X-Rays and Matter

In a diffraction experiment, the X-ray beam interacts with the crystal, giving rise to the diffraction pattern. A crystal is a three-dimensional periodic discontinuum, which can be understood as a lattice. The X-ray beam is a monochromatic electromagnetic wave.

X-Rays

Generating X-Rays

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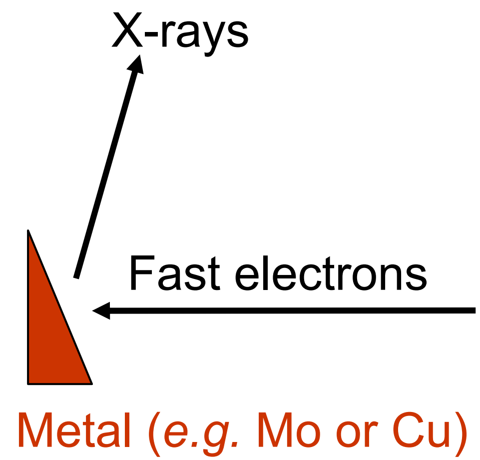
Please see:
Massa, Werner. *Crystal Structure Determination. 2nd ed.* Translated into English by R. O. Gould. New York, NY: Springer, 2004, pp.13. ISBN: 3540206442.

Fig. 3.1



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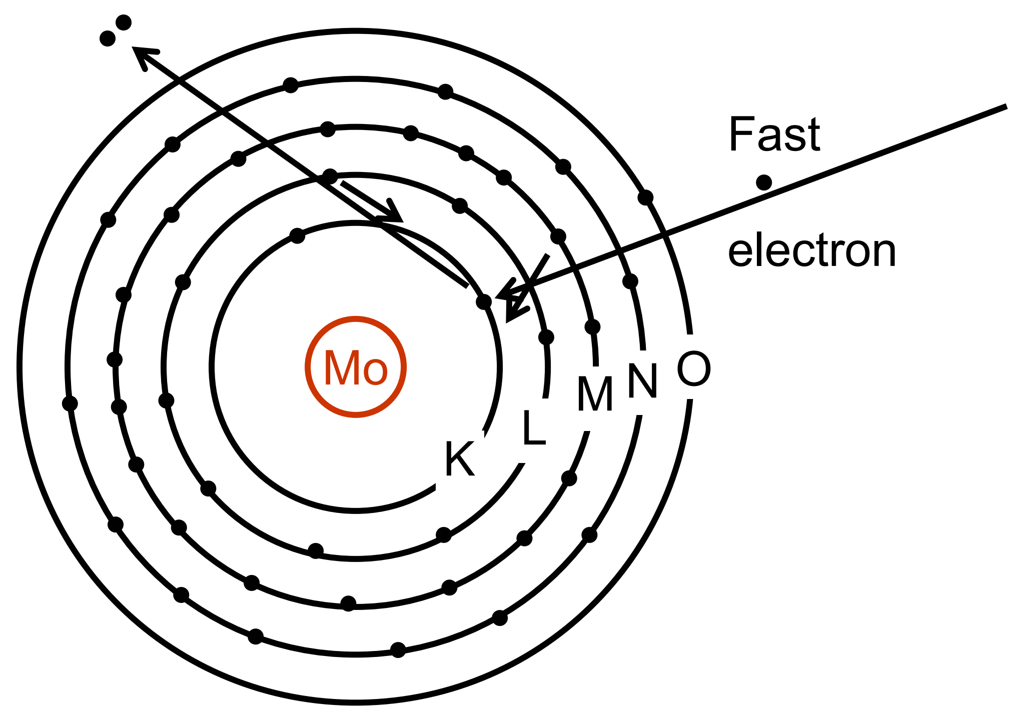
Massa, Werner. *Crystal Structure Determination. 2nd ed.* Translated into English by R. O. Gould. New York, NY: Springer, 2004, pp.14. ISBN: 3540206442.

