What Does a Scattering Pattern Tell Us?

7th X-ray Scattering School

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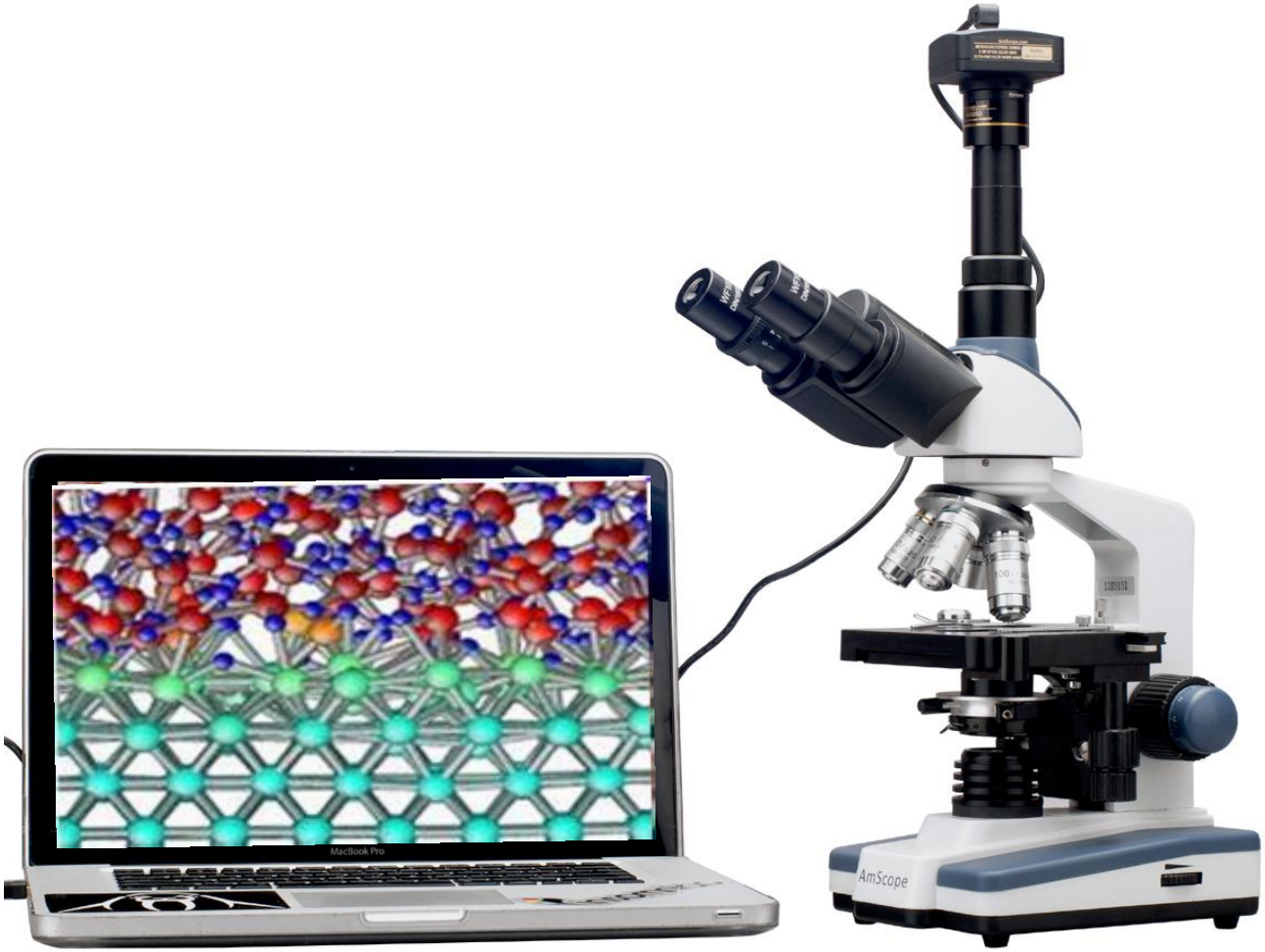
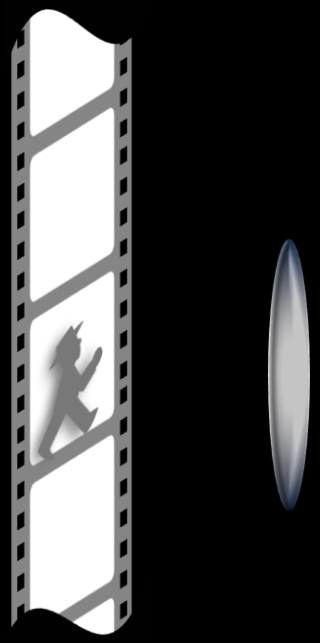
Office of Science
SSRL
SLAC NATIONAL ACCELERATOR LABORATORY

