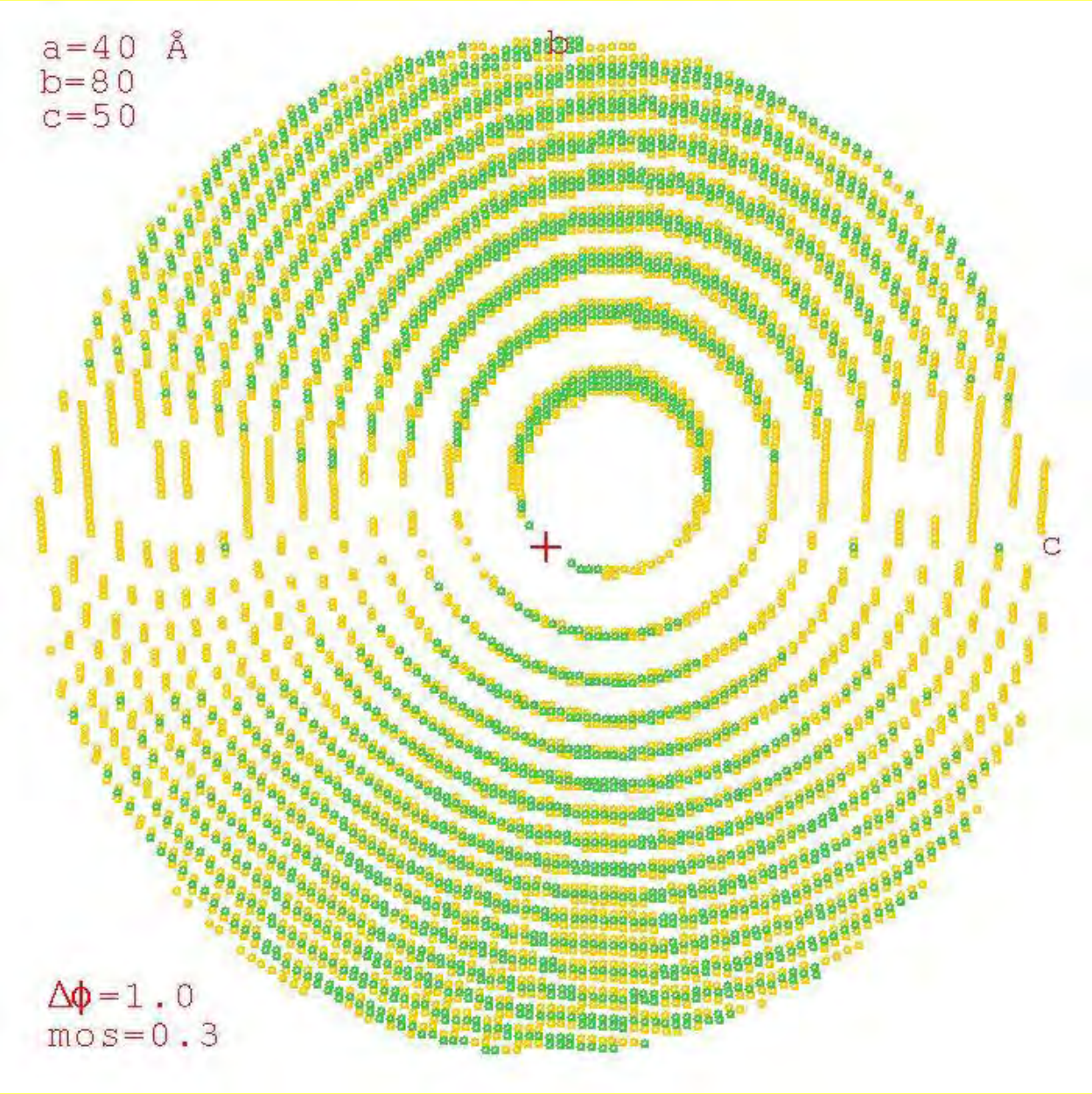


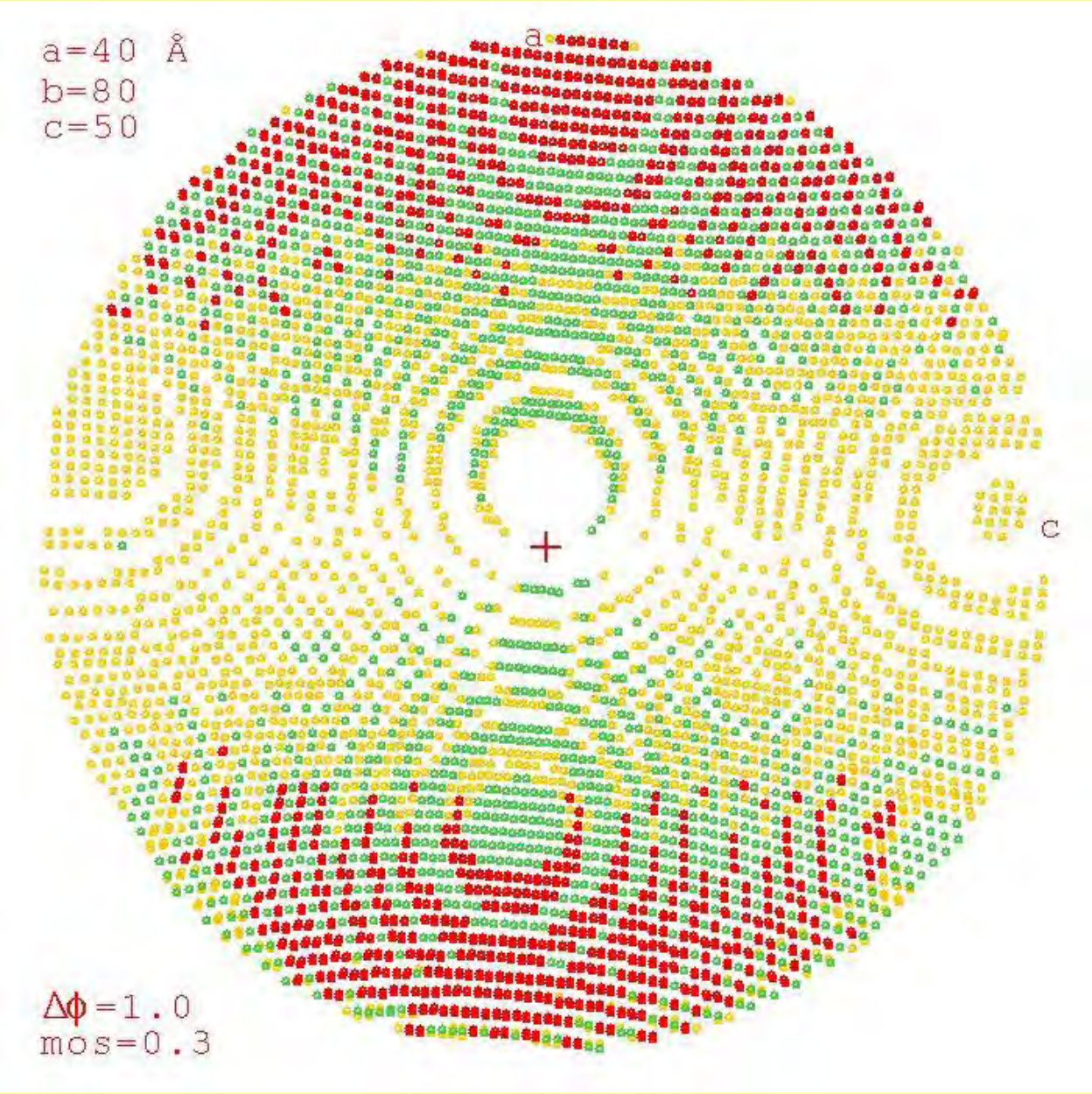


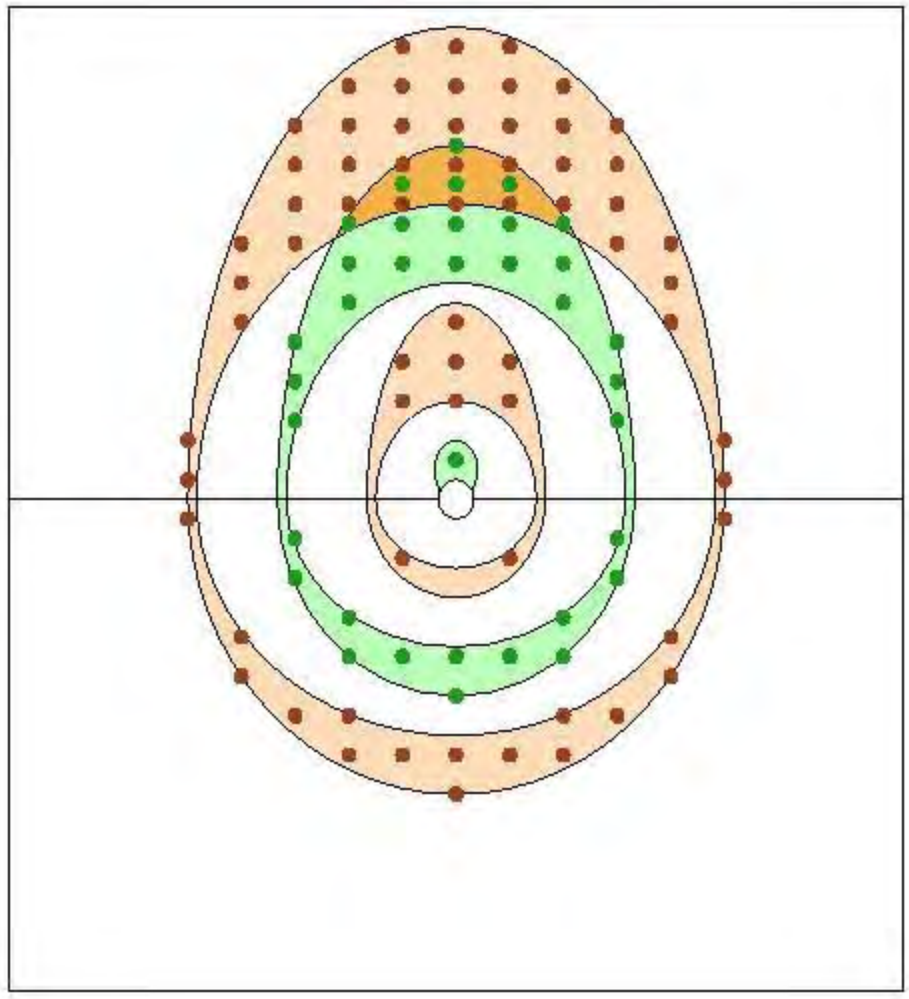

a*
d*
Δφ
θmax
Δφmax = 180/π · d/a − η

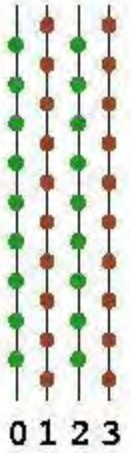