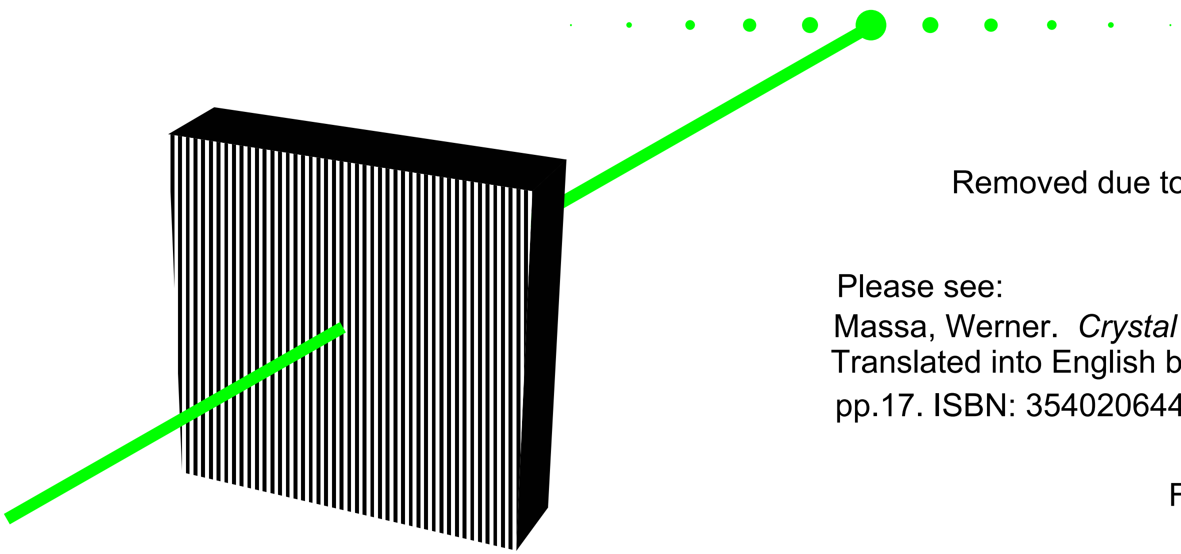
Fig. 3.2



X-Rays and Matter

What happens when a beam of monochromatic electromagnetic waves hits a lattice?

Constructive interference happens only at certain angles, depending on wavelength and lattice constant (spacing between the grid lines).



