Two-Dimensional Diffraction

Your primary learning goals for this lab are

To learn the fundamental physics of crystallography, namely

crystal = lattice plus basis

the convolution theorem

FT(crystal) = FT(lattice) times FT(basis)   (via the convolution theorem)

that all crystals are members of a finite set of symmetries (the 17 2d space groups)

that scattering produces the FT in the far-field limit (via the first Born approximation)

that reciprocal space is momentum space

that crystals contain a discrete set of momenta

that these crystal momenta come from the discretely broken translational symmetry

that the crystal momenta can be, and are, transferred to the photon, electron, etc.

the Bragg formulation of diffraction in position space

The Laue-Ewald formulation of diffraction in momentum space

You should observe and understand the following

How does the diffraction pattern depend on the symmetry of the 2d lattice

How does the diffraction pattern depend on the size of the 2d lattice

How does the diffraction pattern depend on the shape of the basis

How does the diffraction pattern depend on the size of the basis

How do you determine/calculate the size of the 2d lattice from the diffraction pattern

How do you determine the size and the shape of the basis from the diffraction pattern

You should investigate all of the above using optical diffraction (i.e., the laser and the optical crystals) and using computer diffraction (i.e., the applet at http://escher.epfl.ch/fft/)

Learning Goals for Becky's Slides

For Slides 1.1 to 1.4

Compute the optical Fourier transform for her 2d gases composed of large diamonds, small diamonds, large squares, and small squares. Compare each case with the corresponding computer simulation.

Explain how the diffraction pattern depends on the shape of the objects.
Explain how the diffraction pattern depends on the size of the objects.

For Slides 2.1 to 2.4

Compute the optical Fourier transform for her 2d gases composed of triangles, dots, rectangles, and crosses. Compare each case with the corresponding computer simulation.

Explain how the diffraction pattern depends on the shape of the objects.

For Slides 3.1 to 3.4

Compute the optical Fourier transforms for her different size dots on the same rectangular lattice. Compare each case with the corresponding computer simulation.

Explain how the optical diffraction pattern depends on the size of the dots.

For Slides 4.1 to 4.4

Compute the optical Fourier transforms for her different shape objects (squares, dots, triangles, and rectangles) on the same rectangular lattice. Compare each case with the corresponding computer simulation.

Explain how the optical diffraction pattern depends on the shape of the basis elements.

Remember :

Diffraction from a 2d gas is used to boost the intensity of the scattering. Its envelope has the same intensity pattern as a single copy of the object, but is much brighter and thereby easier to observe.

You do not need to create a 2d gas to compute the Fourier transform of the basis using the fast Fourier transform (FFT)---you need only compute the FFT of (one copy of) the object.

Learning Goals for the 1974 Optical Crystals

The Fourier transform of a Bravais lattice is another Bravais lattice.

All crystals can be built using a Bravias lattice together with a basis. The basis element decorates the lattice---there is one copy of the basis located at each point in the Bravais lattice. The Fourier transform of the crystal is the product of the Fourier transform of the lattice times the Fourier transform of the basis.

There are five Bravais lattices in two dimensions: oblique, triangular (also called hexagonal), square, rectangular, and face-centered rectangular. You should understand how to calculate the five reciprocal lattices from the five real lattices.

There are four examples of Bravias lattices on these slides:

2d. A rectangular lattice of dots
3d. A hexagonal lattice of dots
7a. Another rectangular lattice of dots
7b. A rectangular lattice with faced-centered dots
7c. There is also a rectangular lattice with side-centered dots, but this is not a Bravais lattice. Why?

There are two examples of lattices decorated with the basis element “A”

6c. A rectangular lattice, decorated with the basis “A”
6d. A hexagonal lattice, decorated with the basis “A”
6a. There is also a set of randomly located copies of the basis “A” (also called a 2d gas of A’s)

Compute the Fourier transform of the letter A by measuring the optical diffraction pattern for 6a. You will see that the diffraction patterns for 6b and 6c are equal to the Fourier transform of their real space lattice multiplied by the Fourier transform of the letter “A” which is their basis.