a=40 Å
b=80
c=50
b
c
Δφ=1.0
mos=0.0


a=40 Å
b=80
c=50
a
c
Δφ =1.0
mos=0.0


a=40 Å
b=80
c=50
b
c
Δφ=1.0
mos=0.3


a=40 Å
b=80
c=50
a
c
Δφ=1.0
mos=0.3




0 1 2 3

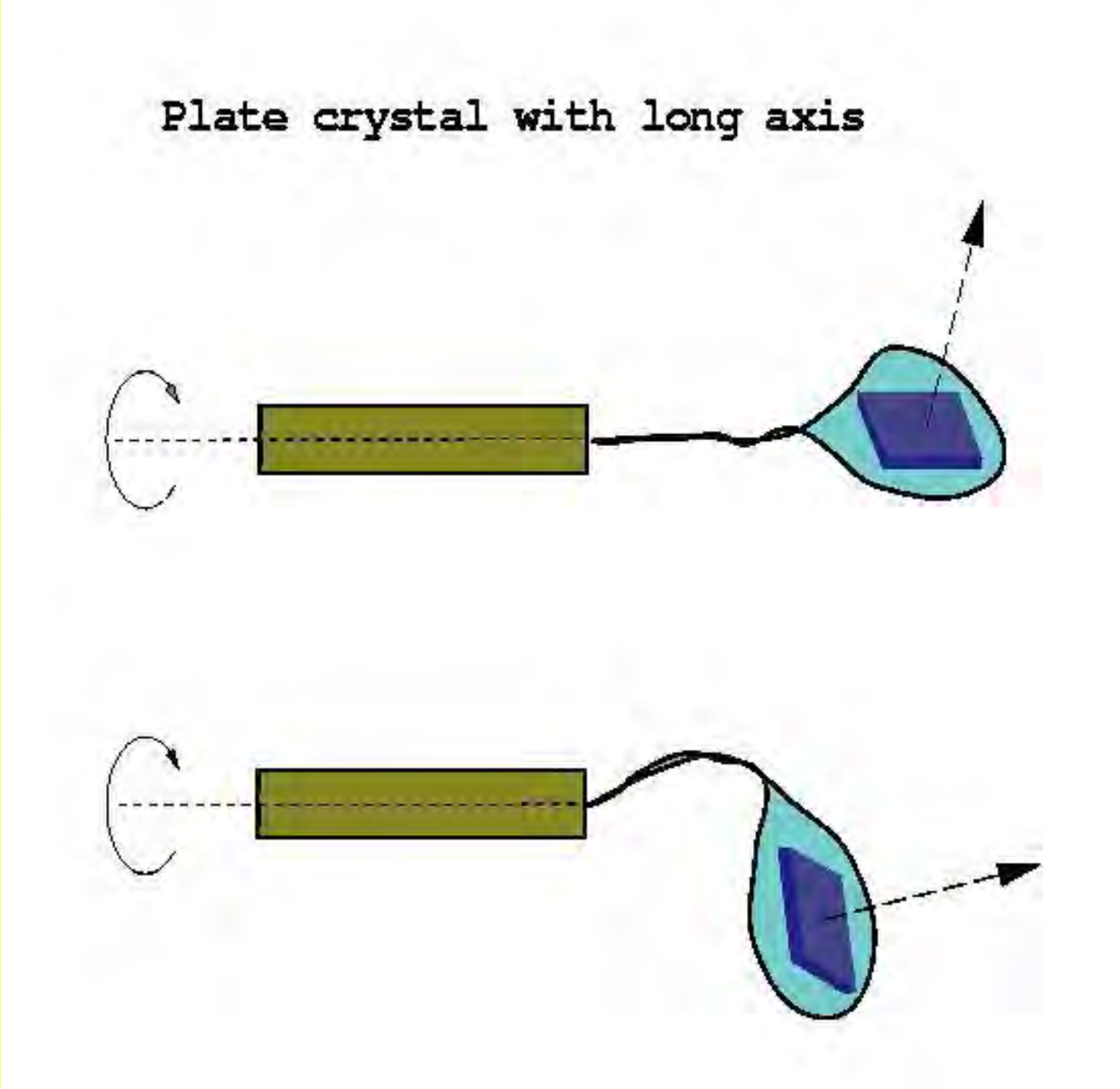
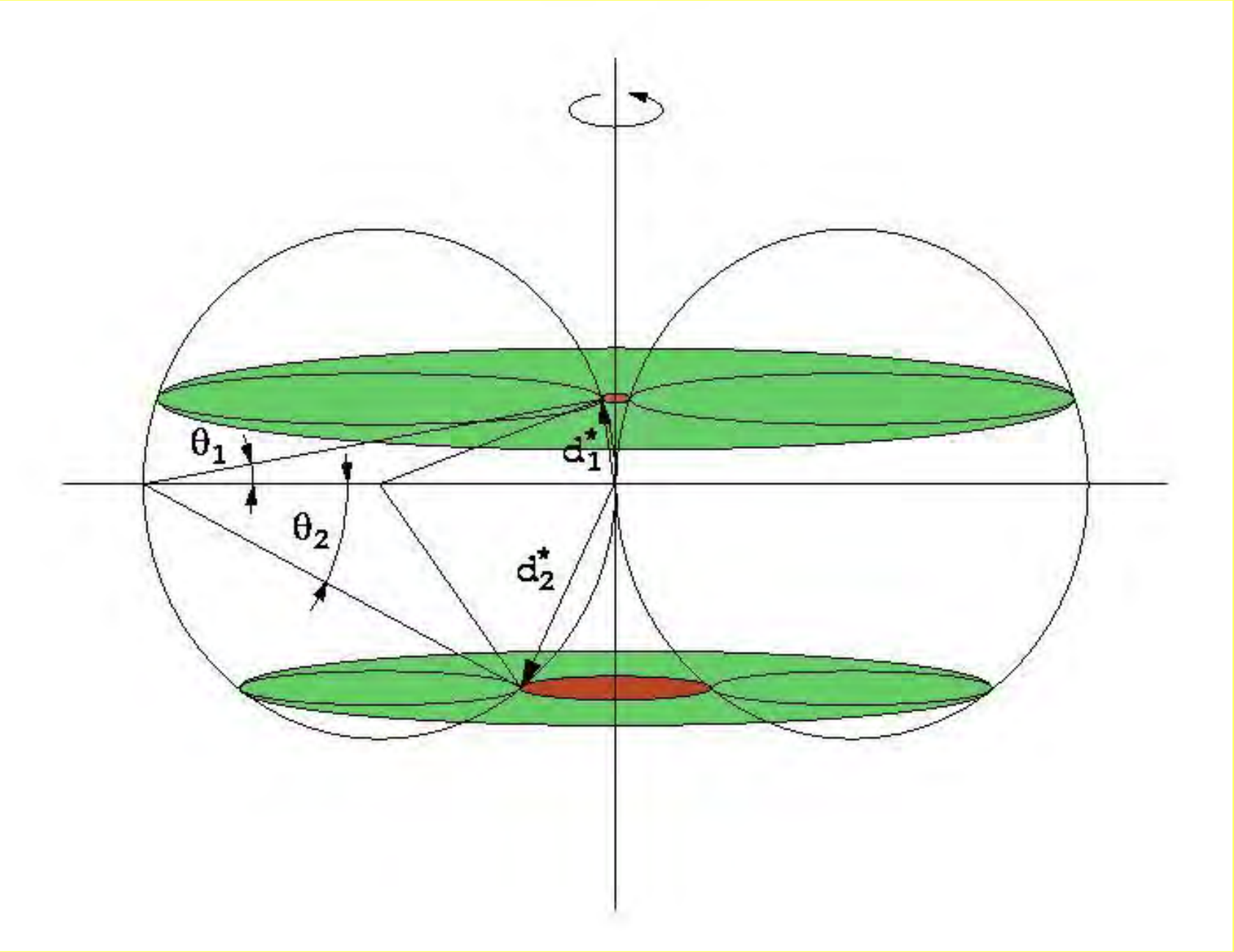
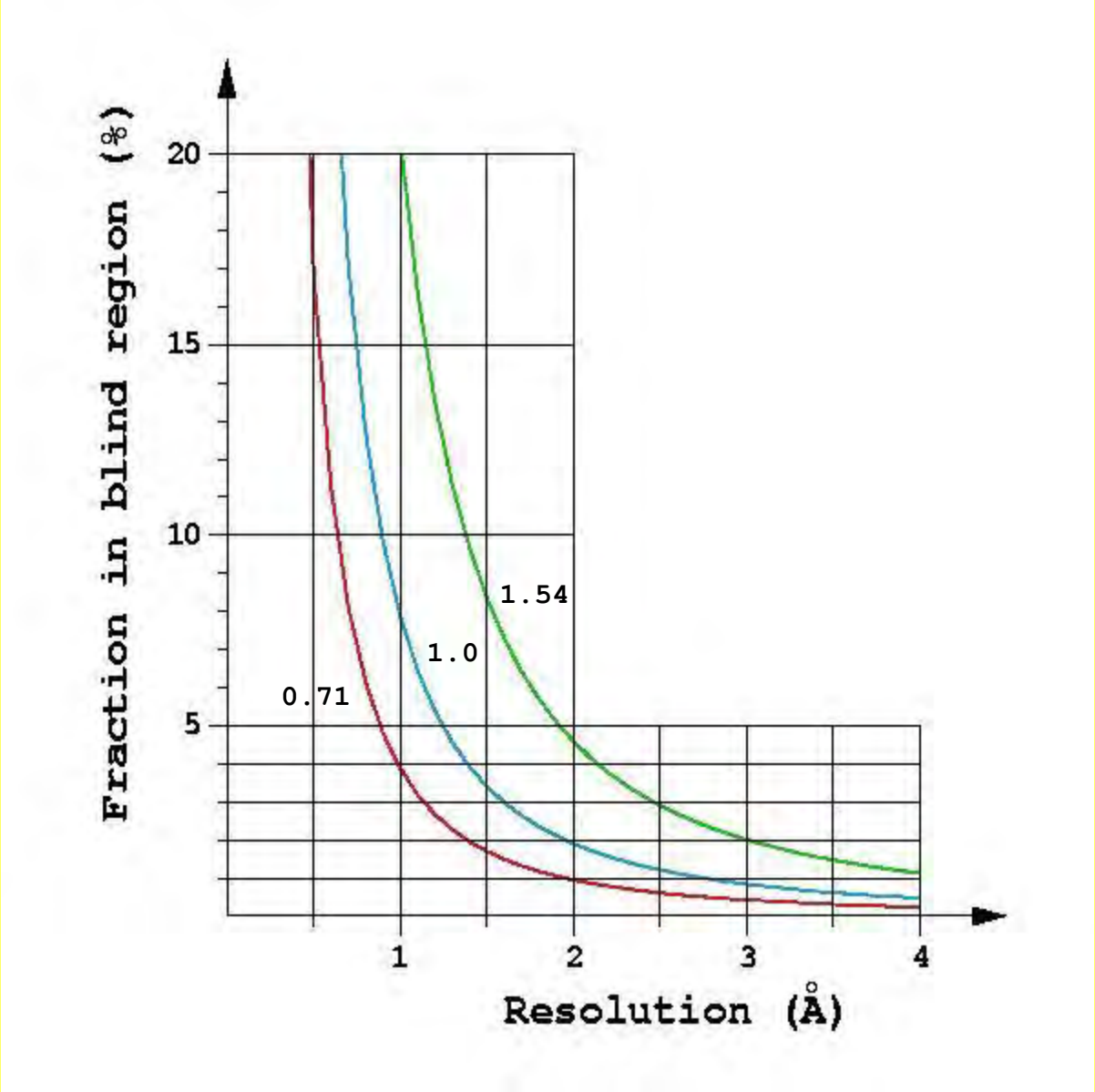
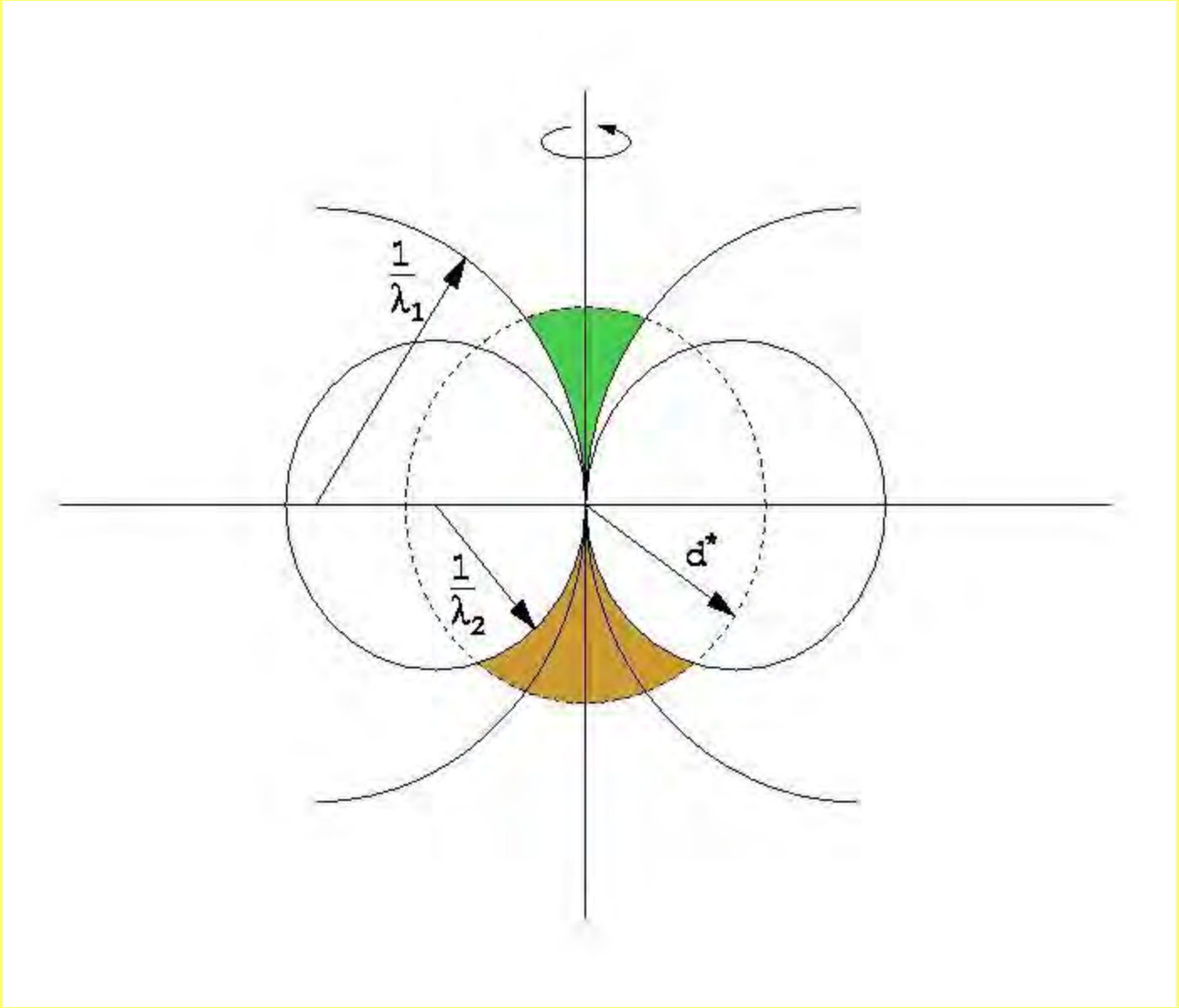
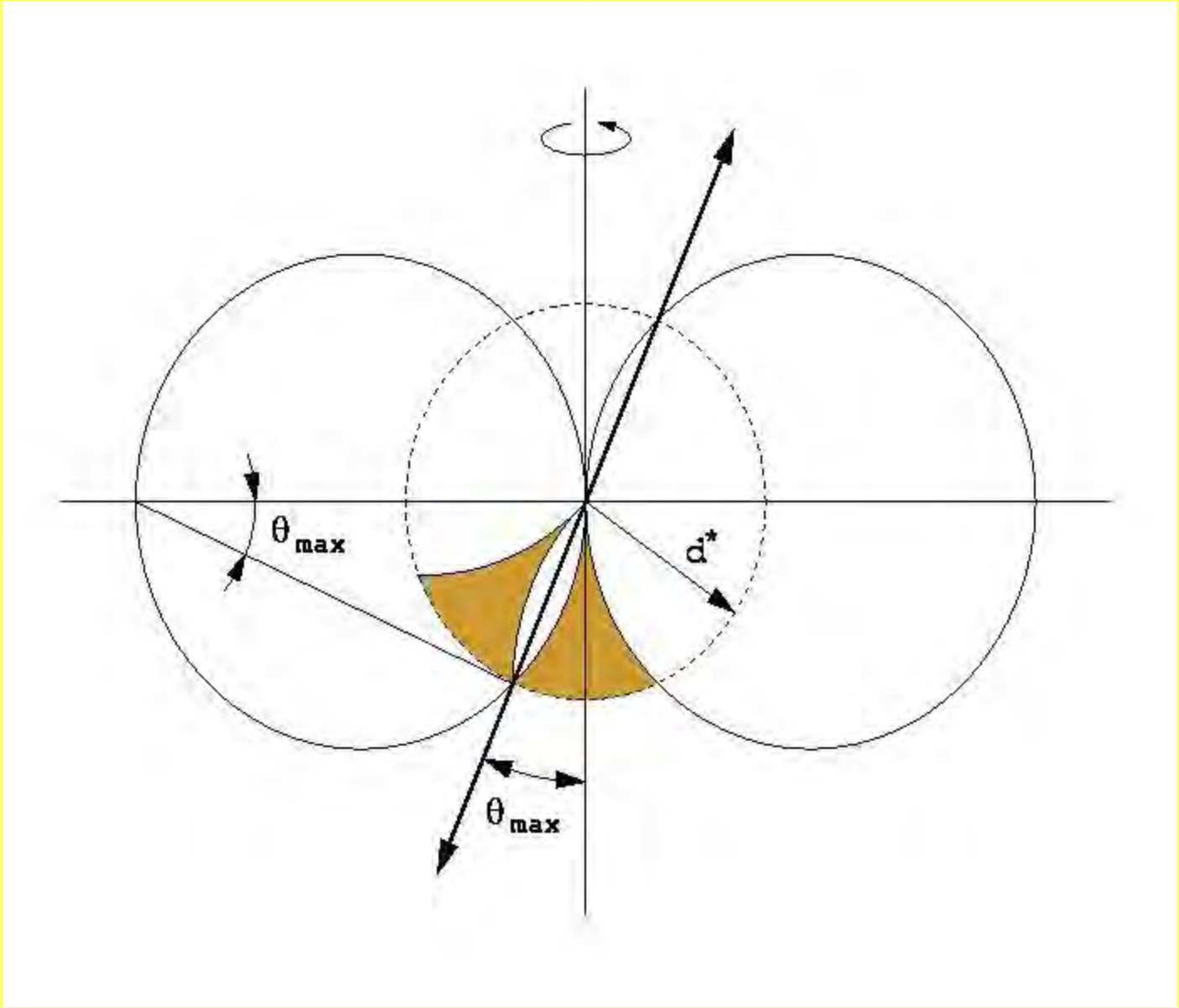