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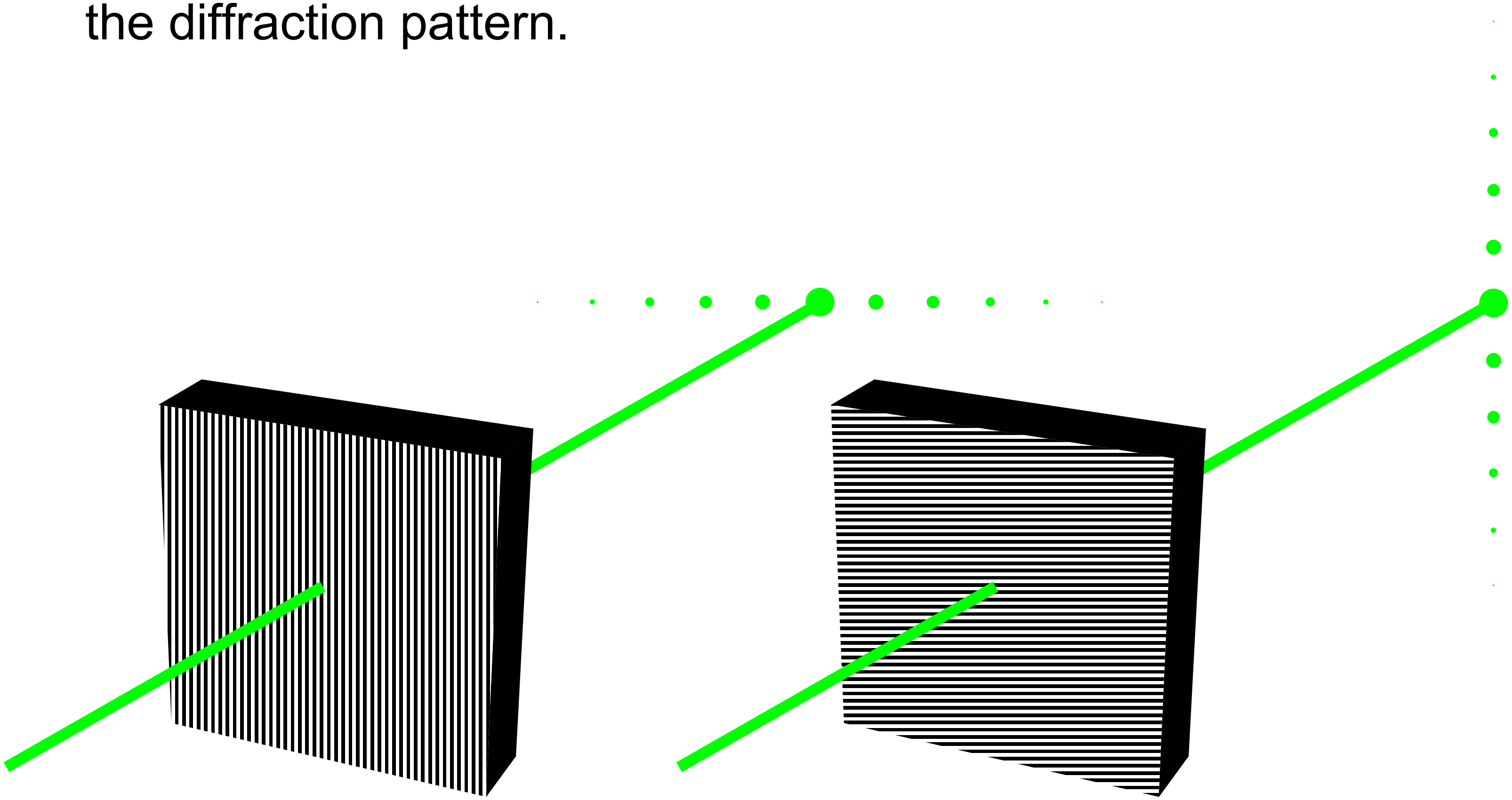
Please see:
Massa, Werner. *Crystal Structure Determination. 2nd ed.* Translated into English by R. O. Gould. New York, NY: Springer, 2004, pp.17. ISBN: 3540206442.

