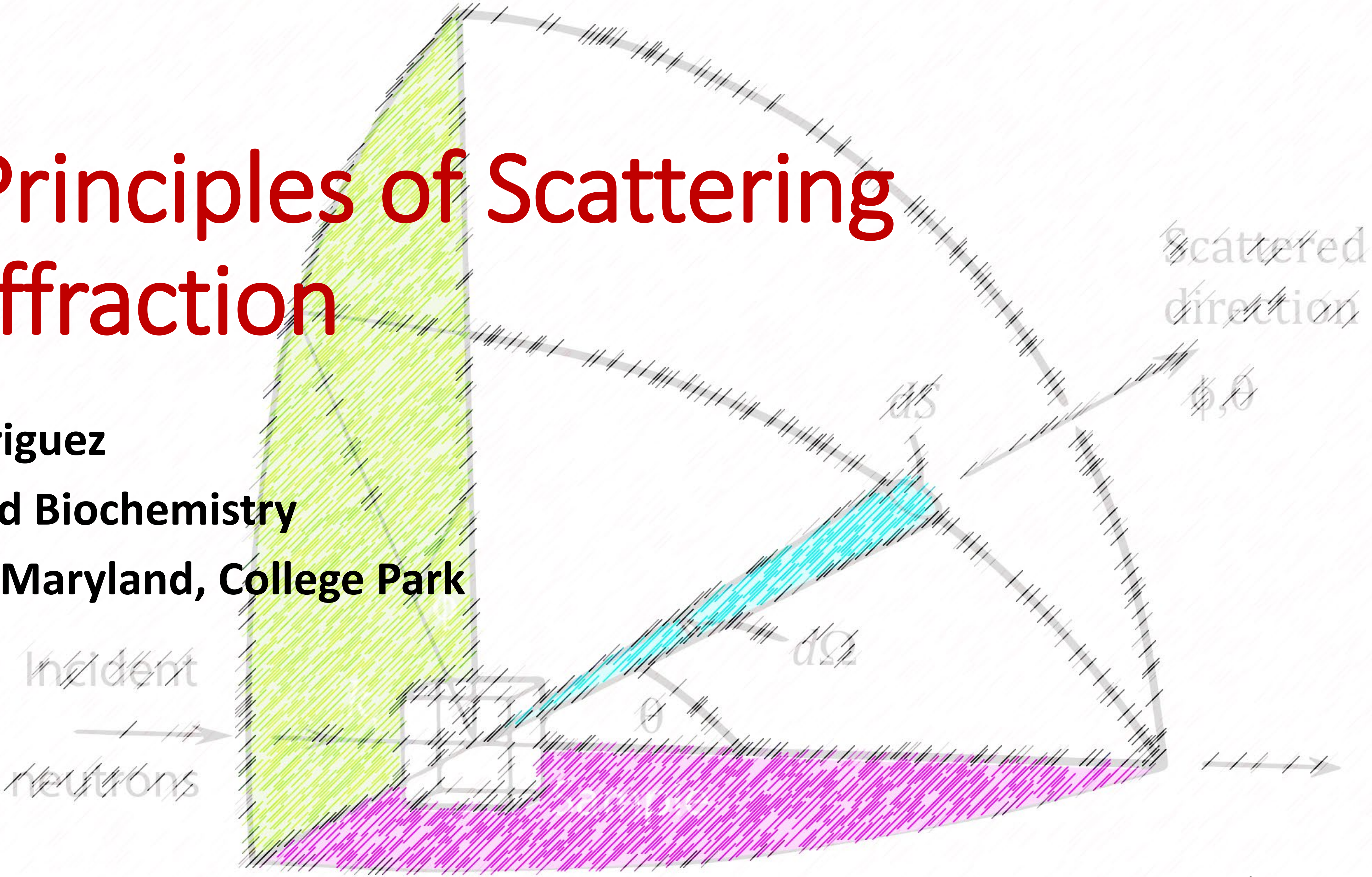
Basic Principles of Scattering and Diffraction

Efrain E. Rodriguez

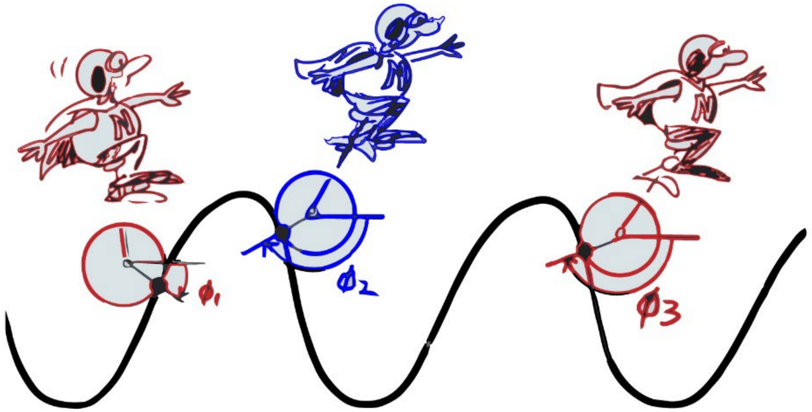
Chemistry and Biochemistry

University of Maryland, College Park



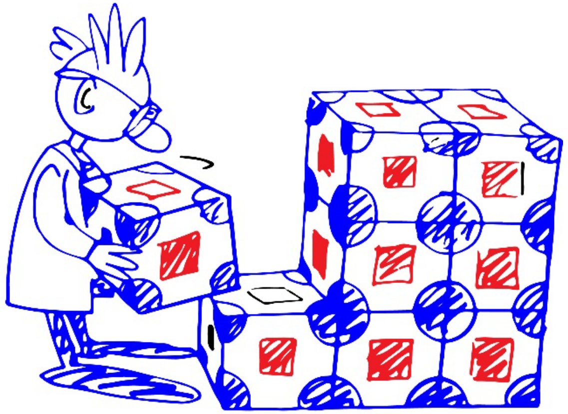
Outline: 15 minute lectures for previewing

1. Going between real space and reciprocal space: Waves and Fourier transforms.

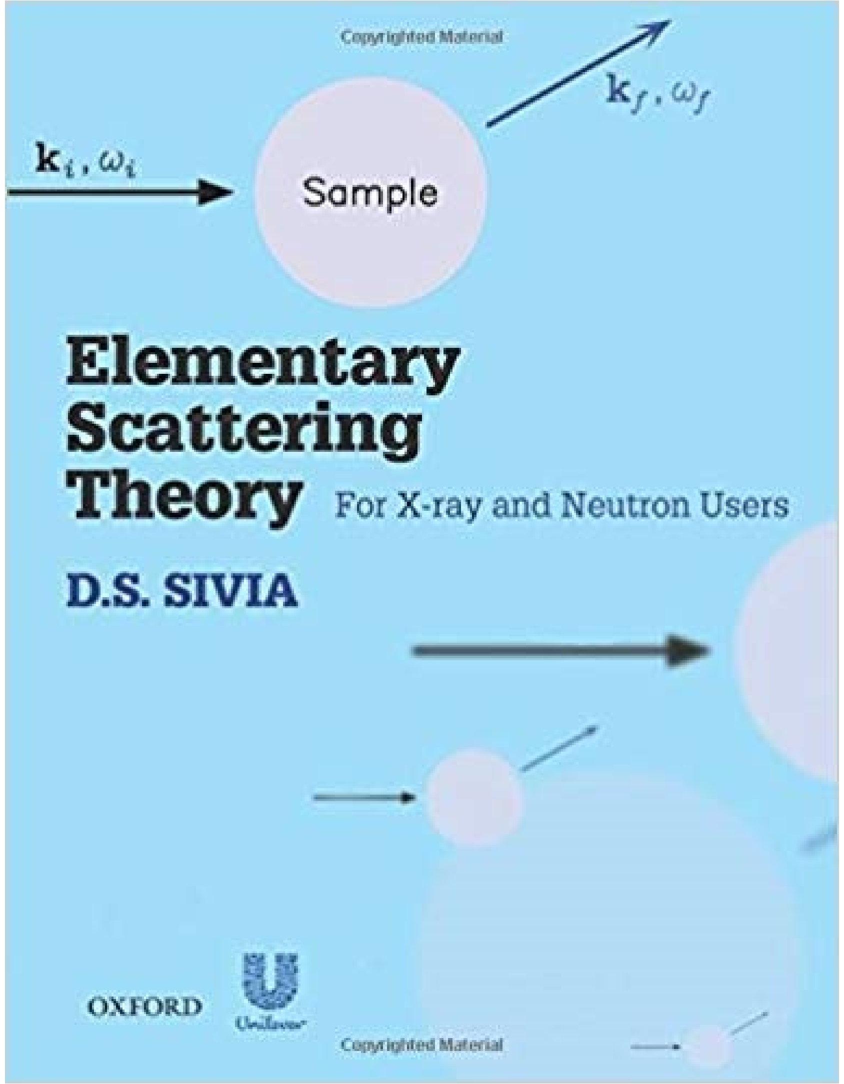


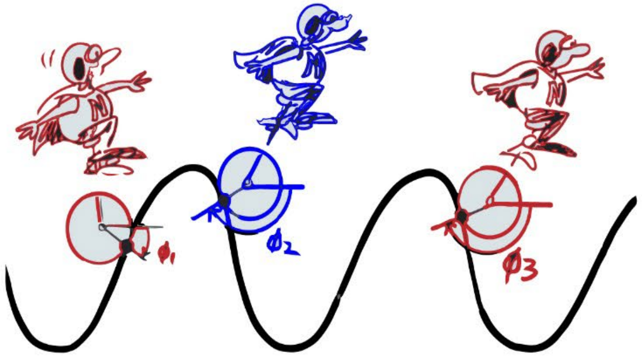
2. Hitting the target: The differential scattering cross section.