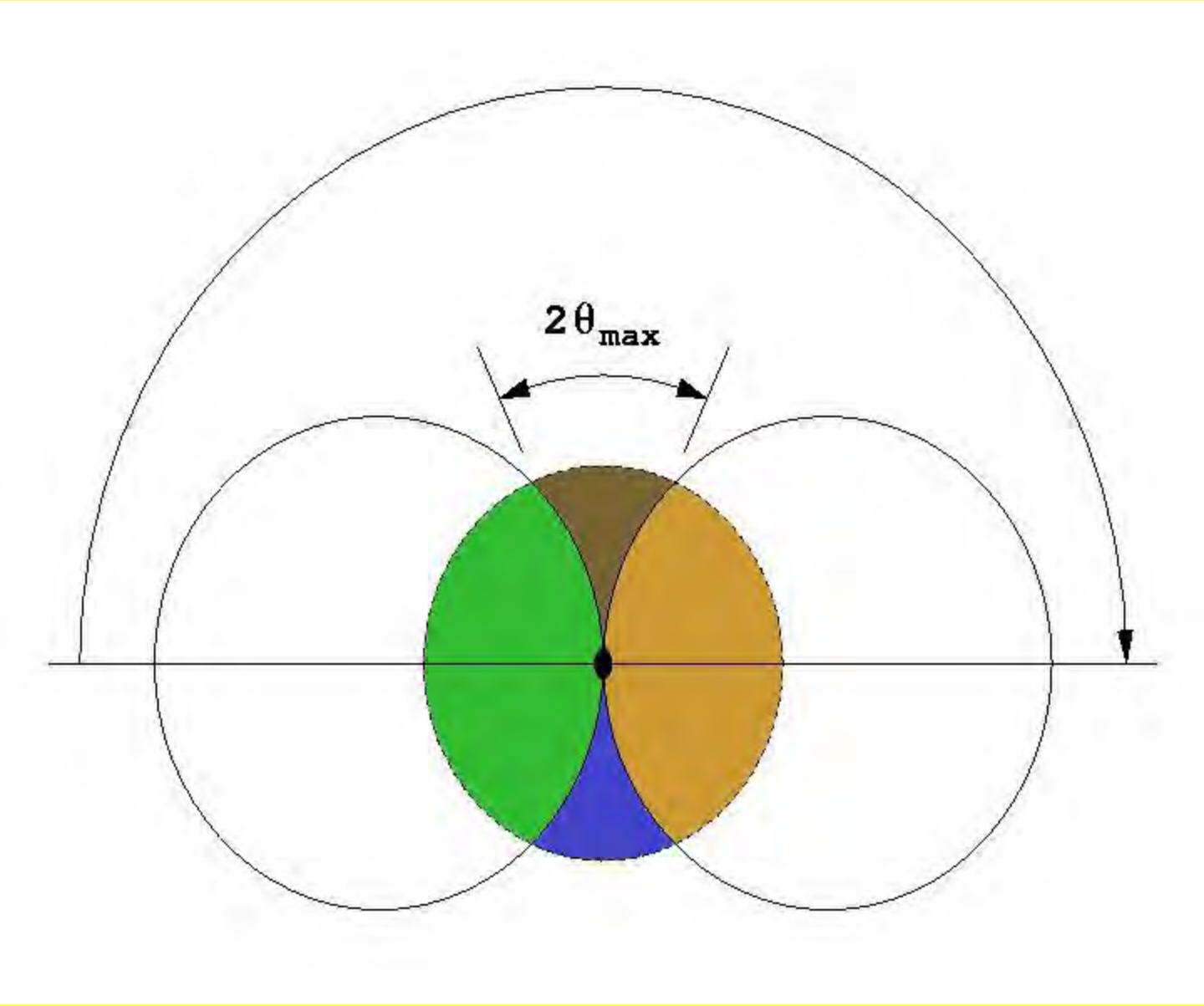
Plate crystal with long axis

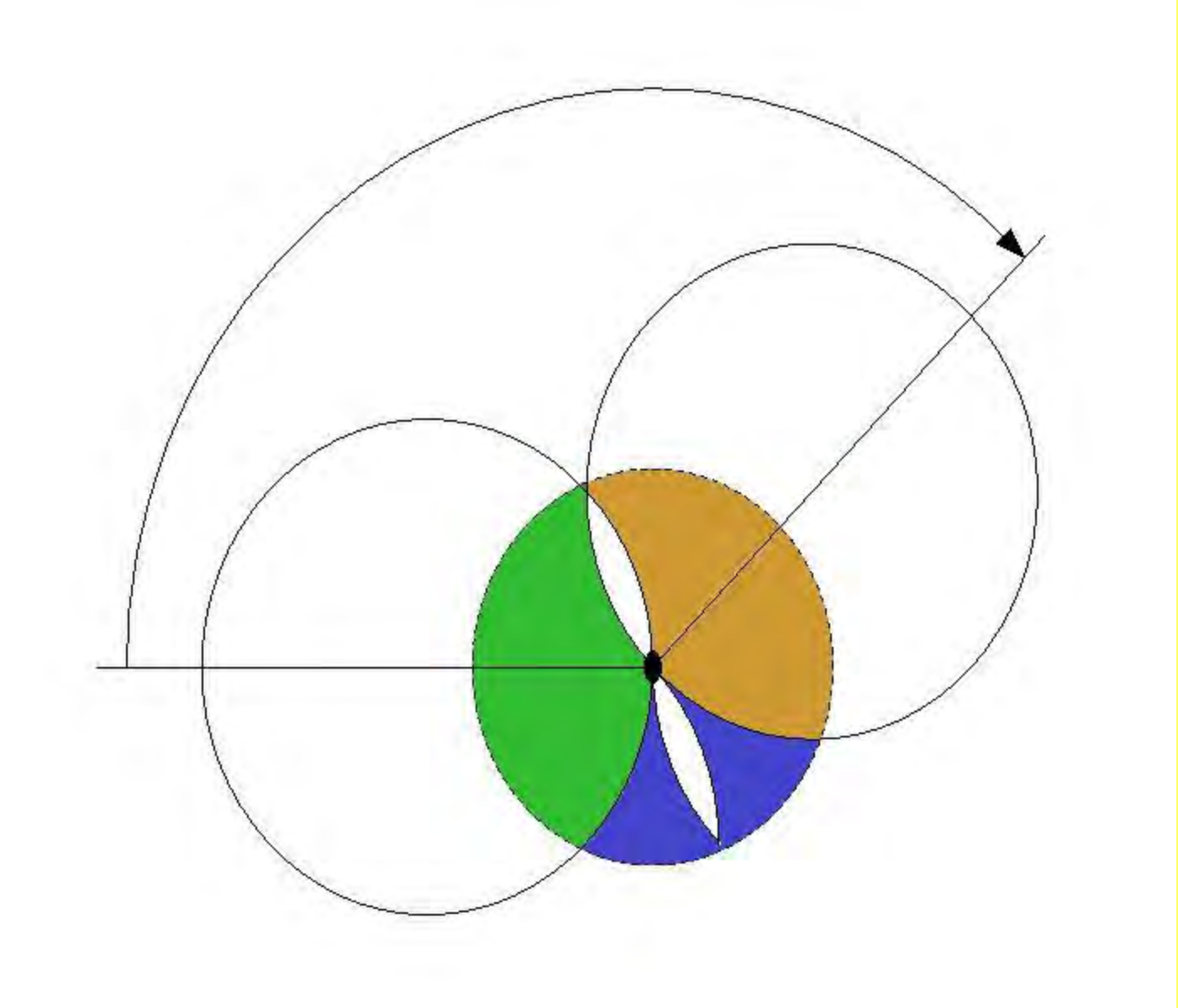

θ1
θ2
d*1
d*2

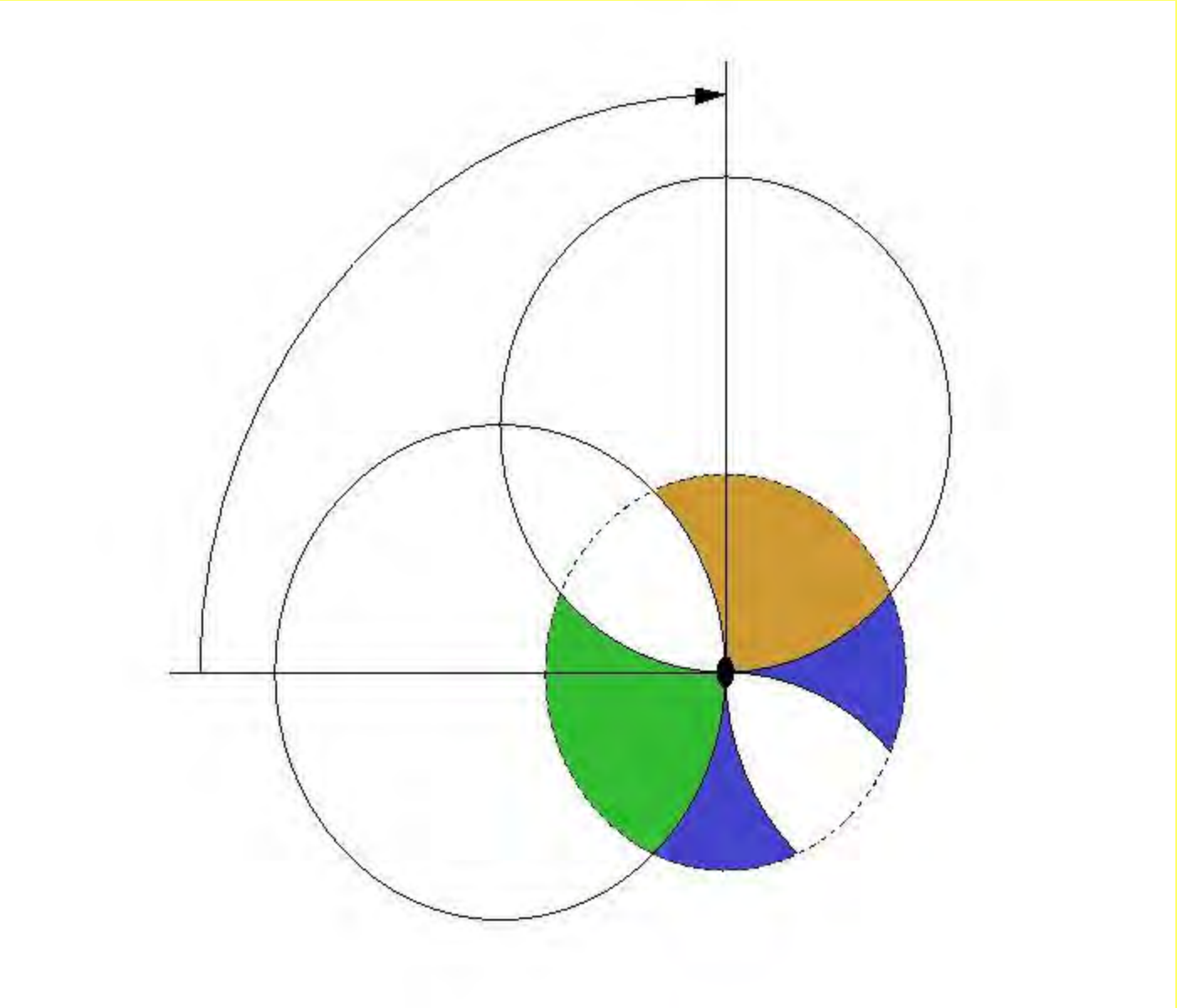

Fraction in blind region (%)
20
15
10
5
1.54
1.0
0.71
1
2
3
4
Resolution (Å)

