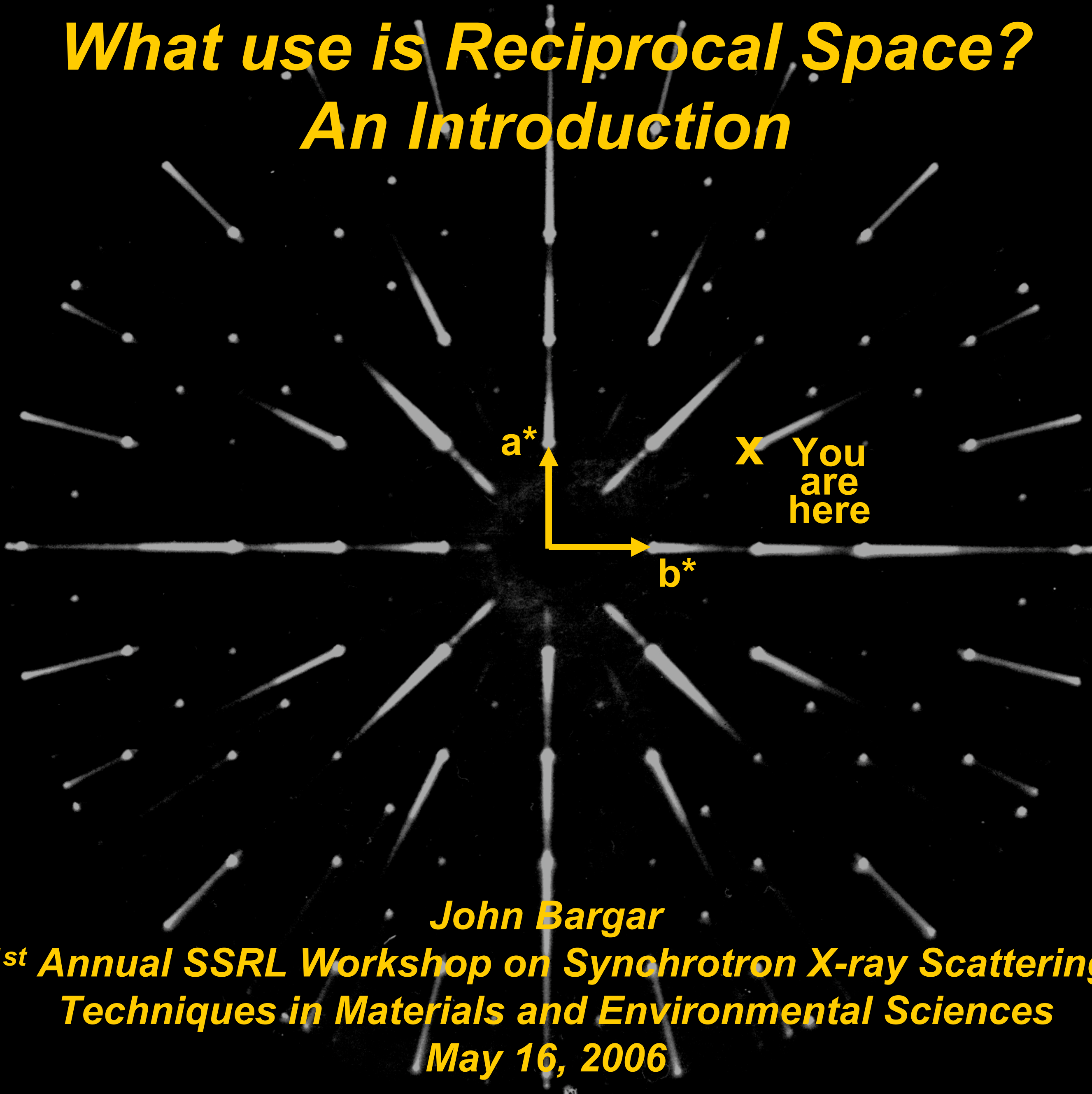
What use is Reciprocal Space? An Introduction



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1st Annual SSRL Workshop on Synchrotron X-ray Scattering Techniques in Materials and Environmental Sciences

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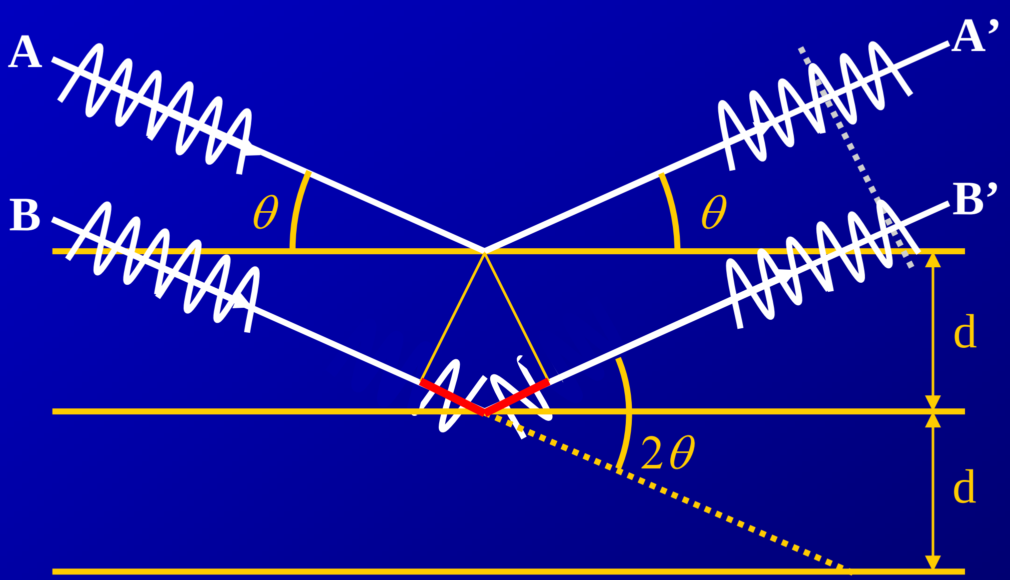
Starting from Braggs' law…

Bragg's Law:
$2d \sin \theta = n \lambda$

- Good phenomenologically
- Good enough for a Nobel prize (1915)

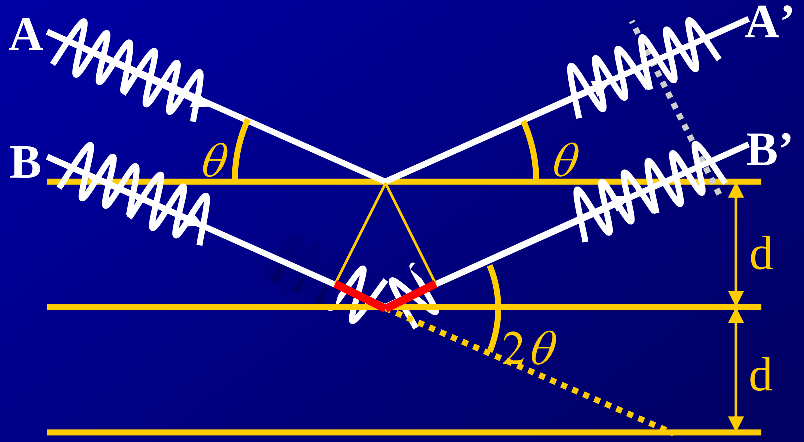


BUT…

- There are a *gabillion* planes in a crystal.
- How do we keep track of them?
- How do we know where they will diffract (single xtals)?
- What are their diffraction intensities?

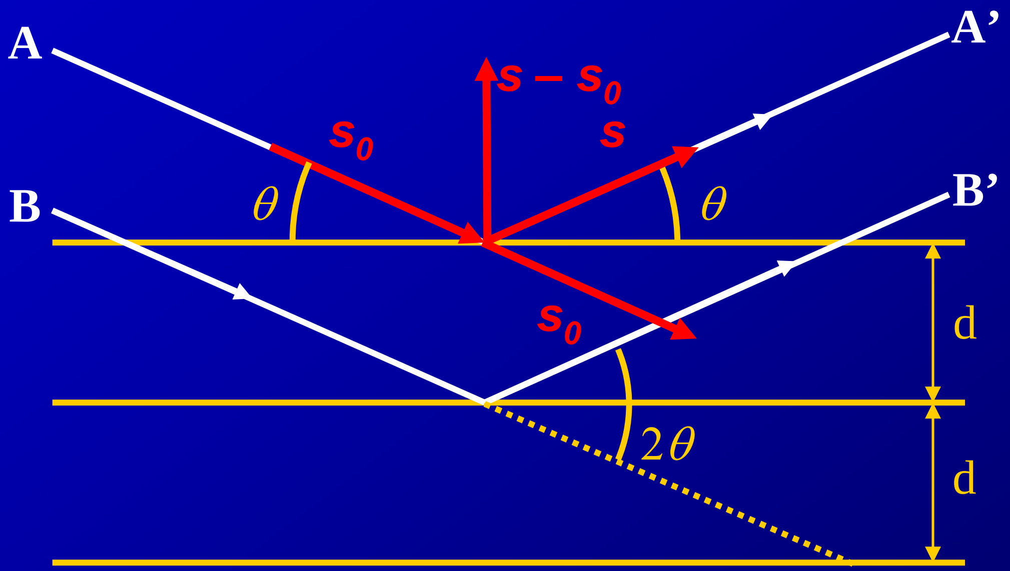
Better approach…

- Make a "map" of the diffraction conditions of the crystal.
- For example, define a map spot for each diffraction condition.
- Each spot represents kajillions of parallel atomic planes.
- 3-D map.
- ***Such a map would provide a facile and convenient way to describe the relationships between planes in a crystal*** – a considerable simplification of a messy and redundant problem.