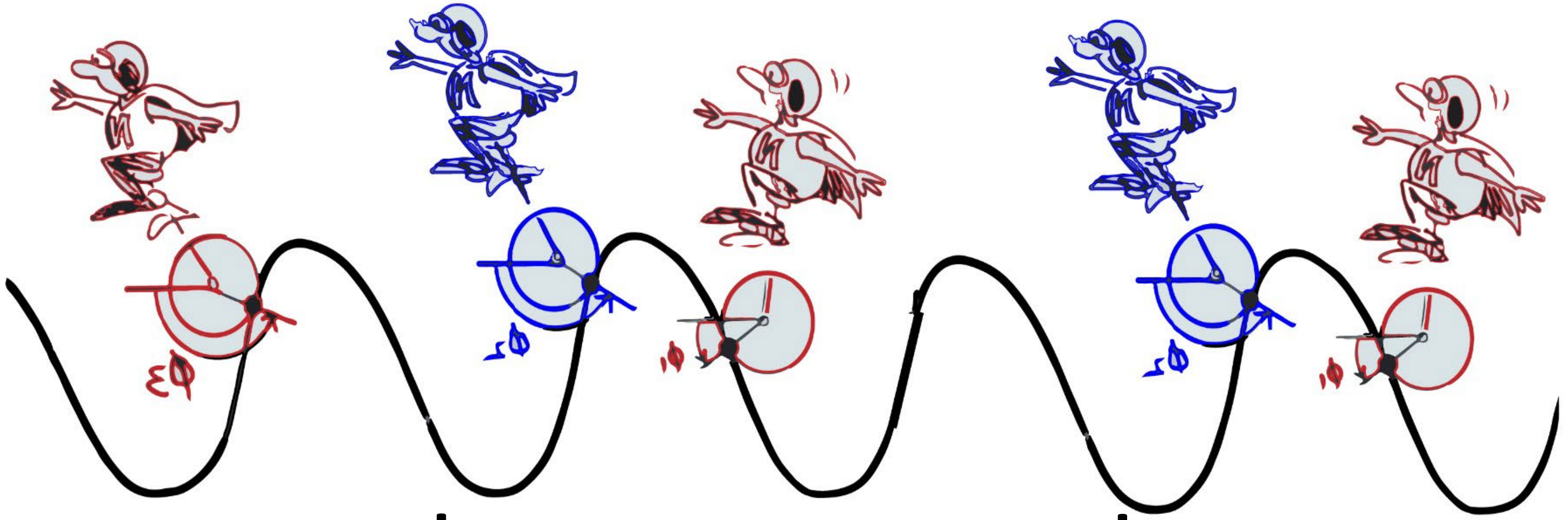
3. Crystals that glitter: Diffraction from materials with translational symmetry.



Acknowledgements



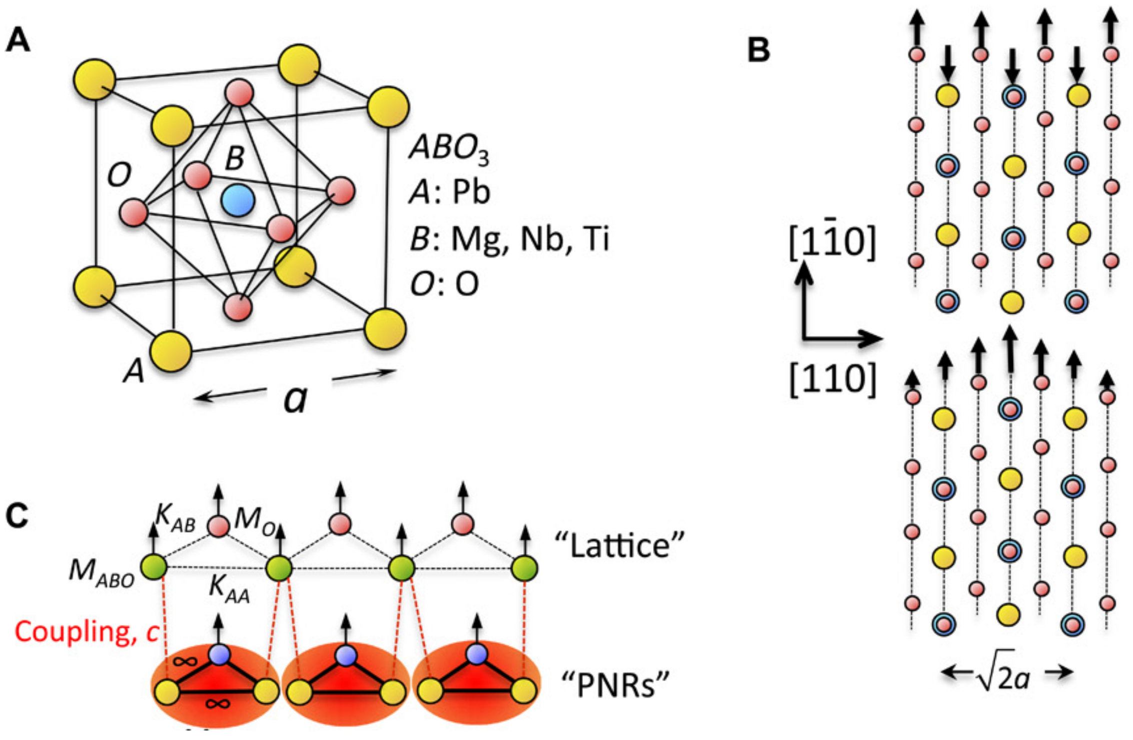




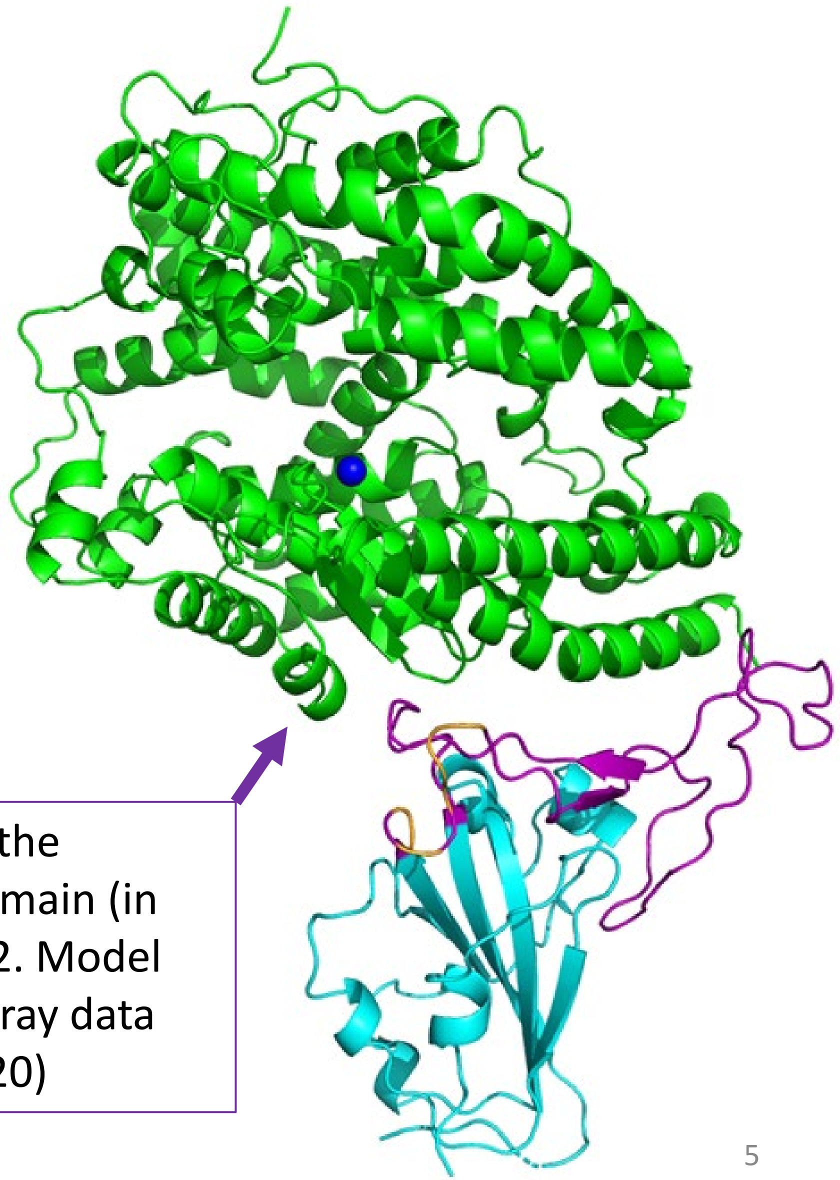
Going between real space and reciprocal space