Fig. 3.4

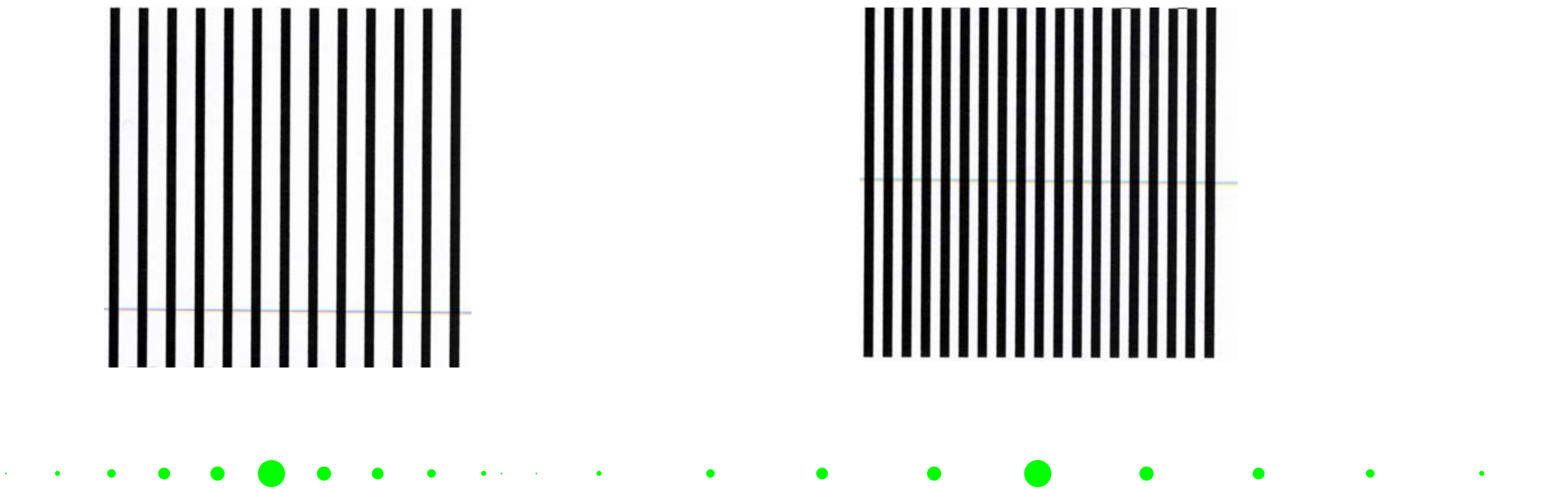
X-Rays and Matter

Diffraction is invariant to translation. But rotation of the lattice rotates the diffraction pattern.



X-Rays and Matter

Halfing the lattice constant doubles