Start again from diffracting planes…

Define unit vectors $\boldsymbol{s_0}$, $\boldsymbol{s}$



- Notice that $|\boldsymbol{s}-\boldsymbol{s_0}| = 2\text{Sin}\theta$
- Substitute in Bragg's law…

$\lambda/d = 2\text{Sin}\theta$…

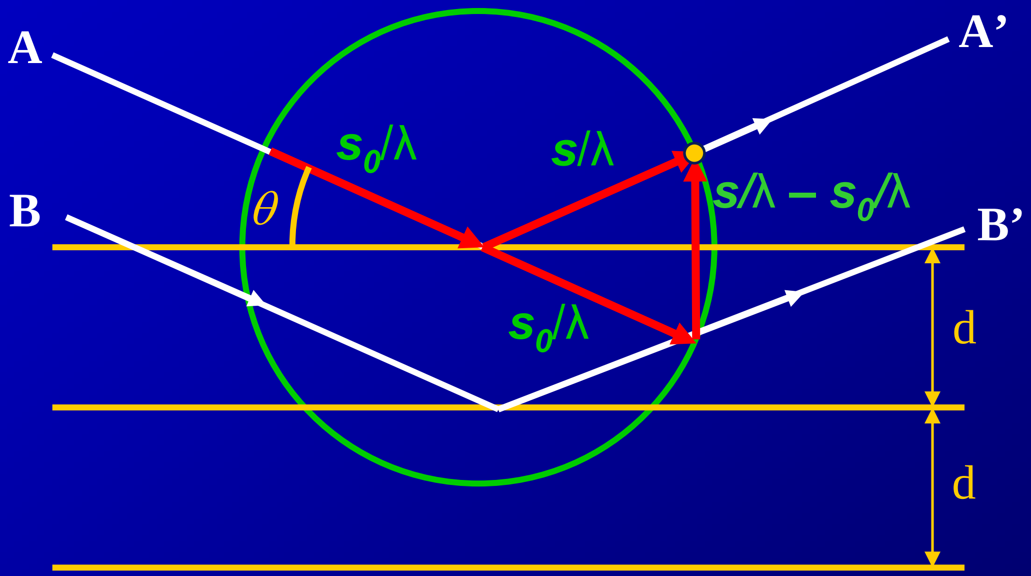
Diffraction occurs when

$|\boldsymbol{s}-\boldsymbol{s_0}| = \lambda/d$

To use Bragg's law in 3D…

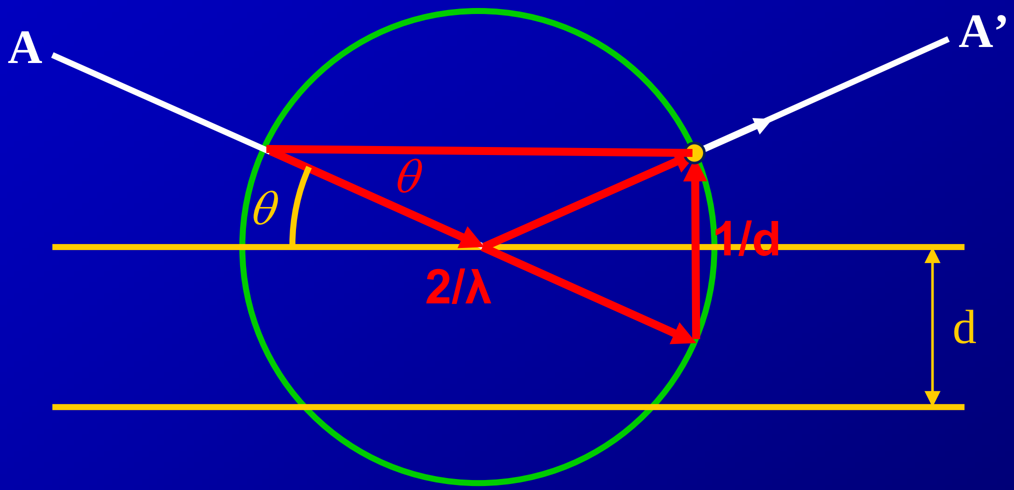
Divide by λ…

- Divide s, s_0 by λ… $(|\boldsymbol{s}\text{-}\boldsymbol{s_0}|)/\lambda = 1/d = 2\mathrm{Sin}\theta/\lambda$
- Define a "map point" at end of $\boldsymbol{s}\text{-}\boldsymbol{s_0}/\boldsymbol{\lambda}$
- Graphical representation of Bragg's law can be obtained by drawing a circumscribing circle of radius 1/λ around vectors…



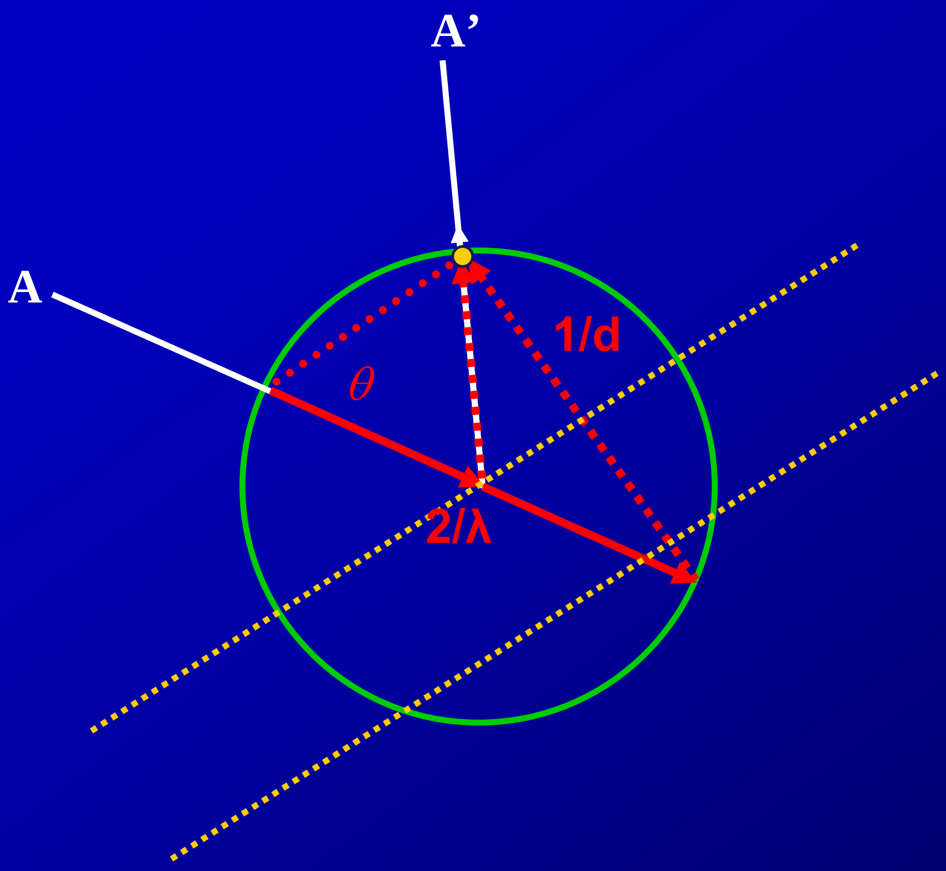
Graphical Representation of Bragg's Law

- Bragg's law is obeyed for any triangle inscribed within the circle: $\sin\theta = (1/d)/(2/\lambda)$
- Note, sample "sits" at center of circle.



Ewald Sphere

- Bragg's law is obeyed for any triangle inscribed within the circle: Sinθ = (1/d)/(2/λ)



Bragg's law is satisfied and diffraction occurs only when map point intersects circle.

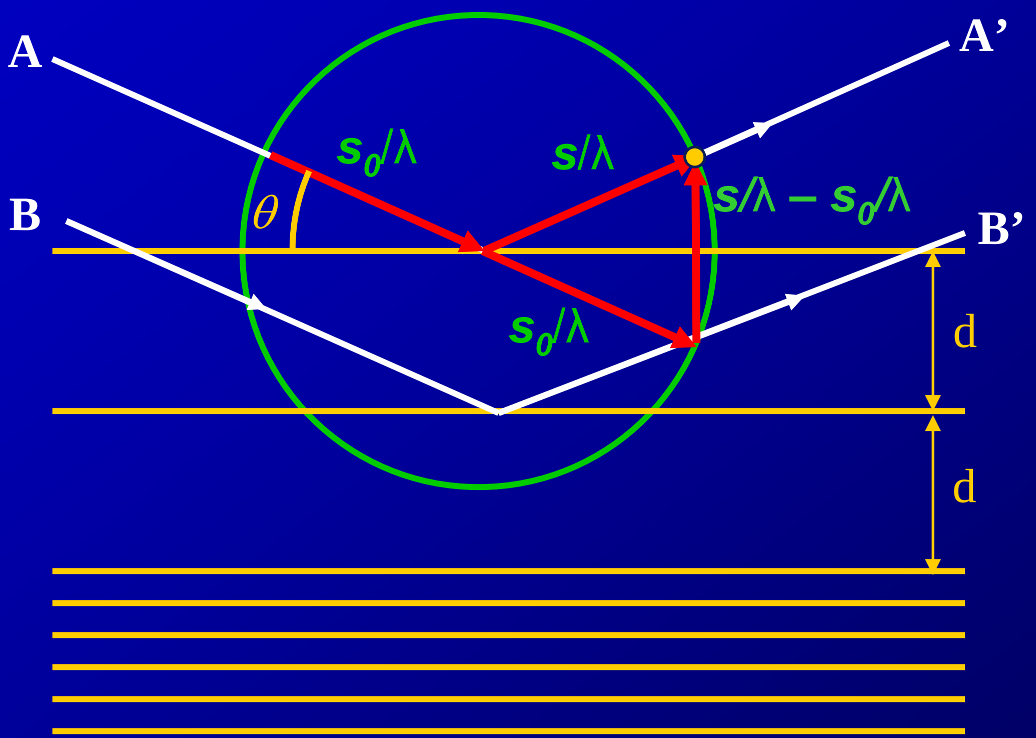
The diffracted beam passes through the map point.

In 3D, circle becomes ***Ewald Sphere***, has units of Å^{-1}. Map points define *a* ***reciprocal lattice***.