Goal : See Atomic Scale Structures



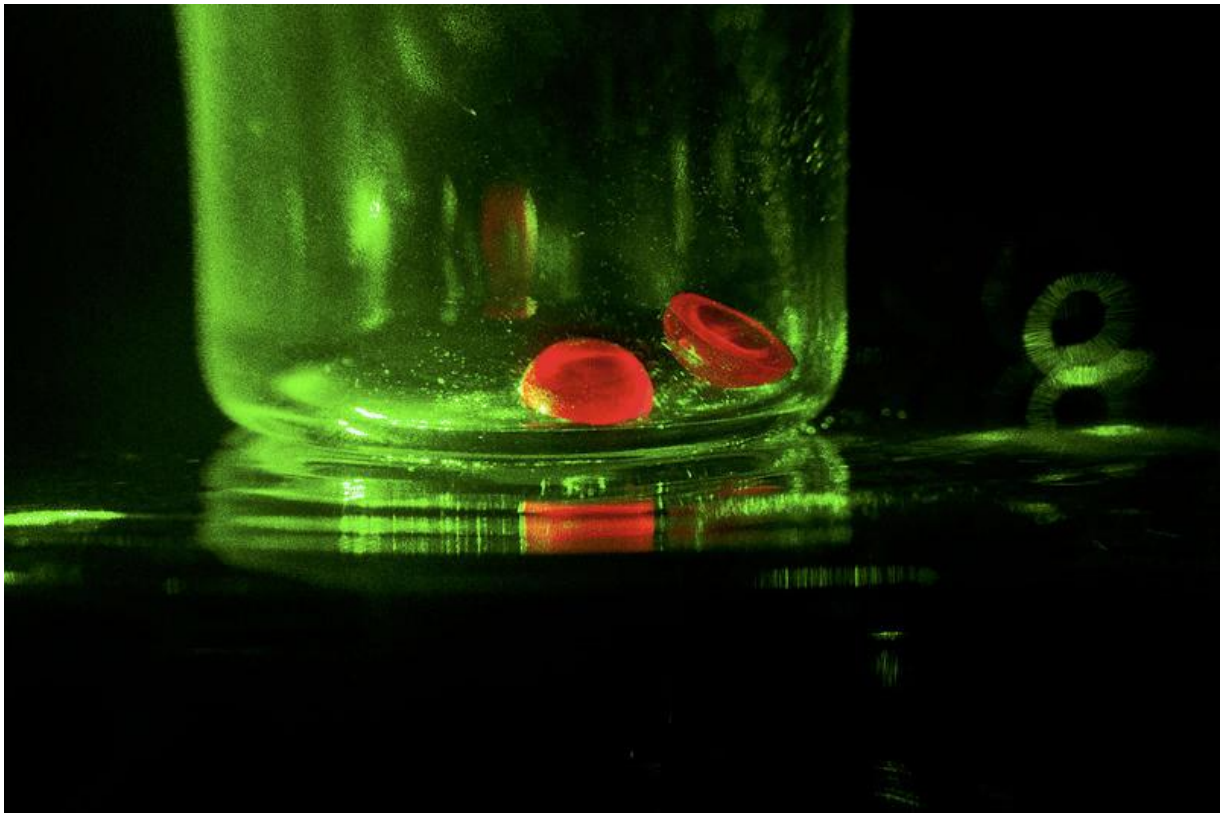
Photography



Camera

Lights

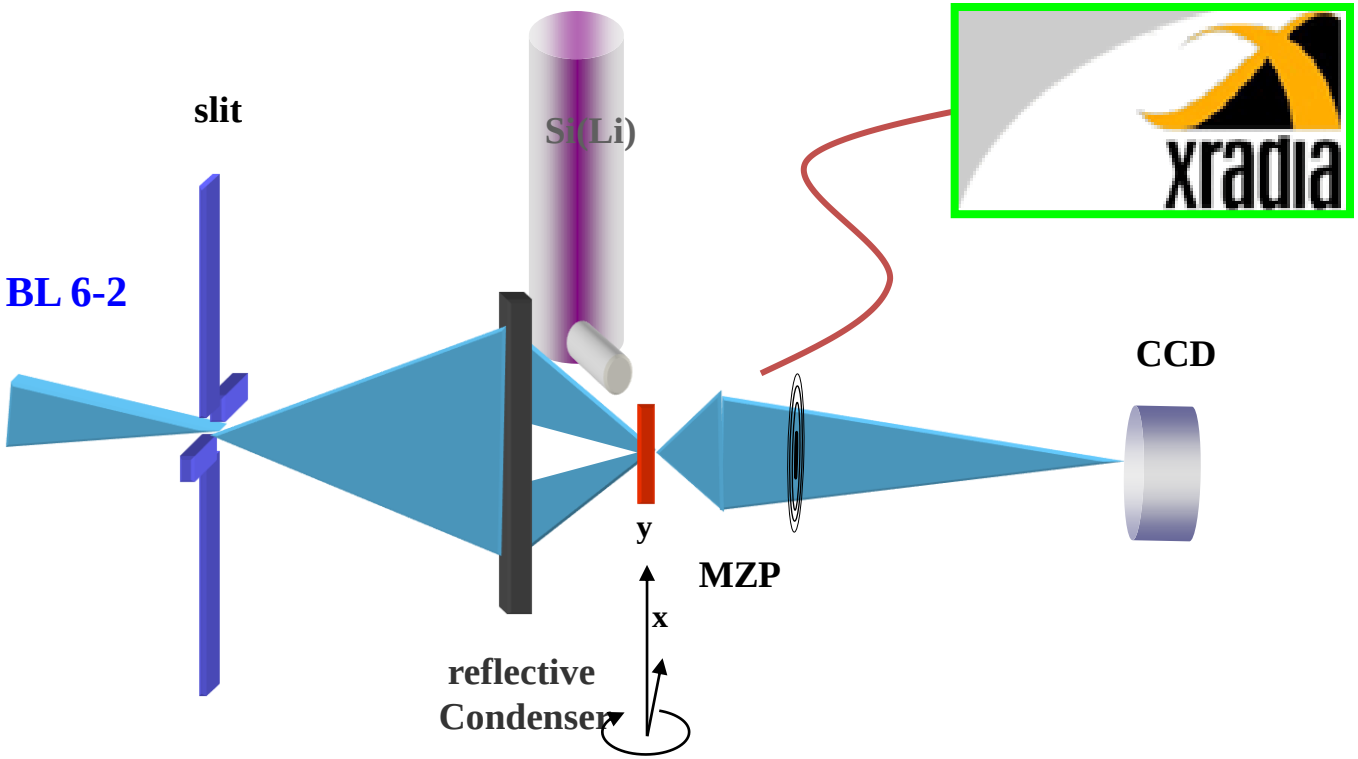
Light



- Interaction of Light with Matter
  - Transparent
  - Scatters
  - Absorbs/re-emits

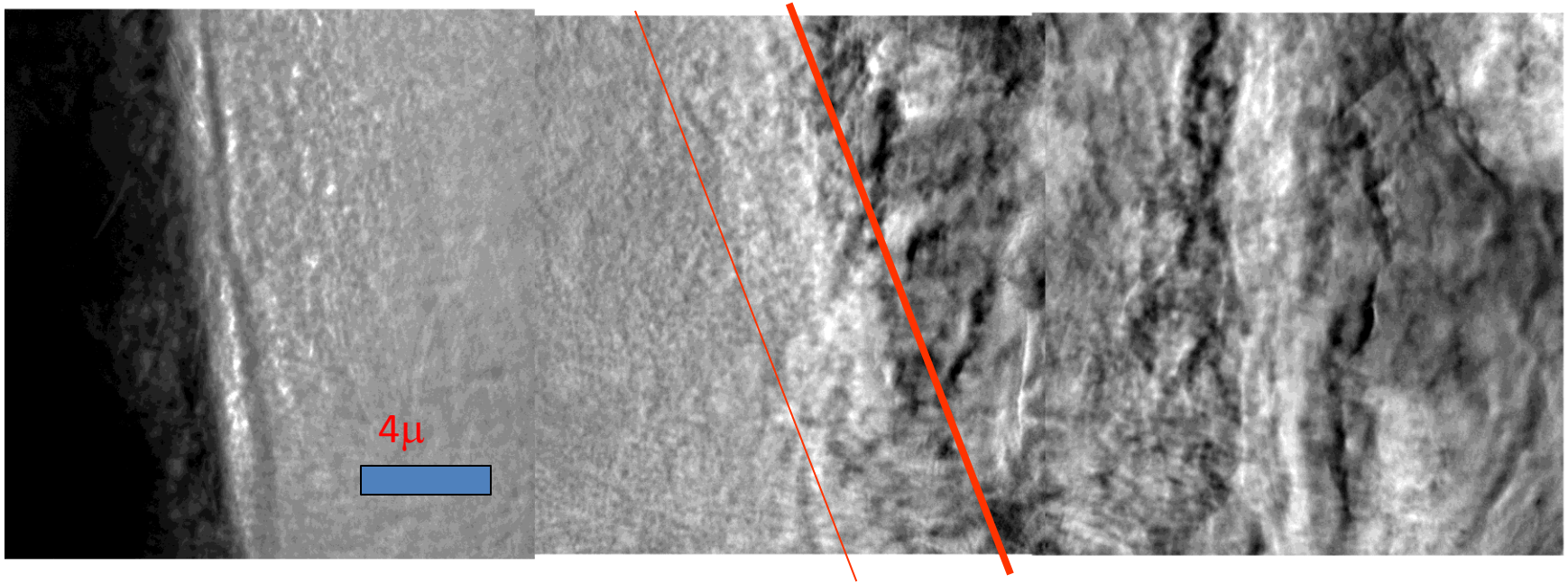
(Resonance)

X-ray camera (microscope) at SSRL

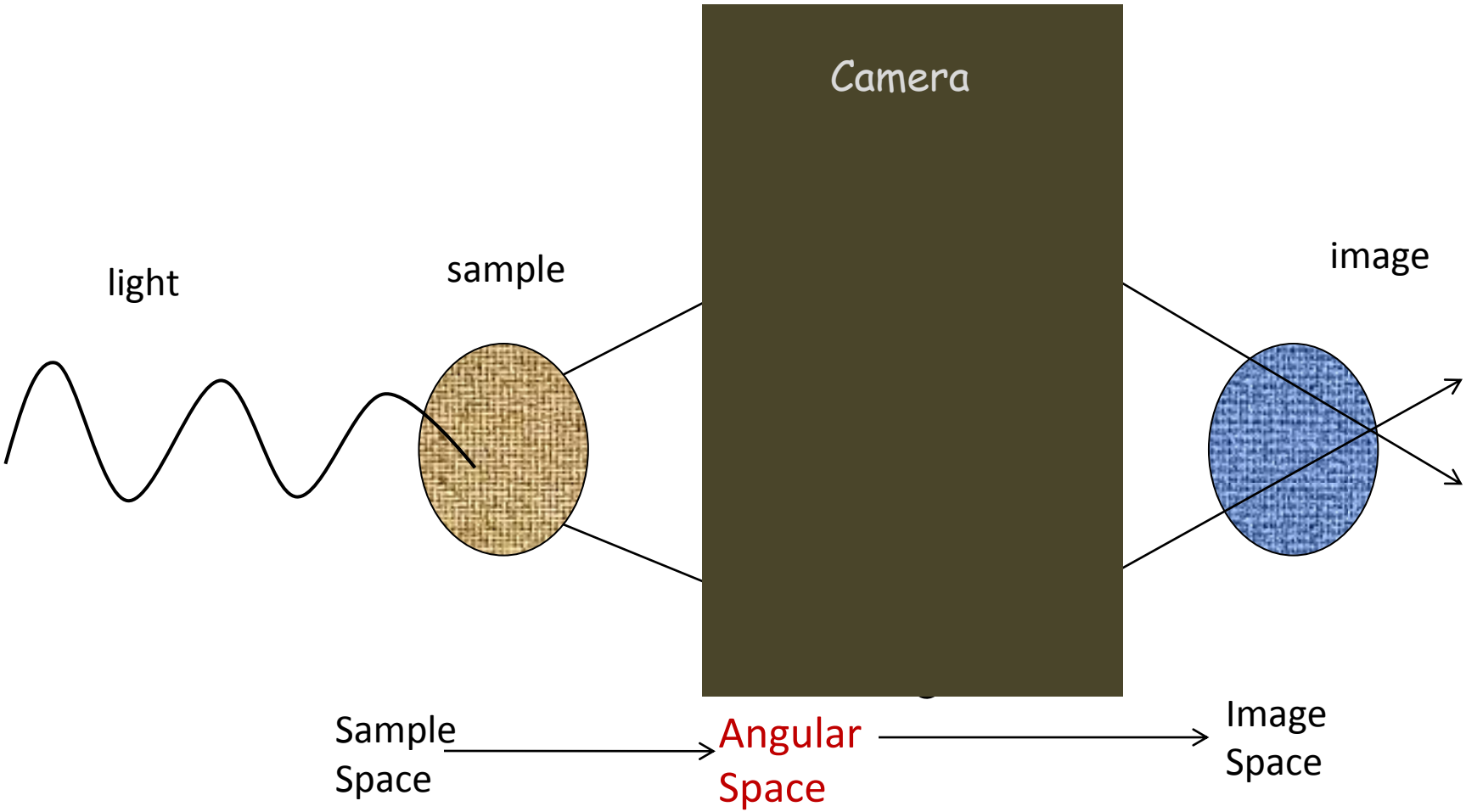


But not for atomic scale.