the distance between the spots.



X-Rays and Matter

Now: Two dimensional case. Shine the laser through a regular array of dots:

X-Rays and Matter

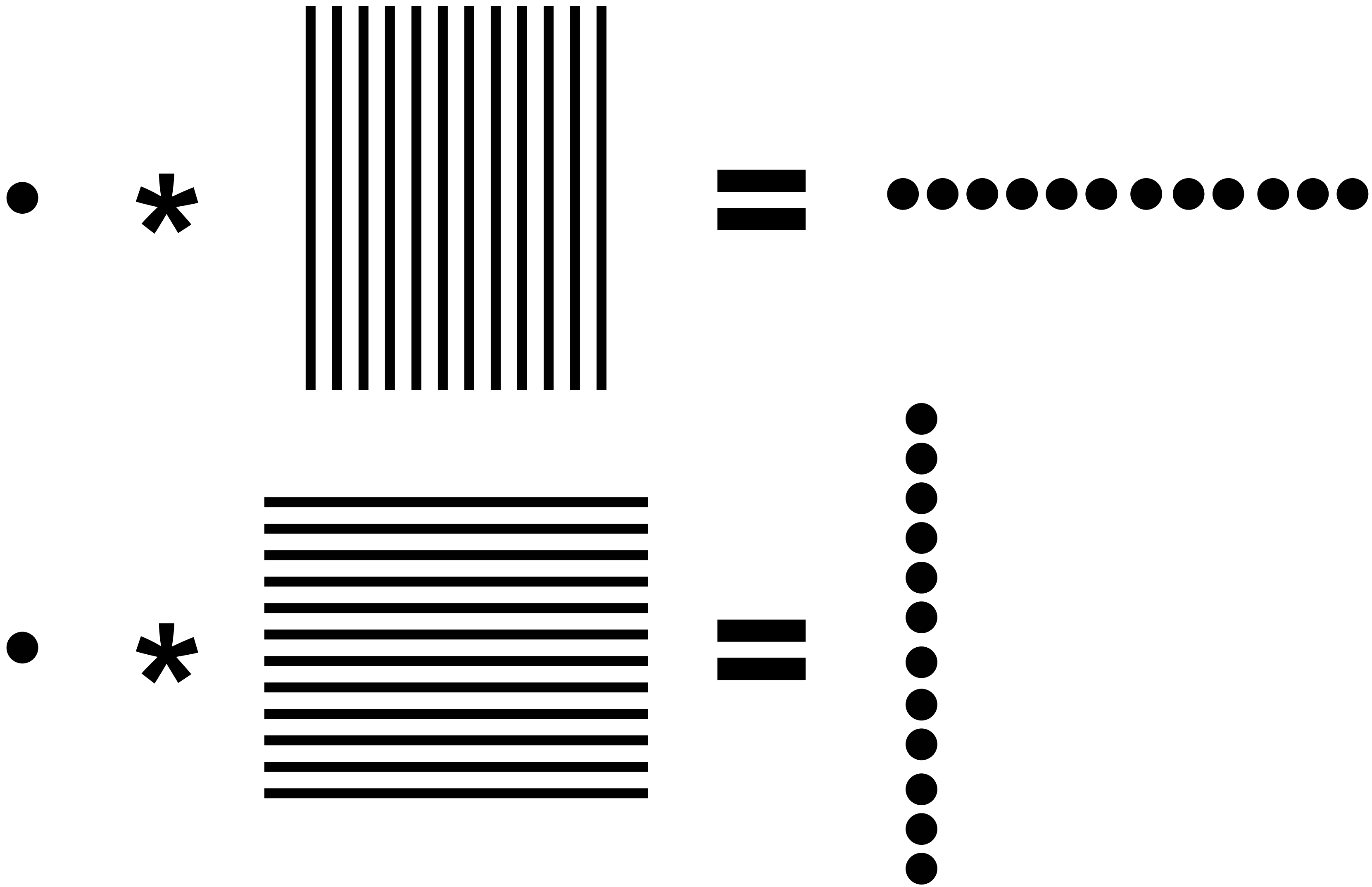
Removed due to copyright restrictions.

