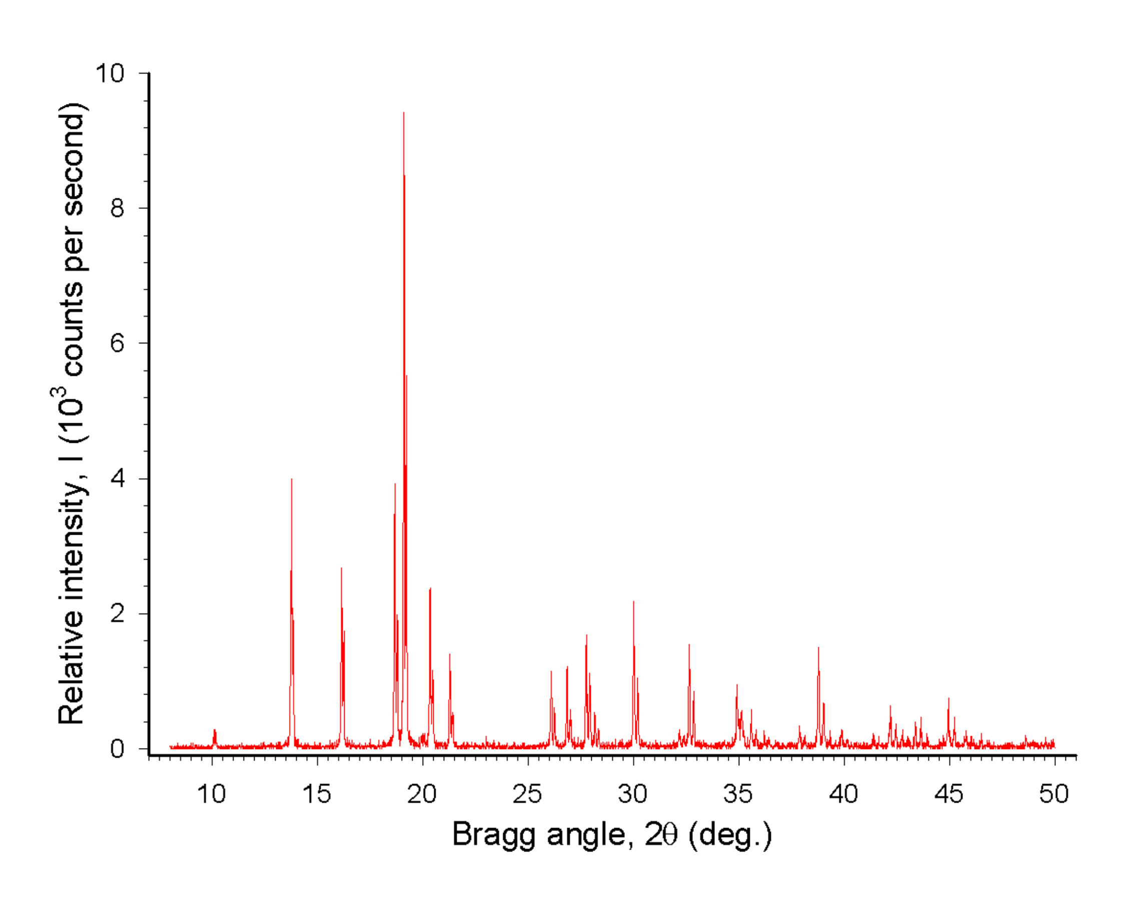
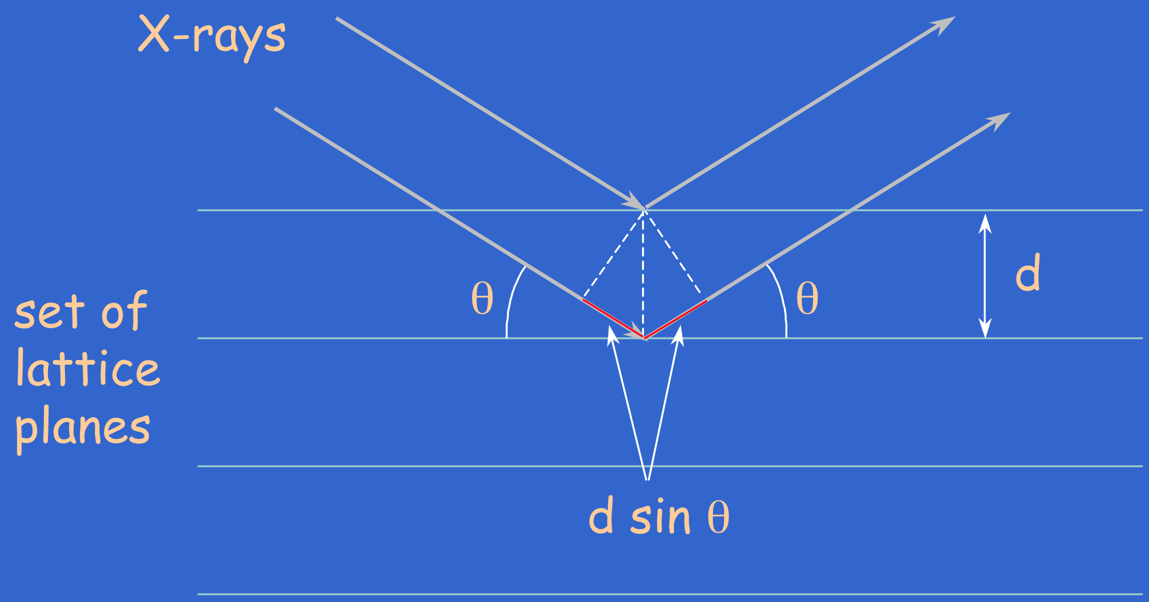
X-ray diffraction