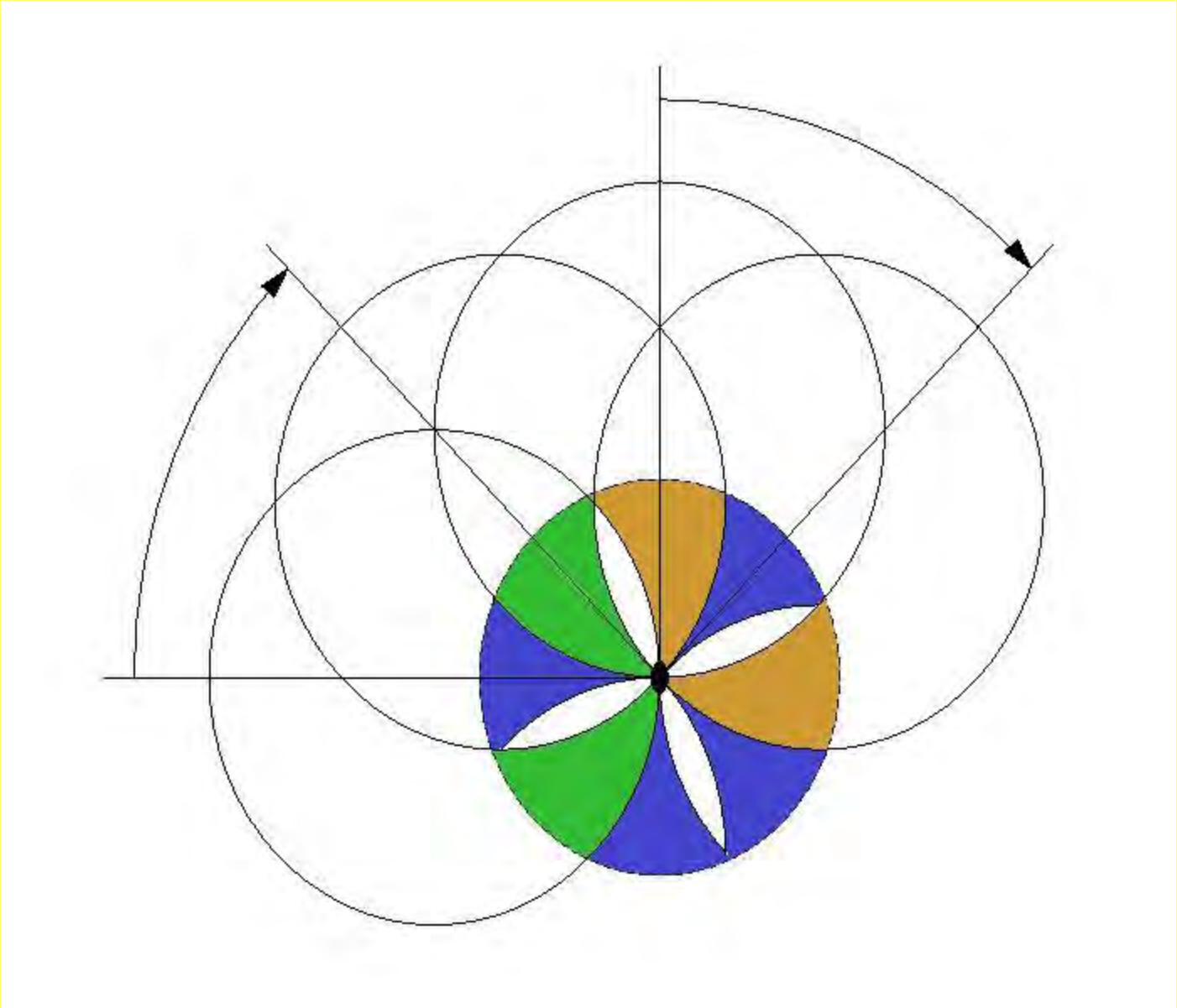

1/λ1
1/λ2
d*

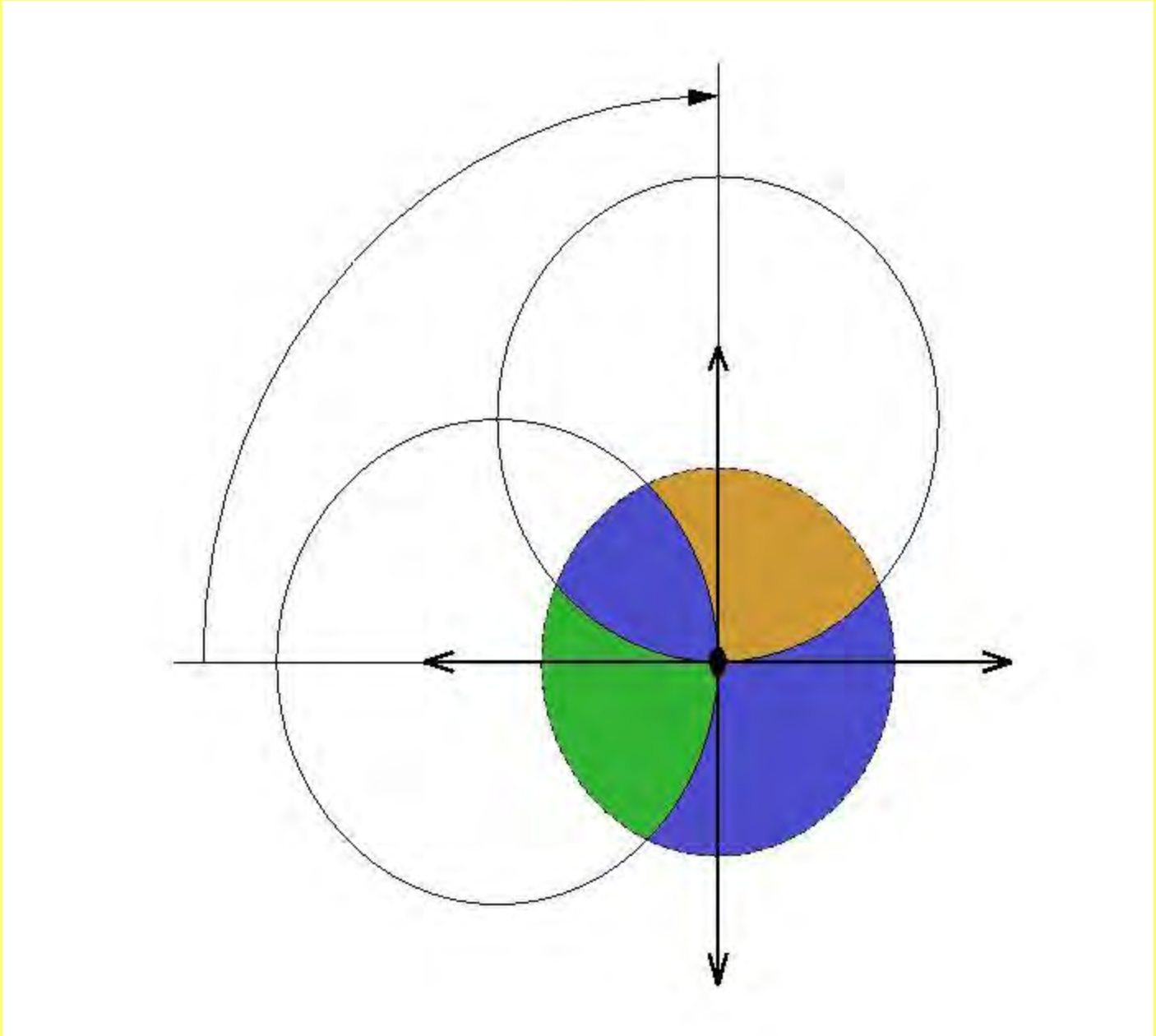

θ max
d*
θ max

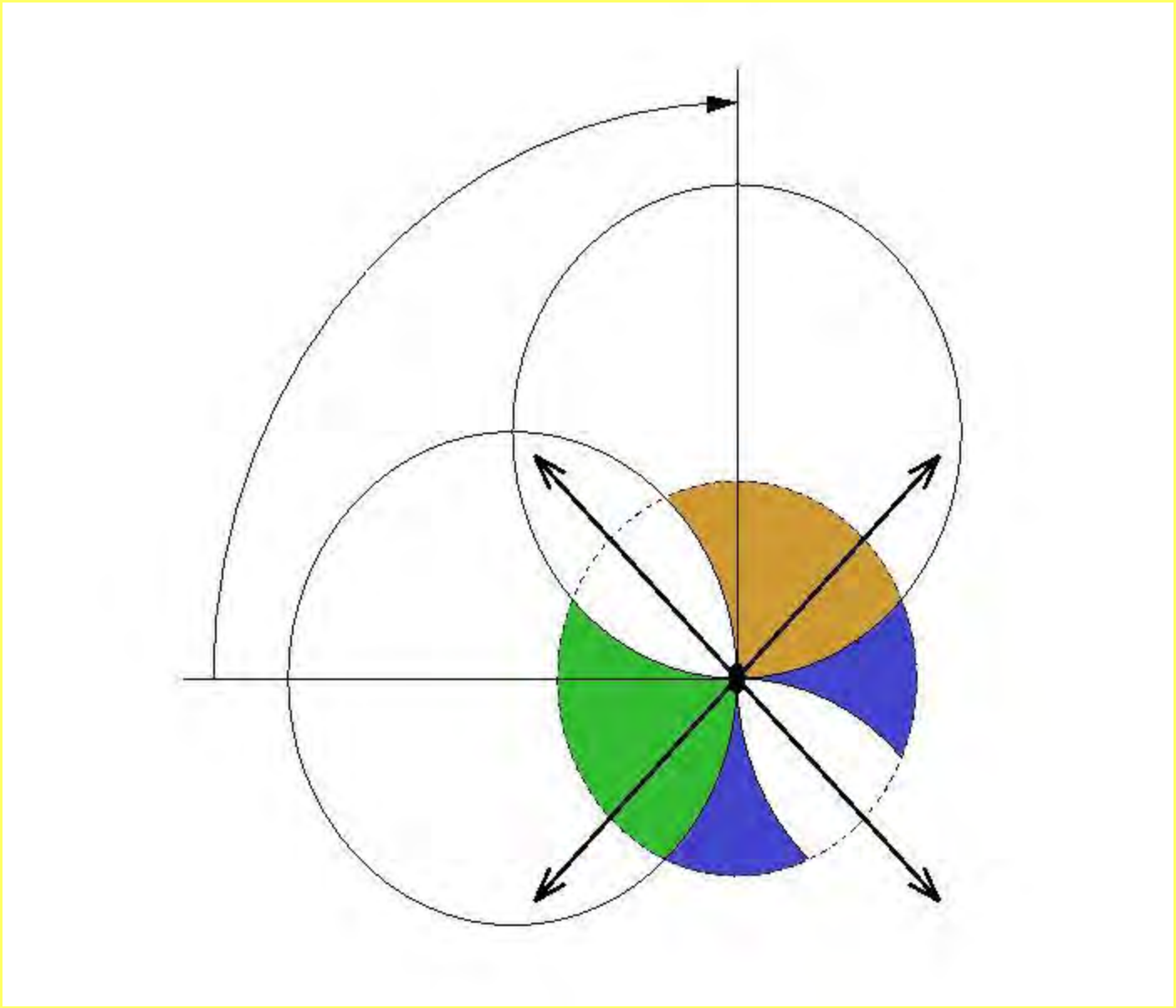

2θmax