Please see:
Lisensky, George C., et al. *Optical Transform Kit*. Madison, WI: University of Wisconsin Board of Regents, Institute for Chemical Education, 1994, pp. 13.

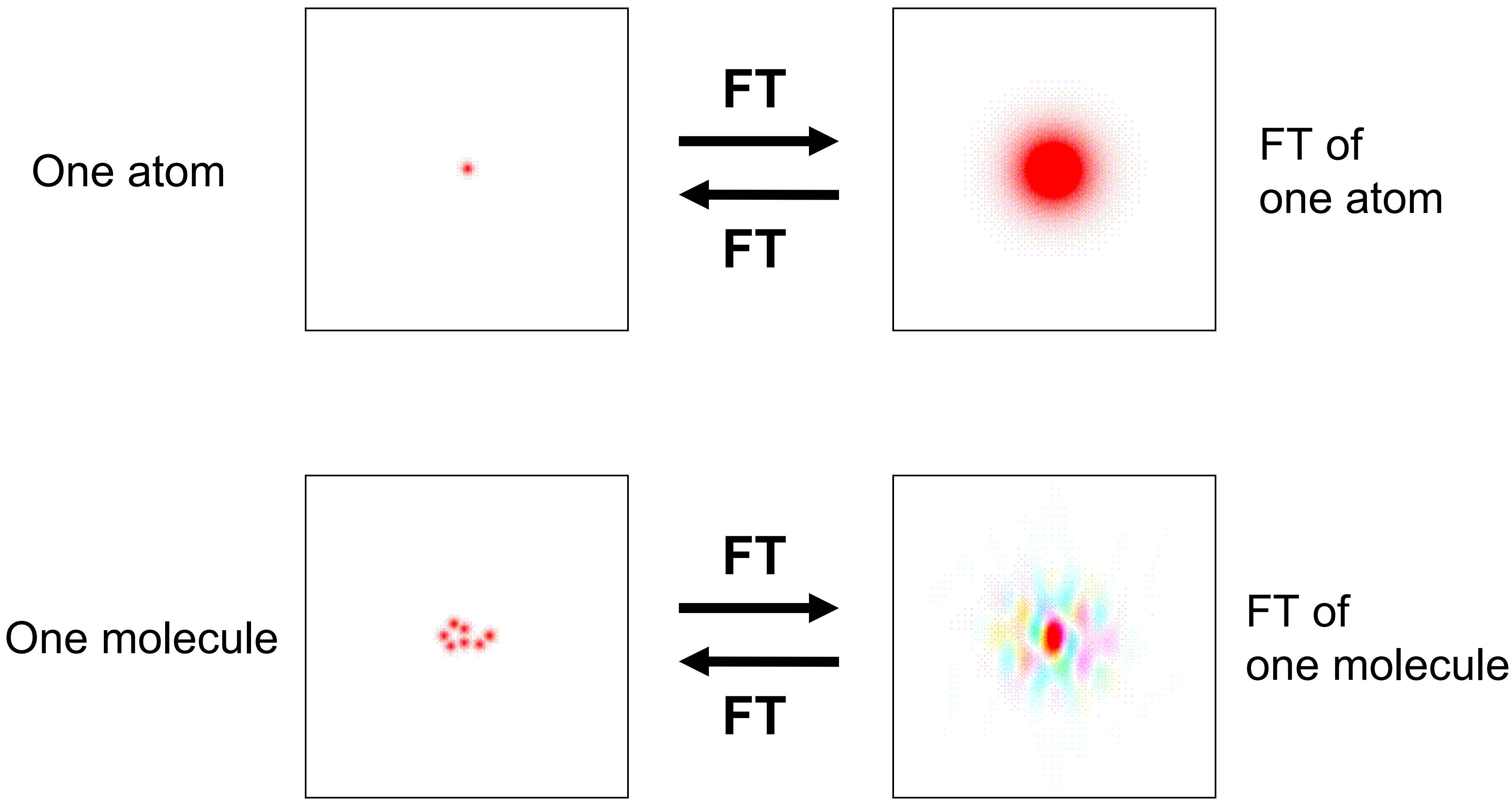
Figs. 2-3

Convolution Theorem

Diffraction is convolution of the beam (dot or sphere) with the lattice:



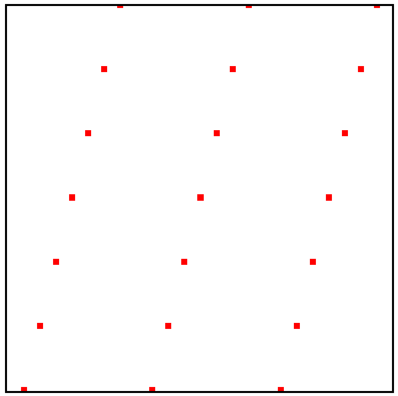
Fourier Transformation



Courtesy of Kevin Cowtan. http://www.ysbl.york.ac.uk/~cowtan/ Used with permission.

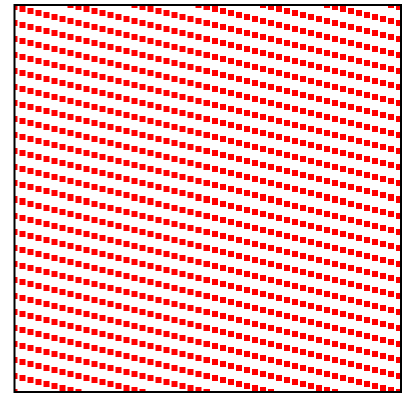
Fourier Transformation

A lattice



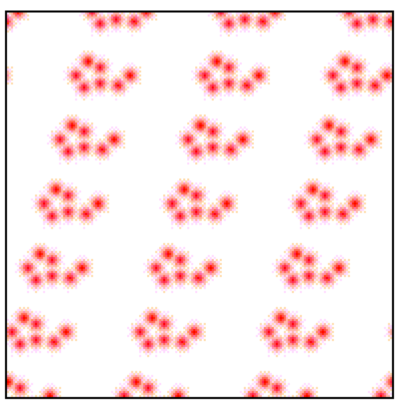
FT

FT



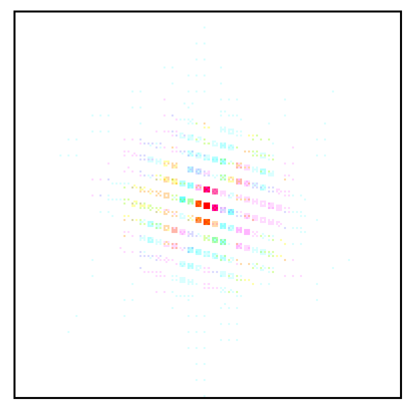
FT of
a lattice

A lattice of
molecules
(a crystal)