Waves and Fourier transforms

What do we want to 'see'? Namely, structure



Crystal structure of a perovskite oxide with relaxor ferroelectric properties. Models reconstructed from neutron scattering data (Nature Comm. Manley, 2014)

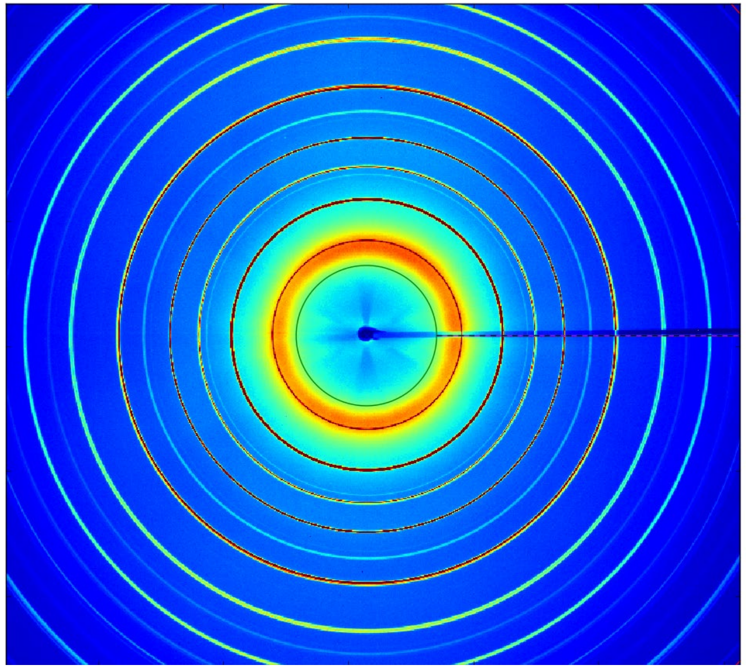


Crystal structure of the receptor binding domain (in green) in SARS-CoV2. Model from synchrotron x-ray data (Nature, Li et al, 2020)

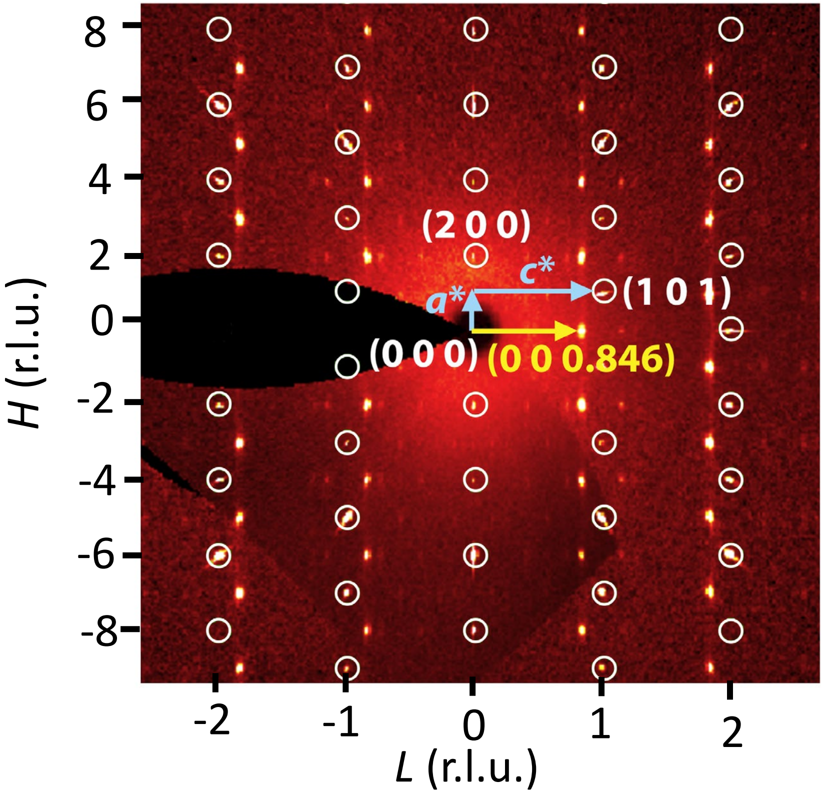
What do we observe? Structure in reciprocal space

In reciprocal space you measure the Bragg peaks known as reflections, but also more than that.

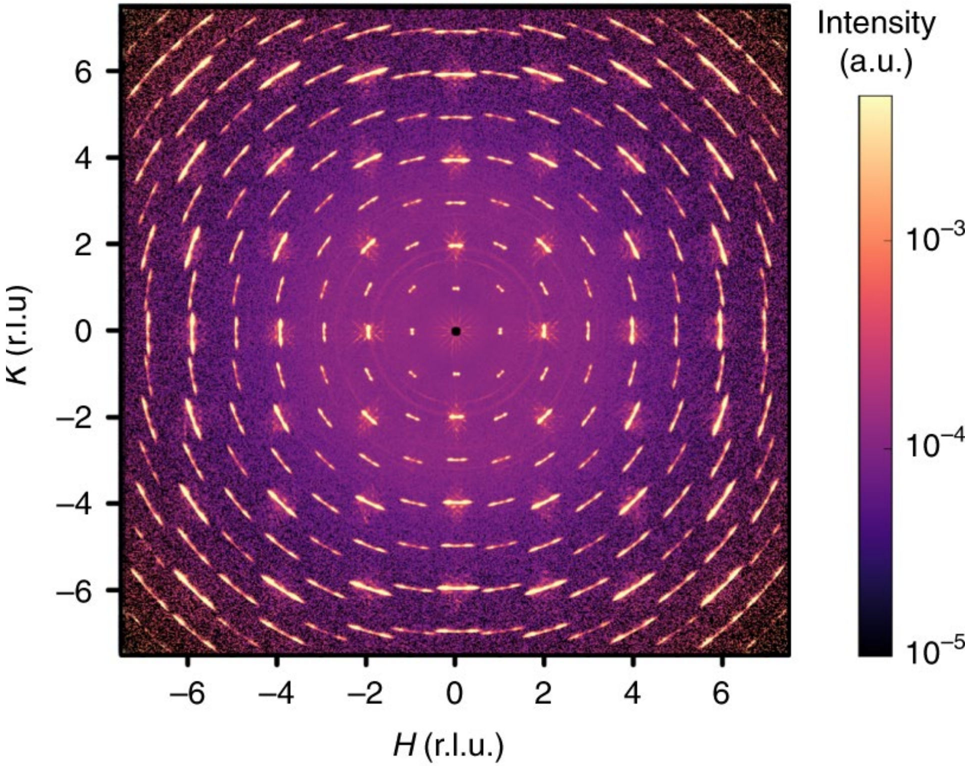
Powder diffraction rings from synchrotron X-ray beamline 17-BM, Advanced Photon Source



X-ray single crystal of $Bi_{1.7}V_8O_{16}$ showing an incommensurate satellite reflections.