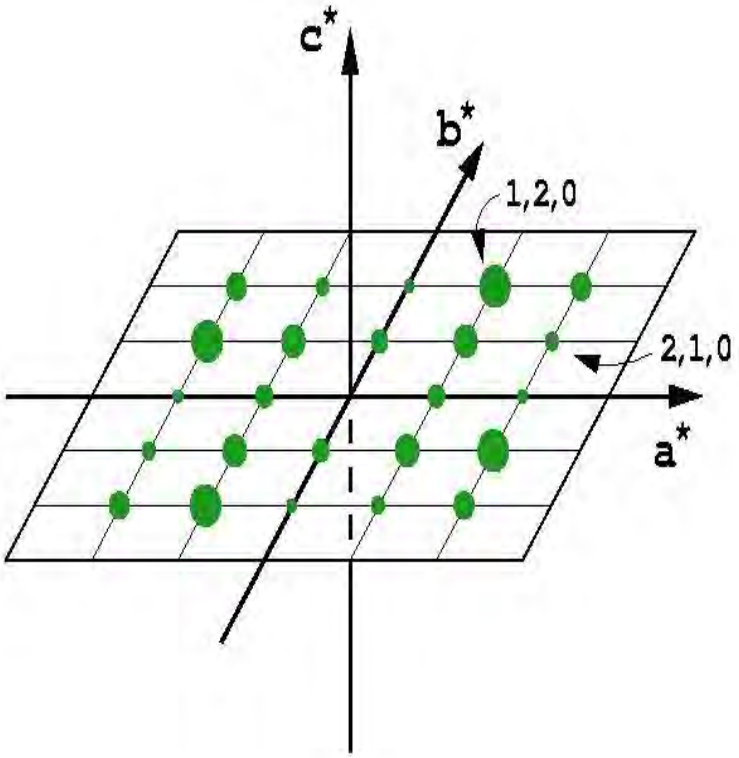


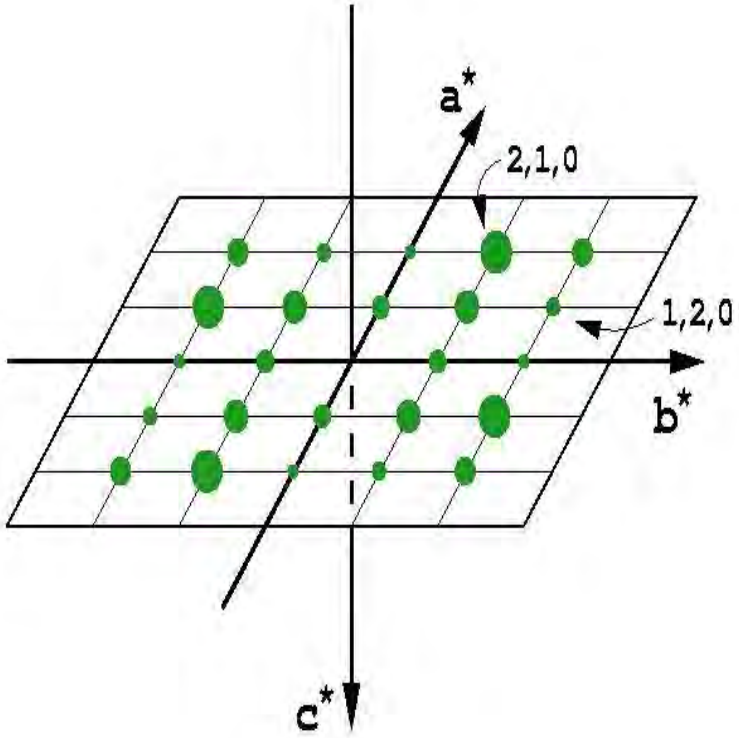






Alternative indexing





Alternative indexing

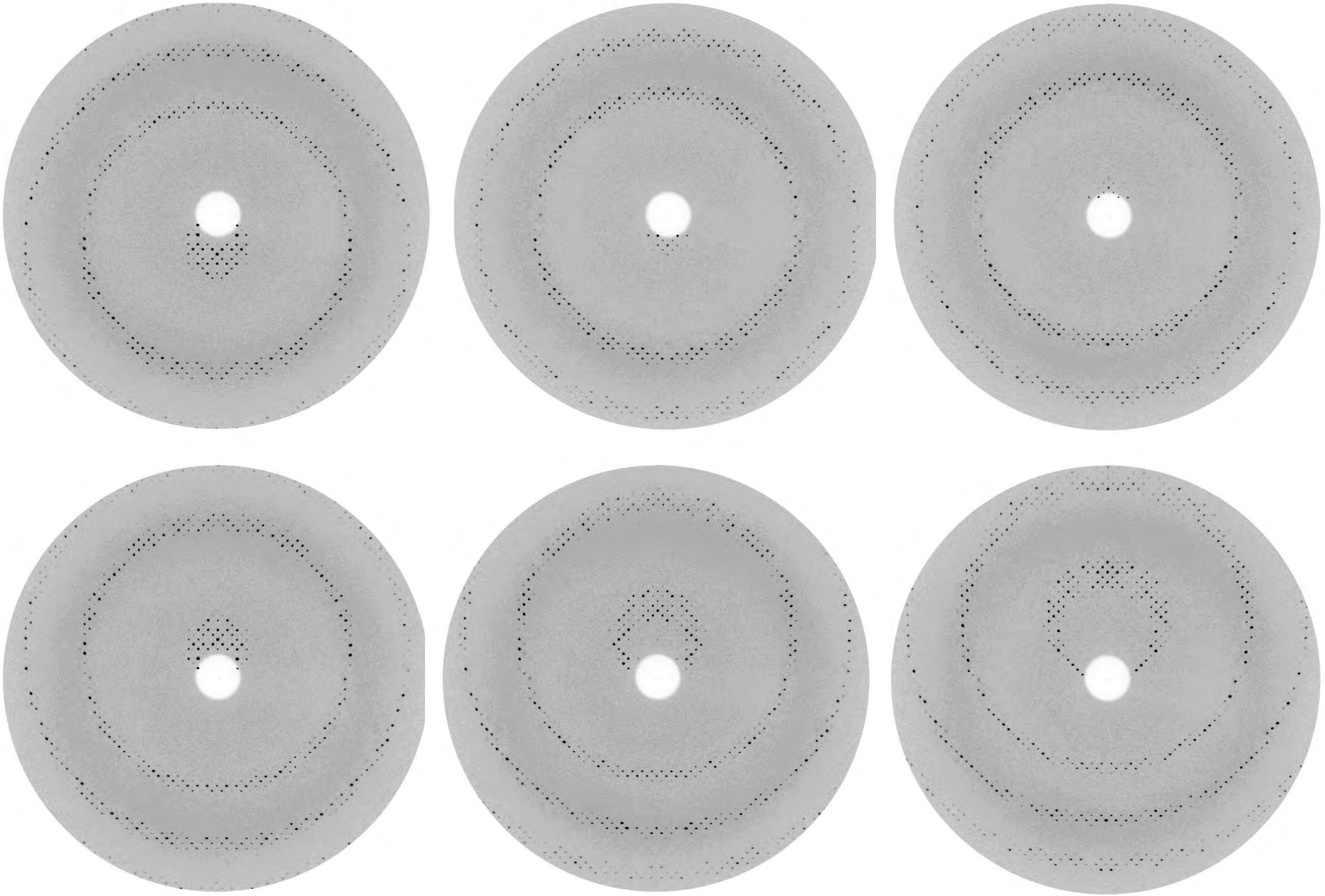
