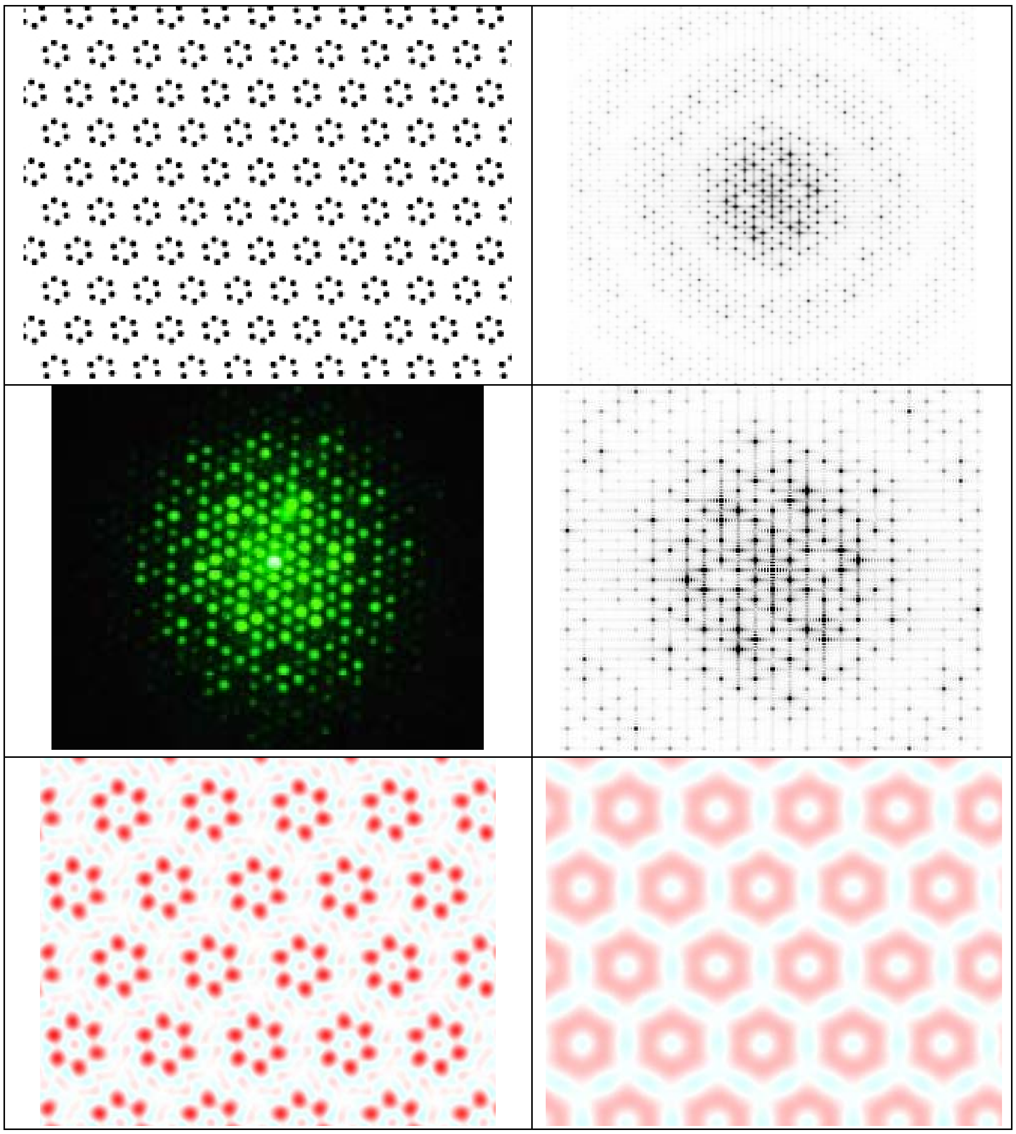
Experiments in Diffraction Using Optical Crystals and Computer Simulation



Rebecca Adams
Evening Physics Masters Project
Advisor: Dr. Larry Sorensen
University of Washington
June 7, 2007

Synopsis

The goal of this project was to develop a laboratory experiment on diffraction which integrated the following elements:

(a) existing and newly developed "optical crystals"

(b) graphics, tutorials, and simulations available on the web

(c) brief overview of some of the key concepts of diffraction and crystal structure, to provide context for the "hands-on" work with the optical crystals and computer simulations.

Most of the material is related to two-dimensional geometry and analysis, although some references are made to three-dimensional crystal geometry, where it's thought that these references would be helpful to allow the students to correlate the analytical or experimental results with real crystals and crystallographic techniques.