X-ray diffraction

Braggs' law $\lambda = 2d_{hkl} \sin \theta_{hkl}$

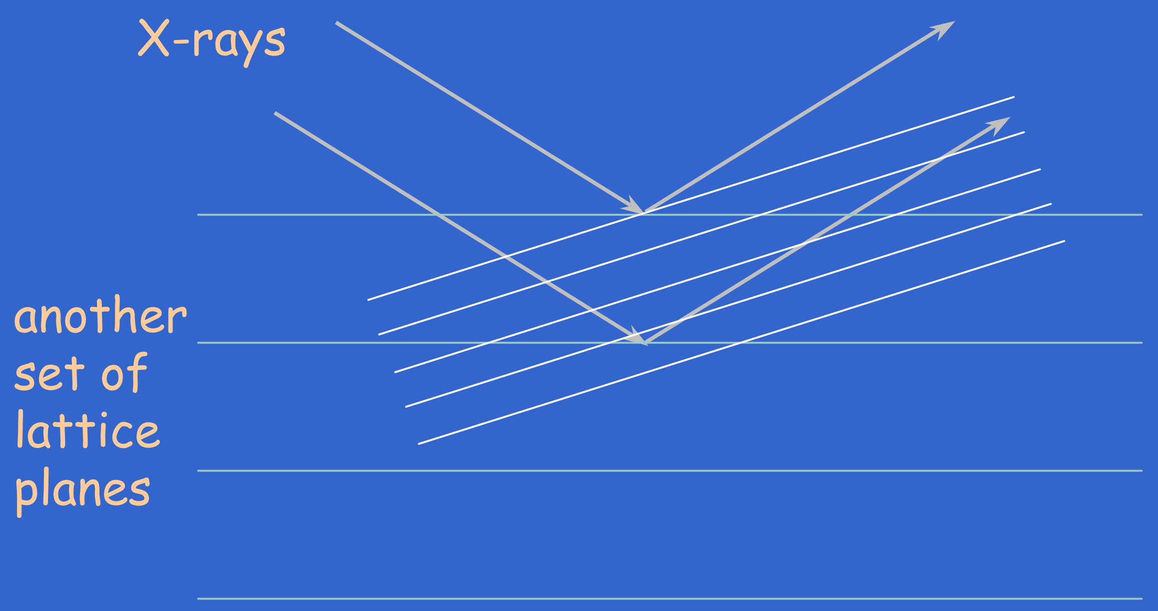


From this set of planes, only get reflection at one angle - θ

X-ray diffraction

Braggs' law

$$\lambda = 2d_{hkl} \sin \theta_{hkl}$$



X-ray diffraction

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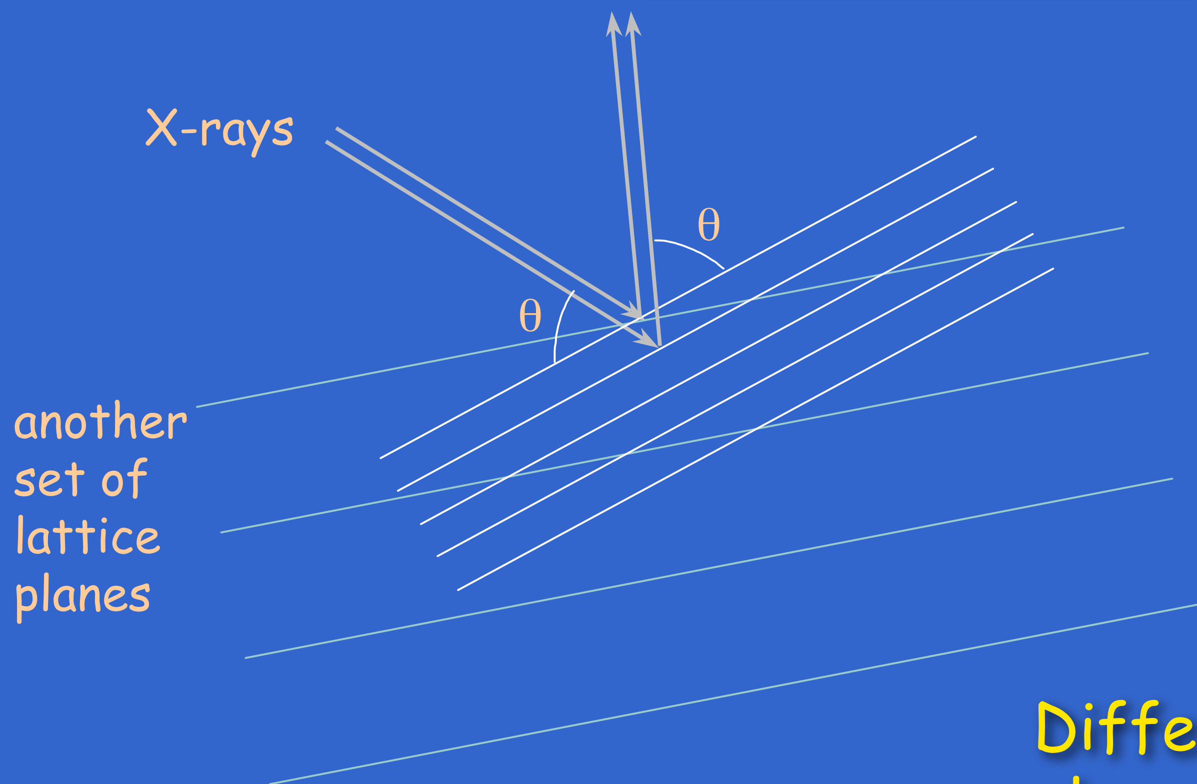
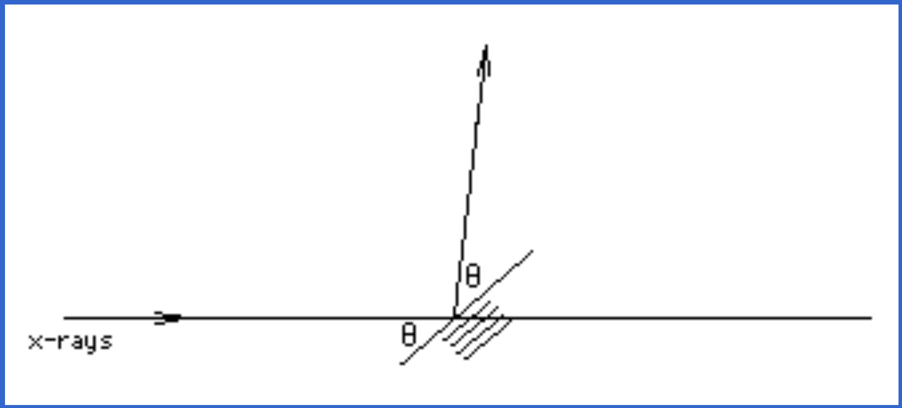


Different sets of planes reflect at different θ angles

As d —> small,
θ —> large (λ is constant)

Ewald construction

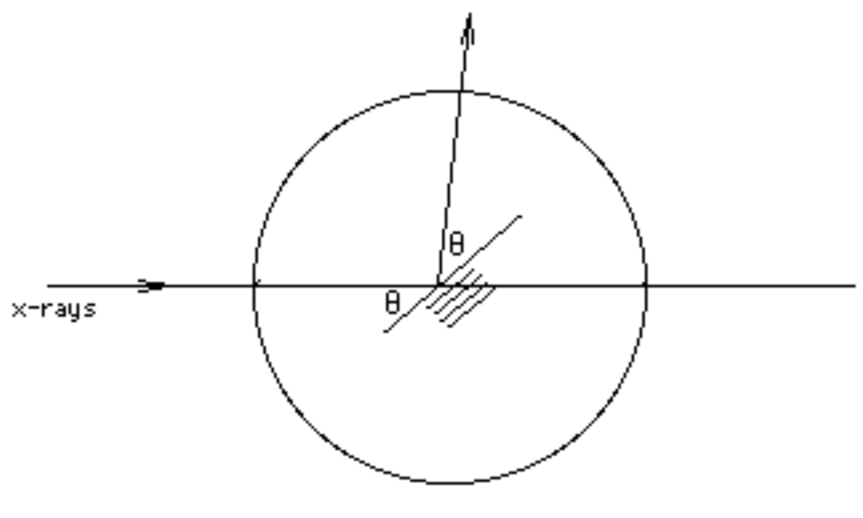
Think of set of planes reflecting in x-ray beam