Why not?

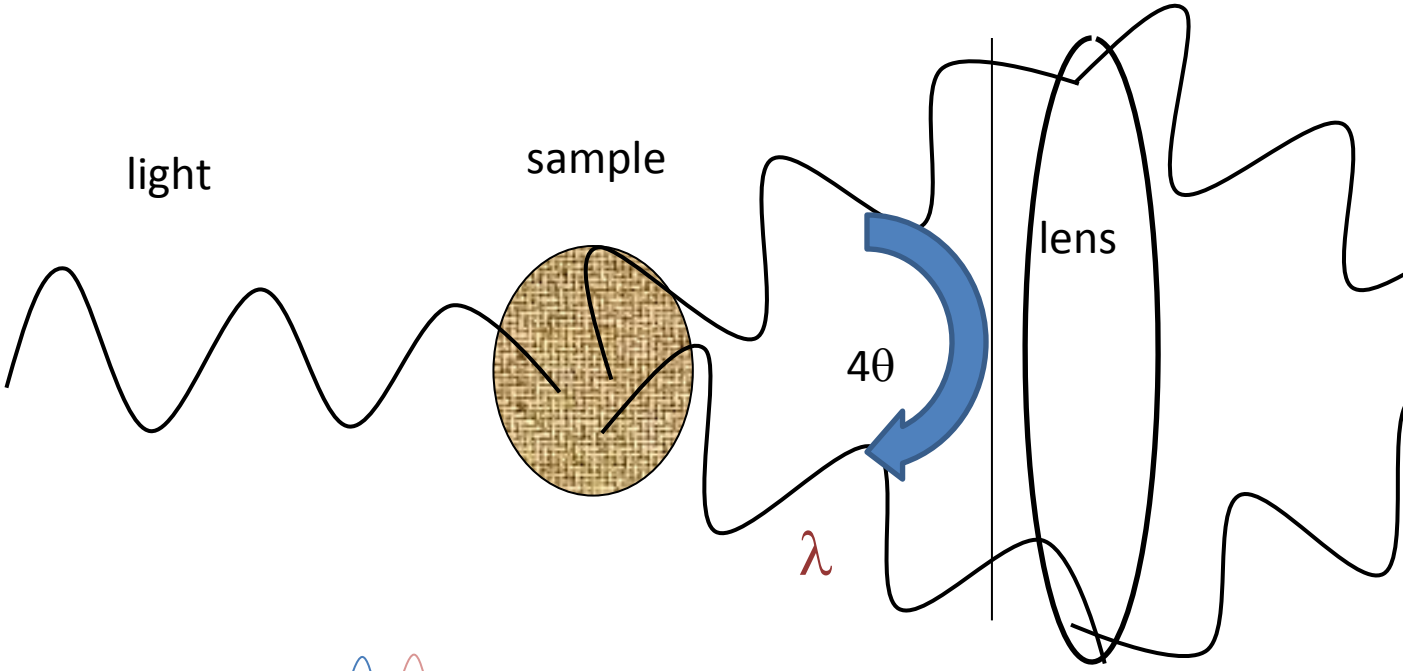


What Does the Camera Do?



Resolution of Full Field Camera

Full Field imaging is a "wave" phenomena -
interference pattern ➔ dark and light stops ➔ image



Rayleigh's Criteria

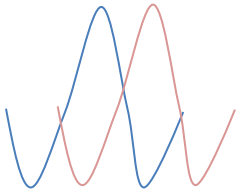
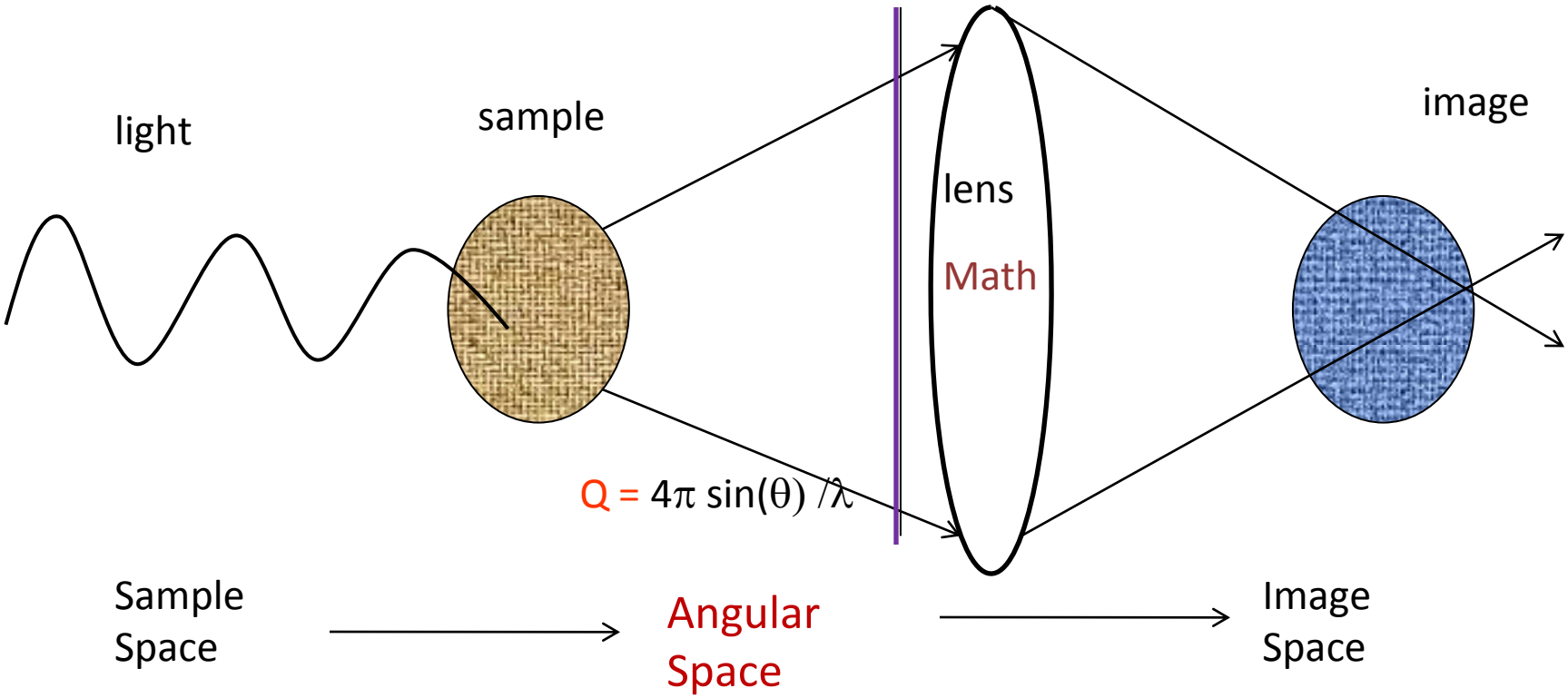


Image Resolution ~ $\lambda/\sin(\theta)$ + lens Aberrations

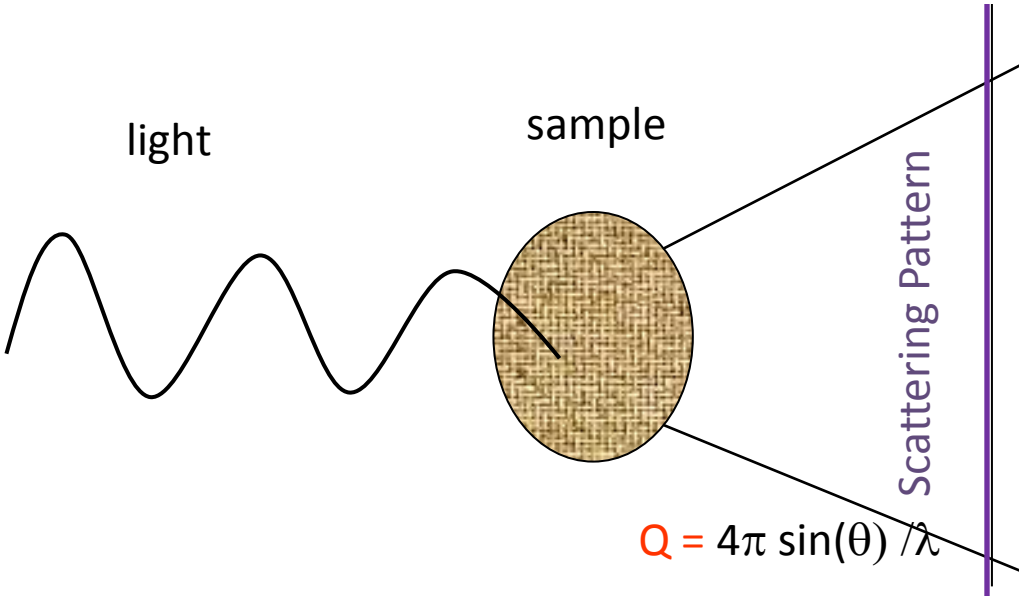
X-ray lens with resolution better than ~10nm don't exist