The intent of including the "overview" material is to re-familiarize students, who have had at least some background in optical physics and materials, with the nomenclature and mathematics relevant to the diffraction experiments. The information is presented assuming only general background or limited recall of these topics. It is not possible to provide a comprehensive treatment of all the necessary topics in a short paper, but references are provided for students who want more background.

The new optical crystal slides developed for this project are described in Appendix A. The patterns on these slides are designed to quickly demonstrate important concepts, by showing the effect of changing one feature at a time. For example, one slide which has four patterns of atoms of slightly different sizes, while the shape of the atom and the lattice geometry is the same. Another example is a slide which has four patterns of atoms of different shapes, while the size of the atoms is approximately the same, and again the lattice geometry is unchanged. See Figure S – 1 for the real space and diffraction pattern photographs from the slide with atoms of different shapes.

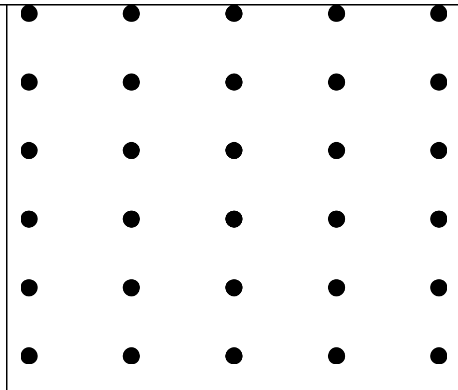
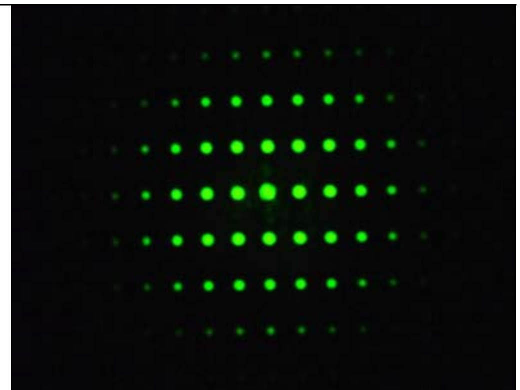
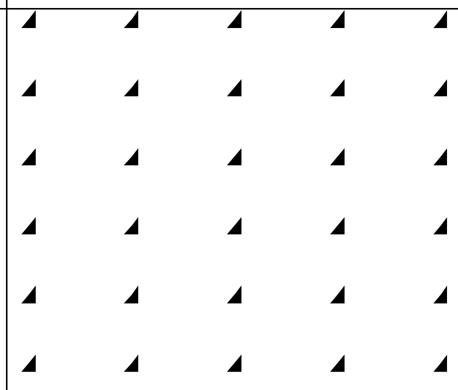
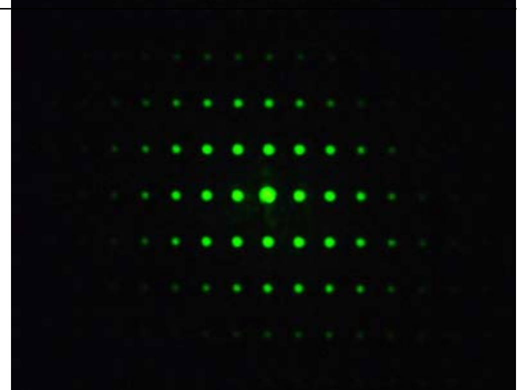
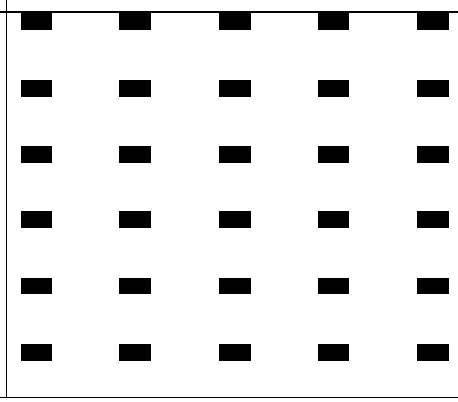
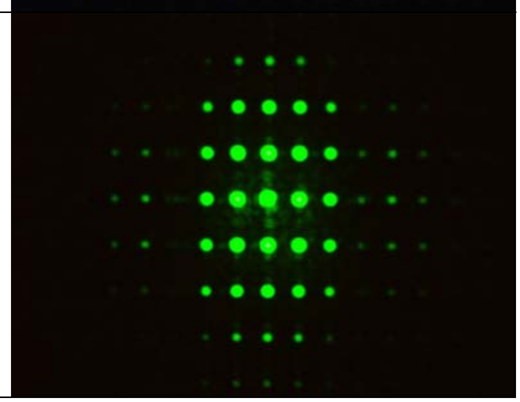
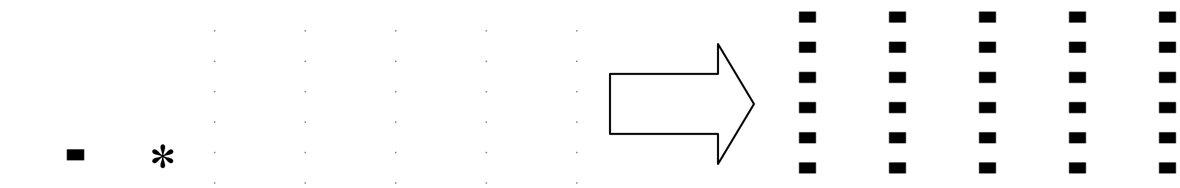
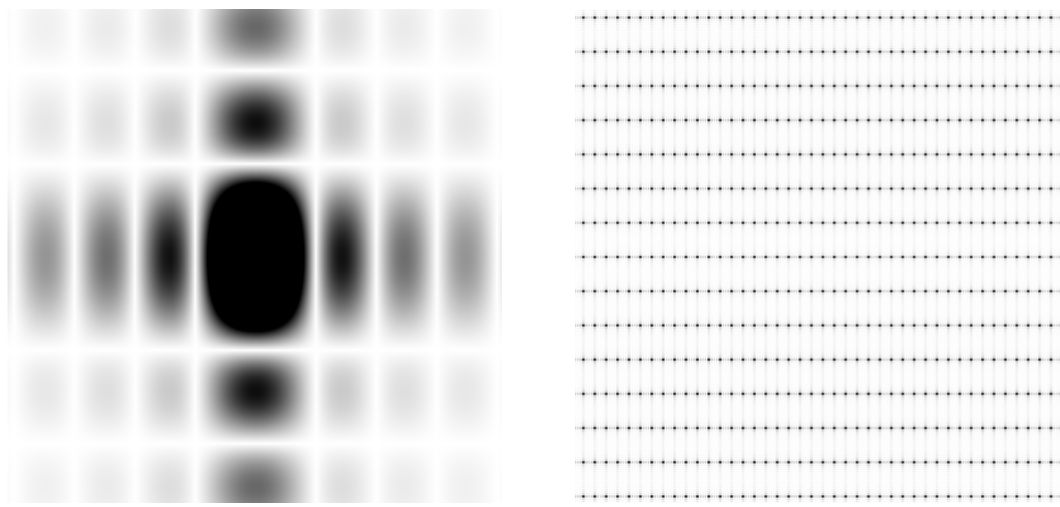
B-4.2 Dots (circles), 0.02 mm in diameter, in a rectangular array, 0.08 mm x 0.12 mm		
B-4.3 Triangles, 0.02 mm in height, in a rectangular array, 0.08 mm x 0.12 mm		
B-4.4 Rectangles, 0.02 mm x 0.04 mm, in a rectangular array, 0.08 mm x 0.12 mm		