Ewald construction

Think of set of planes reflecting in x-ray beam

Center sphere on specimen origin
x-ray beam is a sphere diameter



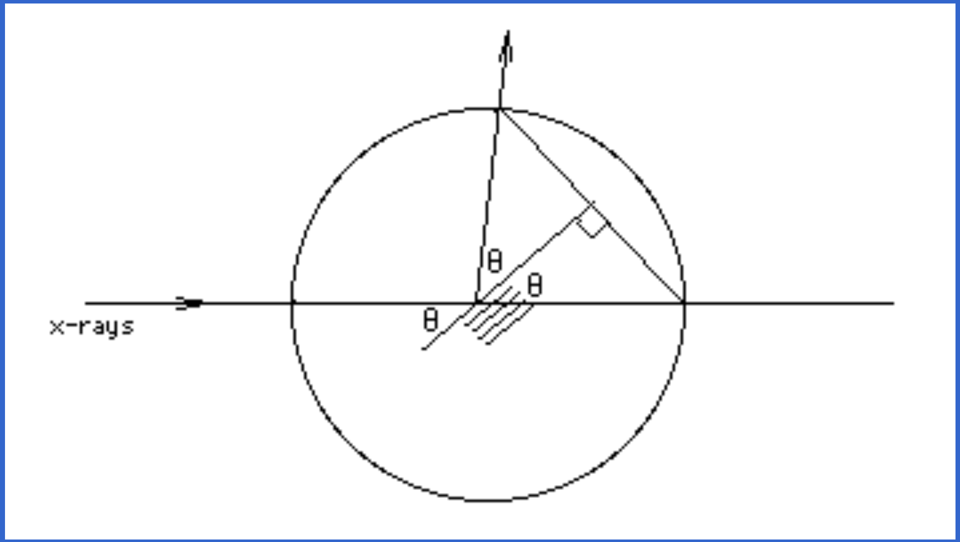
sphere radius = $1/\lambda$

Ewald construction

Think of set of planes reflecting in x-ray beam

Center sphere on specimen origin
x-ray beam is a sphere diameter

Construct lines as below



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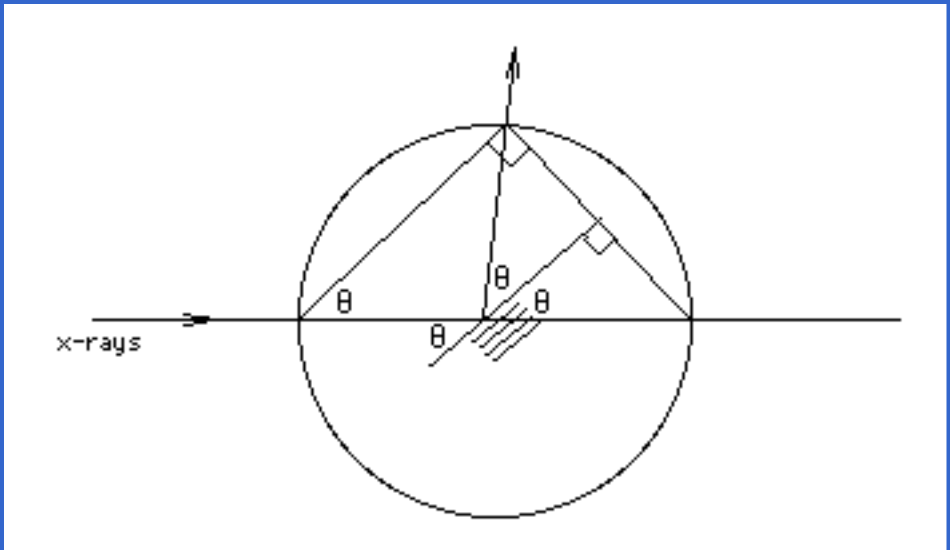
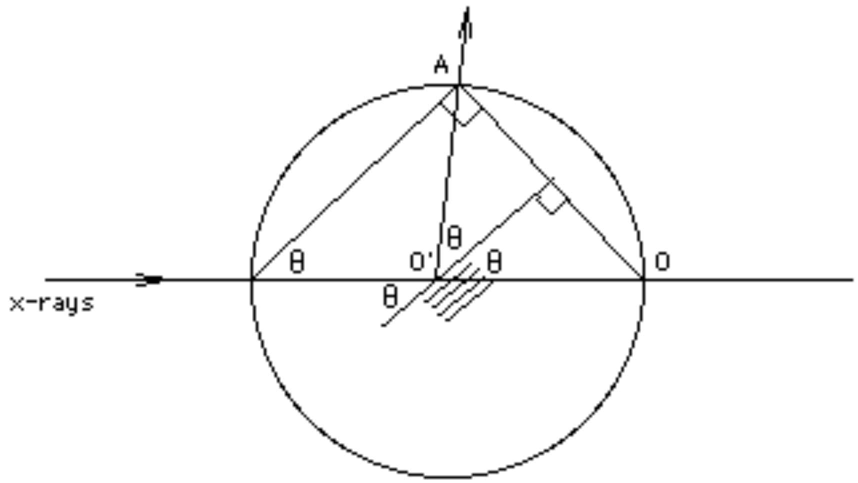