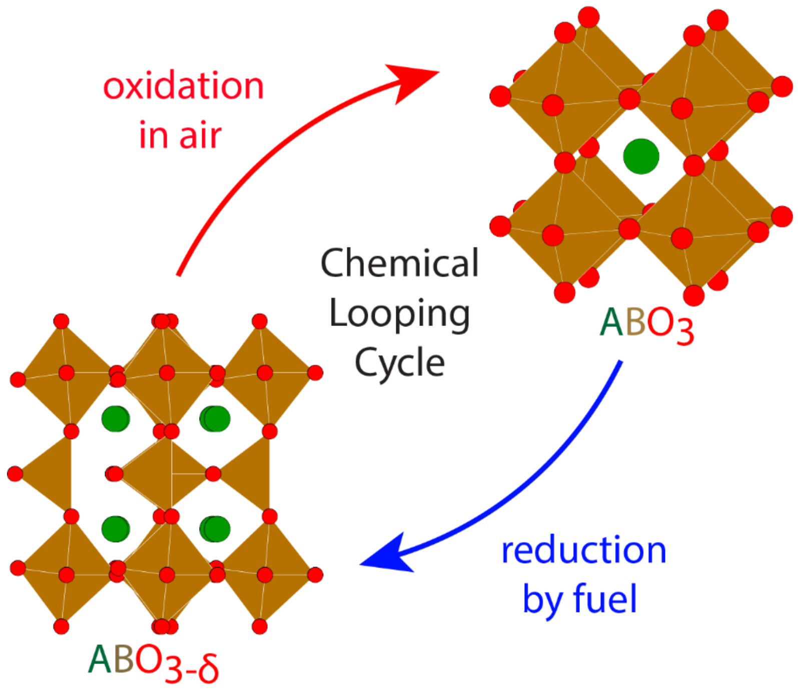


Diffuse neutron scattering from instrument CORELLI (Spallation Neutron Source) on a plastically deformed crystal of $SrTiO_3$.

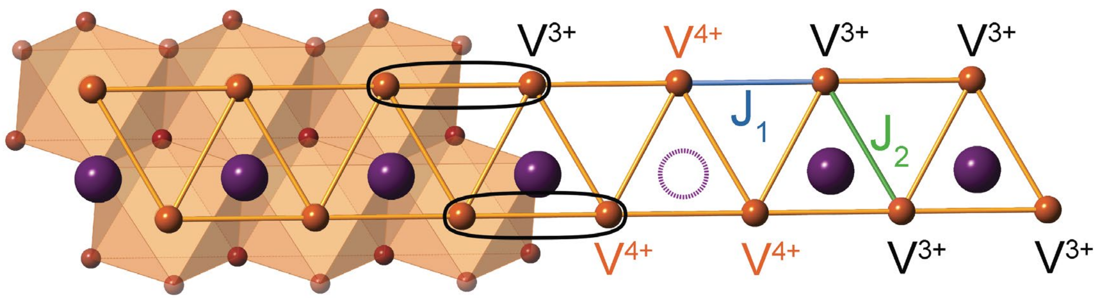


How do we get back from the images in reciprocal space?

Fast powder diffraction (< 5 sec) allows for in situ materials studies

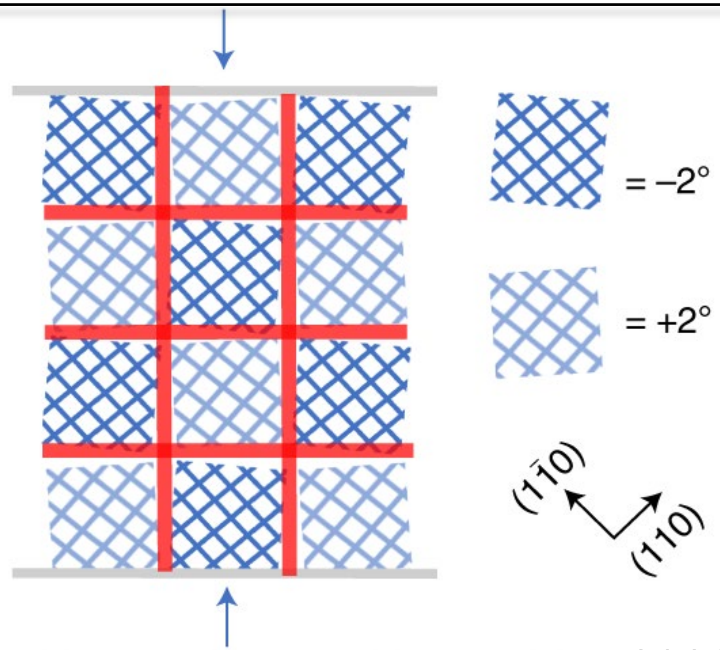


Taylor et al. EER, *Chem. Mater.* **2016**, *28* 3951



Understanding nature of metal-insulator transition through analysis of incommensurate charge order

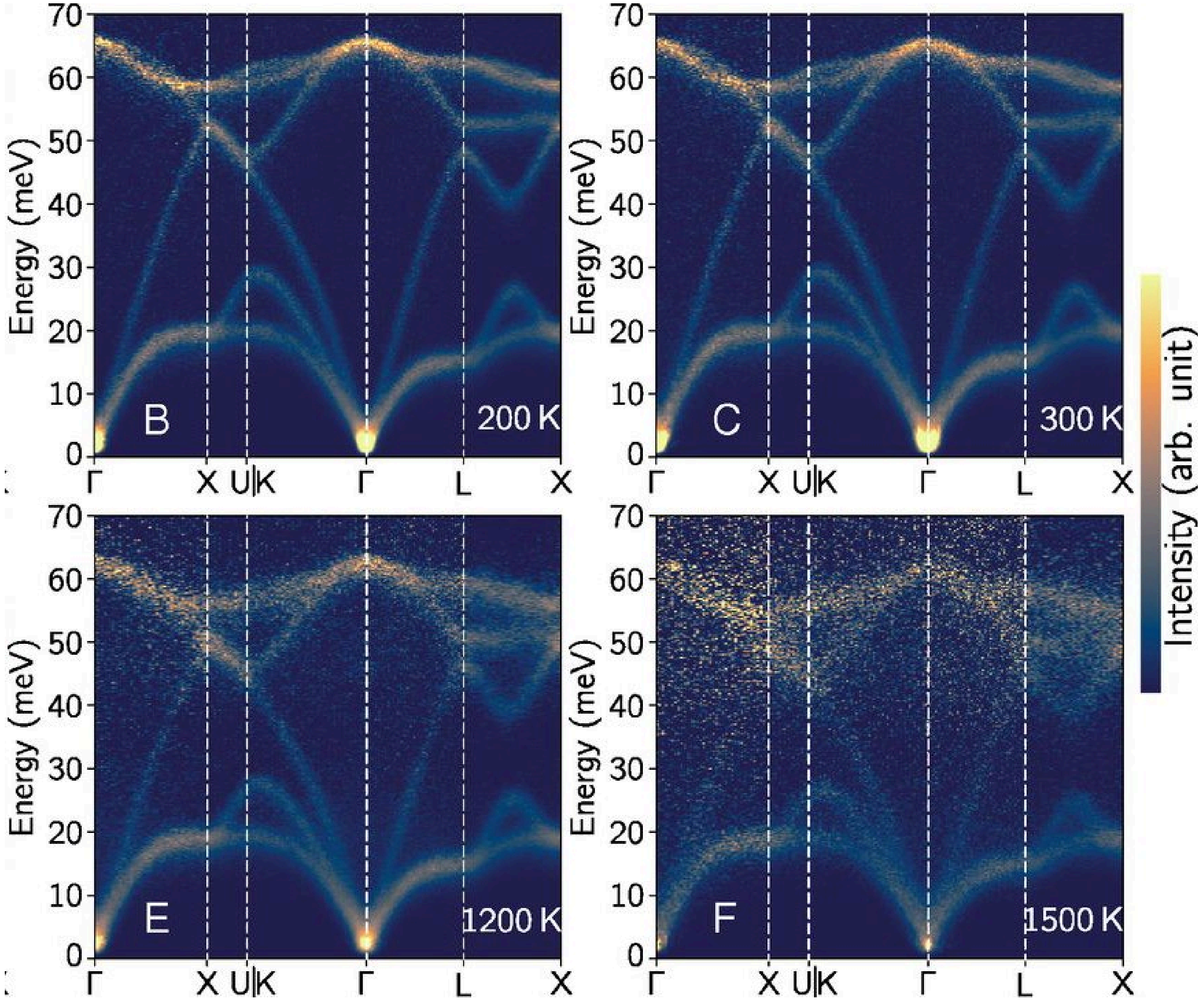
Larson et al. EER, *J. Mater. Chem. C* **2017**, *5* 4967



Plastic deformation of $SrTiO_3$ single crystal with enhanced superconductivity revealed by diffuse scattering