Scattering Physics



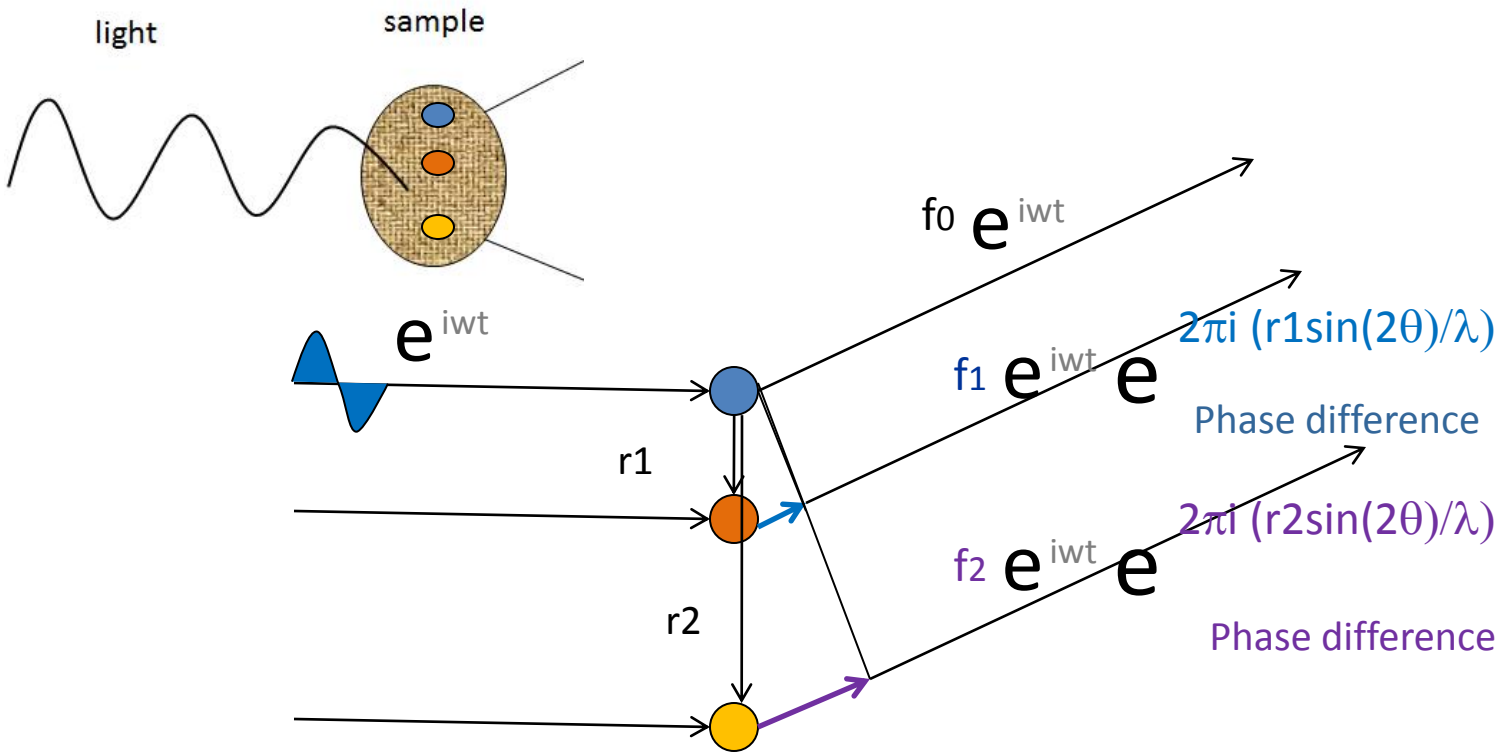
Can we create the image without a lens?

Lensless Imaging



Sample Space → Angular Space

Diffraction Physics



$2\pi i\,(r_i \sin(2\theta)/\lambda)$

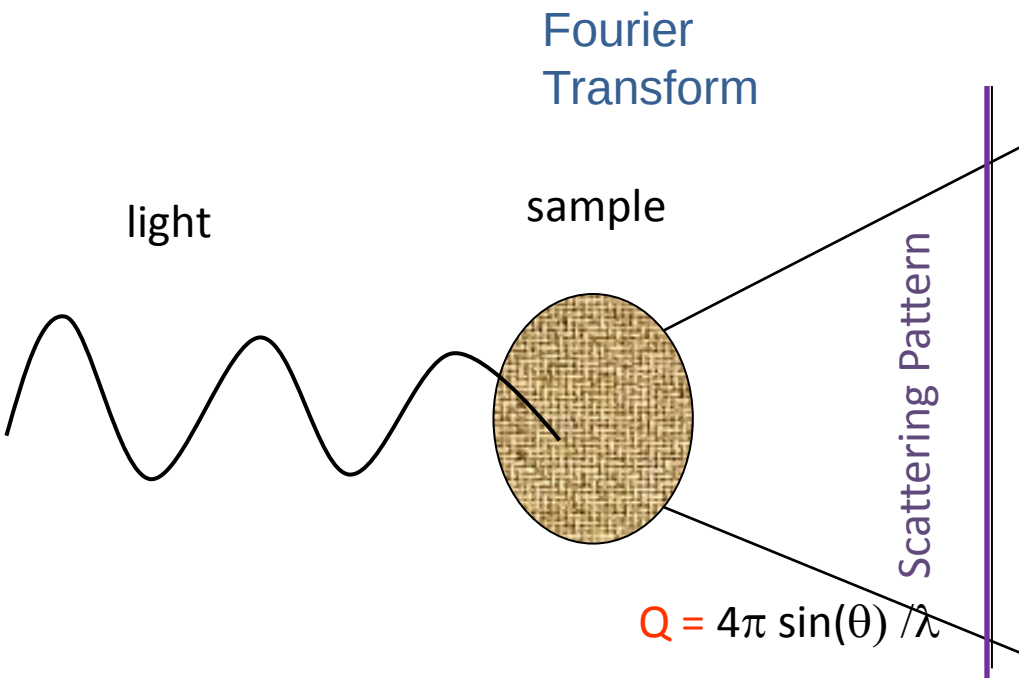
$\Delta K = Q = 4\pi \sin(\theta)/\lambda$

$A(\Delta K = (s-s0)) =$ amplitude $\quad e^{iwt} \sum f_i\, e^{i\,(r_i \bullet Q)}$

$A(\Delta K) = \sum f_i\, e^{i\,(r_i \bullet Q)}$

$A(Q) =$ Fourier Transform (r_i)