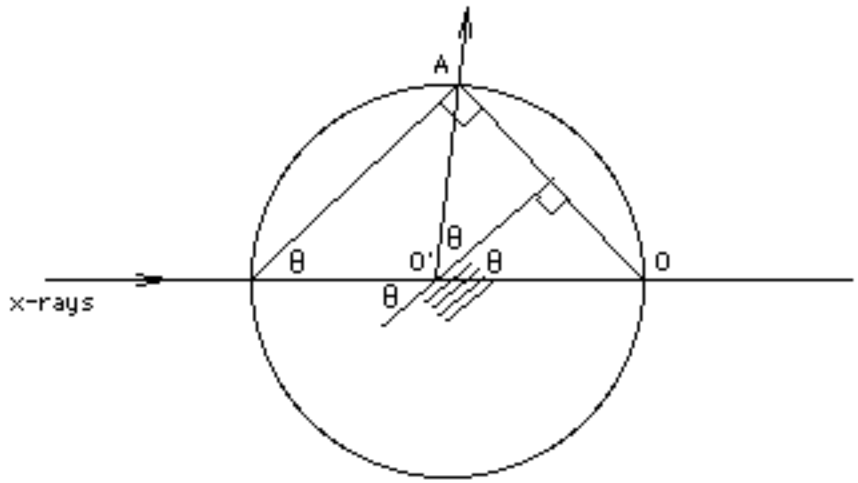
Ewald construction



sphere radius = $1/\lambda$

$$\sin\theta = \frac{AO}{2/\lambda}$$

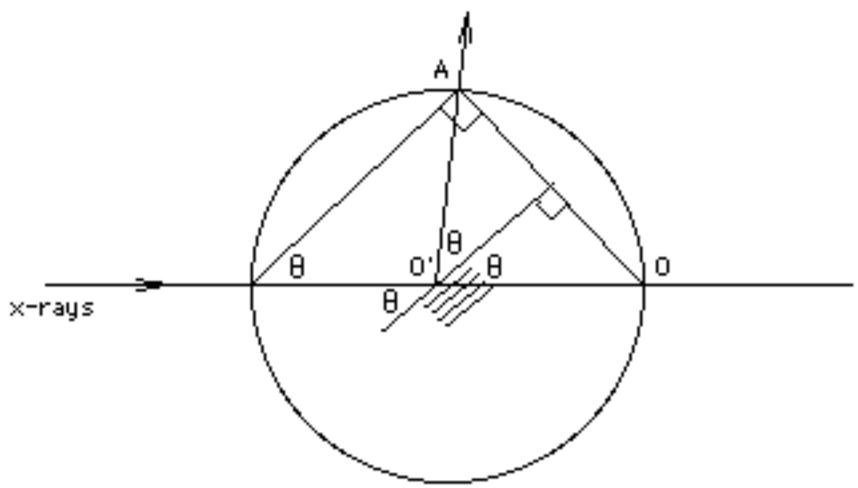
Ewald construction



sphere radius = $1/\lambda$

$$\sin\theta = \frac{AO}{2/\lambda} \qquad 2\sin\theta = AO\cdot\lambda$$

Ewald construction

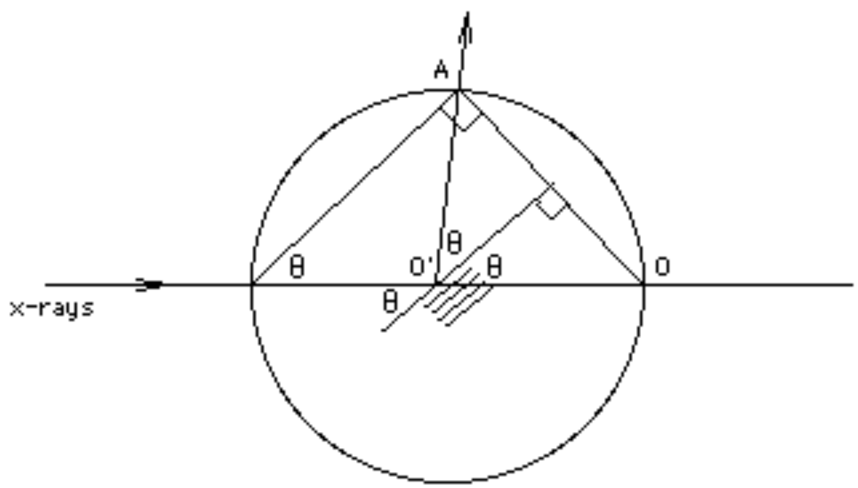


sphere radius = $1/\lambda$

$2 \sin \theta = AO \cdot \lambda$

Braggs' law if $AO = 1/d$
AO is normal to planes

Ewald construction



sphere radius = $1/\lambda$

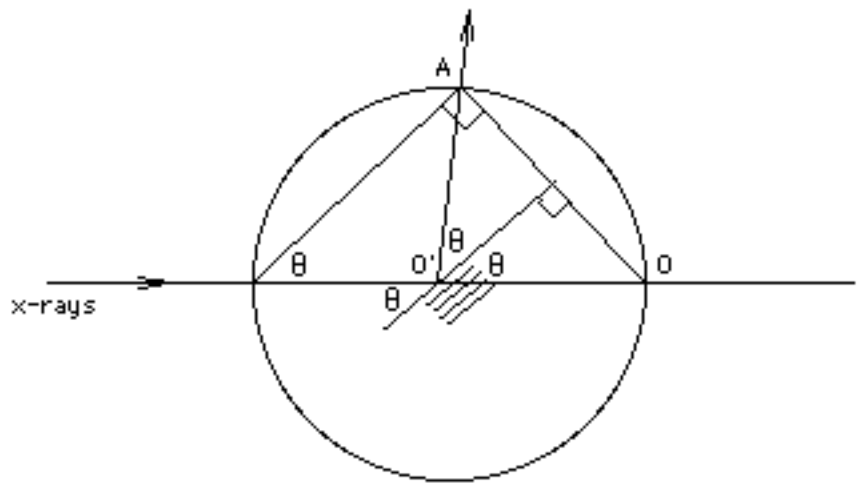
$2 \sin \theta = AO \cdot \lambda$

Braggs' law if AO = 1/d

AO is normal to planes

If O is origin then A is a reciprocal lattice point

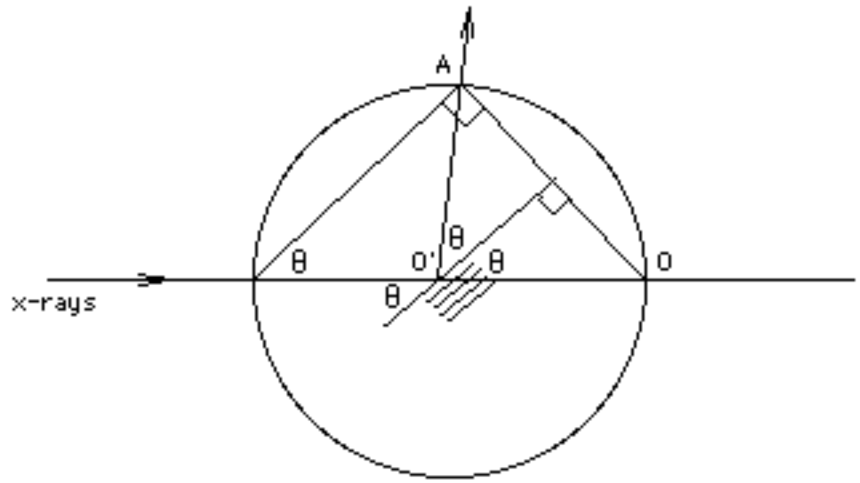
Ewald construction



Criterion: if the origin of the reciprocal lattice is placed at O, then, for any reciprocal lattice point on the Ewald sphere, there be reflection along the direction from the center of the sphere to the point on the sphere.

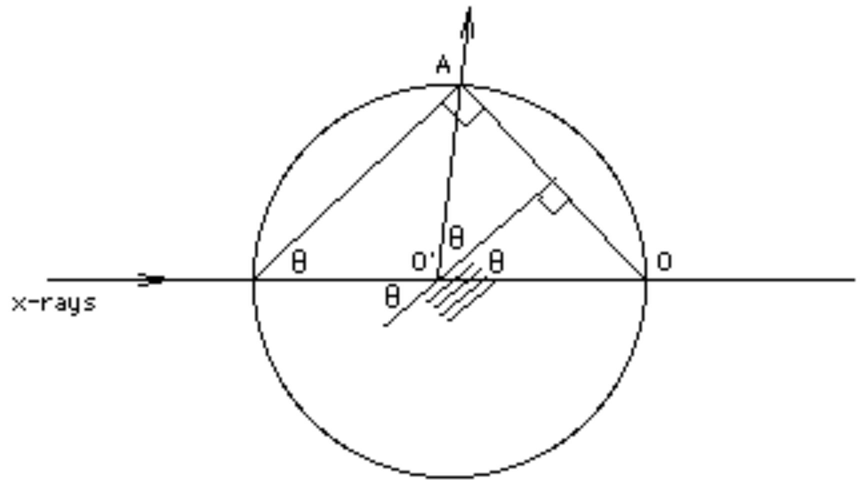
Any point in the reciprocal lattice which does not lie on the sphere corresponds to sets of planes which are not in a position to reflect.

Ewald construction



In general, reciprocal lattice points do not lie on the sphere.