Figure S – 1: Example of one of the new optical crystal slides developed for this project

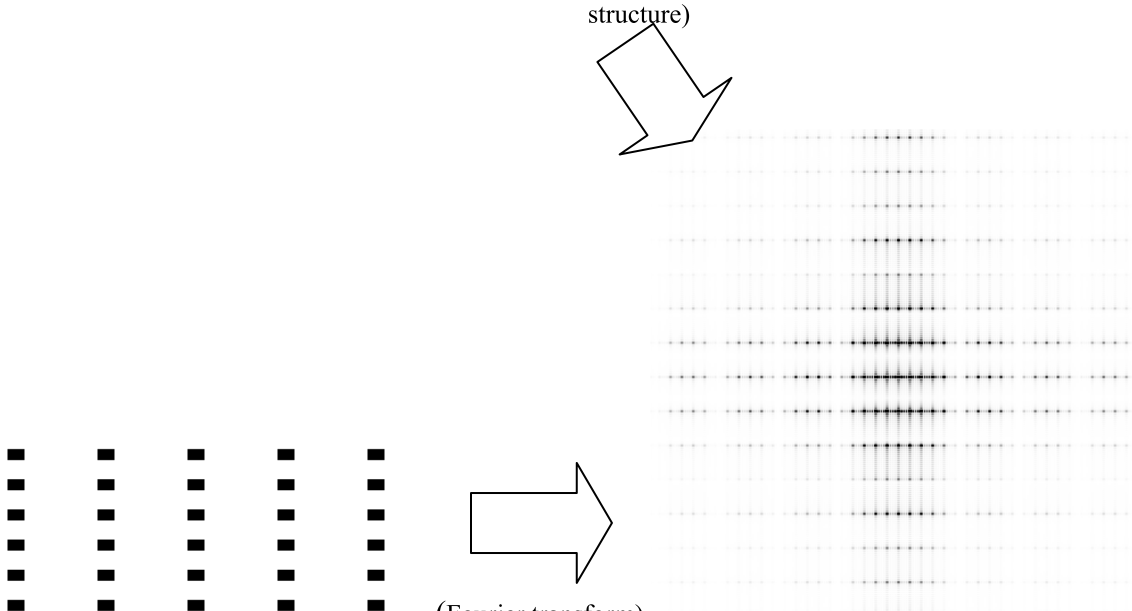
The computer simulations provide even more flexibility than the optical crystals for the student to quickly investigate the effects of changing size or shape of the motif, or the lattice geometry, and other parameters. Figure S – 2 shows an example of how the computer simulation output is used to help demonstrate the relationship between the Fourier transforms of the motif and the lattice, and the “net” Fourier transform of the convolution of the motif and lattice.