when lattice symmetry higher than space group (with polar axes)

also merohedral twinning possible

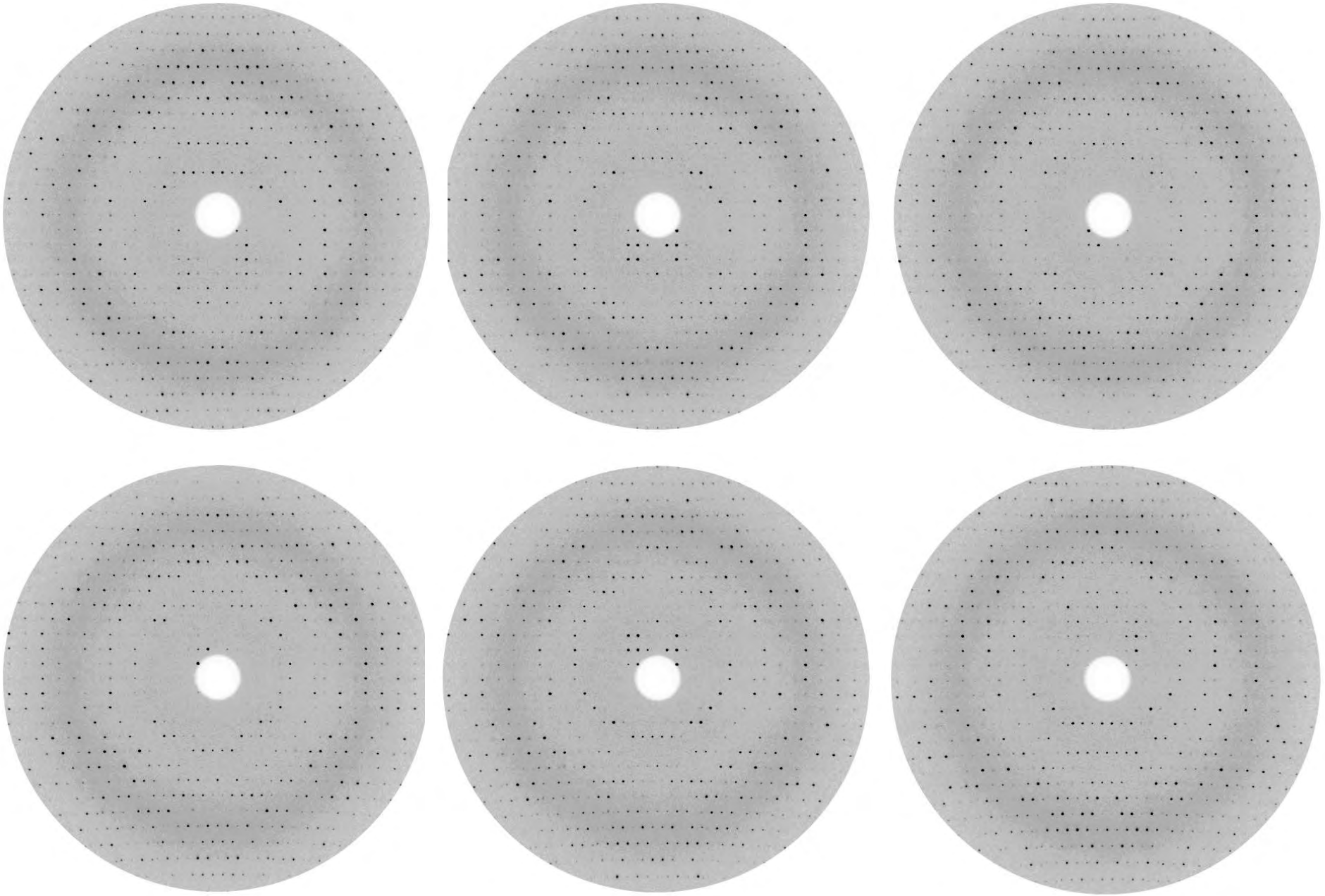
- P4, I4
- P3, R3, P321, P312, P6
- P23, I23, F23