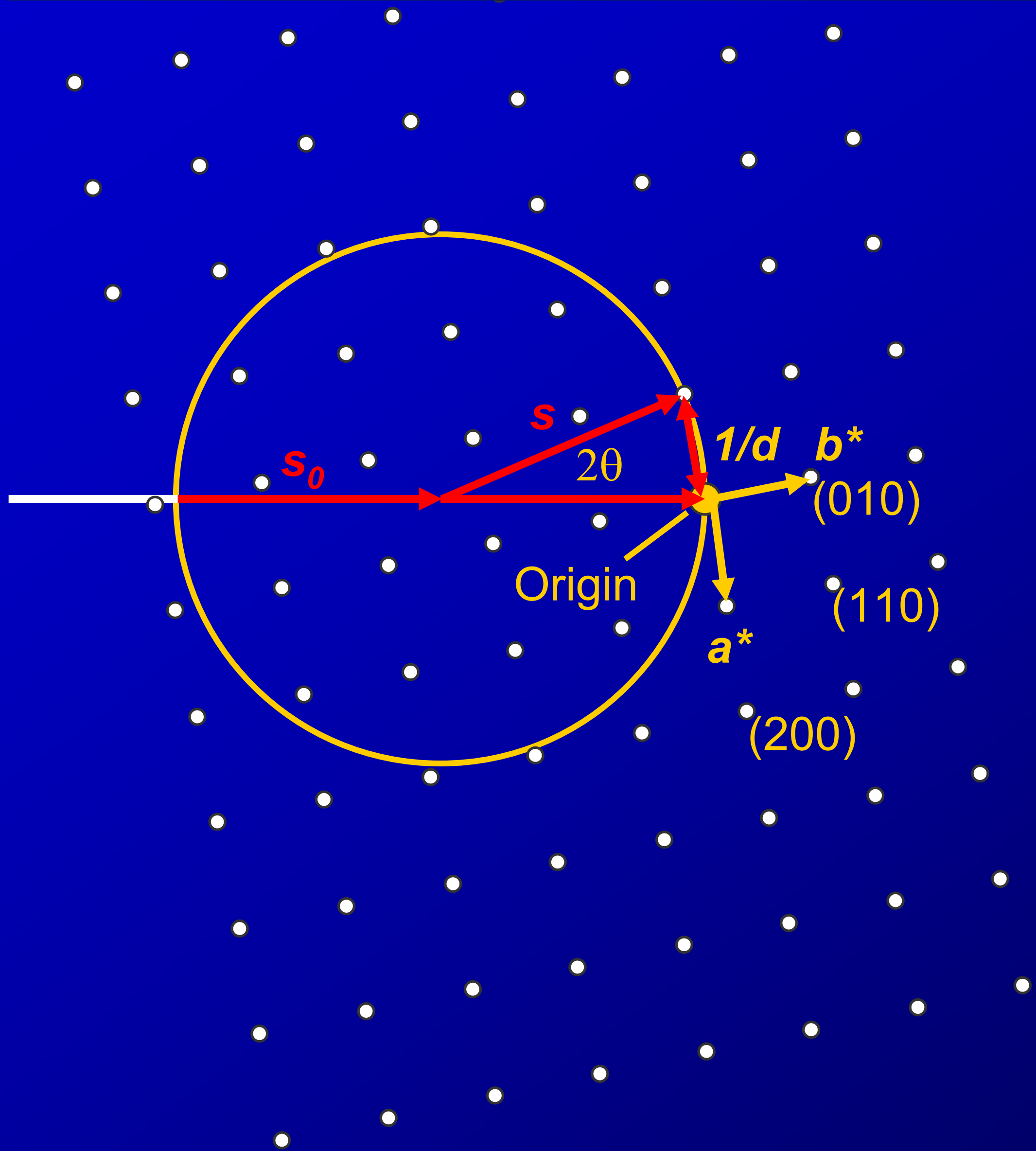
Vector representation carries Bragg's law into 3D.

Families of planes become points!

Single point now represents ***all planes in all unit cells of the crystal*** that are parallel to the crystal plane of interest and have same d value.



Thus, the RECIPROCAL LATTICE is obtained



Distances between origin and RL points give 1/d.

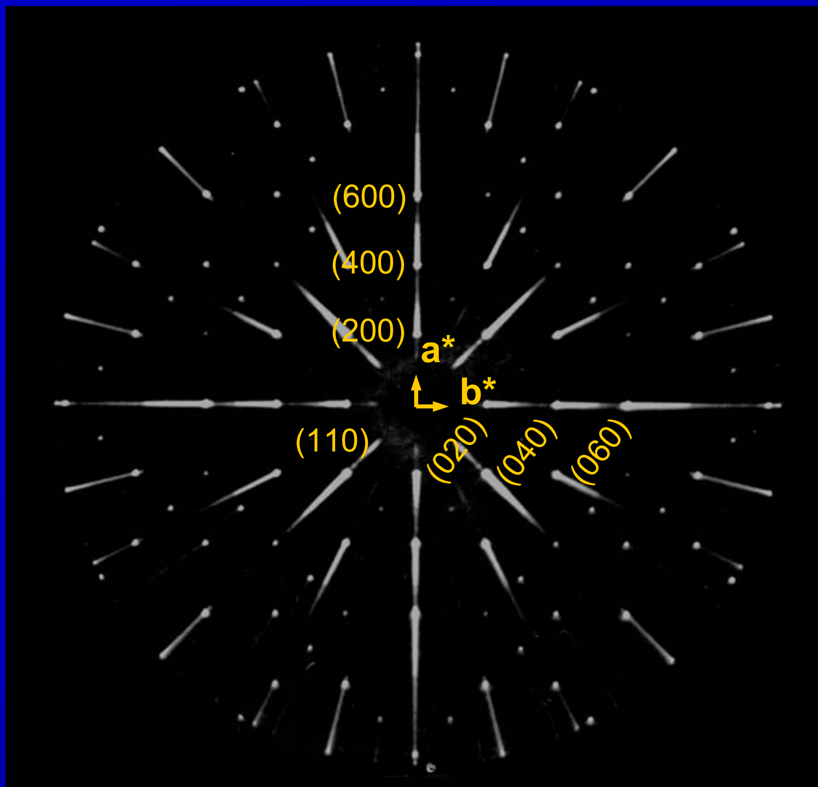
Reciprocal Lattice Axes:
a* normal to a-b plane
b* normal to a-c plane
c* normal to b-c plane

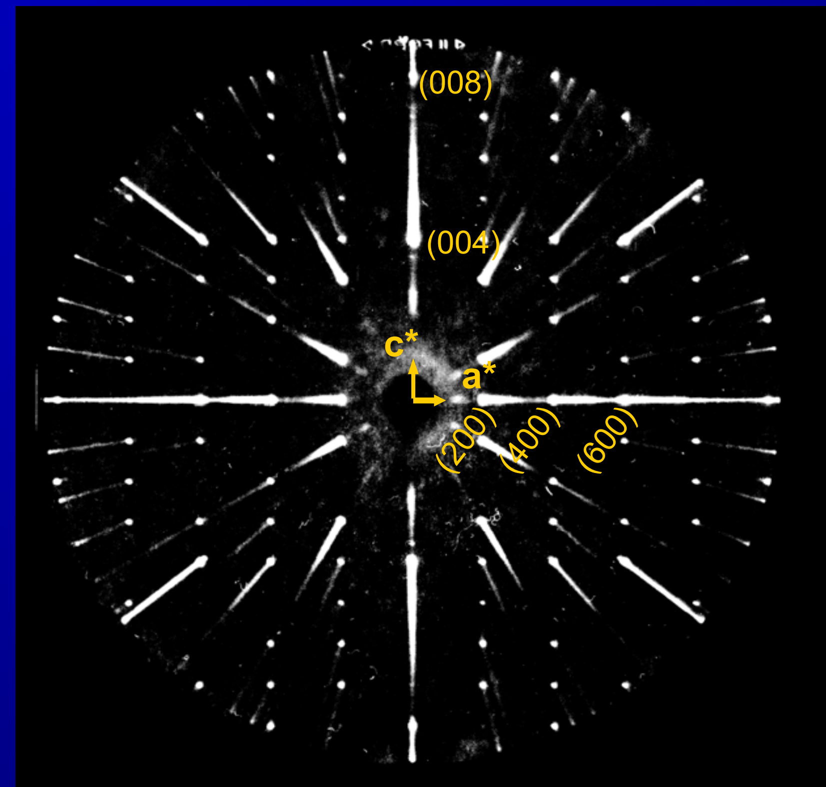
Index RL points based upon axes

Each point represents ***all*** parallel crystal planes. Eg., ***all*** planes parallel to the a-c plane are captured by (010) spot.

Families of planes become points!