(Convolution of the motif and the lattice results in a crystal structure)



(The Fourier transforms of the motif and the lattice are multiplied to obtain the Fourier transform of the crystal structure)



(Fourier transform)

Figure S – 2: Example of how the computer simulation output is used to demonstrate concepts (from Section 6 "Convolution")

One of the important new features of this project was to integrate the use of the computer simulations with the use of the optical crystal slides. This was accomplished by using the same real space patterns for both the optical crystal slides and as input to the computer simulation - see Figure S – 3 as an example. Showing direct correlation between the observed results from the optical crystal slides and the calculated results from the computer simulation (and allowing the students to demonstrate this for themselves), provides the students both better understanding and confidence in the meaning of each.

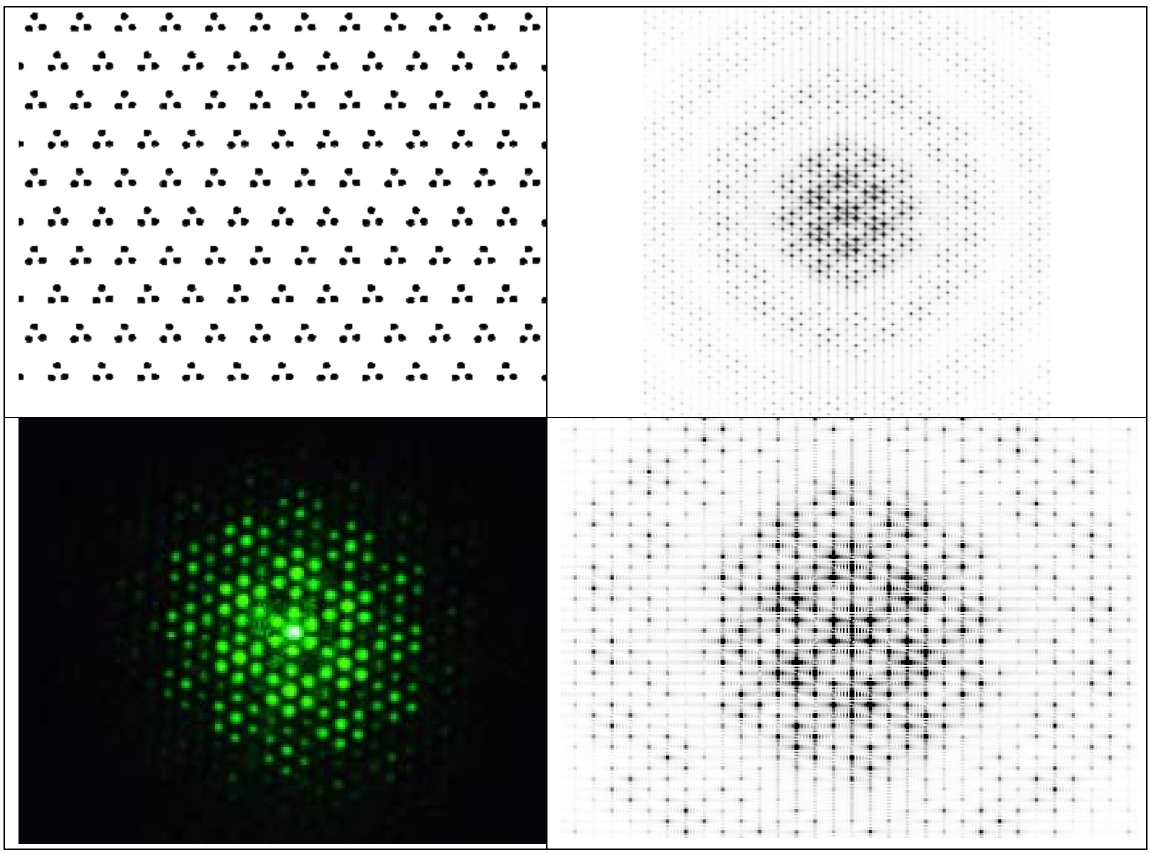


Figure S – 3: Example of how the computer simulation output and the optical crystal slides are integrated (from Section 8 "Symmetry of the Crystal Lattice and the Diffraction Pattern")

Overview

This project was to develop a laboratory experiment on diffraction. My goal in developing this project was to integrate some very useful and interesting interactive material available on the web, with some new slides (two-dimensional "optical crystals") developed by Robert Bachilla, Dr. Larry Sorensen, and myself over the past several months.

Robert and I started meeting with Dr. Sorensen in the fall of 2005, with the original goal of replacing the 1973 "optical crystals" that were being used in the Physics 575 laboratory class. The idea was not just to replace them, but also to expand the patterns, to be able to show additional concepts and to thereby allow the students to gain better and broader understanding of diffraction. In order to strategize what to show, we began researching literature and material on the web. The interactive programs on the web were so helpful, easy to use and yet powerful, that we began discussing how to integrate the web material with the "hands-on" laboratory work with the optical crystals.

Replacing the optical crystals turned out to be far more difficult than we had originally envisioned. The popularity of digital photography has resulted in decreased availability of high resolution "analog" photography materials. Robert Bachilla conducted extensive research into digital methods, but the dynamic range currently available via digital methods is still not sufficient to produce optical crystals usable with lasers. He was successful in finding a high resolution black and white film for generating slides, and his investigation and production was the subject of his Master's thesis last Fall. Several of his photographs are incorporated into this paper, and all of his slides will hopefully be used as part of the laboratory lesson plan.

At Dr. Sorensen's suggestion, I have also investigated commercial microfiche as a way to generate the optical crystals. While fewer and fewer options are commercially available for microfiche (again, due to the popularity of digital mediums for storage), this process was shown to be successful for generating optical crystals.

While Robert was photographing his patterns, he kindly photographed the patterns I had generated. I had developed a small number of patterns designed to quickly show some key concepts in diffraction – the effect of the atom and the lattice size and shape, and the effects of imperfections due to thermal effects or crystal "stacking errors". Robert was wonderful to work with throughout this project, and demonstrated skill and persistence in researching methods and producing several beautiful and interesting new sets of optical crystals.

I owe both Robert and Dr. Sorensen huge thanks for all of their help and patience as we worked together to generate materials for an updated 2-D Diffraction laboratory lesson. Throughout my Master's studies in the Application of Physics, I have been particularly fascinated with light, optics and diffraction, I think because the physics describing light is elegantly simple in theory and yet endlessly complex in real-life applications.

overall background scattering. In the collision of the photon with the electron, momentum is conserved, but the wavelength of the input radiation is changed. There is no well-defined phase relationships between the radiation being scattered from different electrons in the assembly, and with no well-defined phase relationship, the superposition principle discussed above for Thomson scattering, doesn't hold. Sometimes Compton scattering is referred to as incoherent scattering, and Thomson scattering as coherent scattering.

6. Convolution

We've discussed that the diffraction pattern is the Fourier transform of the real space geometry of the crystal, and that this is true whether we're talking about the geometry of the overall crystal (shape function), the crystal lattice (infinite lattice), or the contents of the unit cell (motif).

f(obstacle) = f(motif) * [f(infinite lattice) x f(shape function)]