Ewald construction



In general, reciprocal lattice points do not lie on the sphere.

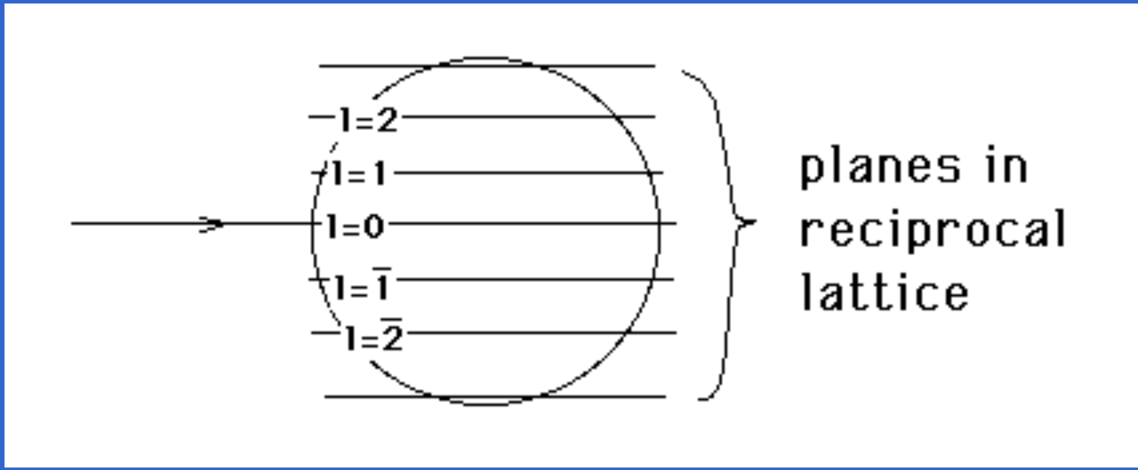
To observe the reflections, then, we must:

1. **move the sphere**
2. **move the crystal (rotate)**
3. **change the size of the sphere**

Ewald construction

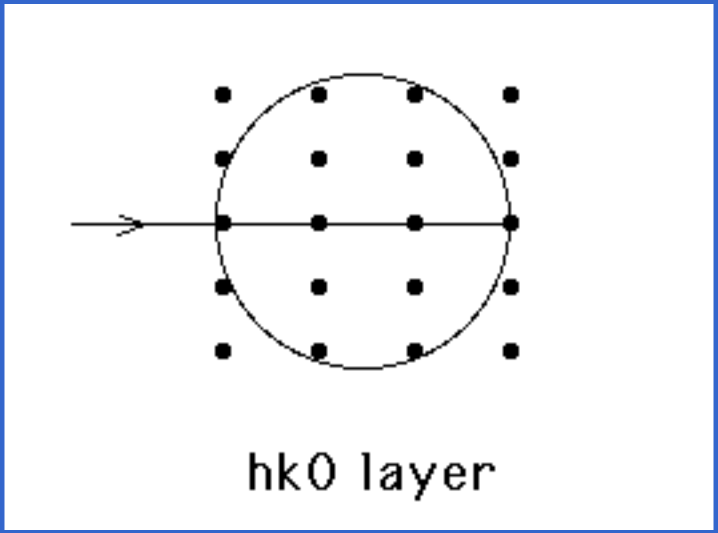
Most common in single crystal studies is to move (usually rotate) crystal

Consider crystal placed at sphere center oriented w/ planes of points in reciprocal lattice as below



Ewald construction

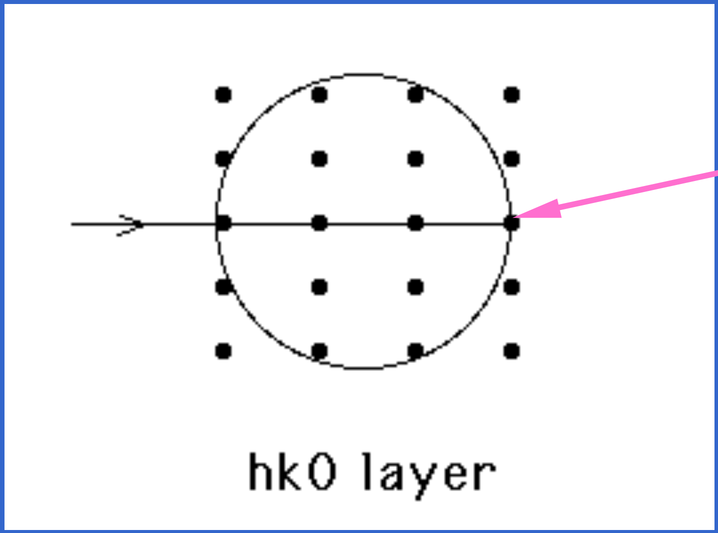
Looking down on one plane of points....
the equatorial plane:



Ewald construction

Looking down on one plane of points....
the equatorial plane

No points on sphere (here, in 2-D, a circle);
must rotate reciprocal lattice to
observe reflections.

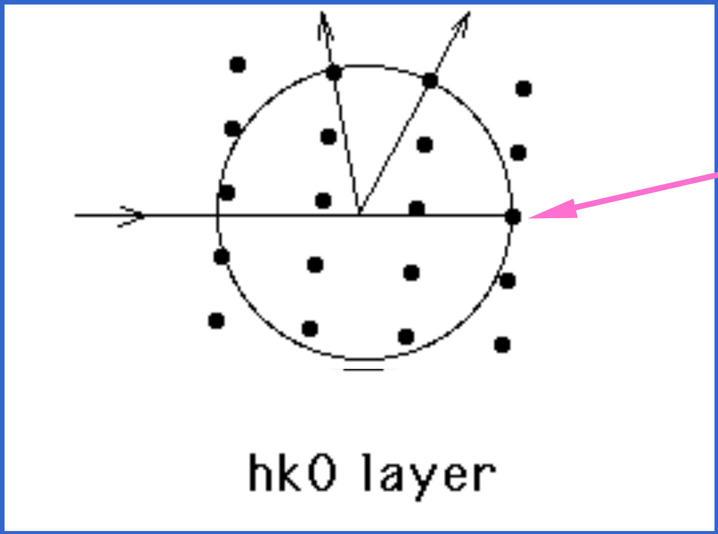


rotate around axis here,
perpendicular to screen

Ewald construction

Looking down on one plane of points....
the equatorial plane

Must rotate reciprocal lattice to
observe reflections.