Reciprocal Lattice of γ-$LiAlO_2$





Projection along c: *hk*0 layer
Note 4-fold symmetry

Projection along b: *h*0*ℓ* layer

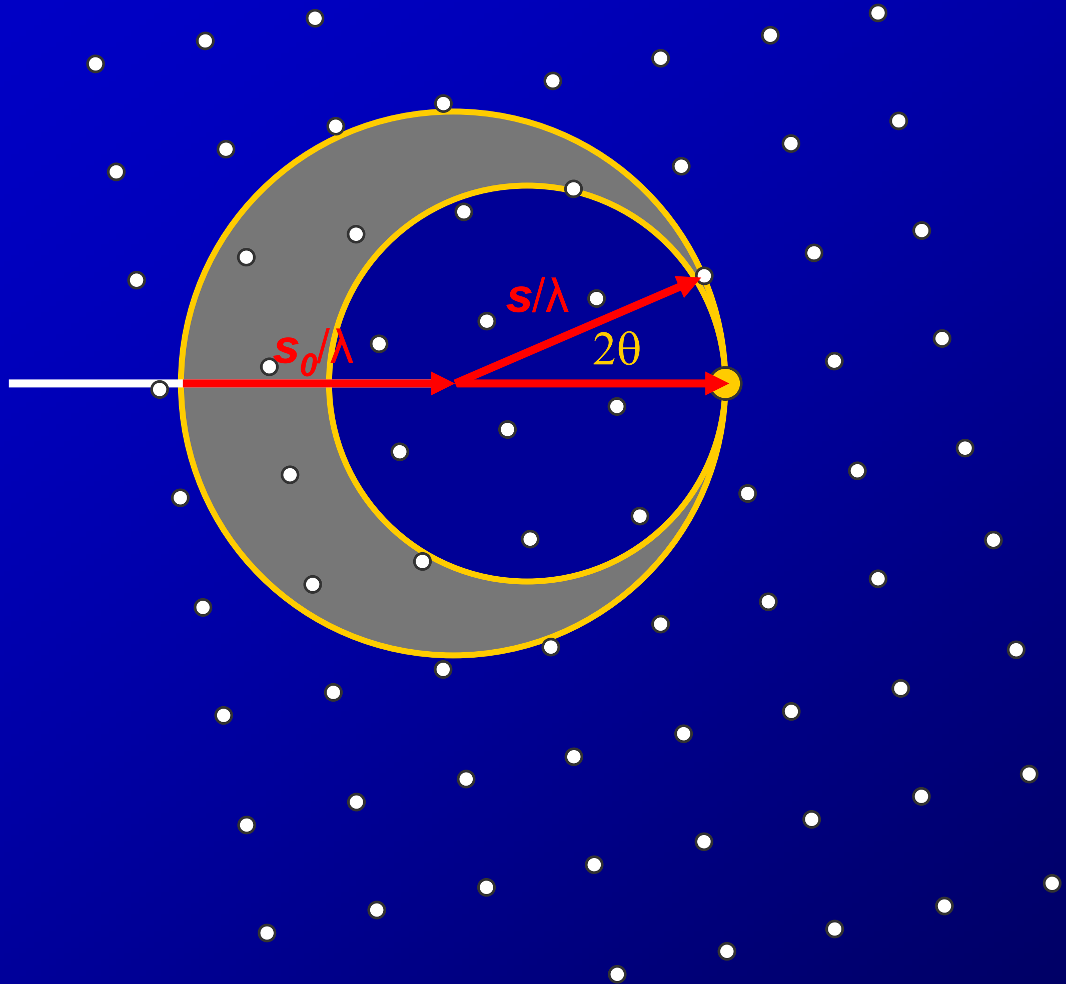
a = b = 5.17 Å; c = 6.27 Å; $P4_12_12$ (tetragonal)

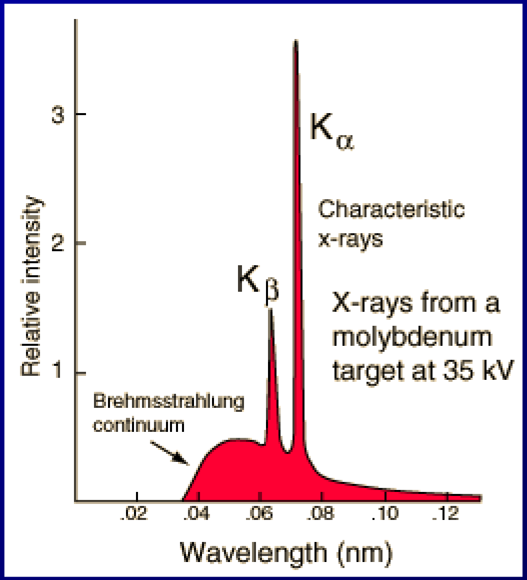
a* = b* = 0.19 $Å^{-1}$; c* = 0.16 $Å^{-1}$

general systematic absences (00ℓn; ℓ≠4), ([2n-1]00)

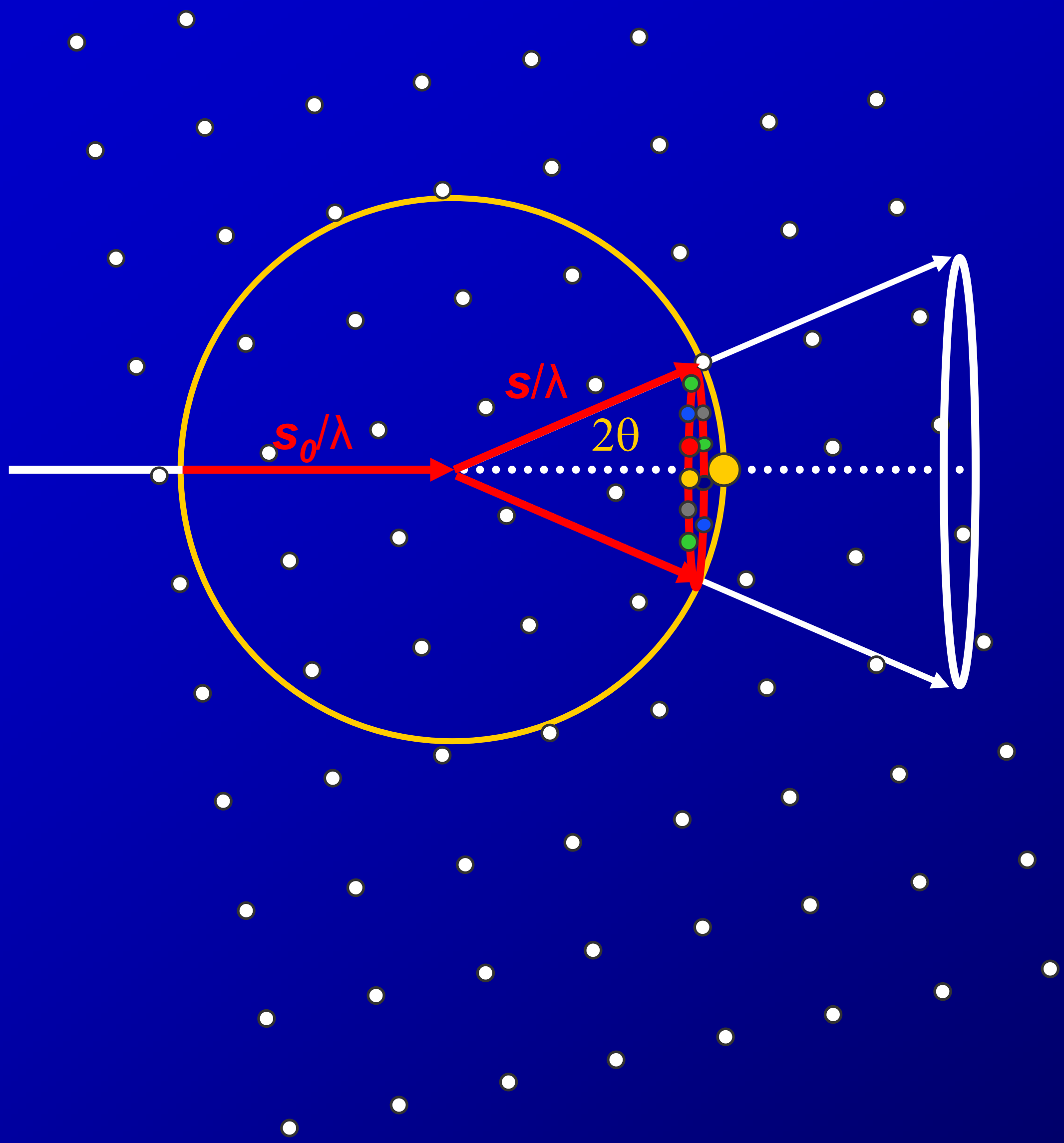
Streaking is caused by finite width of Ewald sphere;

Tube-source contains large energy range due to high-energy bremsstrahlung radiation