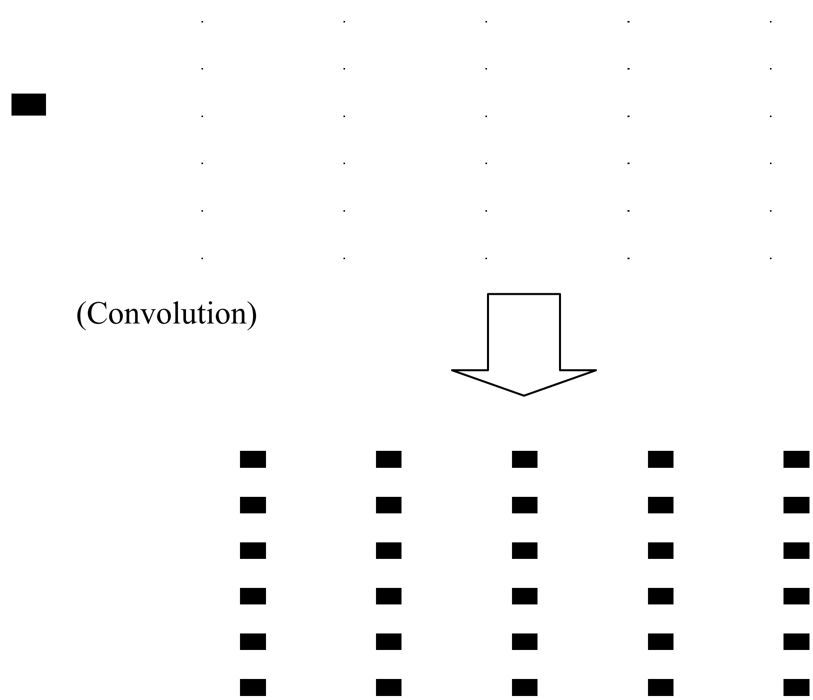


Figure 6 – 1: Convolution of a single rectangle (motif) with a lattice, results in a lattice of rectangles.

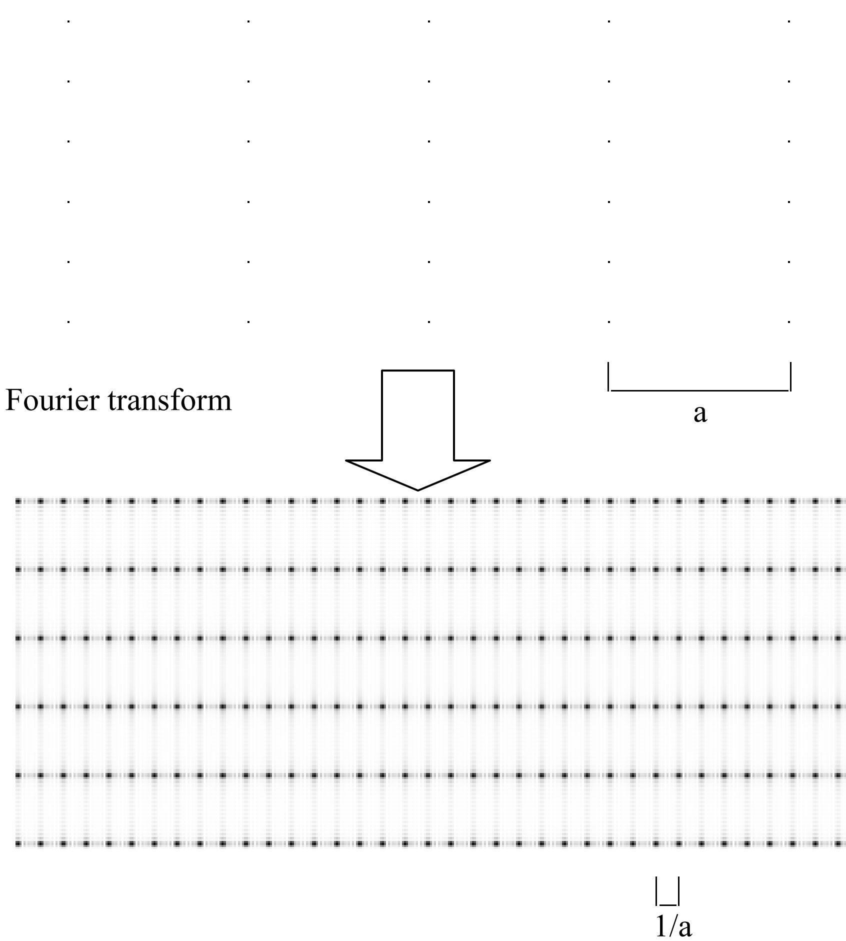


Figure 6 – 2: The Fourier transform operation on a real lattice (top) yields the reciprocal lattice (bottom)