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Ewald construction

Looking down on one plane of points....
the equatorial plane

Must rotate reciprocal lattice to
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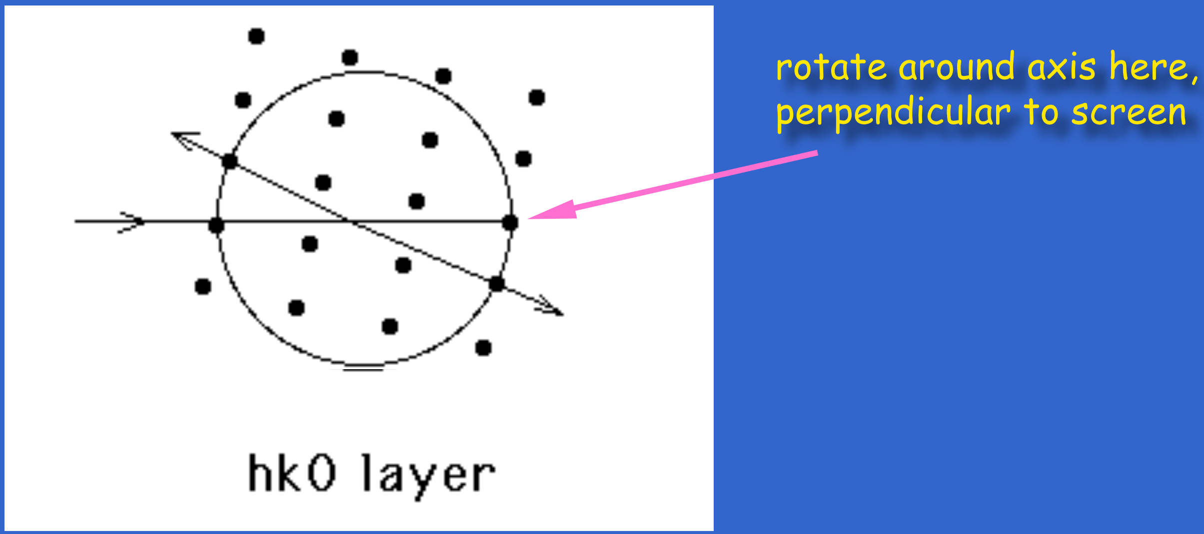

Ewald construction

Looking down on one plane of points....
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Must rotate reciprocal lattice to
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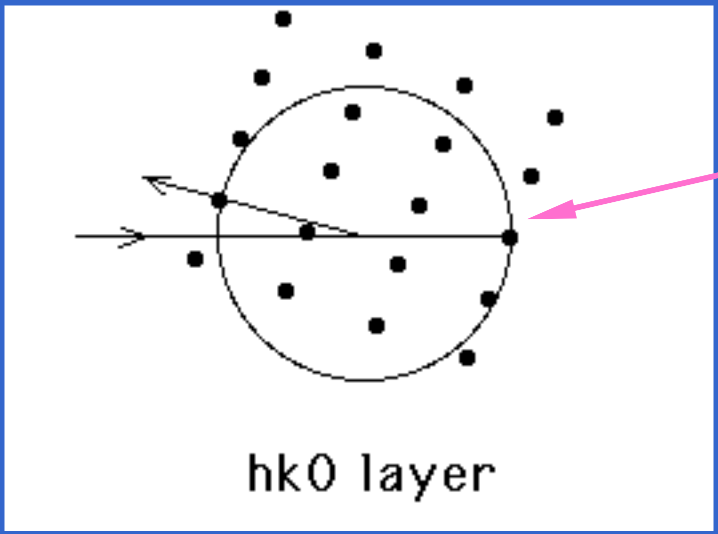
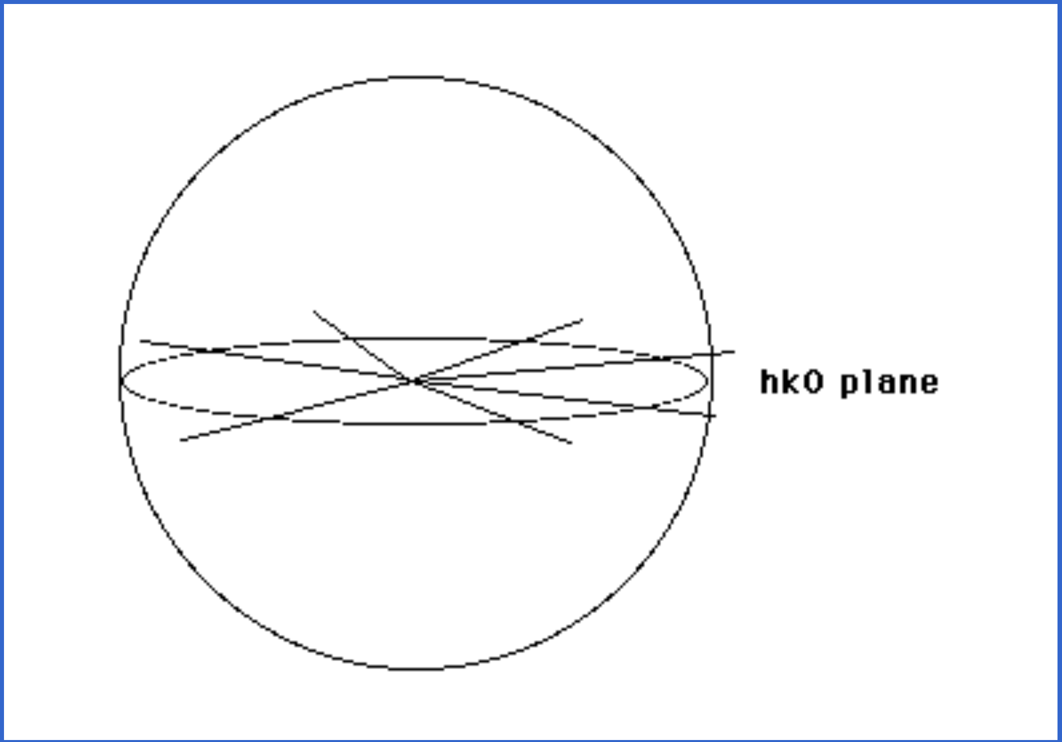


rotate around axis here,
perpendicular to screen

Ewald construction

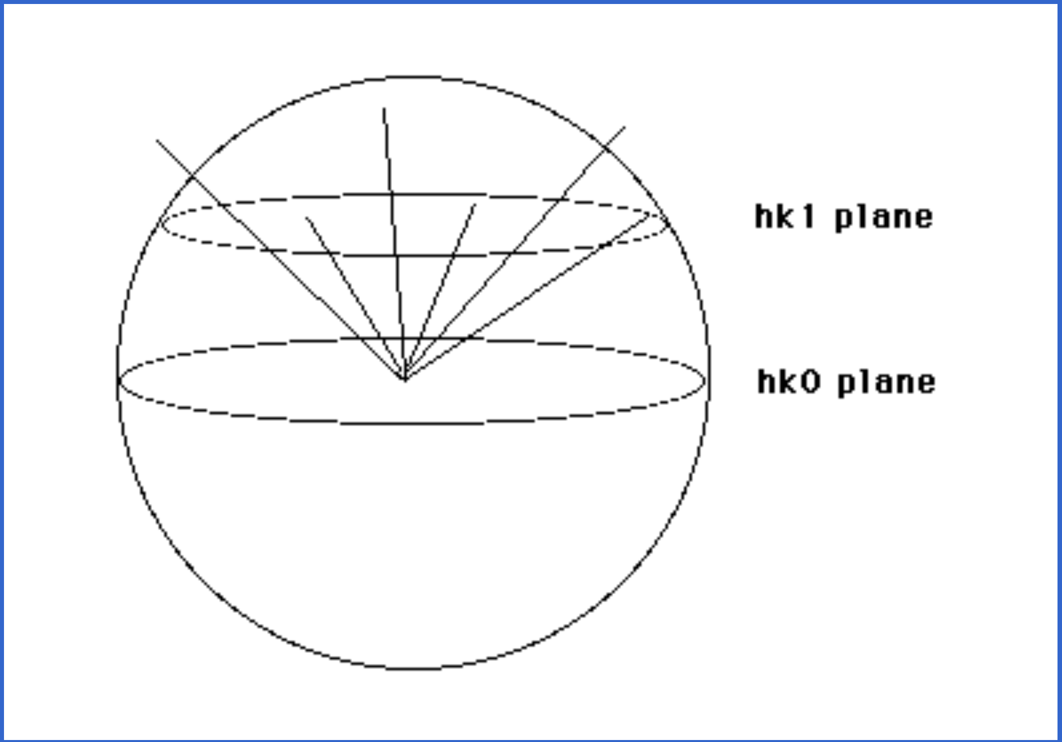
hk0 reflected rays all lie in the equatorial plane.