In a powder, orientational averaging produces rings instead of spots



OUTLINE

I. *What is the reciprocal lattice?*

1. Bragg's law.
2. Ewald sphere.
3. Reciprocal Lattice.

II. *How do you use it?*

4. Types of scans:

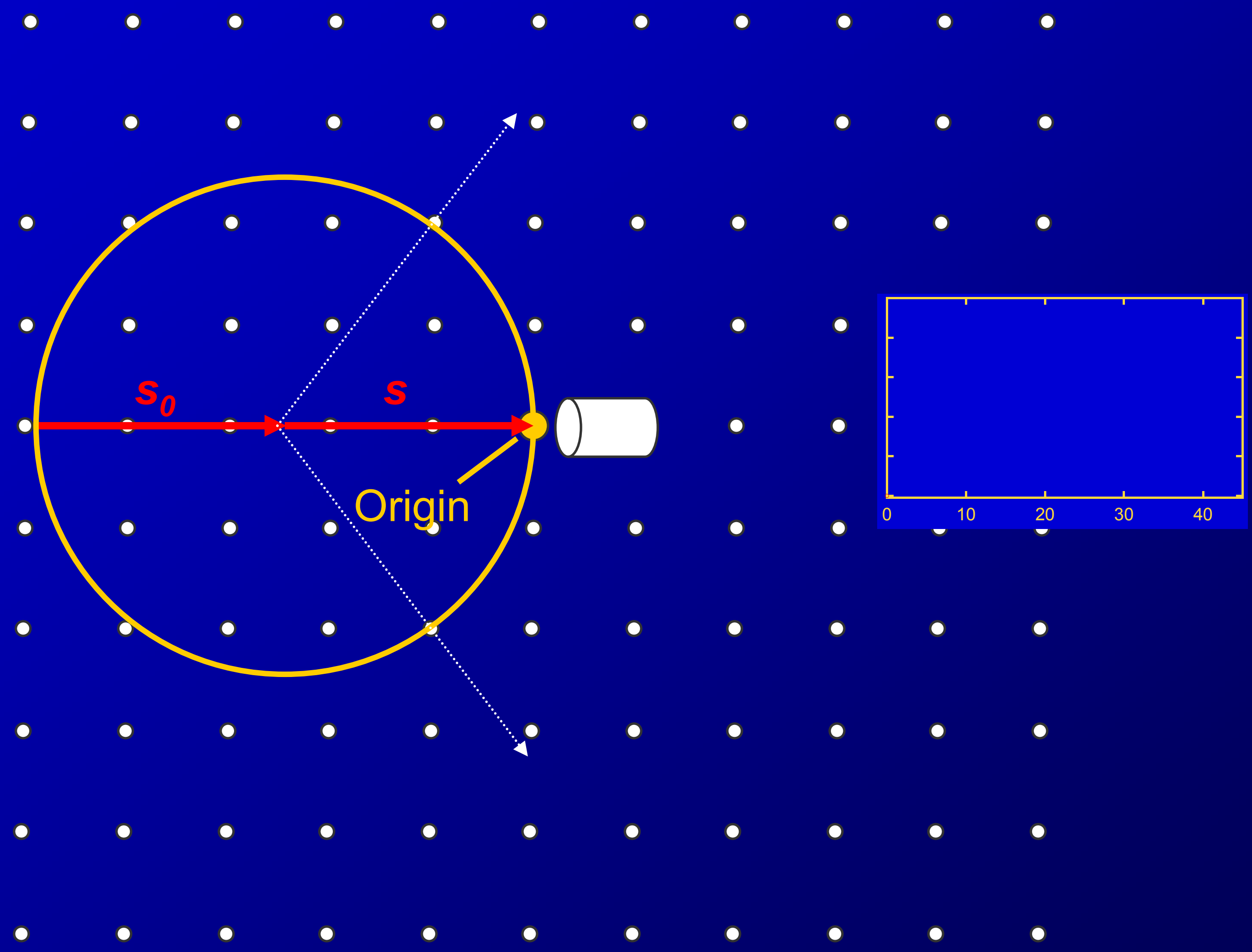
   Longitudinal or θ-2θ,

   Rocking curve scan

   Arbitrary reciprocal space scan

1. Longitudinal or θ-2θ scan

Sample moves on θ, Detector follows on 2θ



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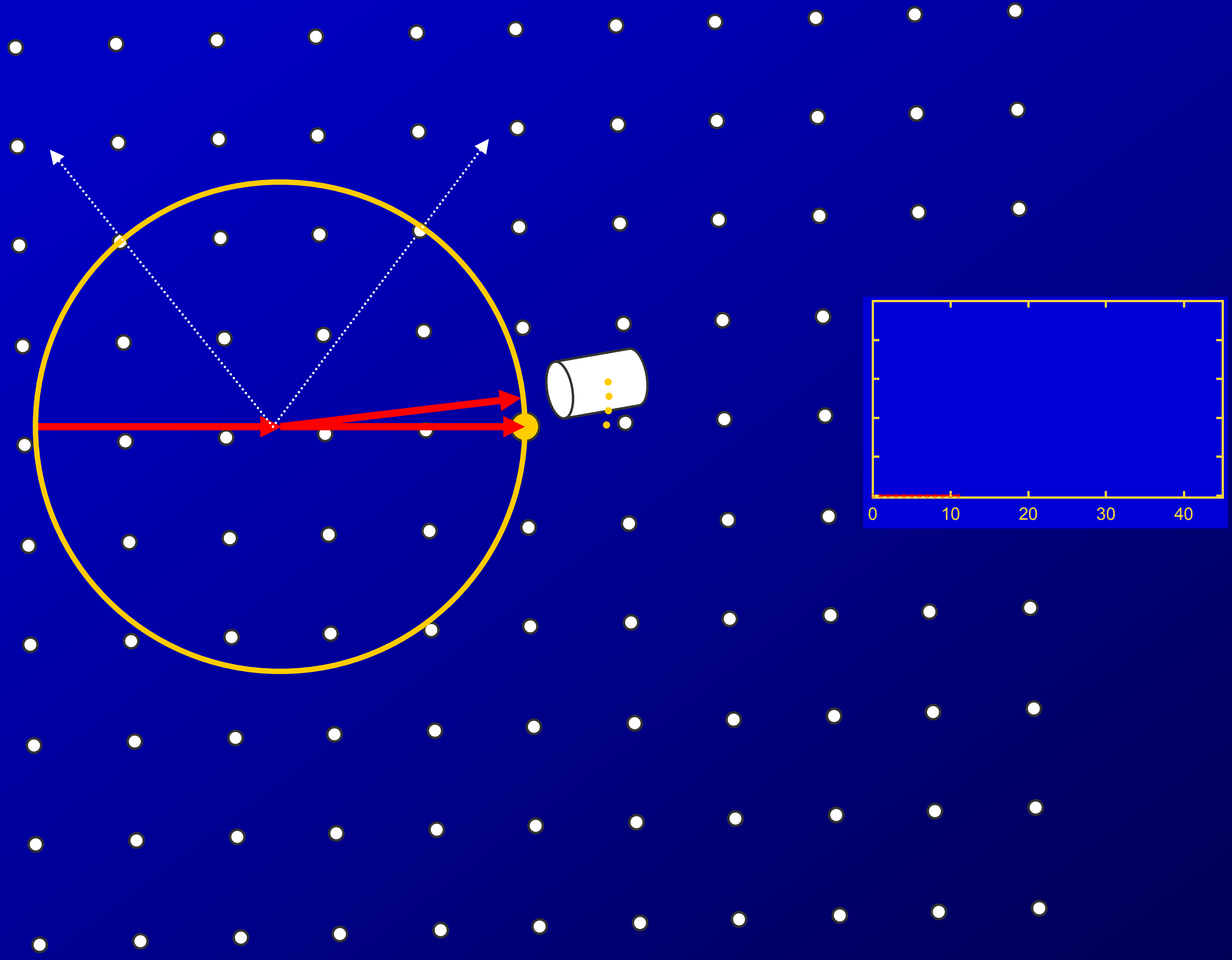

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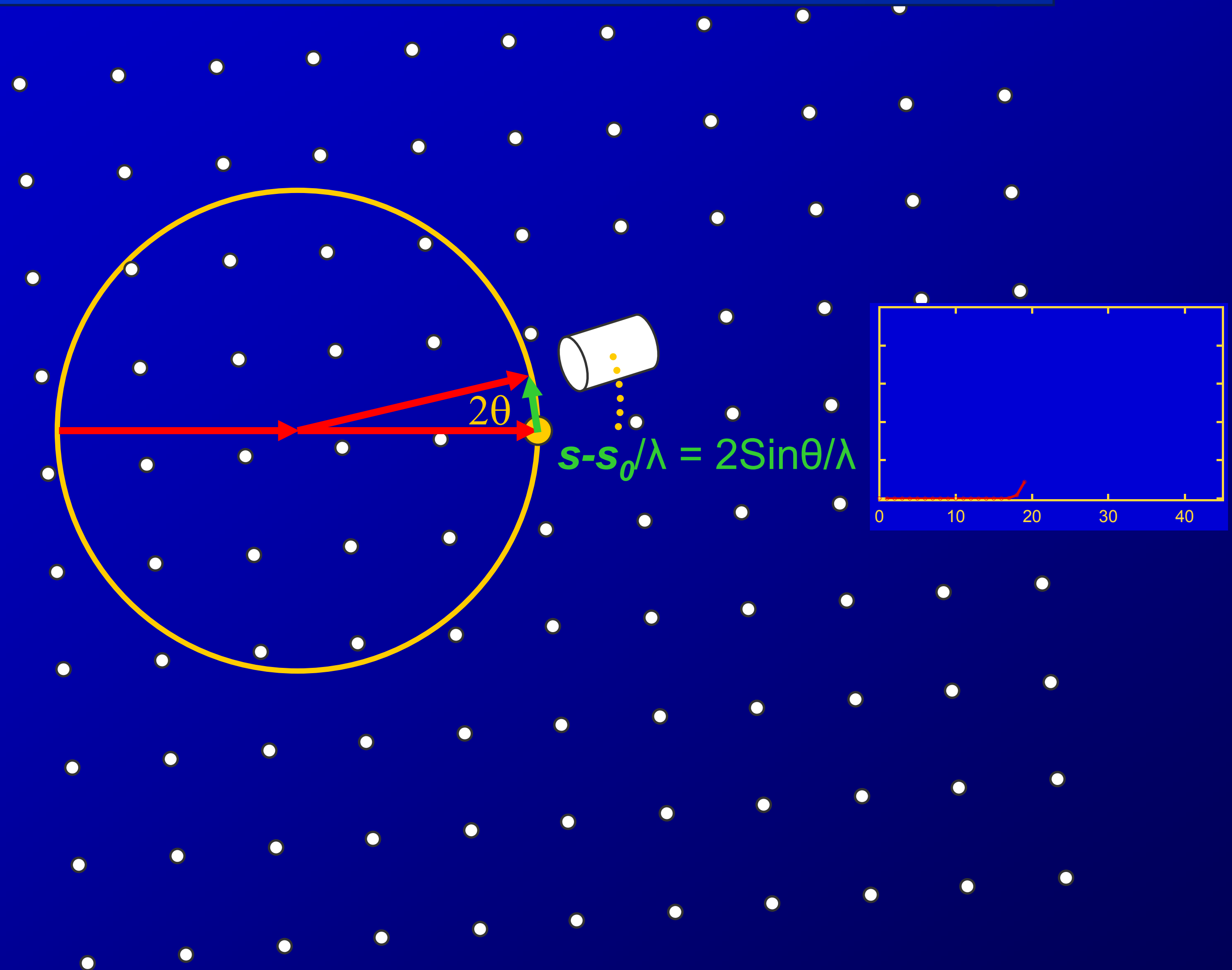