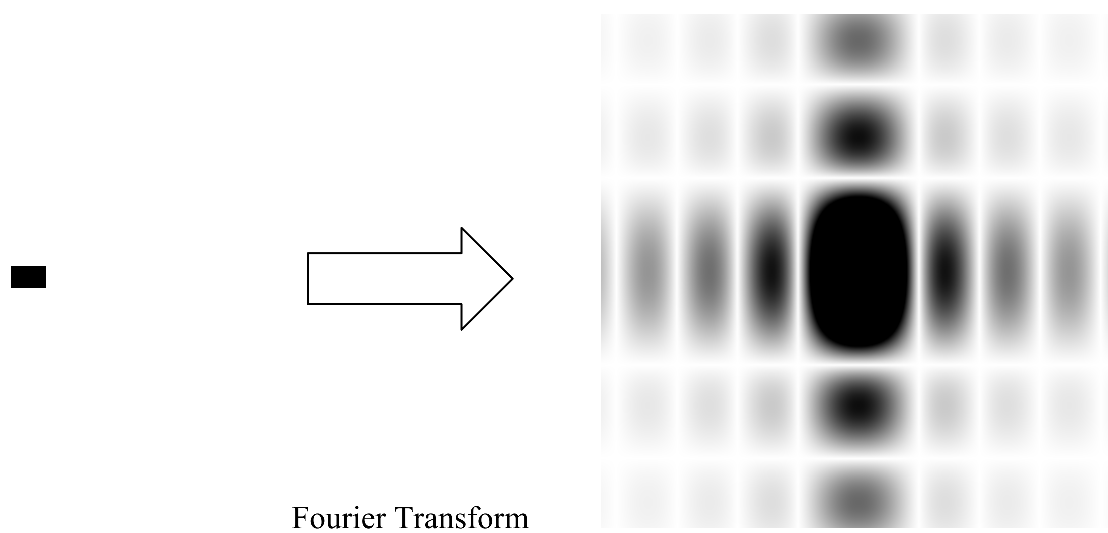


Figure 6 – 3: The Fourier transform of a single rectangle yields the pattern on the right.