Hameed et al., *Nature Mat.* **2022**, *21* 54-61

Add time or energy to the map

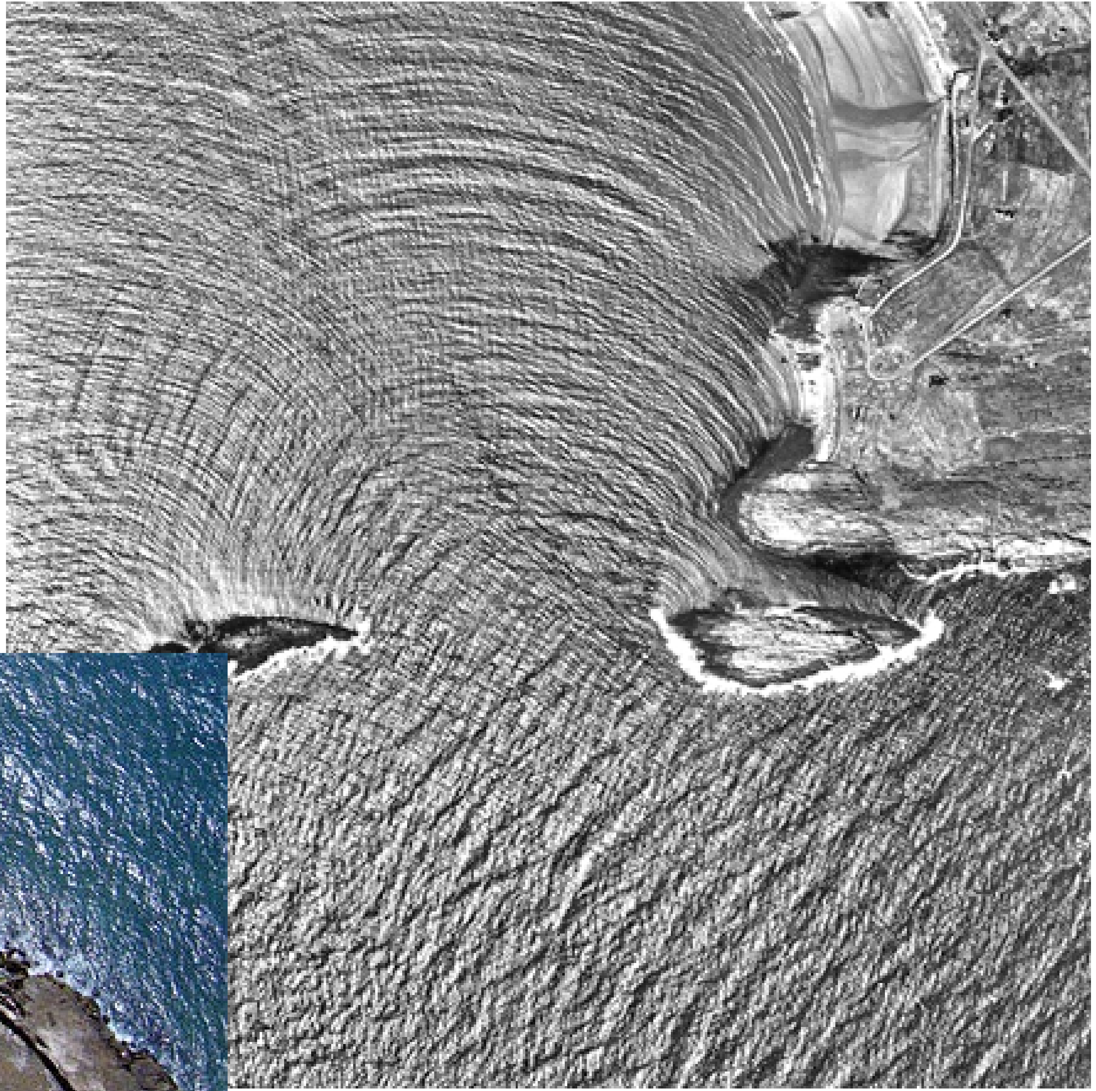


Energy , or $\hbar\omega$

Reciprocal space, or Q

We directly visualize excitations in condensed matter. **Example:** Phonon dispersion curves of silicon taken. Data taken on ARCS spectrometer at SNS (PNAS, Fultz et al, 2018)

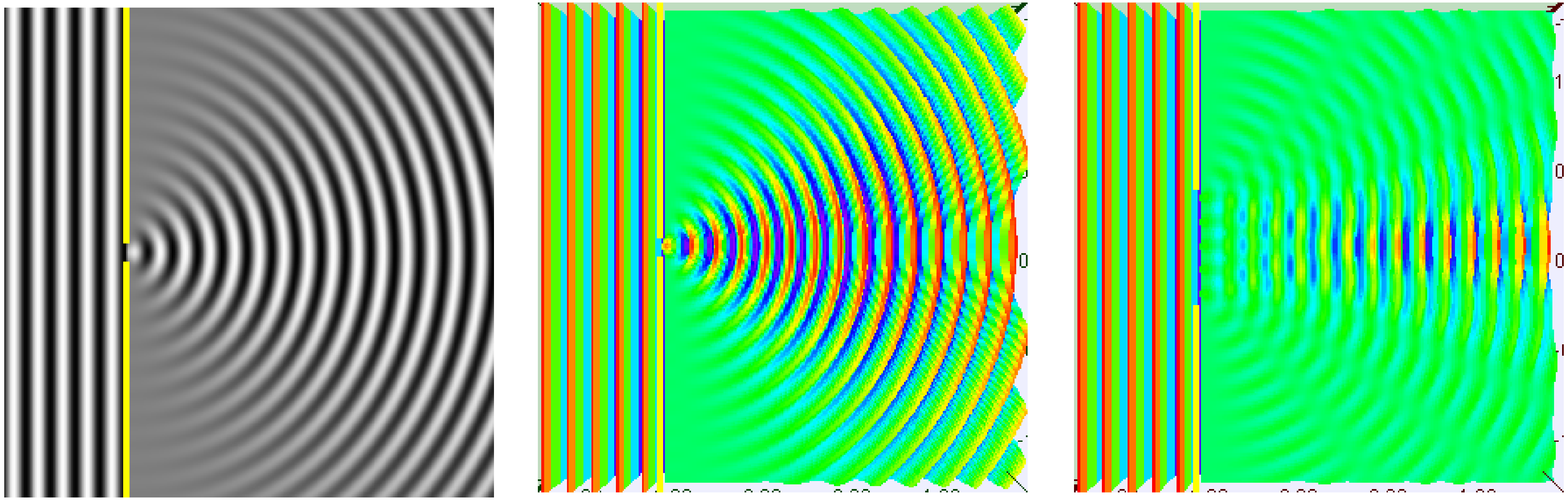
Diffraction at
the beach!



