Simulating and Visualizing X-Ray Diffraction from Crystall Lattices

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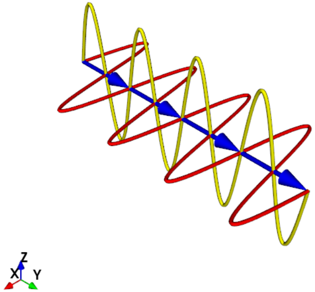
X-Ray Crystallography, kinda a big deal

Bababooey

What is Light?

When you have a changing electric field, a changing magnetic field will be created.

- A changing magnetic field will also create a changing electric field.
- This creates a cycle between the two fields.
- This cycle between the electric and the magnetic fields of the wave is why light is also known as electromagnetic radiation.



Electromagnetic Spectrum

Light (Electromagnetic Radiation) exists on a variety of different wavelengths

- Light with a smaller wavelength, and thus a higher frequency, will carry more energy.
- Wavelength and frequency are connected with the relationship $\lambda f = c$, where λ is the wavelength of the wave, f is the frequency of the wave, and c is the speed of light.

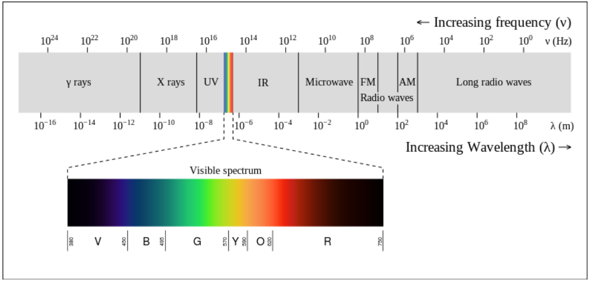


Figure 2: A diagram of the electromagnetic spectrum

Thomson Scattering

Becuase light has an electric field, it will "wiggle" a charged particle, such as an electron.

- This wiggling of the electron will create a changing electric field.
- This will create a changing magenetic field, thus forming a new light wave.
- This forms the phenomenon of Thomson scattering, where light with relitively low energy (such as an X-Ray), will be scattered by an electron.
- The force acting on the electron is specifically the Lorentz force, which is a combination of the electric and magnetic fields. This force is oscilatory, which is why the electron is "wiggled".

Modeling Thomson Scattering

To model Thomson scattering, we can use the following equation:

$$E_{rad}(R,t) = -E_{x0} r_0 \frac{e^{i(kR-\omega t)}}{R} cos\psi$$

Figure 3: An equation to model Thomson scattering

- R represents the distance between the electron and the point of observation.
- t represents the time of observation.
- e_{x0} represents the amplitude of the incident electric field.
- r_0 represents the classical electron radius, which is about 2.82x10-15 m.
- e is Euler's number, and i is the copmlex number.
- k is the wavenumber of the incident electric field.

Thomson Scattering Visualizations

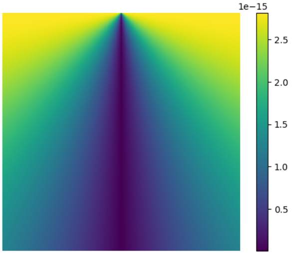


Figure 4: A graph of the amplitude of thomson scattering over space

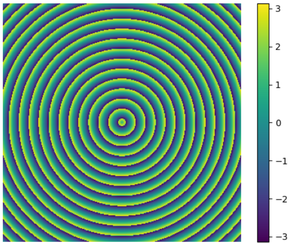


Figure 5: A graph of the phase of thomson scattering over space

Eulers Formula

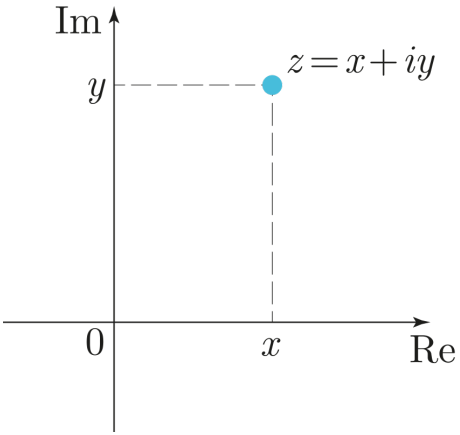
In the Thomson Scattering Equation, e^{ix} represents the incident oscilitory electric field, using Euler's formula.

- Eulers formula is defined by the identiy $e^{ix} = \cos x + i \sin x$
- In the context of our wave, when converted to polar coordinates, the length of the value represents the amplitude of the scattered wave, and the angle represents the phase of the wave

Complex Number Review

As you are probably aware of, you can describe $\sqrt{-1}$ with the letter *i*

- Any number multiplied by *i* is an imaginary number
- You can combine real numbers and imaginary numbers to form a complex number (for example, 2+3i)



Complex Polar Coordinates

To describe a wave, we can use complex polar coordinates.