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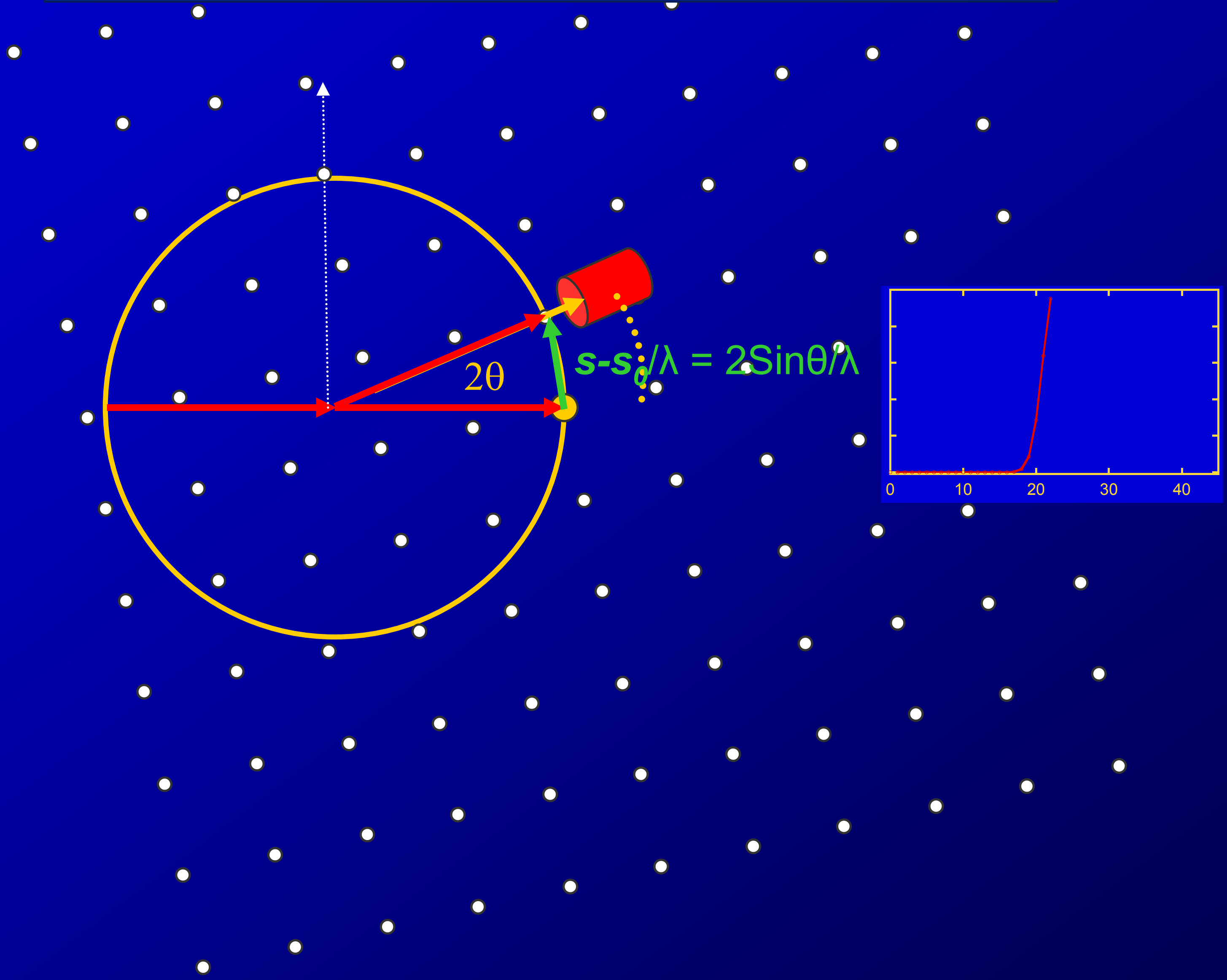

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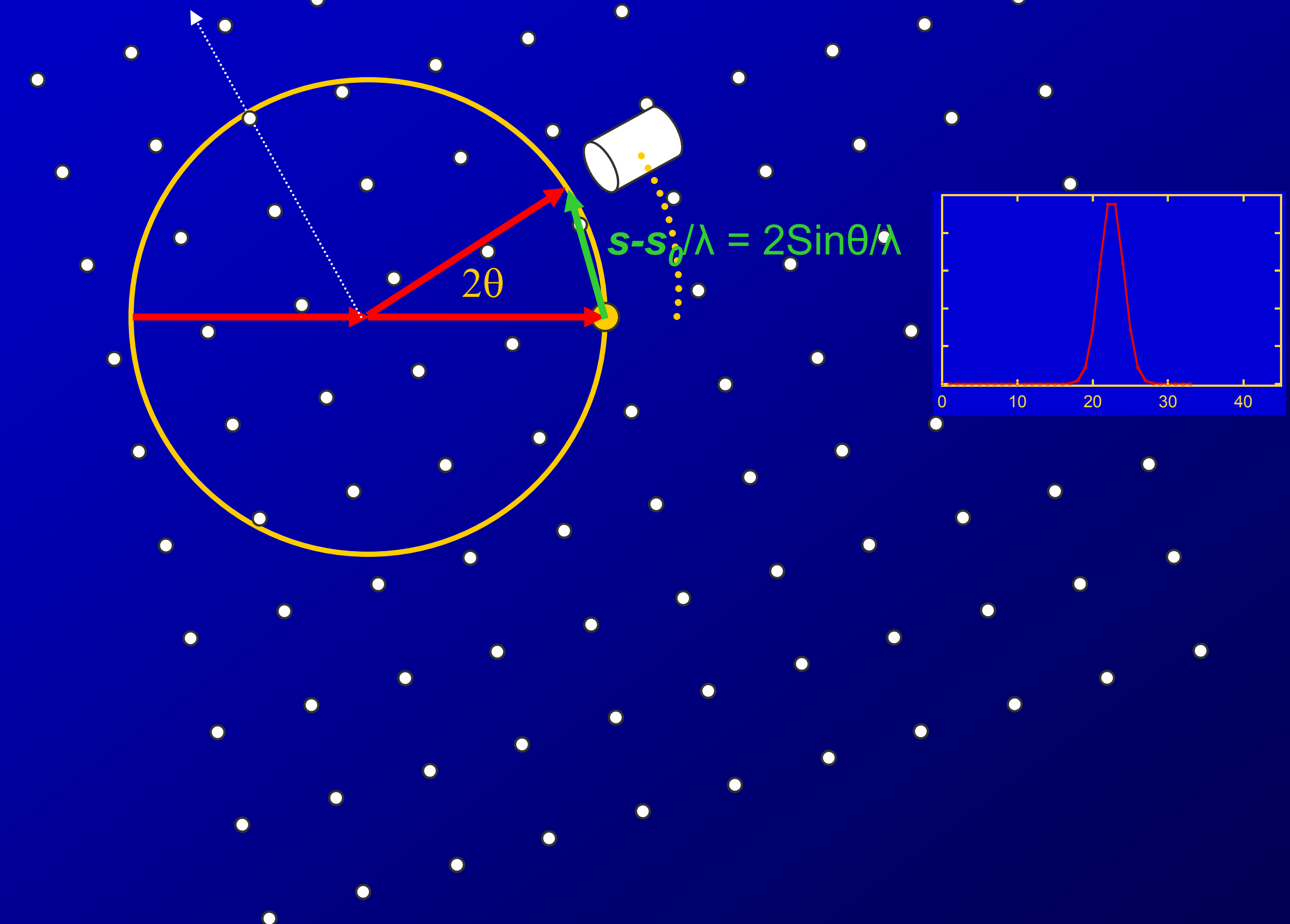

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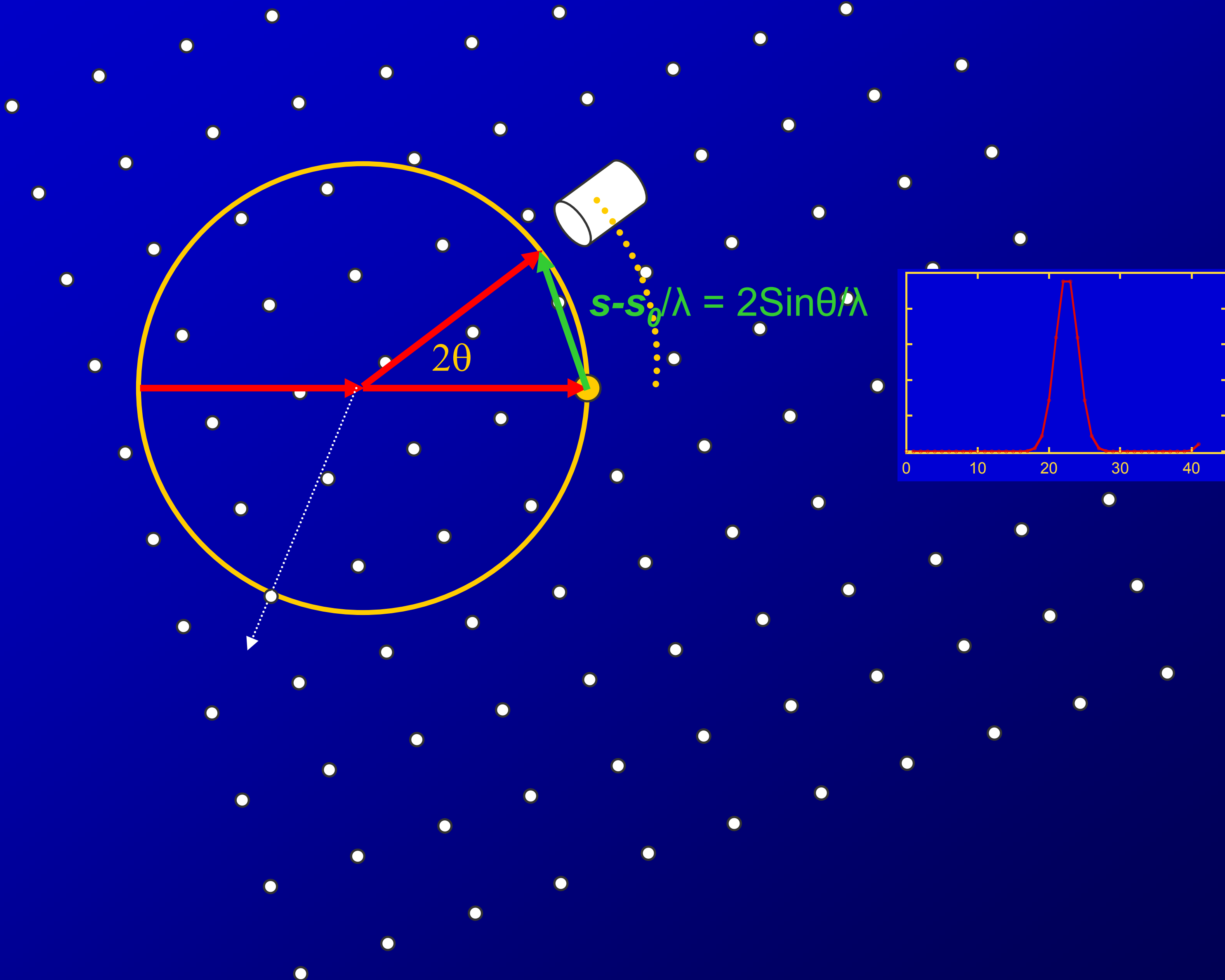