Lensless Imaging

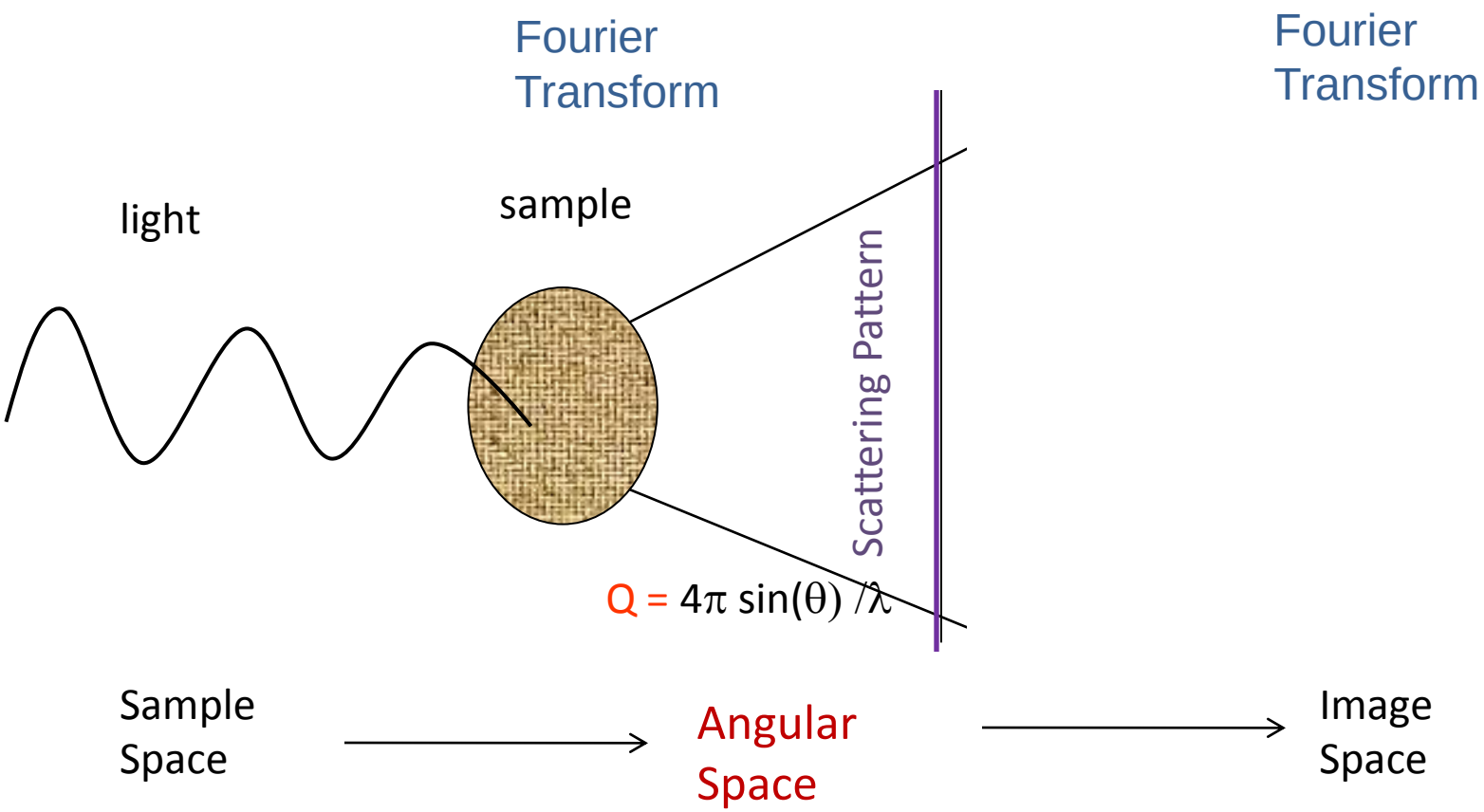


Sample Space → Angular Space

Fourier Transform Recap

- 1: FT (FT (S)) ~ S

Lensless Imaging



Fourier Transform Recap

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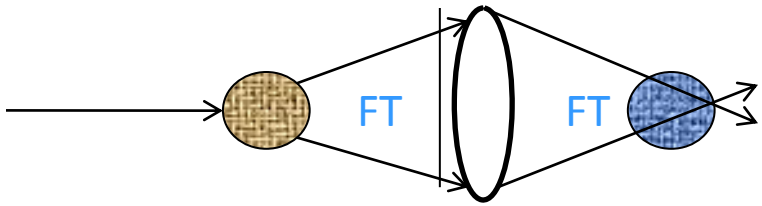
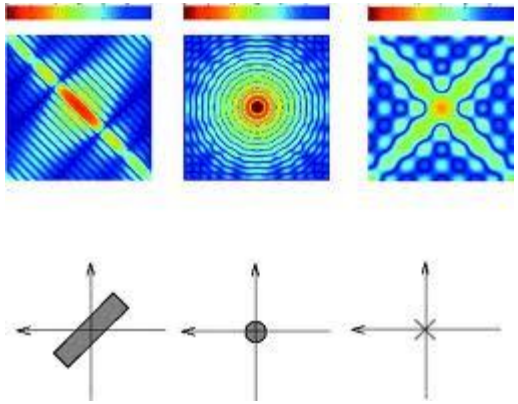


- 2: FT (large) ~ 1/large ➔ small



Fourier Transform Recap

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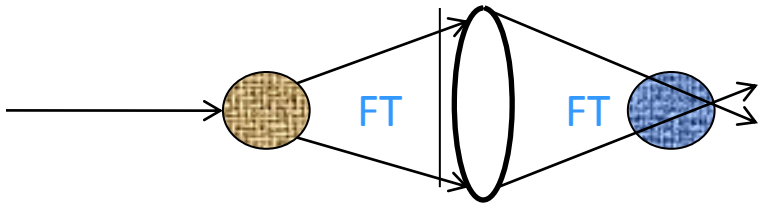

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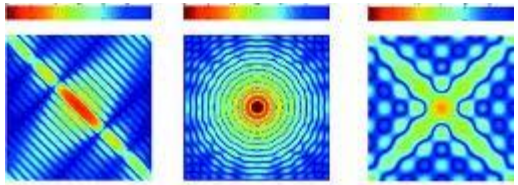
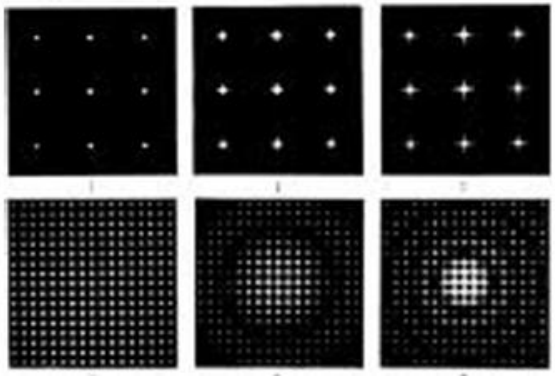


- 3: FT (periodic fn) ~ periodic



Fourier Transform Recap

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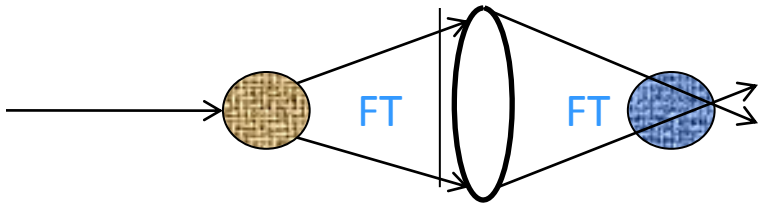

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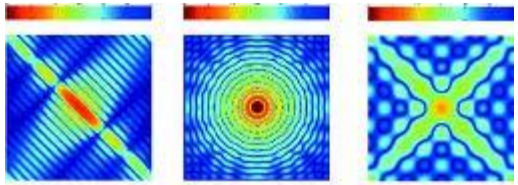
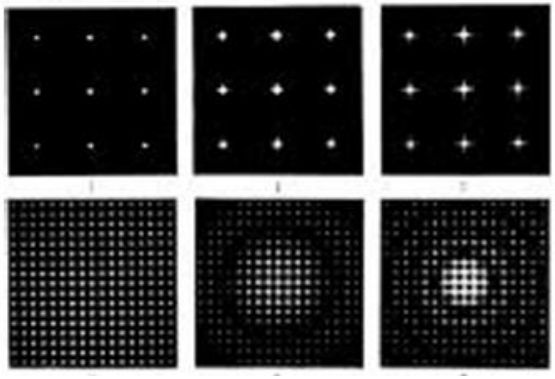
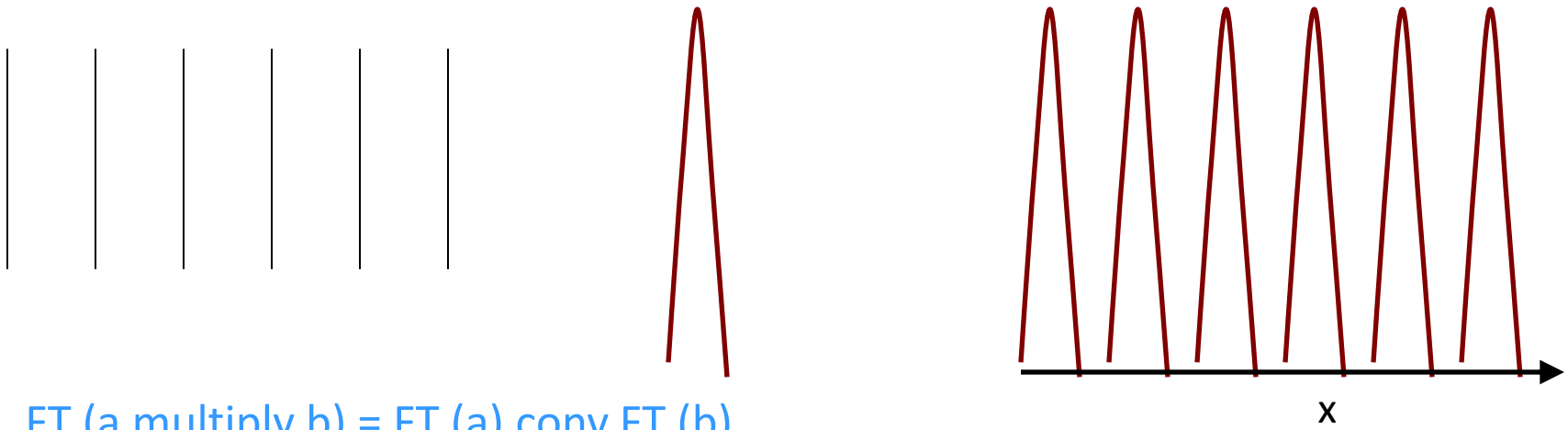


- 3: FT (periodic fn) ~ periodic

- 4: Convolution Theorem:
  - FT (a multiply b) =
    - FT (a) conv FT (b)
  - FT (a conv b) =
    - FT (a) multiply FT (b)