interference
of waves

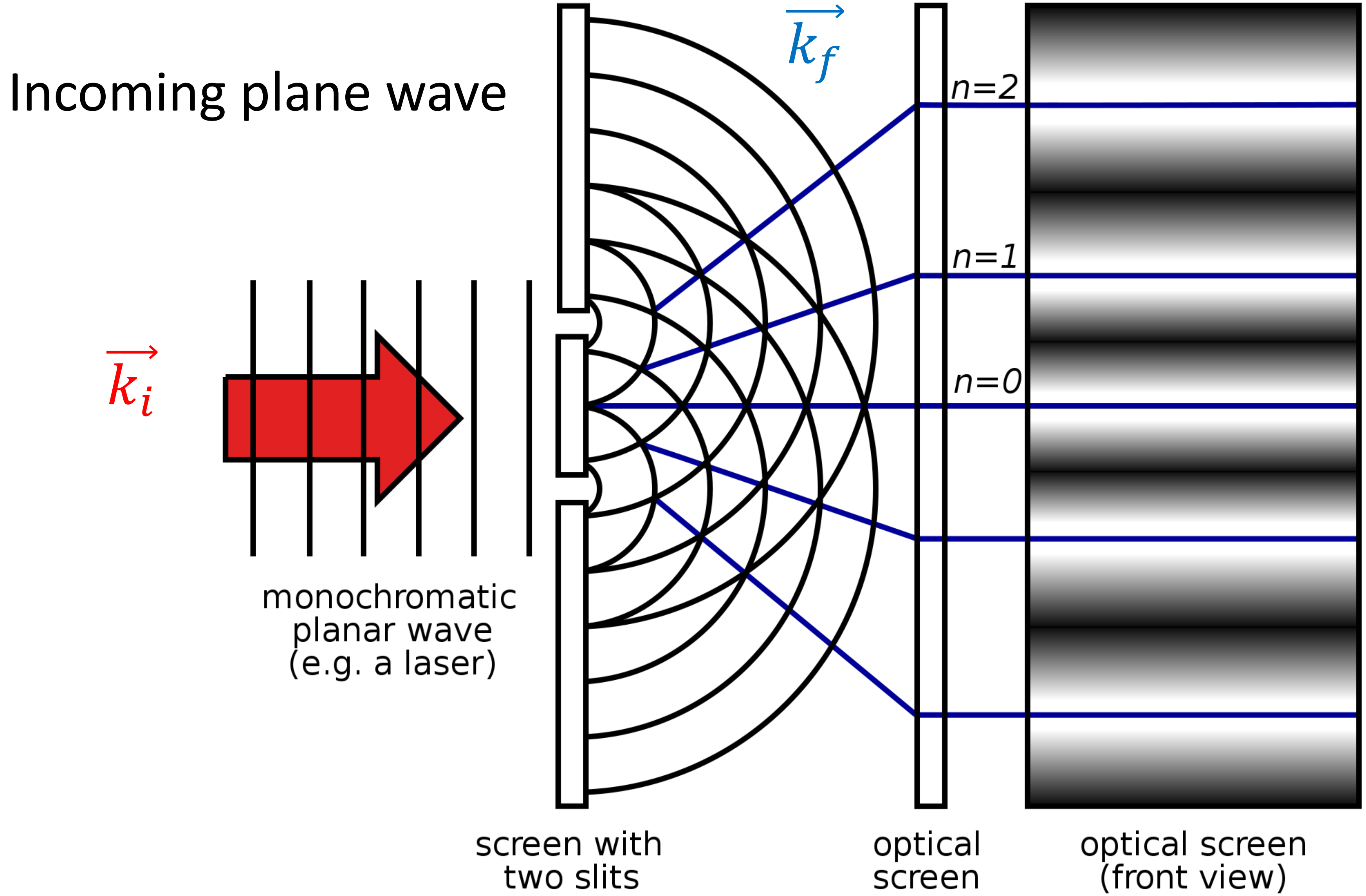
What is diffraction?

- Scattering of a wave from an object, so that it becomes like a point source of a radial wave.
- Example a slit diffracts a plane wave.
- Circular waves emerge from the slit.
- Key is that slit size must be similar in scale to wavelength of wave!



GIFs of plane wave arriving at a slit

Young’s double slit experiment



The scattered waves are radial waves and destructively and constructively interfere to make a diffraction grating.

The scattering is described as ***elastic***, since no energy transfer leads to the same wavelength.

$$|\vec{k_i}| = |\vec{k_f}| = \frac{2\pi}{\lambda}$$

Scattering geometry basics: The plane wave

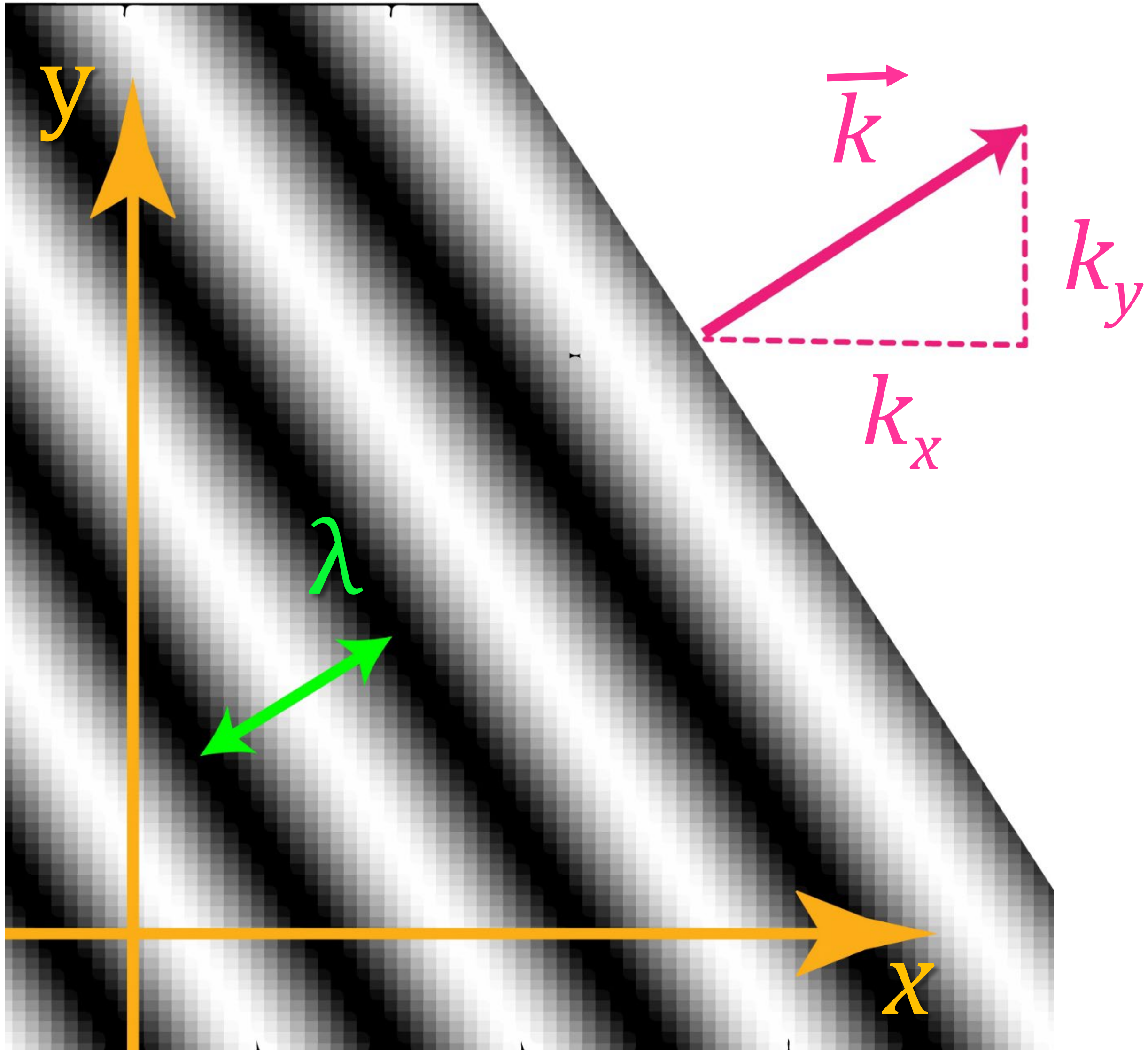
We define a plane wave:
Amplitude in the *z*-direction,
Propagates in *y*- and *x*-directions.