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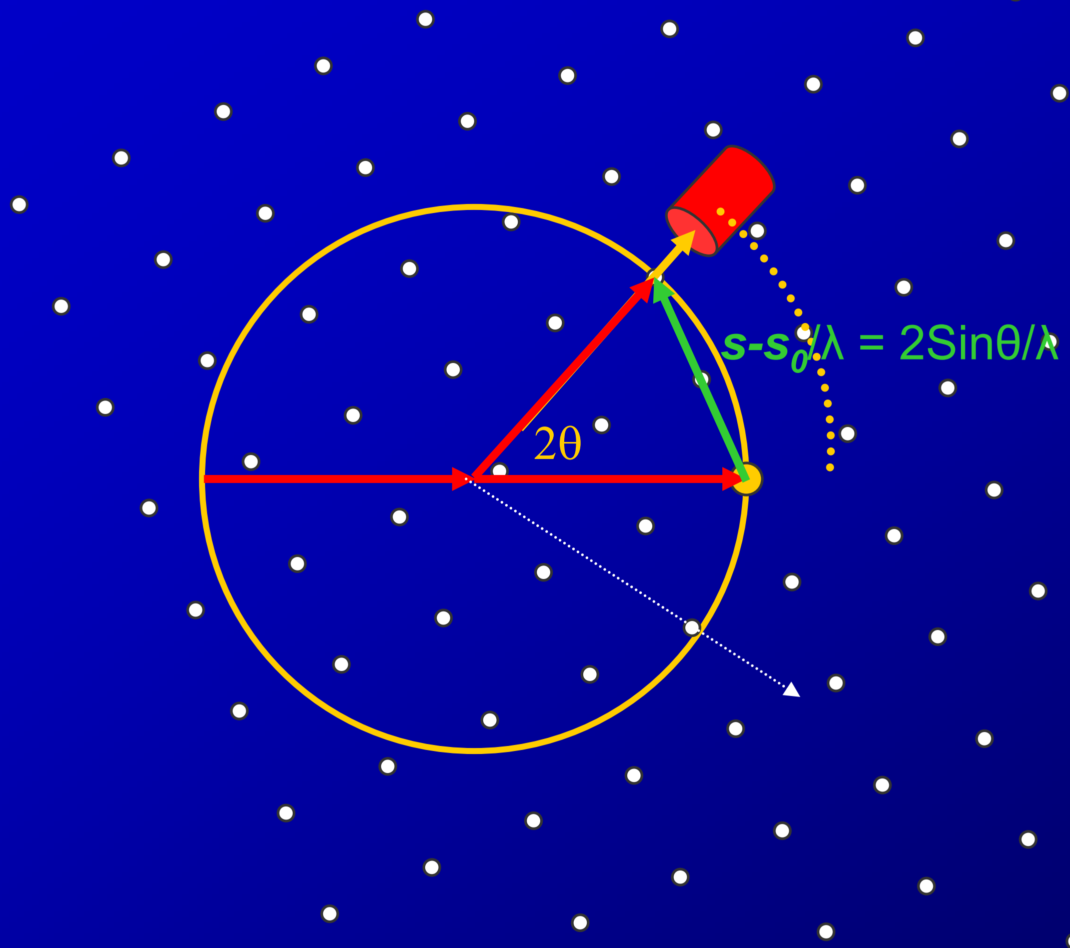
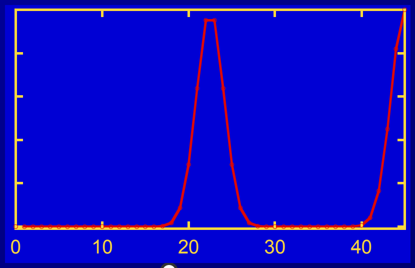


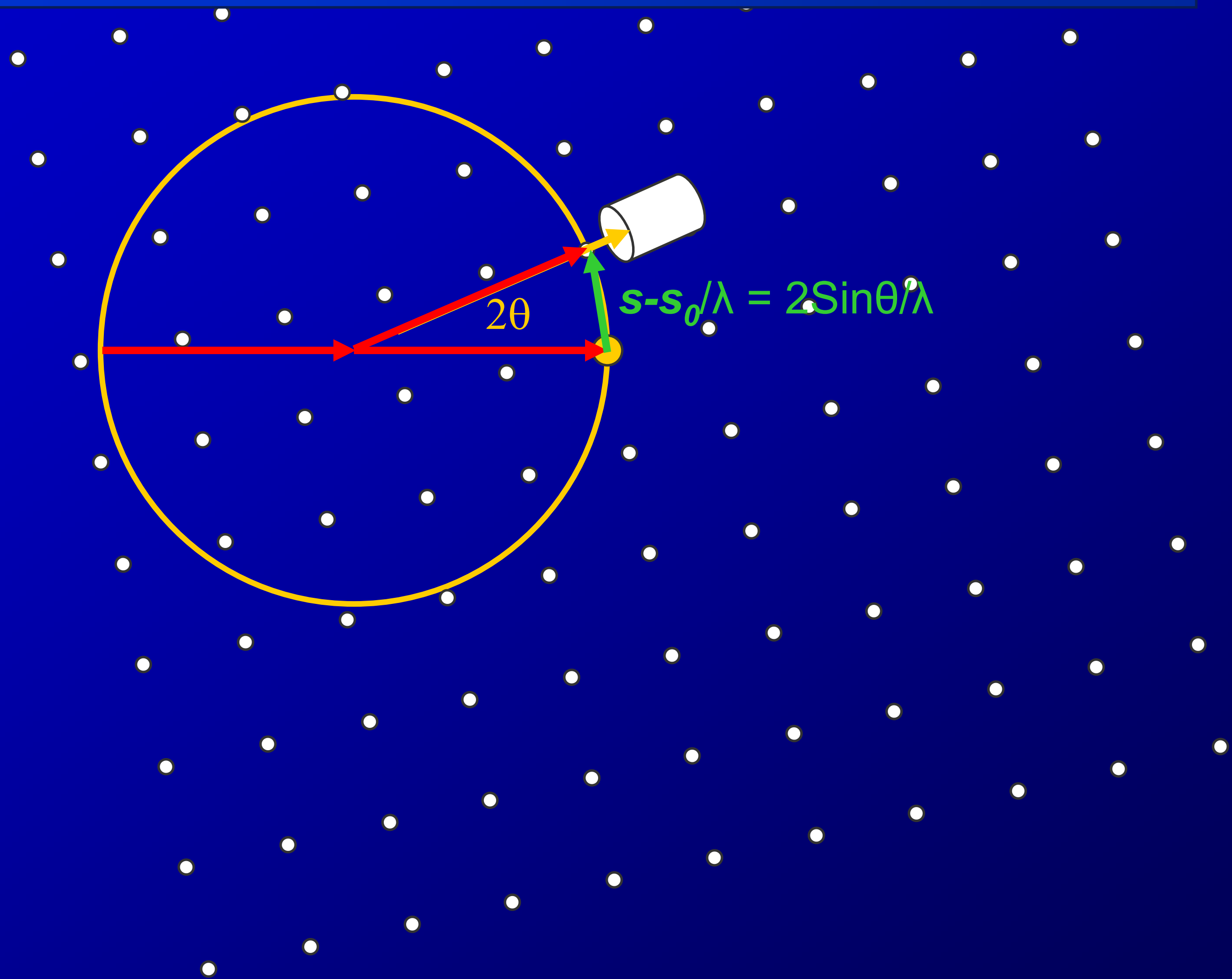


- Note scan is linear in units of Sinθ/λ - *not θ*!
- Provides information about relative arrangements, angles, and spacings between crystal planes.

2. Rocking Curve scan

Sample moves on θ, Detector fixed

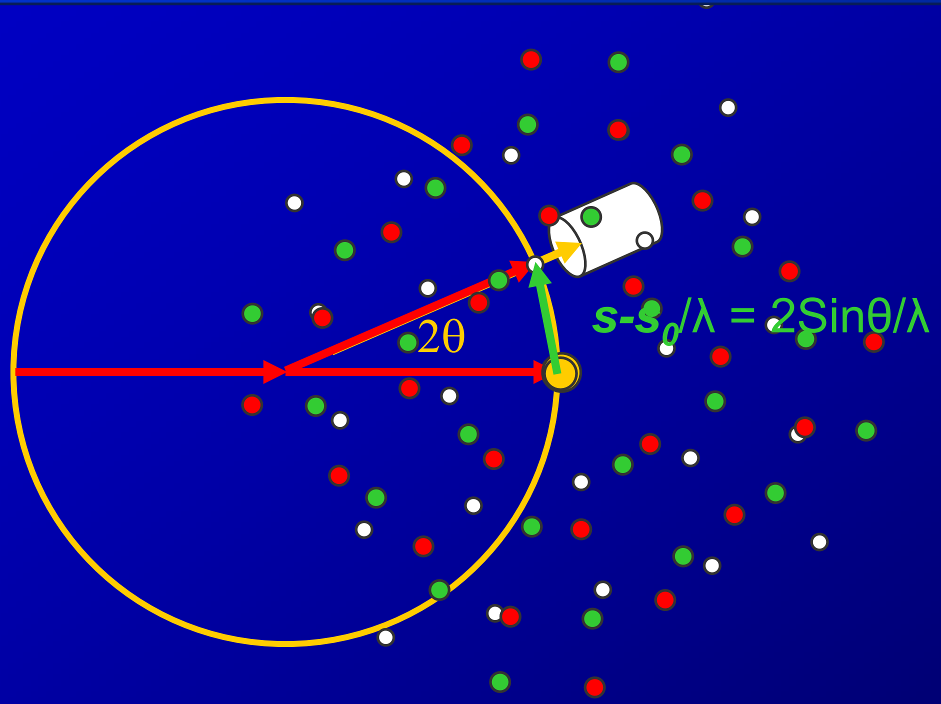
Provides information on sample mosaicity. Tells about quality of orientation