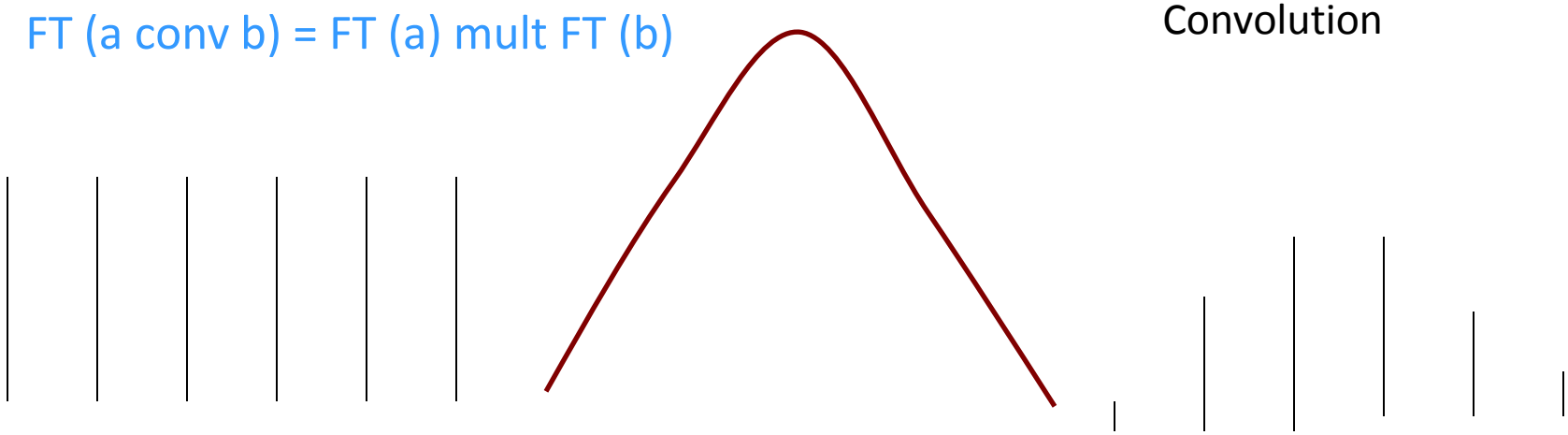


Multiplication vs Convolution



Convolution

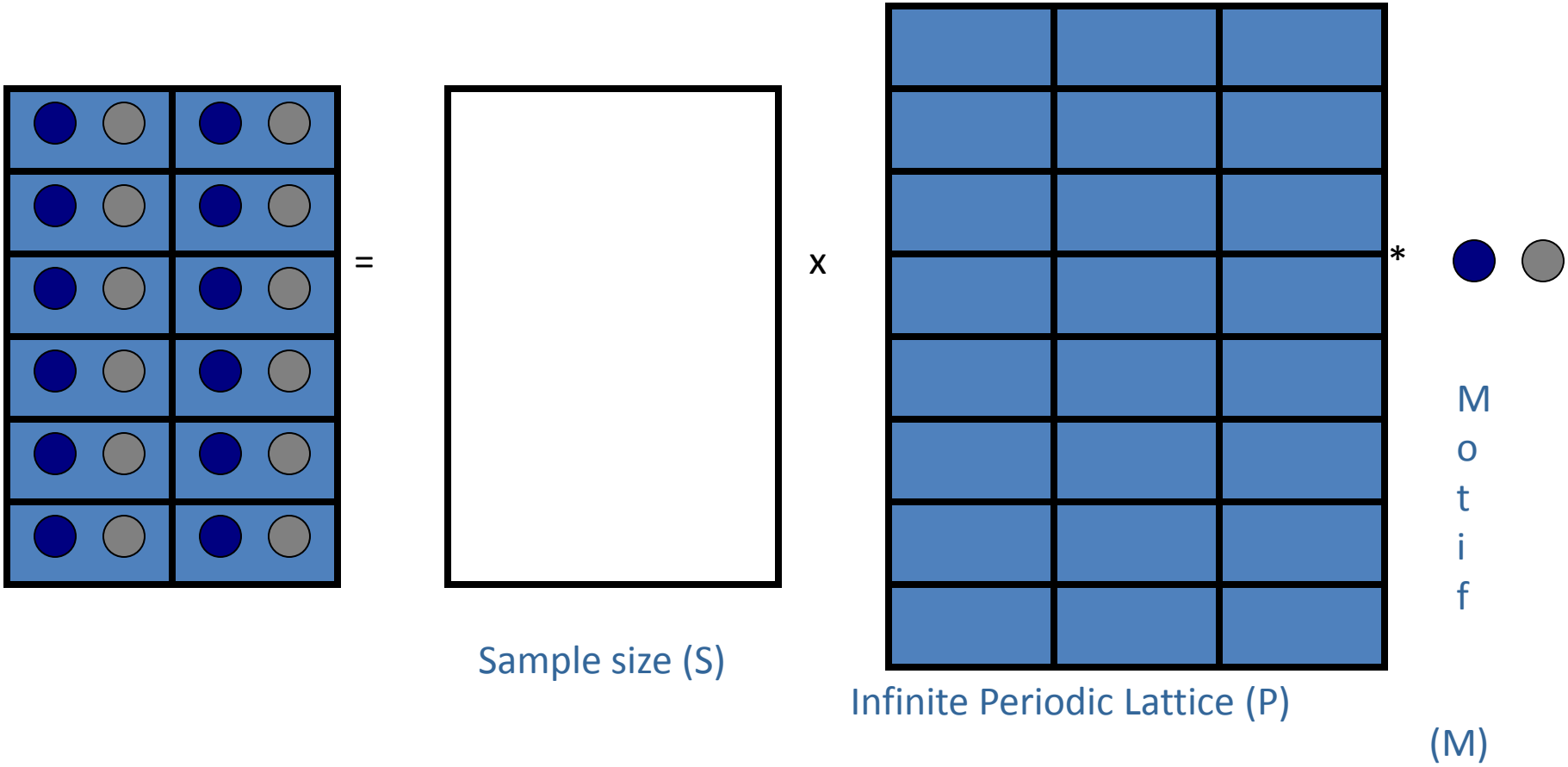
FT (a multiply b) = FT (a) conv FT (b)
FT (a conv b) = FT (a) mult FT (b)