$\vec{r}$ = direction of propagation

$\vec{k}$ = wavevector

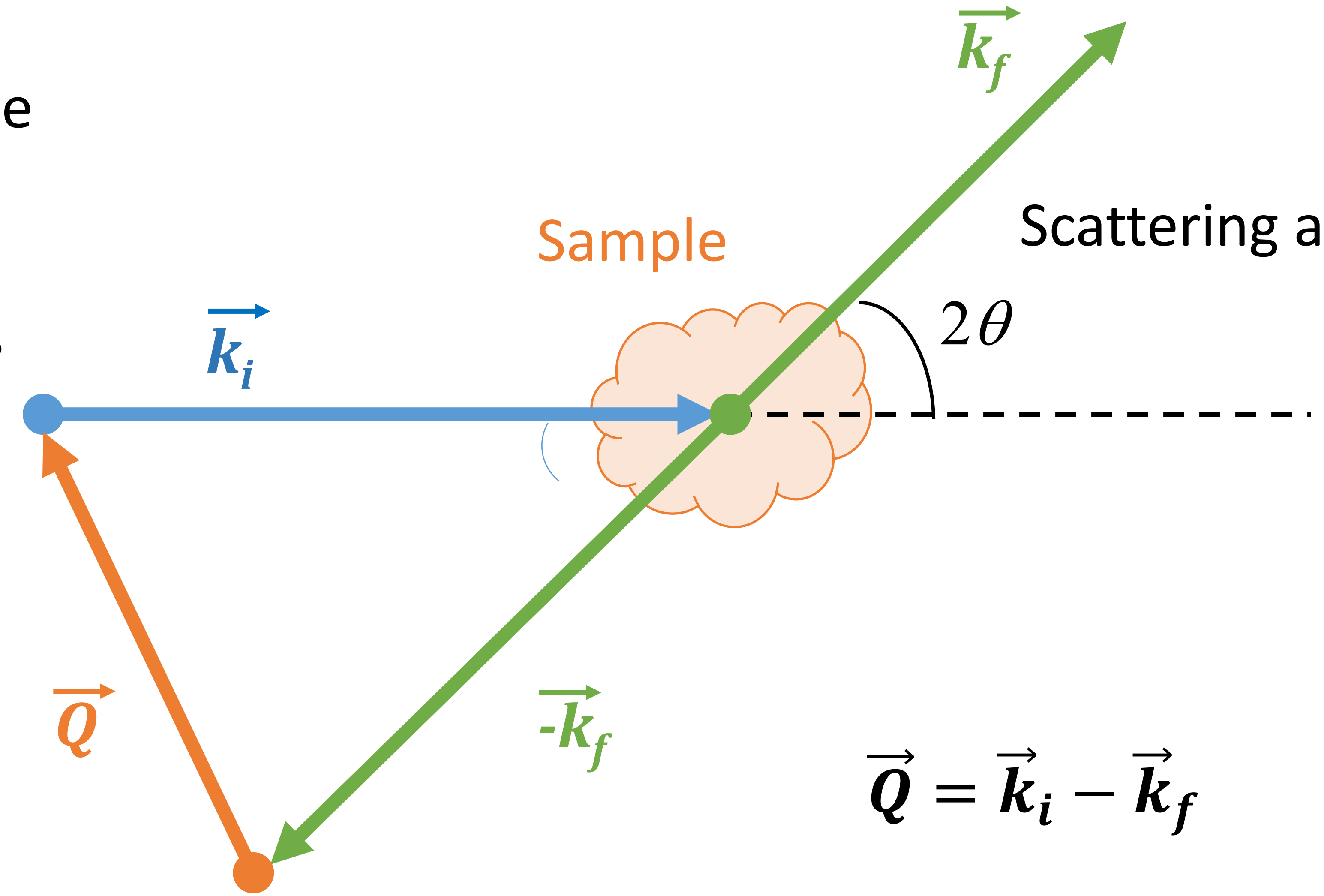
$$|\vec{k}| = \frac{2\pi}{\lambda}$$

$$\psi = A\sin(\vec{k}\cdot\vec{r}+\varphi)$$



Momentum transfer or Q

- k_i is the incident wavevector and k_f is the scattered wavevector
- Useful to work with another vector besides k_i or k_f
- We define $\vec{Q}$, as our **momentum transfer**



$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

Momentum transfer, or Q-space

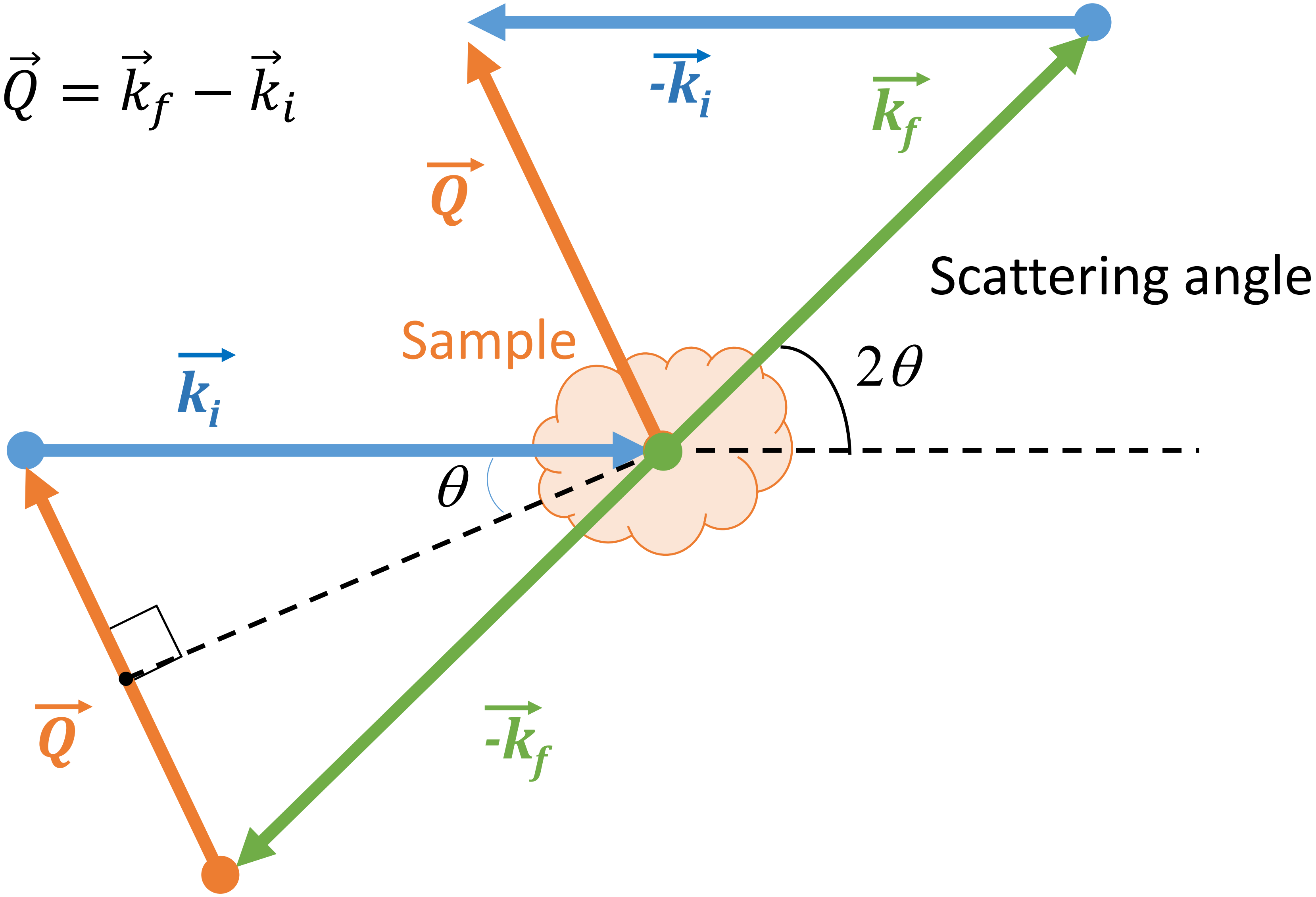
$$\vec{Q} = \vec{k}_i - \vec{k}_f \quad \text{or} \quad \vec{Q} = \vec{k}_f - \vec{k}_i$$