There is one example of a non-Bravais lattice (namely 7c). It uses 3 dots as its basis

Compute the Fourier transform of its 3 dot basis by measuring the diffraction pattern for 7d. Compute the Fourier transform of its Bravais lattice by measuring the diffraction pattern for 7a. You will see that the diffraction pattern for 7c is equal to the Fourier transform of its real space lattice (7a) multiplied by the Fourier transform of its basis (7d)

Slide 5 shows how the Fourier transform of the basis depends on the size and shape of the basis

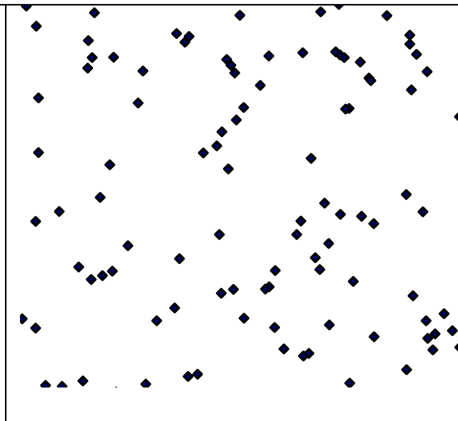
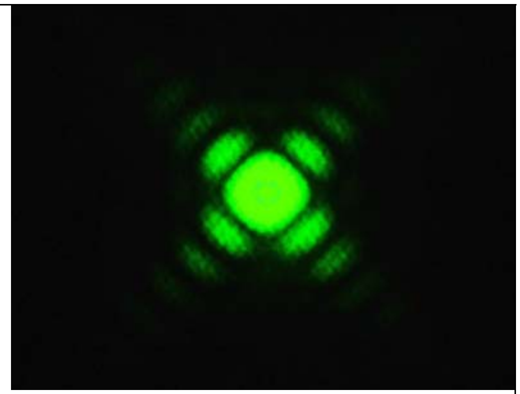
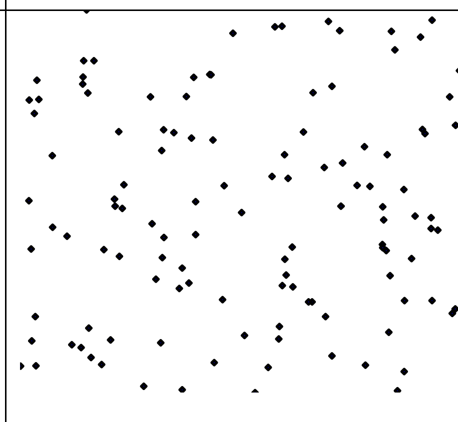
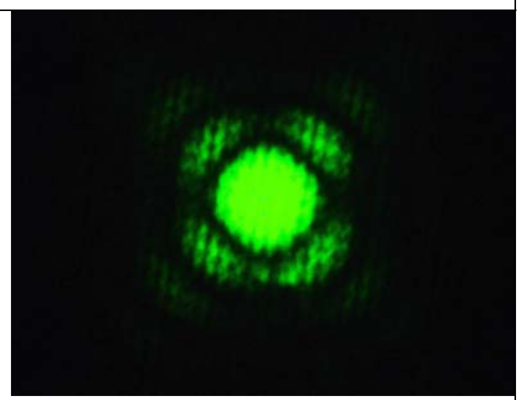
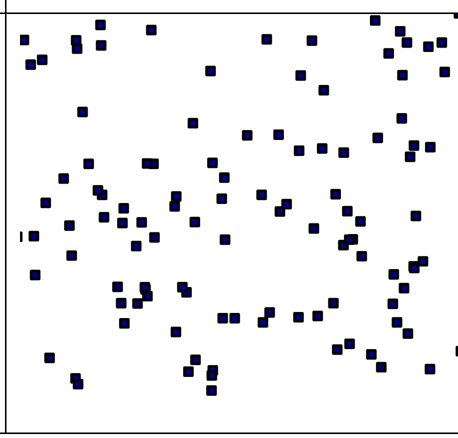
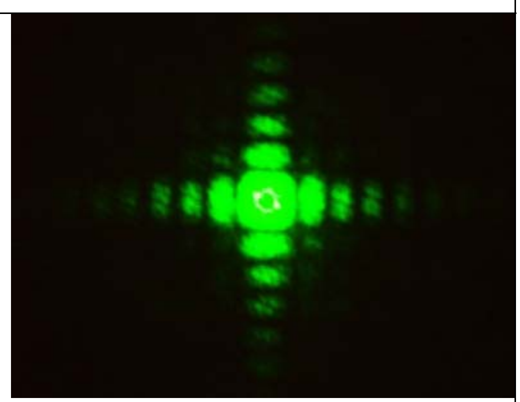
5a. Randomly located copies of asterisks, the size of each * is 0.1 mm
5b. Randomly located copies the size of each * is 0.05 mm
5c. Randomly located copies upper case S’s, the size of each S is 0.1 mm
5d. Randomly located copies of upper case S’s, the size of each S is 0.05 mm