Ewald construction

hk0 reflected rays all lie in the equatorial plane.

hk1 reflected rays lie on a cone.



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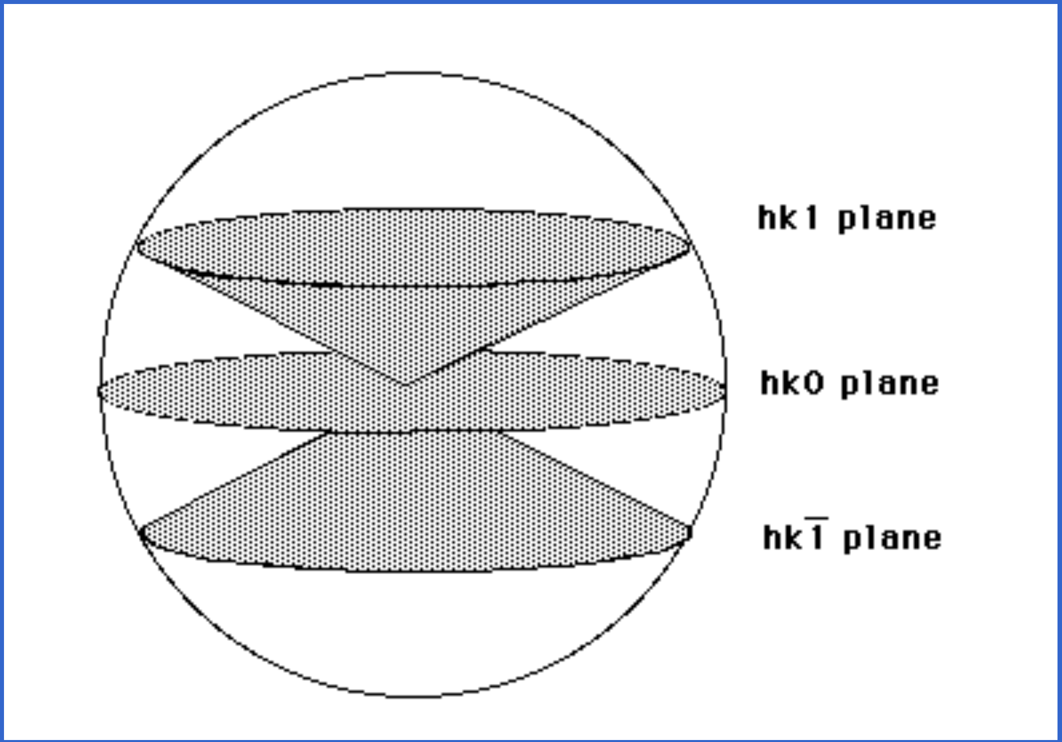
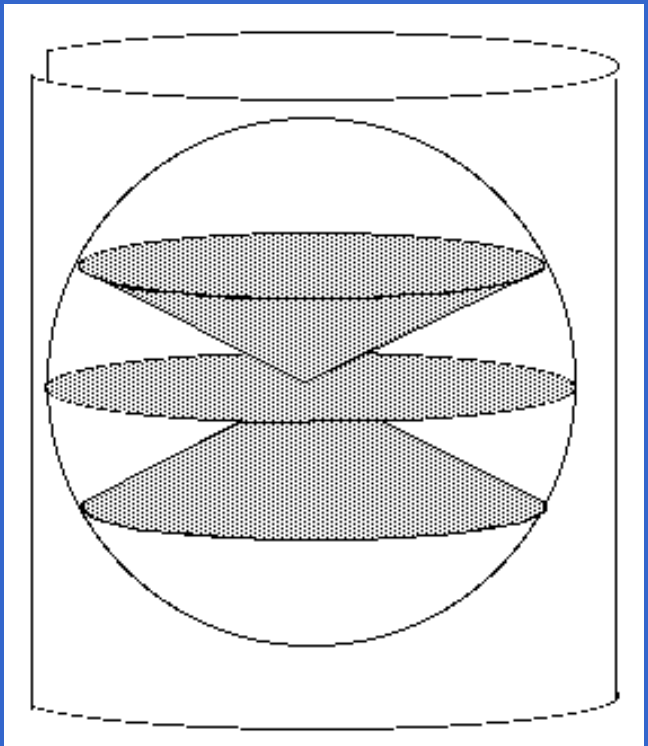