$$|\vec{k}| = \frac{2\pi}{\lambda}$$

For elastic scattering, no energy transfer

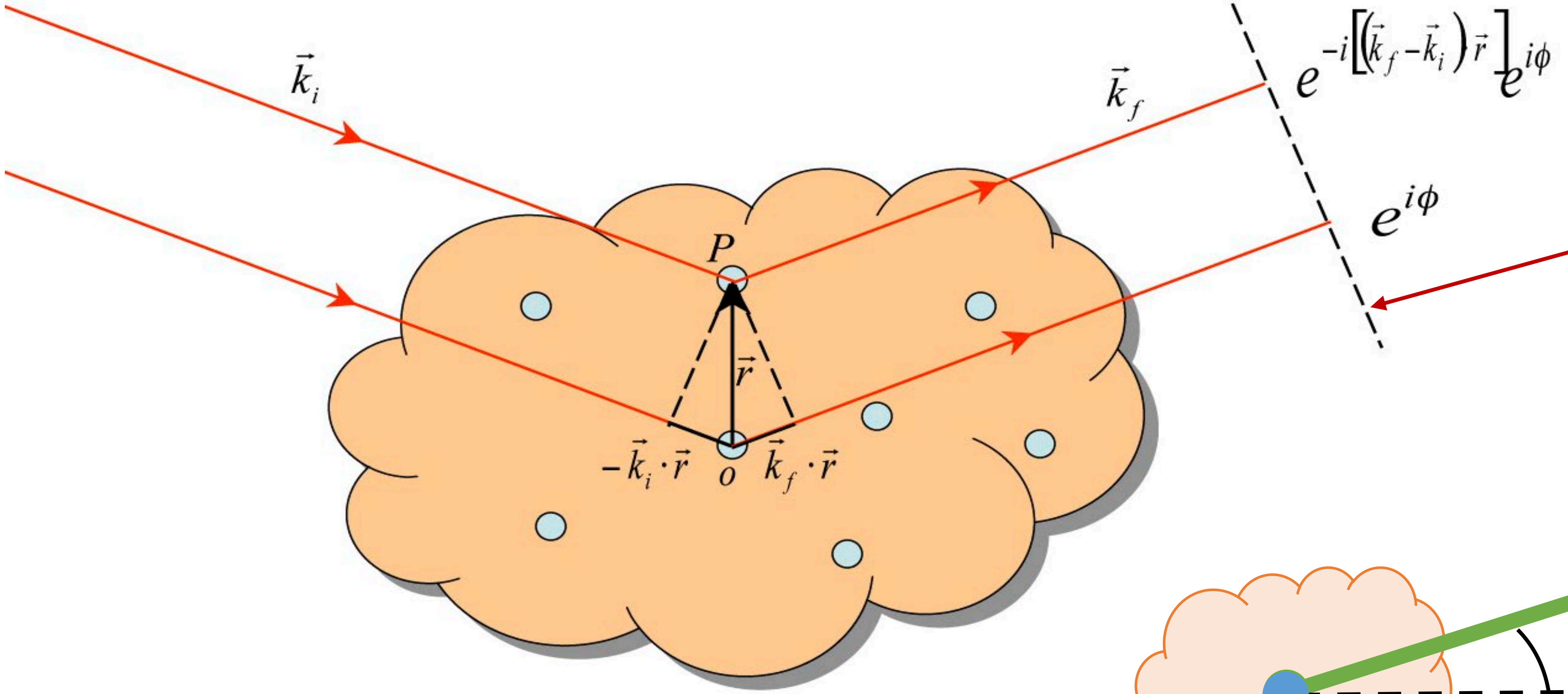
$$|\vec{k}_i| = |\vec{k}_f|$$

$$\frac{|\vec{Q}|}{2} = |\vec{k}| \sin\theta$$

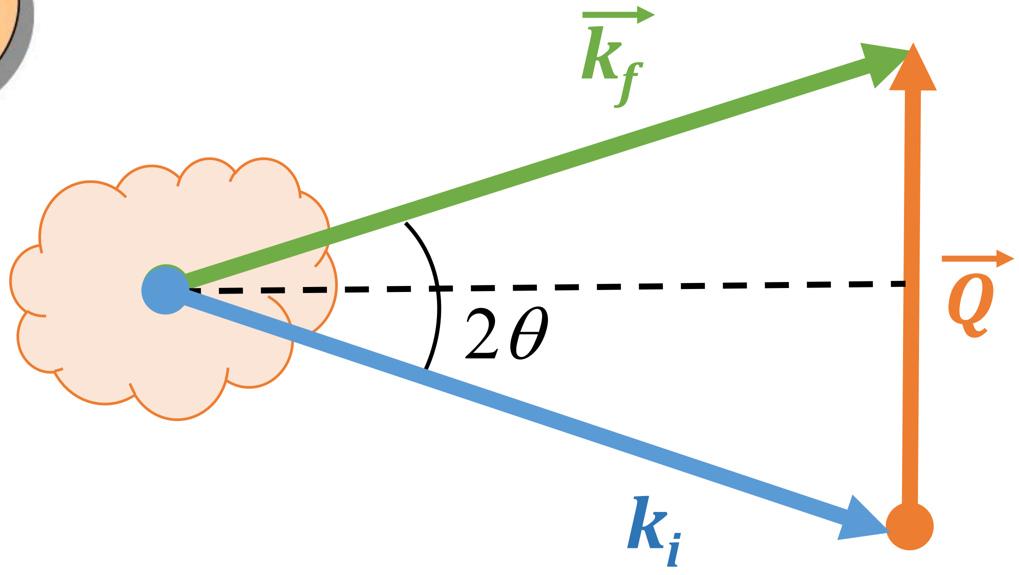


Scattering from an ensemble of atoms

$$\vec{Q} = \vec{k}_f - \vec{k}_i$$



Waves scattered can add up in phase



$$|\vec{Q}| = \frac{4\pi \sin\theta}{\lambda}$$

The Fourier transform

- We call $F(k)$ the Fourier transform of $f(x)$, and vice versa
- We can toggle between real space (x) and reciprocal space (k)

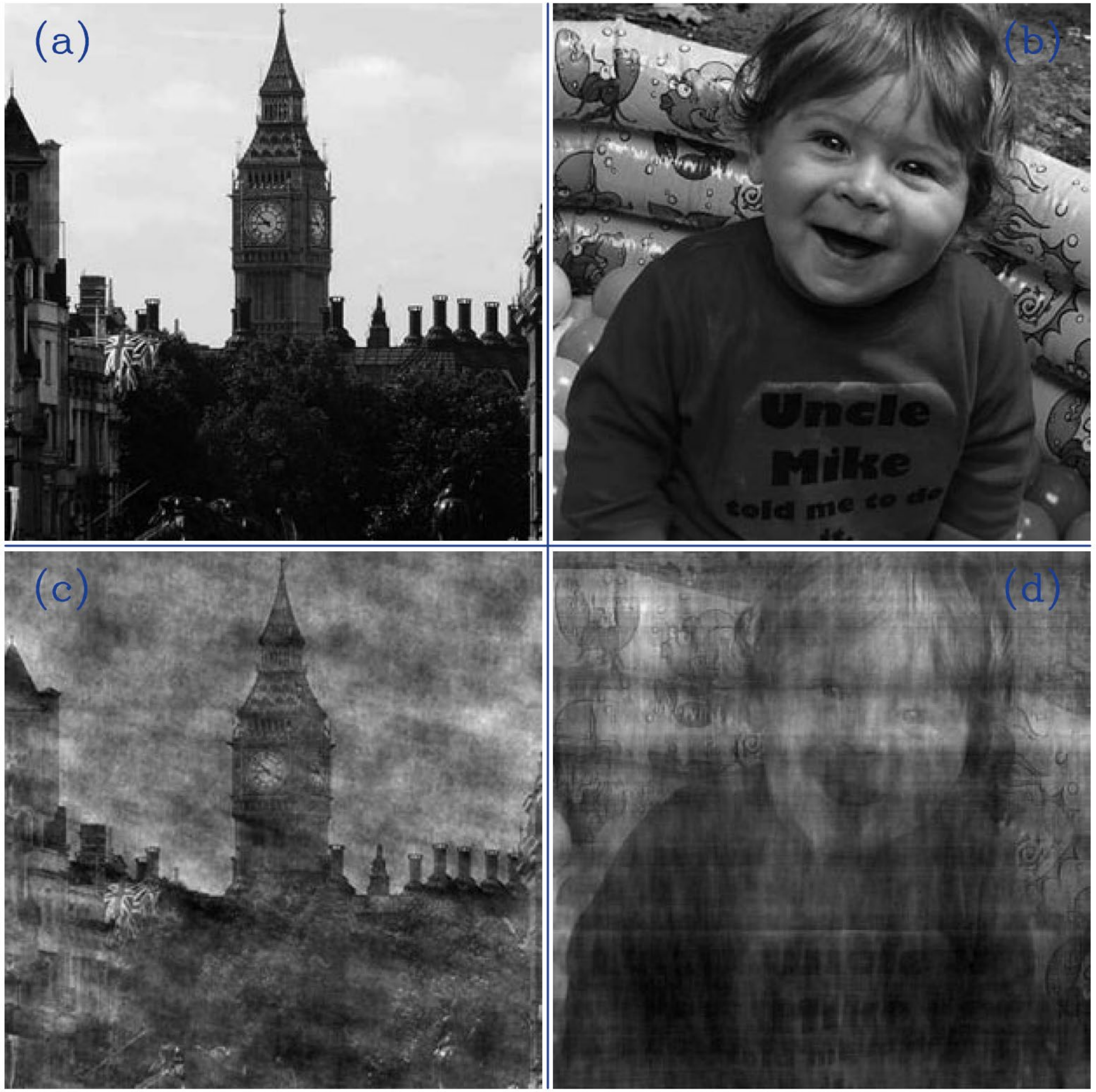
$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{\mathrm{i}kx} \mathrm{d}k$$

Real space function as Fourier transform of function *F*(*k*)

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-\mathrm{i}kx} \mathrm{d}x$$

k-space function as an inverse Fourier transform of real space function *f*(*x*)

The phase problem in scattering experiments



- The Fourier transform includes information on the amplitude and phase (or argument) of the function.
- Pictures of (a) Big Ben and (b) Lil' Ben.
- In (c) the amplitude from Lil' Ben is mixed with the phase information of Big Ben. The resulting inverse Fourier transform looks like Big Ben.
- In (d) the amplitude form Big Ben is mixed with the phase information of Lil' Ben, resulting inverse Fourier transform is Lil' Ben.

From D. S. Sivia, Elementary Scattering Theory