Or when some cell dimensions coincidentially equal

Important with derivatives or data from more than one crystal

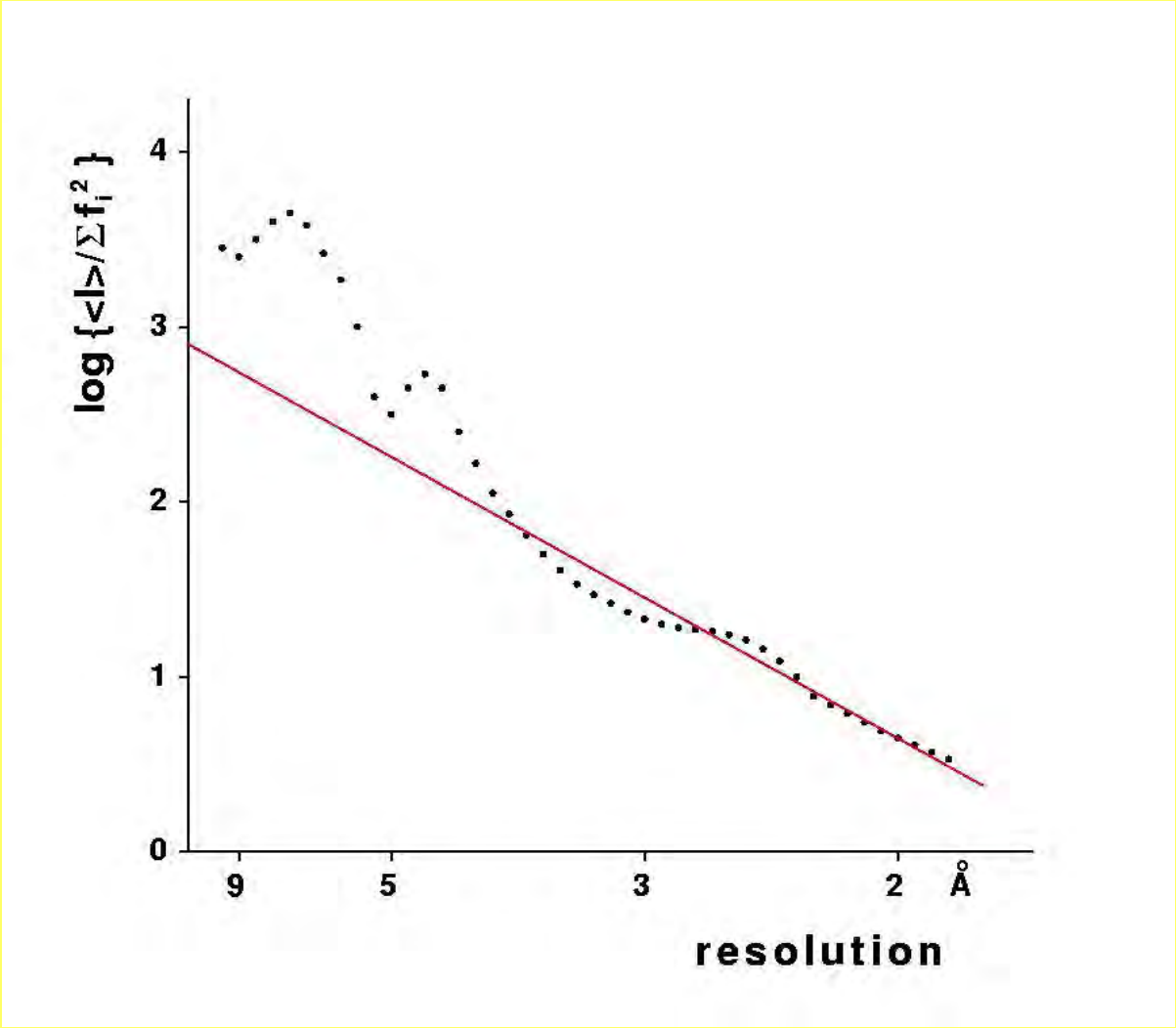


NCI, Macromolecular Crystallography Laboratory, Synchrotron Radiation Research Section @ BNL

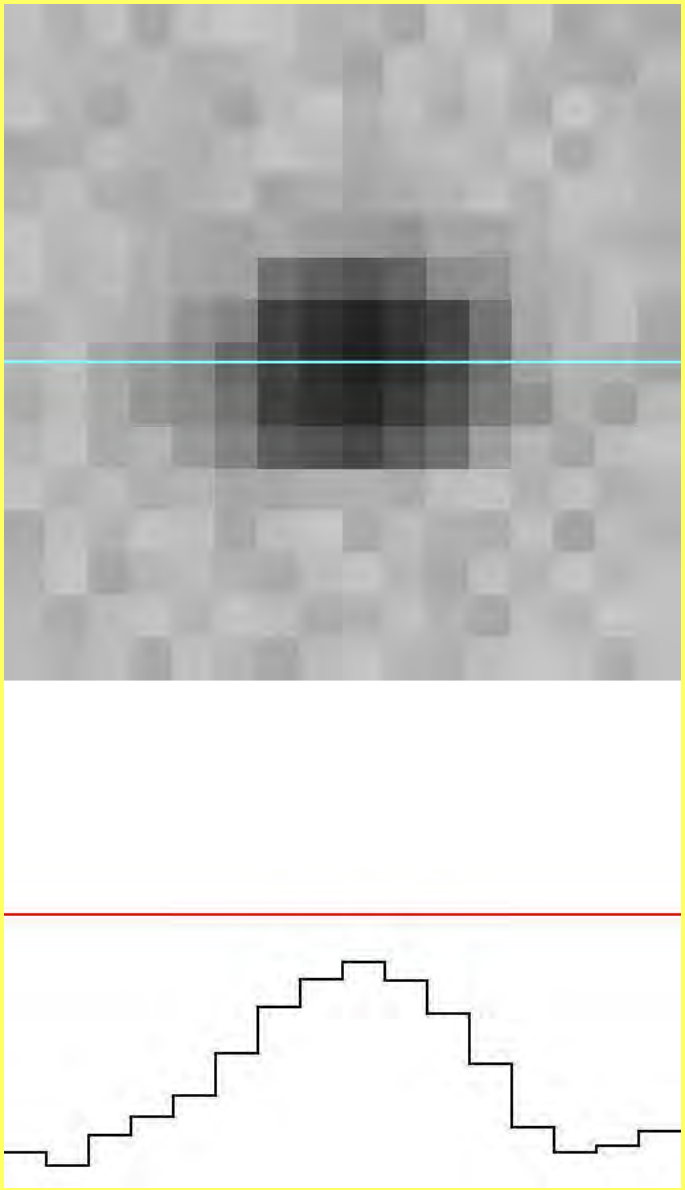


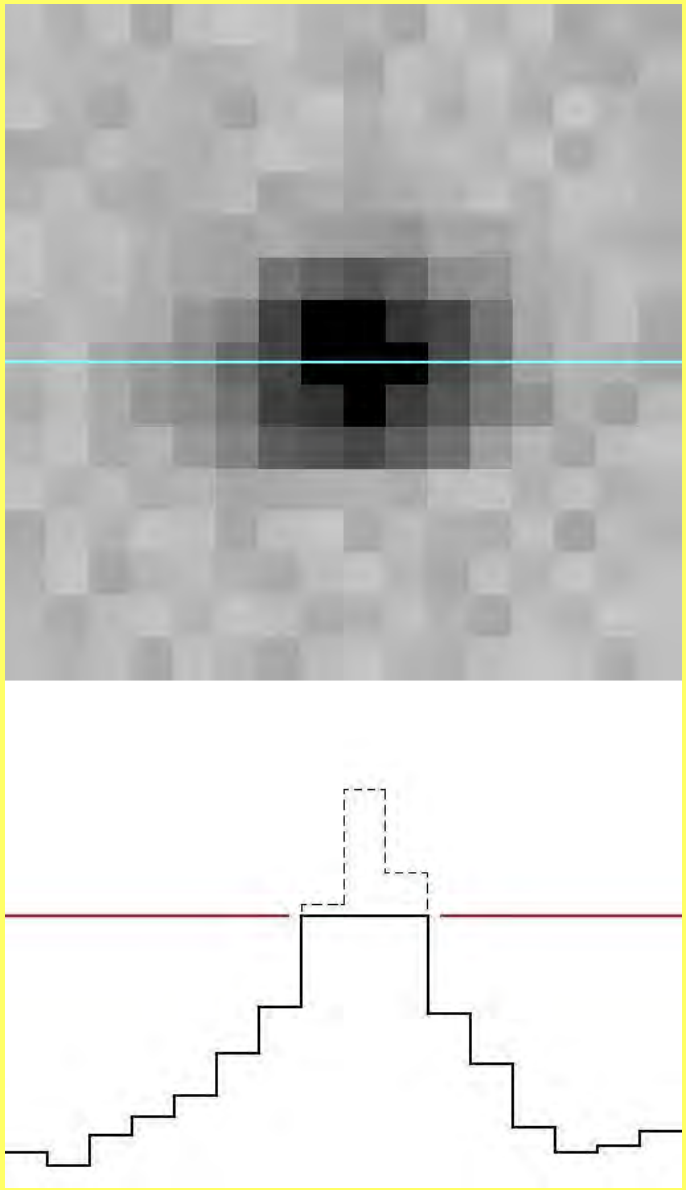
NCI, Macromolecular Crystallography Laboratory, Synchrotron Radiation Research Section @ BNL

Wilson plot



Reflection profile with overloaded pixels





Strongest reflections are important

- for all methods based on Patterson and MR
- for direct methods
- they modulate Fourier maps
- not so crucial for refinement

Weak reflections

- bias results, if absent
- informative in pseudosymmetric cases

$$R_{merge} = \frac{\Sigma\{\langle I \rangle - I_i\}}{\langle I \rangle}$$

$$R_{meas} = \frac{[n/(n-1)]^{1/2} * \Sigma\{\langle I \rangle - I_i\}}{\langle I \rangle}$$

$I/\sigma(I)$ - better,

but σ's must be estimated correctly

2-D detectors do not provide counting statistics –

– σ′s must be corrected

- by t-plot = $\frac{\langle I \rangle - I_i}{\sigma(I)}$

- or $\chi 2$ criterion

important for programs based on maximum likelihood

Data collection

- scientific process
  not technicality

- irreversible consequences
  (often)

- even more important due to
  progress in automation,
  phasing, refinement etc.