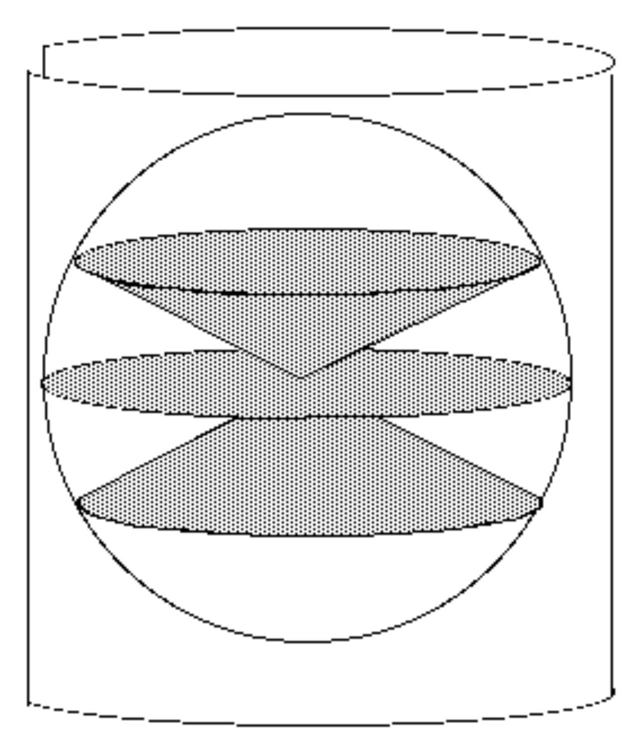
Ewald construction

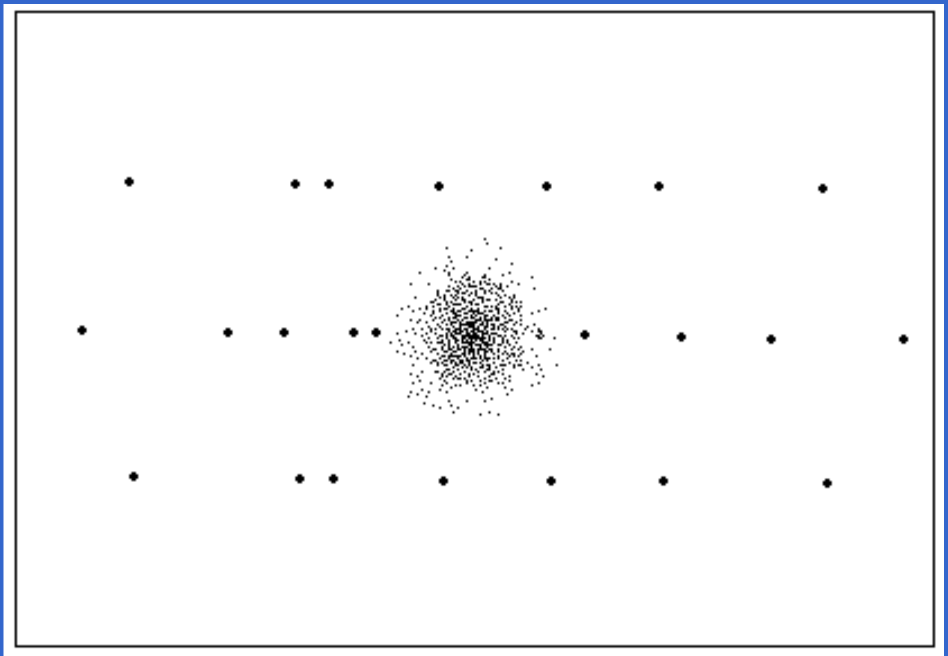
Sheet of film or image paper wrapped cylindrically around crystal....



Ewald construction

Sheet of film or image paper wrapped cylindrically around crystal.... looks like this after x-ray exposure of oscillating crystal .....when flattened:



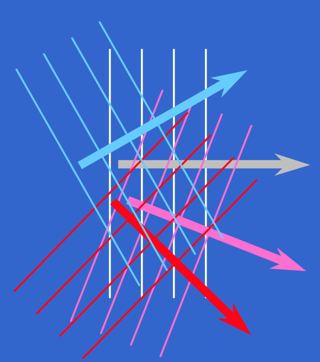


Ewald construction

To see reflections:

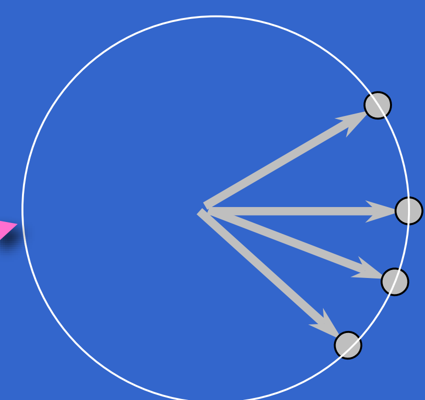
- move sphere
- move crystal
- change sphere size
- use polycrystalline sample

real space

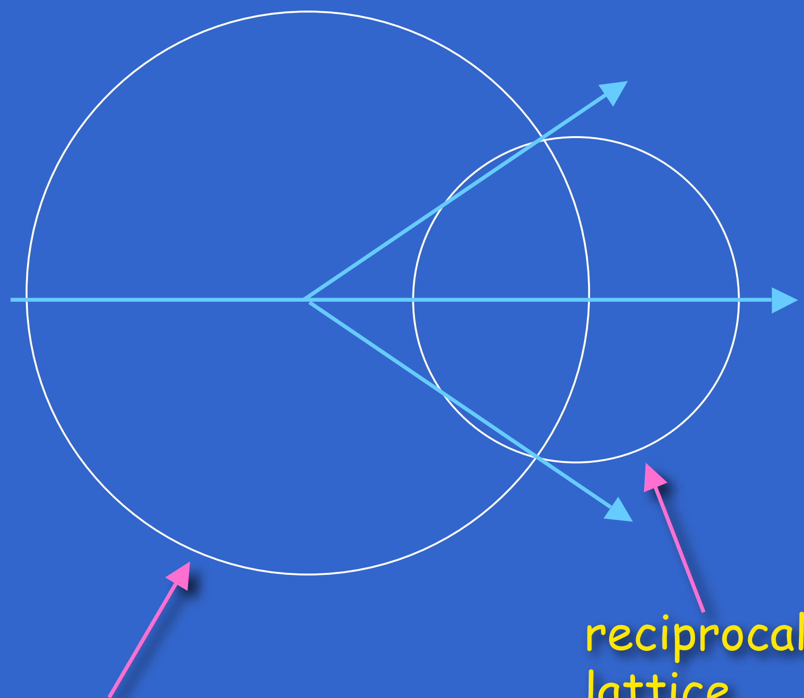


only one set of planes - one (hkl)

reciprocal space

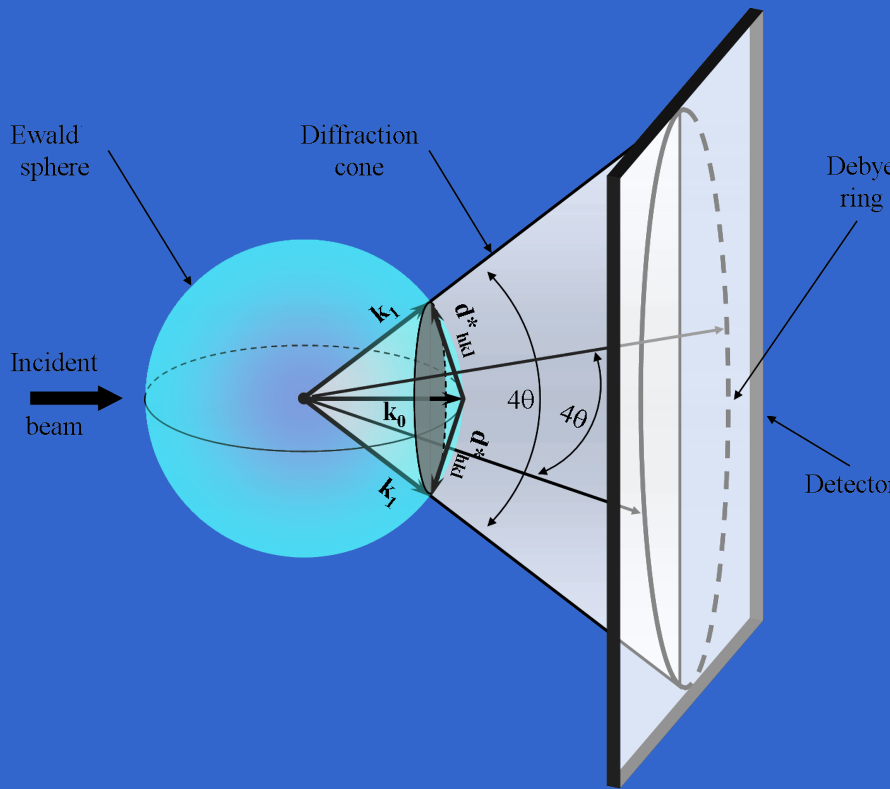


Ewald construction



Ewald sphere

reciprocal lattice representation



Ewald construction