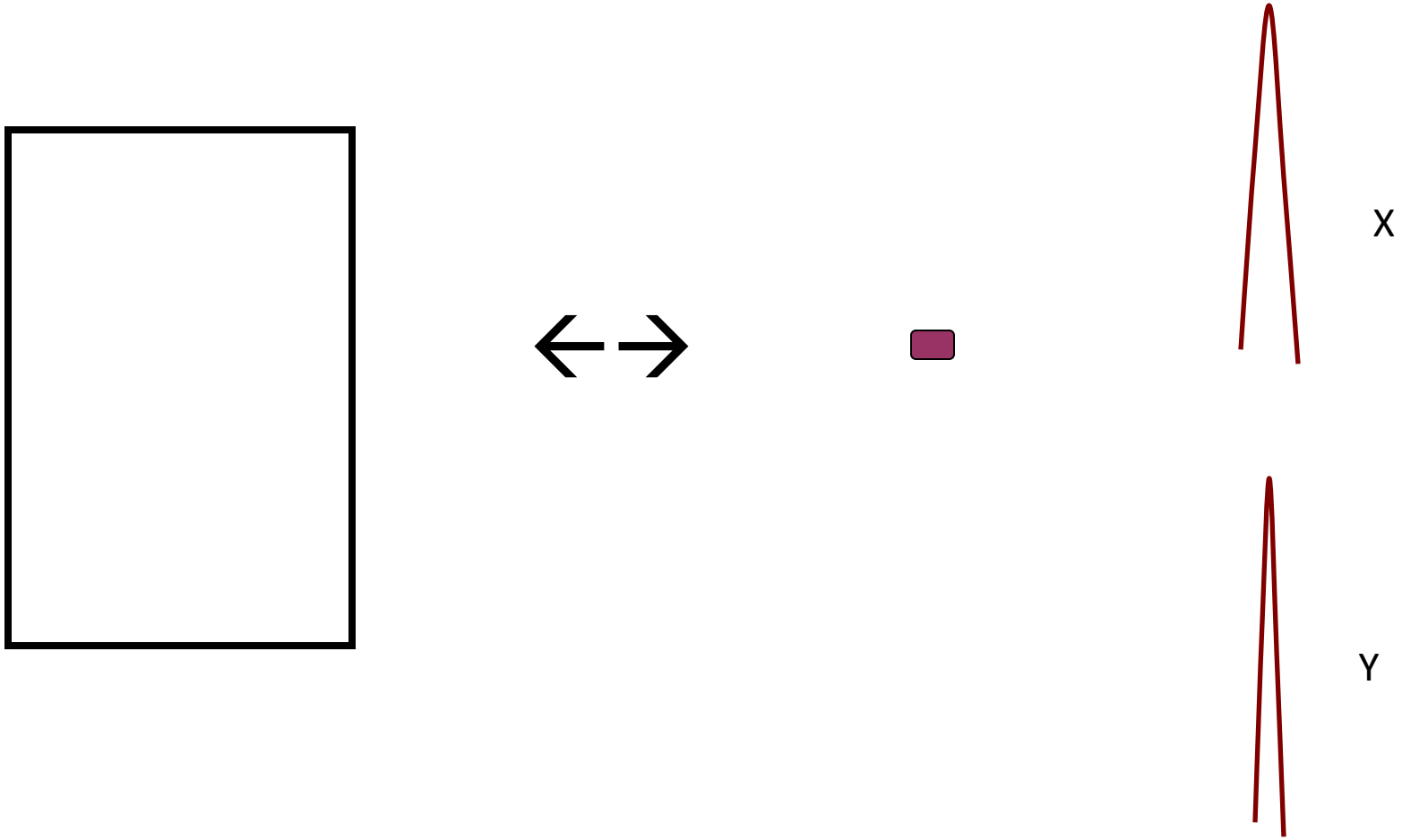
Multiplication

Deconstructing the Sample space

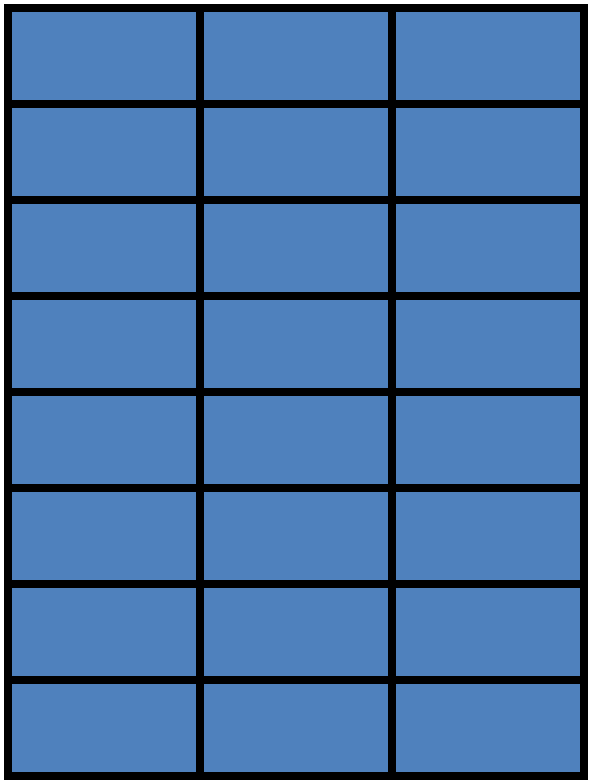
Sample = S x P * M



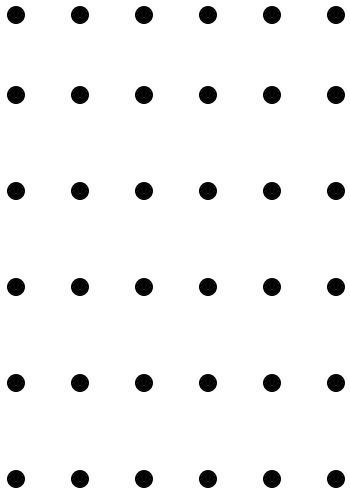
FT(S)



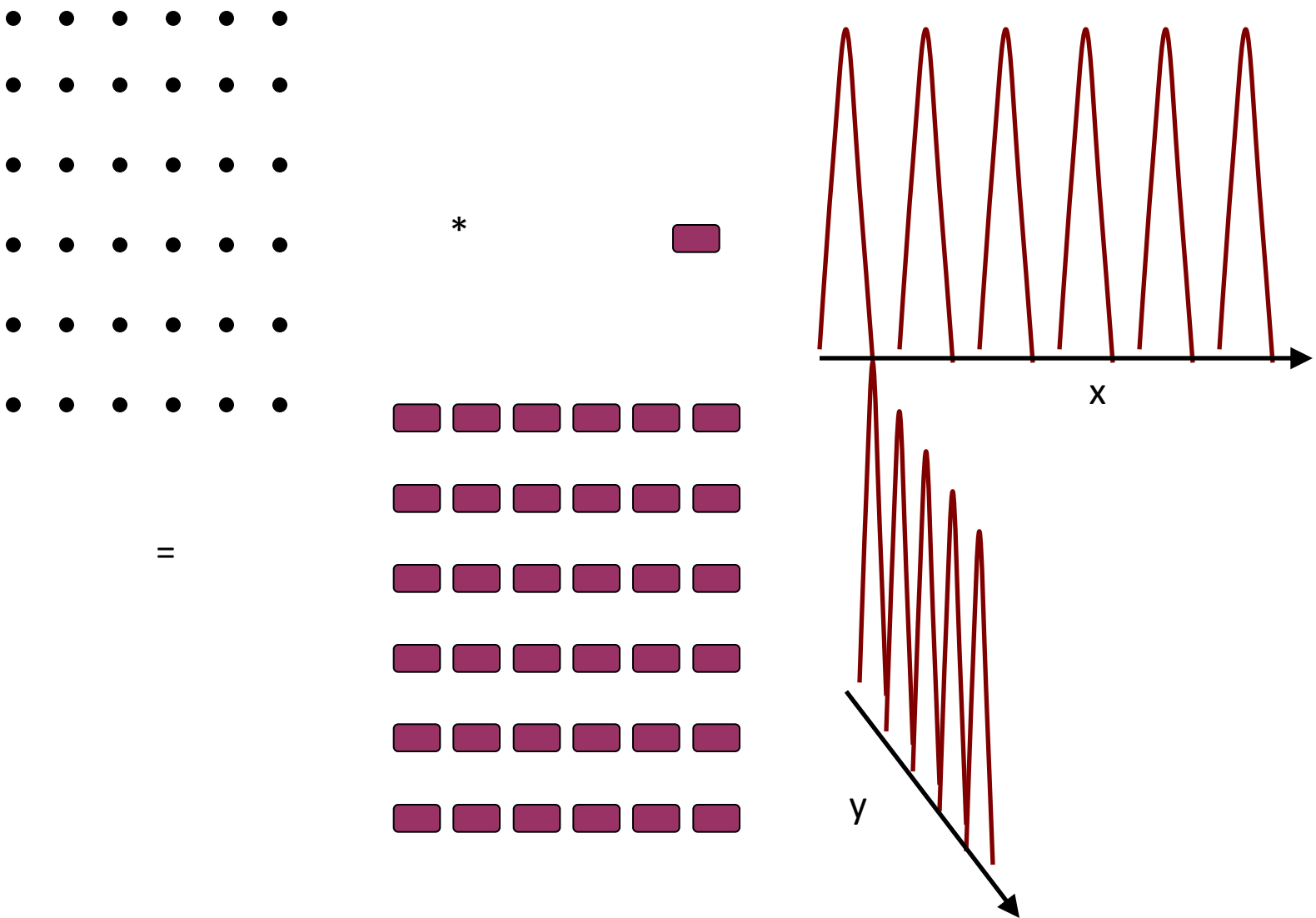
FT(P)



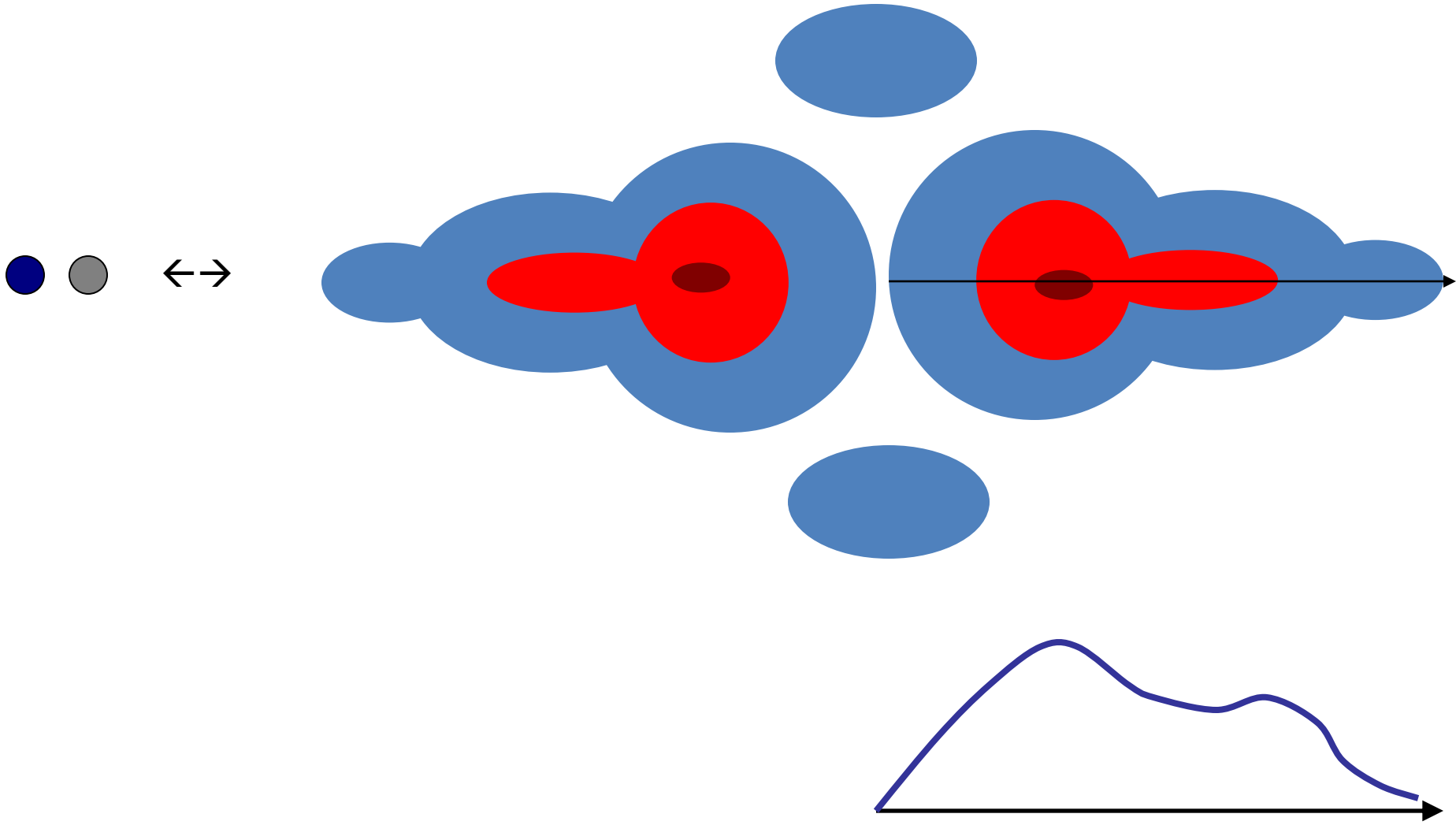
↔



FT (S x P) = FT(S) * FT(P)