FT

FT

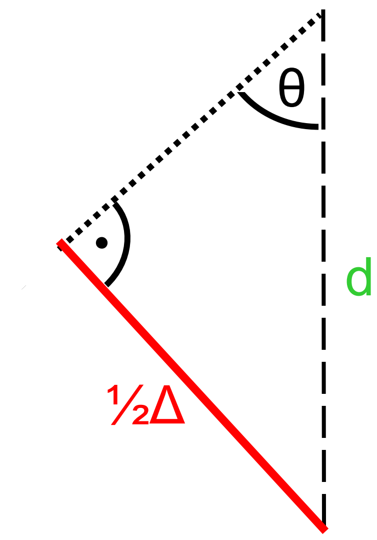


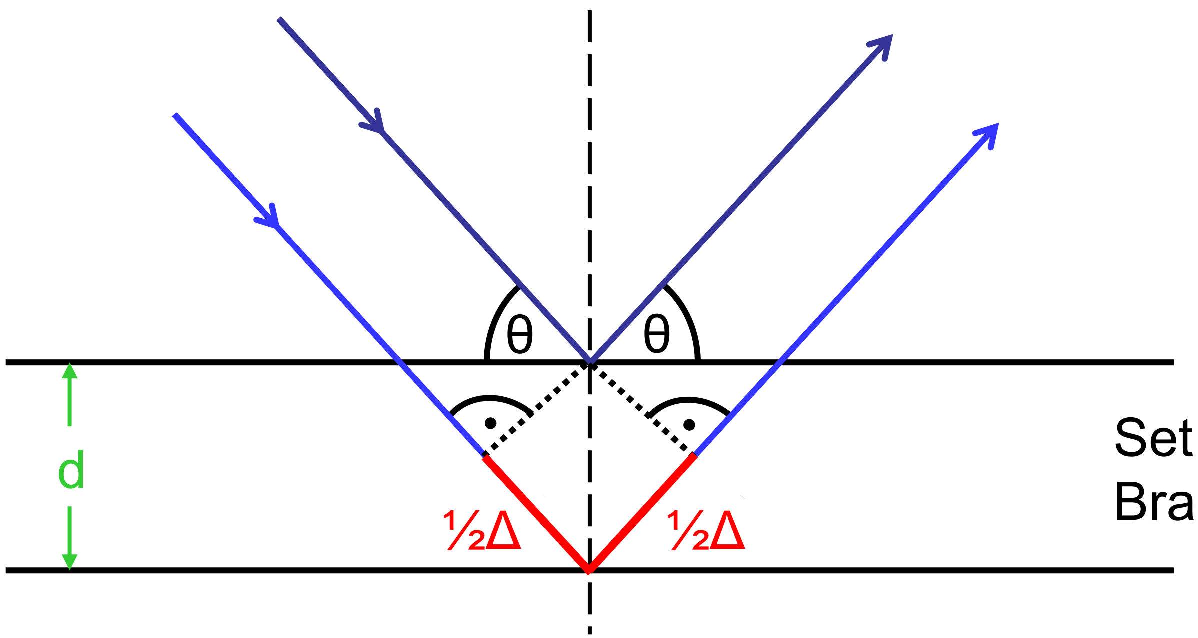
FT of
a crystal

Reflection on Lattice Planes

$$\sin\theta = \frac{\tfrac{1}{2}\Delta}{d} = \frac{\Delta}{2d}$$

Bragg's Law: $\Delta = \boxed{2d\sin\theta = n\lambda}$

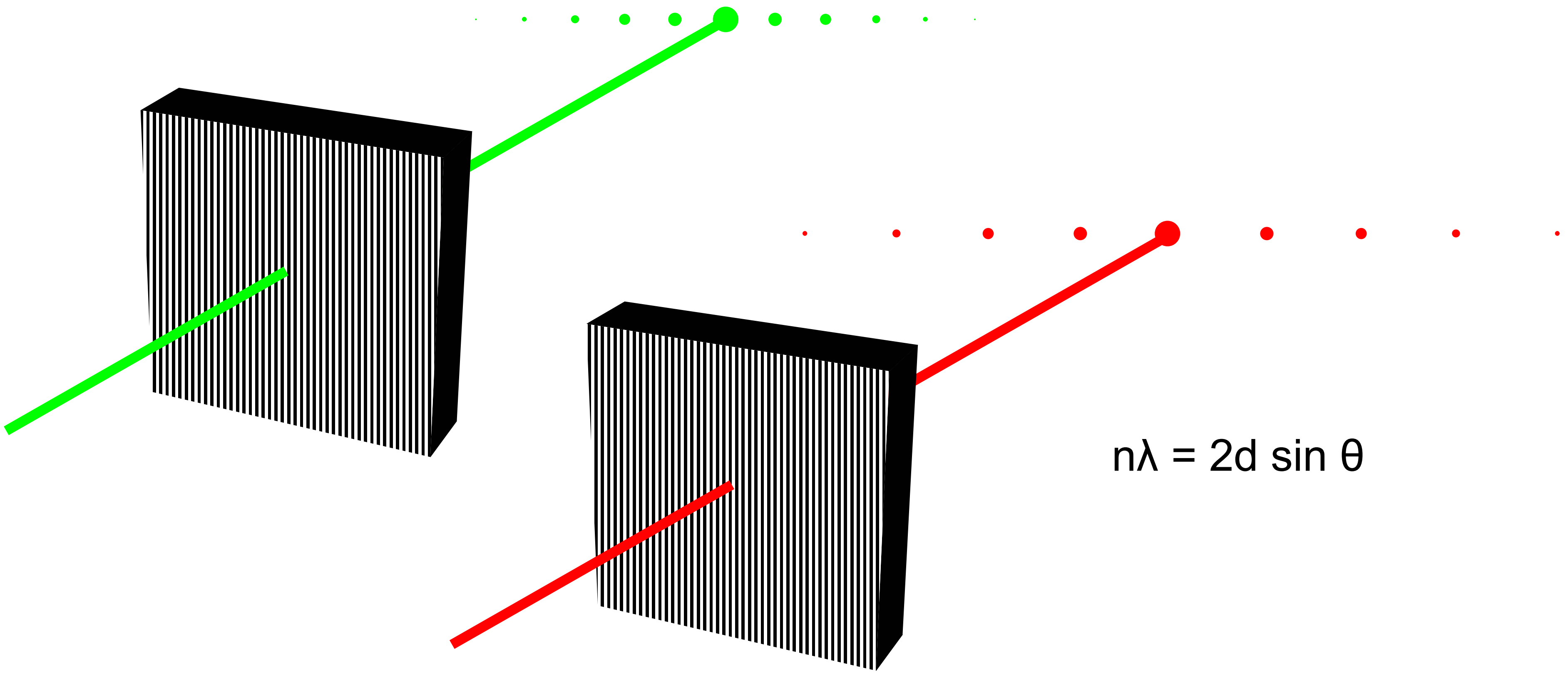




Set of parallel planes:
Bragg planes

X-Rays and Matter

What does the wavelength do?



$n\lambda = 2d \sin \theta$

3D Bragg Planes: Miller Indices (h, k, l)

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Please see:
Massa, Werner. *Crystal Structure Determination. 2nd ed.* Translated into English by R. O. Gould. New York, NY: Springer, 2004, pp. 21. ISBN: 3540206442.

Fig. 3.8, 3.9

3D Bragg Planes: Miller Indices (h, k, l)

Please see:
Massa, Werner. *Crystal Structure Determination. 2nd ed.* Translated into English by R. O. Gould. New York, NY: Springer, 2004, pp. 21. ISBN: 3540206442.

Fig. 3.8, 3.9

Real Space → Reciprocal Space

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Massa, Werner. *Crystal Structure Determination. 2nd ed.* Translated into English by R. O. Gould.
New York, NY: Springer, 2004, pp. 21. ISBN: 3540206442.
Fig. 3.8, 3.9

Between the points of a crystal lattice in real space, we have Bragg planes.
Each set of Bragg planes corresponds to one reflection.
Each set of Bragg planes corresponds to one set of Miller indices.
Each reflection is identified by the corresponding Miller indices (h, k, l).
The reflections form another lattice, the reciprocal lattice.

Real Space → Reciprocal Space

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Please see:
Massa, Werner. *Crystal Structure Determination. 2nd ed.* Translated into English by R. O. Gould.
New York, NY: Springer, 2004, pp. 21. ISBN: 3540206442.

Fig. 3.8, 3.9

The vector d is perpendicular to a set of Bragg planes.
Its length is equivalent to the distance between two Bragg planes.
Each reflection (h, k, l) marks the endpoint of the vector d* = 1/d = s.
The length of s is inversely related to the distance between the Bragg planes.

The Reciprocal Lattice: Ewald Construction