Compare each case above with the corresponding computer simulation
The simulation applet is located at http://escher.epfl.ch/fft/

Slide 4 shows how three-dimensional diffraction emerges from interference between its 2d sub-lattices. There is interference because of the periodic spacing in the third direction.

4a. Two identical layers of dots, each layer has dots at random locations
4b. Two identical layers of dots, each layer is a hexagonal lattice
4c. Two identical layers of dots, each layer is a 2d rectangular lattice (spacing 0.12 by 0.18 mm)
4d. Two identical layers of dots, each layer is a 2d rectangular lattice (spacing 0.08 by 0.12 mm)

Becky's Slides

B-1.1 A gas of large diamonds		
B-1.2 A gas of small diamonds		
B-1.3 A gas of large squares		

The 1974 Slides

TABLE I. Description of optical crystals.

Sample	Composition	Diffraction Pattern
1a	A random array of dots.	The sample demonstrates the amorphous form factor of the characters used in Samples 1a–4d.
1b	A single row of dots making a one-dimensional crystal.	The sample produces a line diffraction pattern due to a one-dimensional lattice that can be aligned perpendicular or nearly perpendicular to the incident radiation. (See Fig. 2.)
1c	A one-dimensional crystal having a smaller spacing than Sample 1b.	The sample produces a pattern similar to that of Sample 1b except that the lines are spaced farther apart showing the reciprocal relationship between the lattice spacing and the spacing of the diffraction pattern.
1d	A one-dimensional crystal having a smaller spacing than Sample 1c.	See Sample 1c.
2a	Two parallel rows of dots.	Each of the lines of the diffraction pattern produced by one row of dots is broken into a dashed line. The variation in intensity along each line is similar to that produced by a double slit. (See Fig. 3.)
2b	Three parallel rows of dots.	Each of the lines of the diffraction pattern produced by one row of dots is broken into primary and secondary maxima resulting in an intensity variation along each line similar to that of a triple slit.
2c	Four parallel rows of dots.	Each of the lines of the diffraction pattern due to one row of dots is altered in intensity so as to be similar to that of a quad slit.
2d	Many parallel rows of dots (simple rectangular lattice).	The primary maxima produced by Samples 2a–2c reduce to bright spots and the secondary maxima vanish, leaving a spot pattern similar to the composition of the sample but rotated 90° due to the reciprocal relationship between the lattice and the diffraction pattern. (See Fig. 4.)
3a	One row of dots.	See Sample 1b.
3b	Two rows of dots at a 60° angle.	The diffraction pattern consists of two sets of lines with an angle of 60° between the sets. The pattern is brighter where the two sets of lines intersect.
3c	Three rows of dots, each row making a 60° angle with the other rows.	The diffraction pattern consists of three sets of lines. Each set makes a 60° angle with the other two sets. The intensity is much brighter where the lines intersect.
3d	More dots are added to Sample 3c to produce a full hexagonal array.	The diffraction pattern consists of bright spots (corresponding to the intersections of the lines of Sample 3c). The array of bright spots is similar to the array of dots in the sample except rotated 90°.
4a	Two identical layers of dots randomly distributed in each layer.	Corresponding dots of the two layers can be aligned with the incident radiation. The resulting pattern consists of circular rings as predicted by Laue theory for two scattering centers aligned with the incident radiation. When the sample is rotated, the rings open up and approach straight lines similar to those produced by Samples 1b–1d. (See Fig. 5.)
4b	A three-dimensional crystal consisting of two layers, each layer containing a hexagonal array of dots.	The spot pattern produced is quite similar to that produced by Sample 3d except that the interference due to the alignment of one dot from each layer with the incident beam removes some of the spots (see Sample 4a), thus limiting the spots to Laue zones. The pattern is typical of an electron diffraction pattern due to a thin monoclinic crystal.