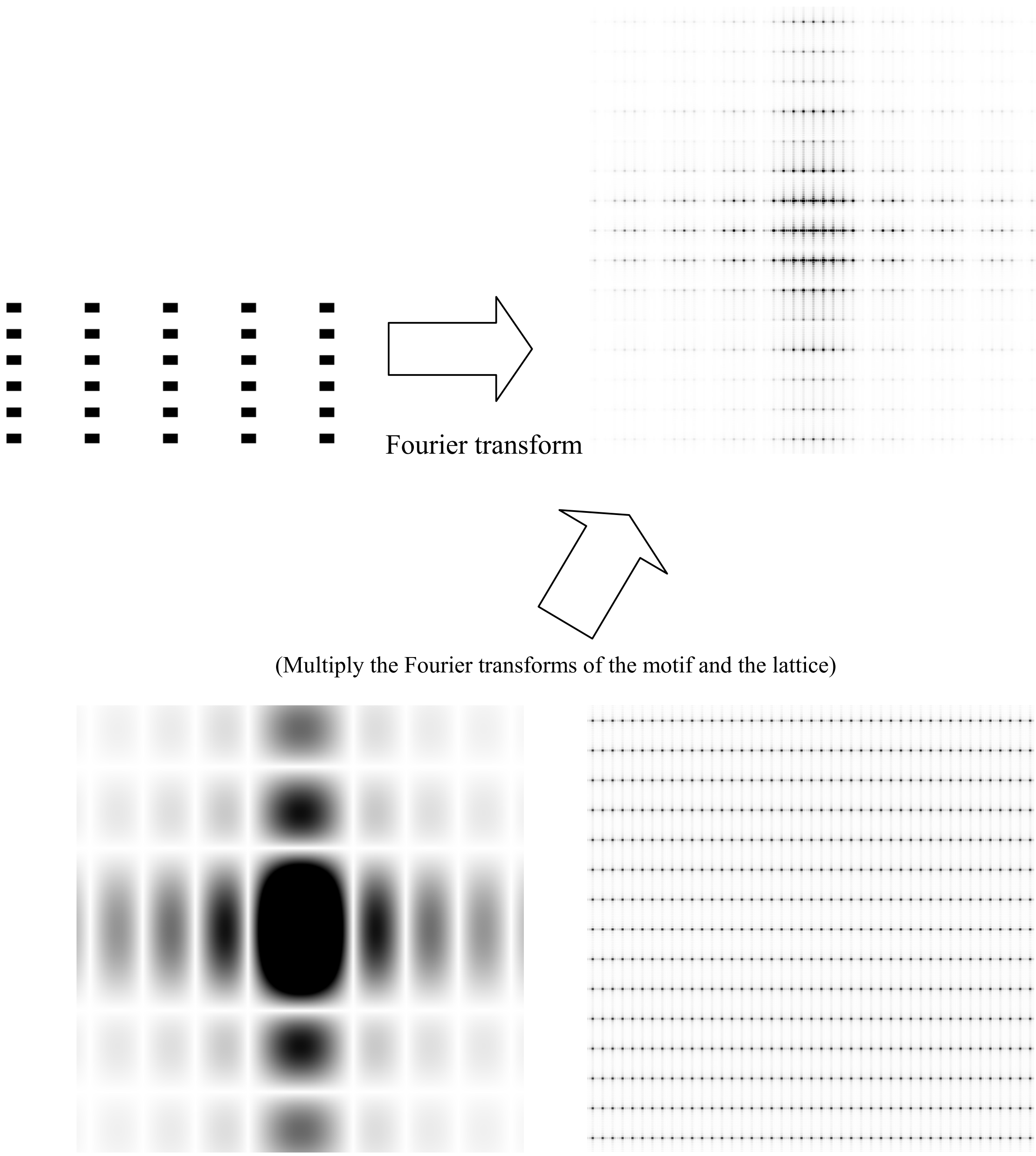


Figure 6 – 4: The Fourier transform of the lattice of rectangles is shown in the upper right hand corner. It is the product of the Fourier transform of the rectangle and the Fourier transform of the lattice.

The above figures show pictorially that the Fourier transform of the convolution of the motif with the lattice is the product of the individual transforms of the motif and the lattice. More generally:

Diffraction pattern amplitude $F(\sin\theta) = T\, f(\text{motif}) \times [Tf(\text{infinite lattice}) * Tf(\text{shape function})]$

Recall the definition and view an animated example of the convolution theorem by visiting this website:

http://mathworld.wolfram.com/Convolution.html

The effect on convolution can be seen in the diffraction pattern as an "enveloping" of the transform of the infinite lattice (idealized with perfect point scatterers) with the transform of the motif (assumes the transform of the shape function isn't affecting the result).

See a graphical example at this website:

http://www.mineralogie.uni-wuerzburg.de/crystal/teaching/conv_a.html

Below are some additional pictorial examples, from the "Diffraction and Fourier Transform" program at the following website:

http://escher.epfl.ch/fft/

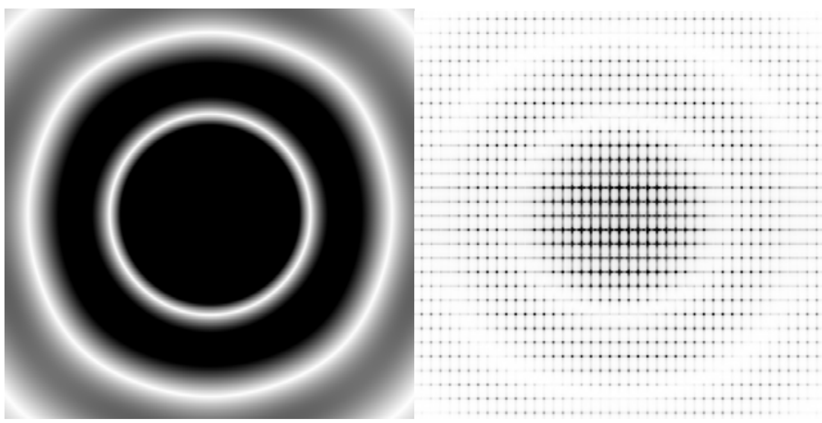


Figure 6 – 5: Fourier Transform of a single dot, and of a rectangular array of dots

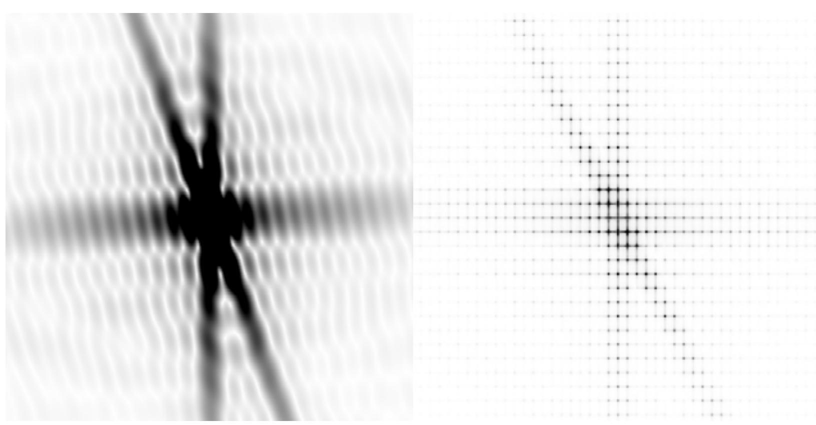


Figure 6 – 6: Fourier Transform of a single right triangle, and of a rectangular array of right triangles