2. Rocking Curve scan

Sample moves on θ, Detector fixed

Provides information on sample mosaicity & quality of orientation



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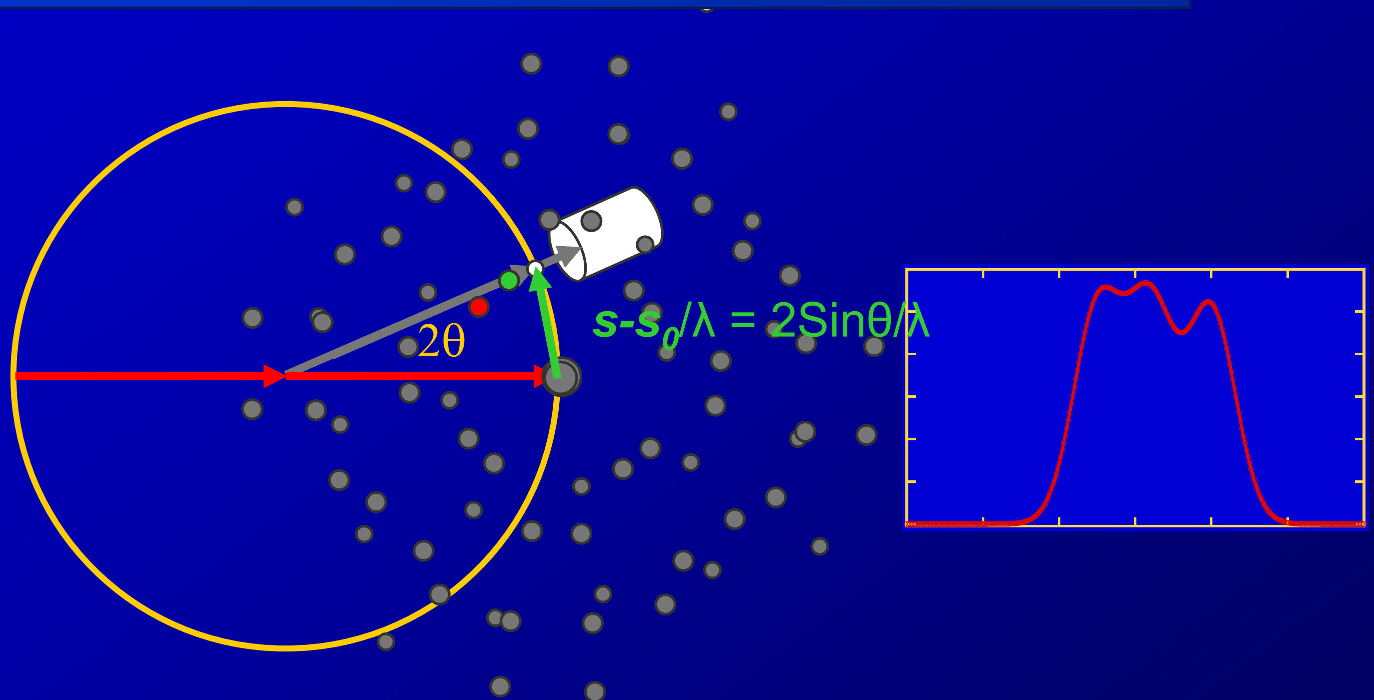
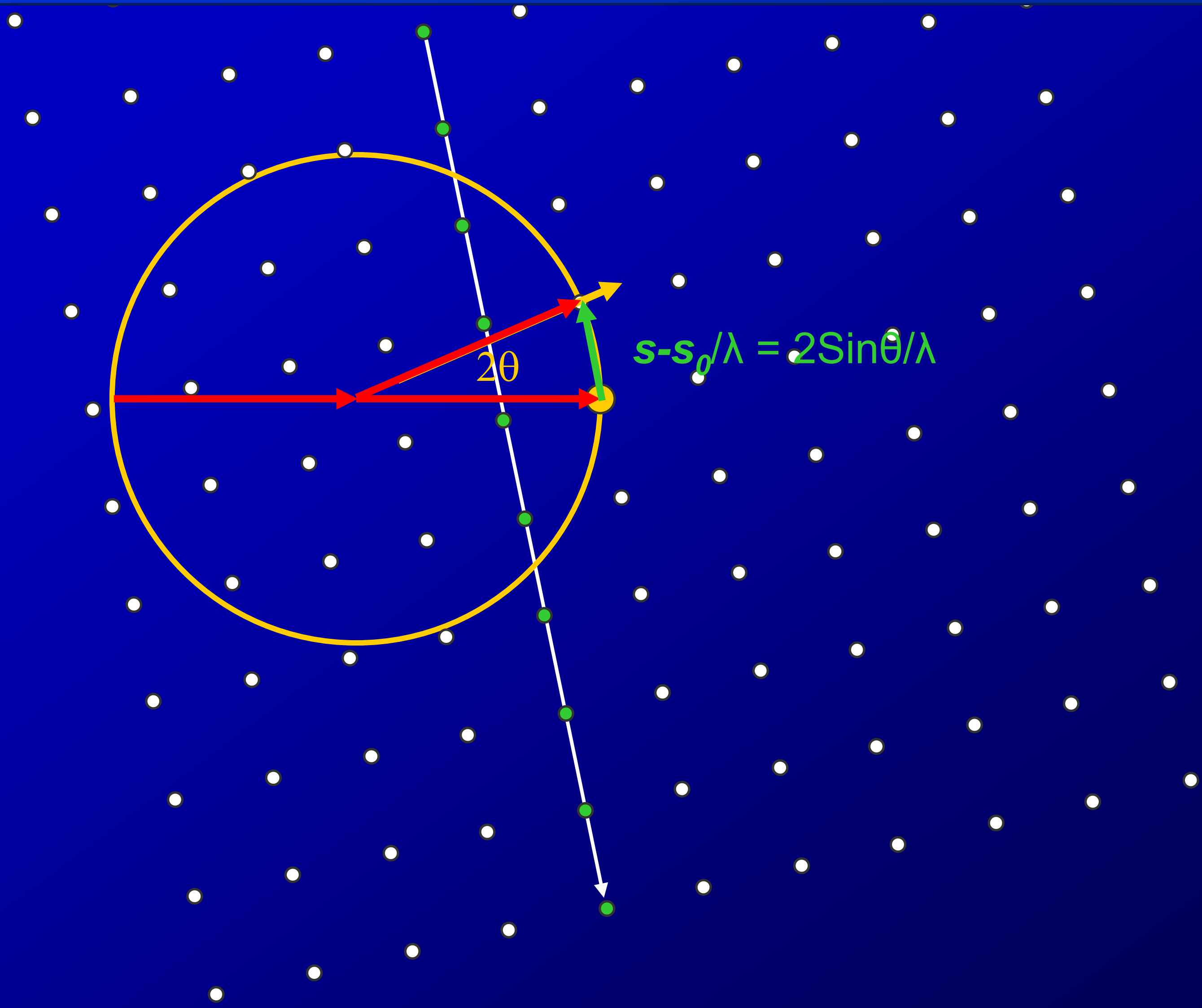


3. Arbitrary Reciprocal Lattice scans

Choose path through RL to satisfy experimental need, e.g., CTR measurements

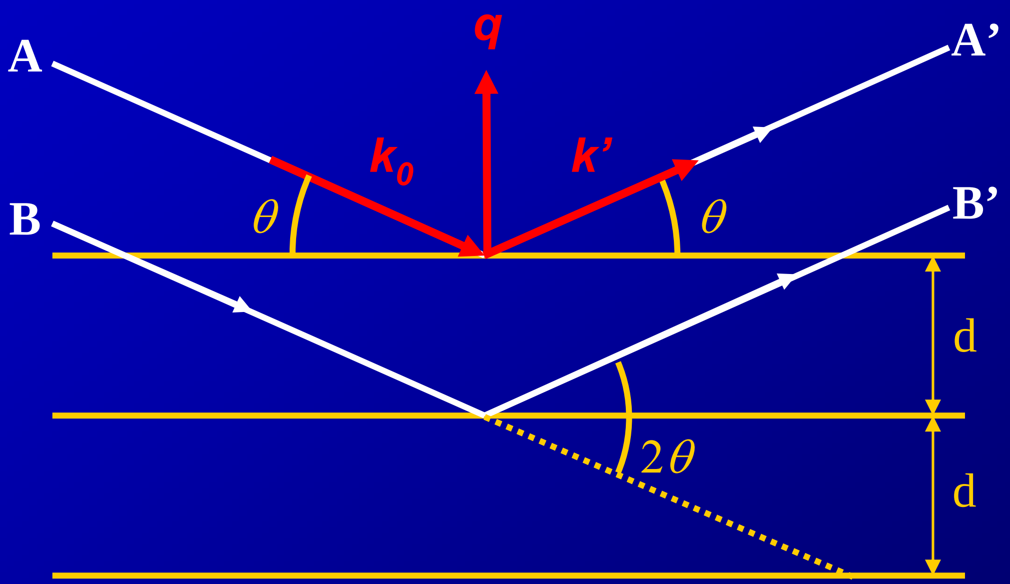


A note about "q"

In practice ***q*** is used instead of ***s-s₀***

|***q***| = |***k'-k₀***| = 2π * |***s-s₀***|

$$|\boldsymbol{q}| = 4\pi \sin\theta/\lambda$$




~~The End~~
The Beginning…