Ronald Bergsten

TABLE I—(*Continued*)

Sample	Composition	Diffraction Pattern
4c	A three-dimensional crystal consisting of two layers, each layer containing a rectangular array of dots.	The diffraction pattern is similar to that produced by electrons incident on a thin simple orthorhombic crystal. The rectangular array of diffraction spots due to one layer is restricted to Laue zones which are produced due to the near alignment of one dot from each layer with the incident radiation (see Sample 4a). As the sample is rotated, other sets of Laue zones move across the field of bright spots causing each spot to blink. (See Fig. 6.)
4d	Similar to Sample 4c except different spacings.	See Sample 4c.
5a	A random array of asterisks.	The diffraction pattern illustrates the form factor associated with an asterisk.
5b	Similar to 5a except the asterisks are smaller.	The diffraction pattern is similar to that produced by 5a except that the diffraction pattern is larger, indicating the reciprocal relationship between the size of the symbol and the size of the diffraction pattern.
5c	A random array of S's.	The diffraction pattern illustrates the form factor associated with an S.
5d	Similar to 5c except the S's are smaller.	The diffraction pattern is similar to that produced by Sample 5c except that the pattern is larger.
6a	A random array of A's.	The diffraction pattern is characteristic of an A (form factor). (See Fig. 7.)
6b	One row of A's (one-dimensional crystal).	The resulting pattern combines the form factor and structure factor. A series of lines are produced characteristic of the periodicity of the crystal. (see Samples 1a–1d). These lines are only visible where there is brightness due to the form of the A (see Sample 6a and Fig. 8).
6c	A two-dimensional rectangular crystal made up of A's.	The resulting pattern combines the structure factor illustrated by Sample 2d with the form factor illustrated by Sample 6a.
6d	A two-dimensional hexagonal crystal of A's.	The resulting hexagon spot pattern as illustrated by Sample 6d is restricted by the diffraction patterns produced by Sample 6a.
7a	A simple rectangular crystal of dots.	A diffraction pattern characteristic of a rectangular array is produced (see Sample 2d). The resolution is increased since many more dots are used. (See Fig. 9.)
7b	Dots are added to the array of Sample 7a to produce a face-centered rectangular crystal.	The resulting pattern indicates Sample 7b does constitute a unique Bravais lattice. As is typical of x-ray diffraction by a face-centered crystal, the pattern is similar to that of a simple crystal except that some of the orders are missing. (See Figs. 9, 10.)
7c	Dots are added to the array of Sample 7a to make a side-centered rectangular crystal. (See Fig. 13.)	The resulting pattern is similar to that of Sample 7a with no orders missing, indicating that this sample does not constitute unique Bravais lattice. It is a simple rectangular crystal. The intensity of the spots corresponding to every other row and column is greater. This variation in intensity is due to the form factor of the element which is arranged in a rectangular manner. (See Figs. 11, 12, 13.)
7d	A random array of sets of three dots that constitute the element from which Sample 7c is made (see Fig. 13).	The resulting pattern should be compared to those produced by Samples 7a and 7c. This comparison clearly illustrates that the form factor of a set of the three dots as circled in Fig. 13 causes the variation of intensity of the spot pattern produced by Sample 7c. (See Figs. 12, 13.)