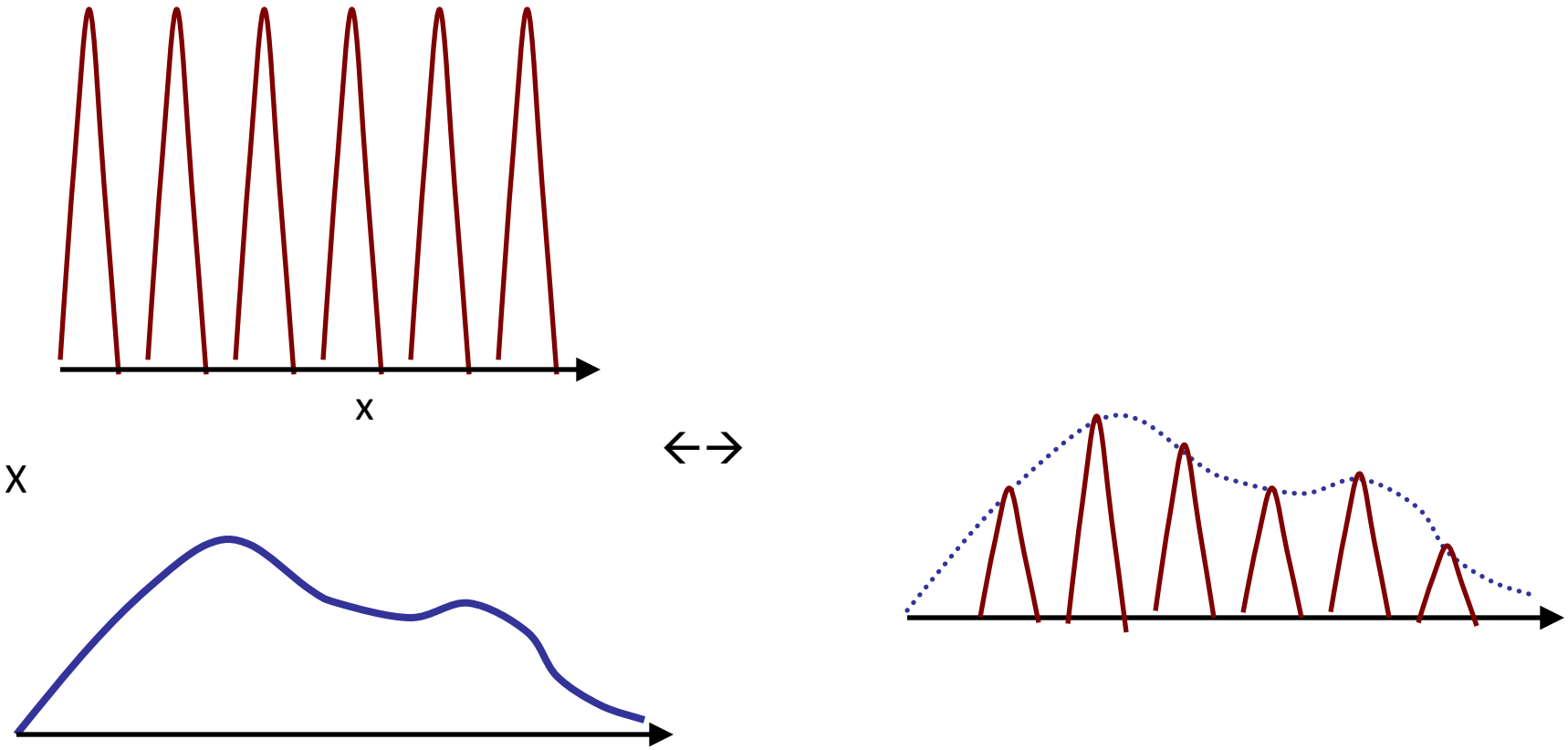


FT(M)

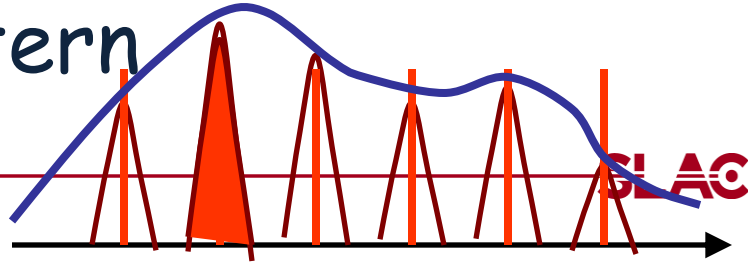


FT(sample) = FT(S x P) x FT(M)

Along X direction



What does a diffraction pattern tell us?

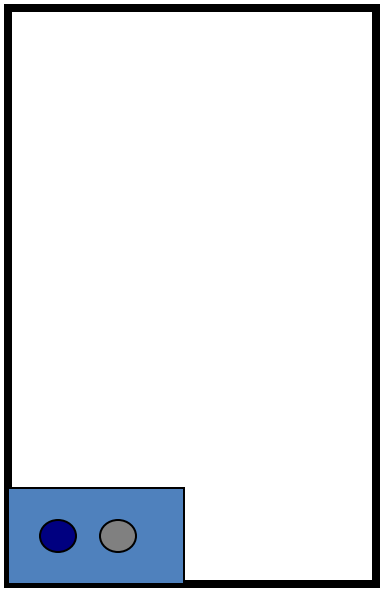


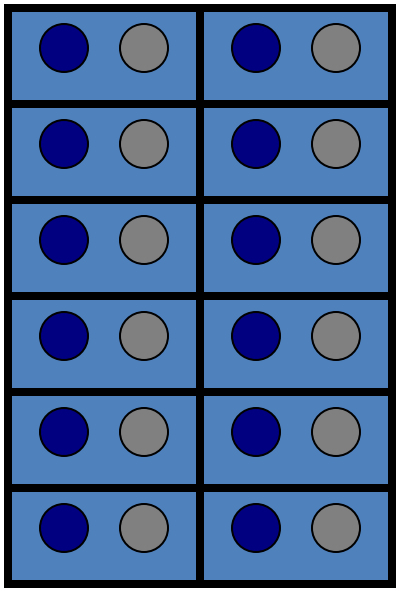
- Peak Shape & Width:
  - Zero order peak

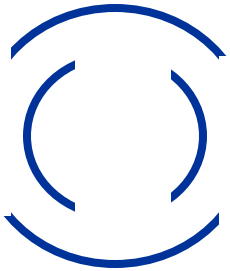
Small Angle Scattering & Reflectivity

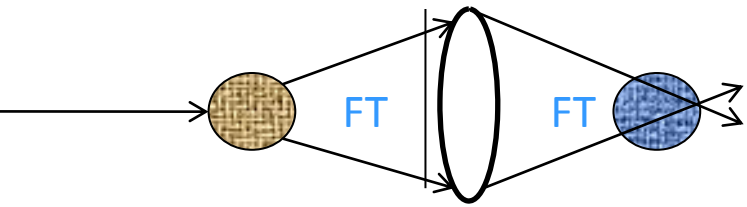
  - Higher order peaks
    - crystallite size
    - Strain gradient
- Peak Positions:
    - Phase identification
    - Lattice symmetry
    - Lattice strain
- Peak Intensity:
    - Structure solution
    - Crystallite orientation

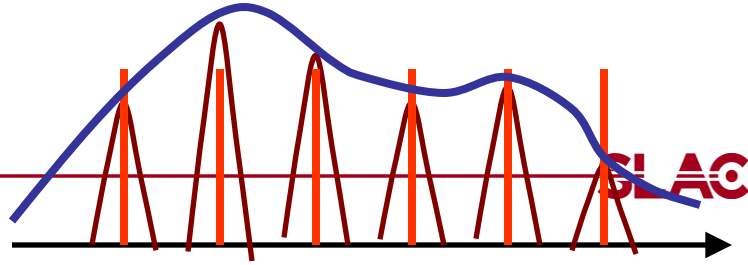
Wide Angle Scattering











Questions?

1: FT (FT (S)) ~ S

2: Scattering Pattern (large) ~ 1/large ➔ small features

3: Scattering Pattern (periodic lattice) ~ periodic