- With polar coordinates, instead of describing the complex number with cartesian coordinates in an x, y plane (like we did on the previous slide), we describe it with an angle it with an angle and magnitude.

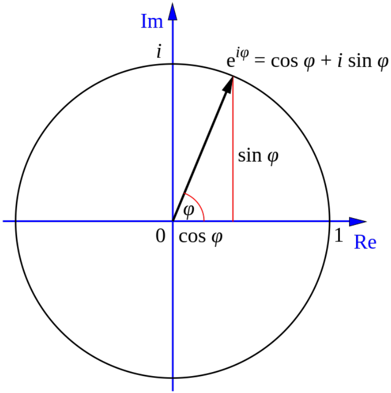


Figure 6: A diagram of the complex polar coordinates resulting from Euler's formula.

Complex Polar Coordinates to describe a wave

We can use the complex coordinates from Euler's formula to describe a wave

- The magnitude of the polar coordinate represents the amplitude of the wave
- The angle of the polar coordinate represents the phase of the wave

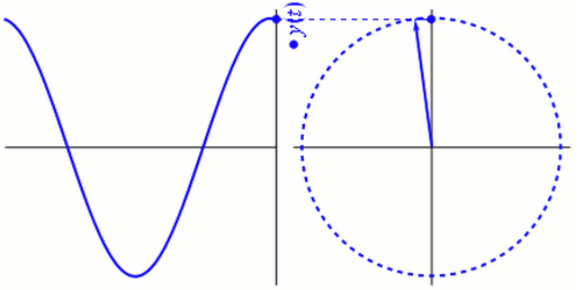


Figure 7: An animation of a phasor

Thomson scattering from an atom

In most cases, we are not interested in the scattering from a single electron, but rather from an atom.

- To do this, we have to integrate over the area of an electron, while taking into account the probability than an electron as at each point

$$E_{rad} = 2\pi \int_{R=0}^{R=\infty} \int_{\psi=0}^{\psi=\pi} f_{Thomson} \times (R, \psi, E_{in}, \lambda) \times p(R) \times (r^2 \sin \psi) dr d\psi$$

Figure 8: An equation to model Thomson Scattering from an atom

- R represents the distance from the center of the atom
- ψ repersents the angle at which the scattering is being observed, on the plane of polarization
- E_{in} represents the incident electric field
- λ represents the wavelength of the incident light

Charge Probability Density Function

We, of course, cannot know exactly where an electron is while orbiting an atom.

- However, we can have some idea where an electron is likely to be. For example, it is more likely to be 20 picometers from the nuclues, than 20 meters from it.
- In my simulations, the following equation for charge probability density was used. Note that it is a very rough approximation, and many more accurate techniques exist.

$$p = \frac{e^{-(2r/a)}}{\pi a^3}$$

Figure 9: A simple charge probability density function

- p represents the relitive probability that an electron is at the described point
- e is Euler's number (a constant)
- r is the distance of the electron from the center of the atom
- a is the typical distance of the electron from the center of the atom, based on the shell/orbital the electron is in.

Wave Interference

Figure 10: Destructive Interference Occuring Between two Waves in a Pond

Wave interference

When two waves meet, interference occurs.

- This interference is just the sum of the two waves.
- This means that when the waves are in phase with eachother, their valleys and peaks will line up, and the waves will constructively interfere.
- When the waves are perfectly out of phase, the valleys of one wave will line up with the peaks of another, and the waves will cancel eachother out.

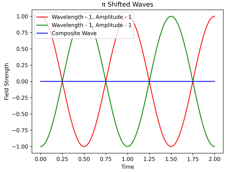


Figure 11: Destructive Interference Between Two Sinesoids

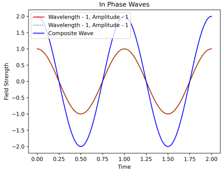


Figure 12: Constructive Interference Between two Sinesoids

Crystal Lattices

In a crystal structure, atoms are organized into a grid we call a lattice.

- The most basic repreating unit in a crystal structure is known as the unit cell.
- This unit cell is then repreated to form an entire crystall
- Note that in most real crystals, the lattice is not perfect, unlike what is shown in these diagrams.

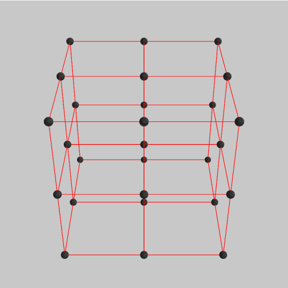


Figure 13: An animation of a simple cubic lattice

More Crystall Lattices

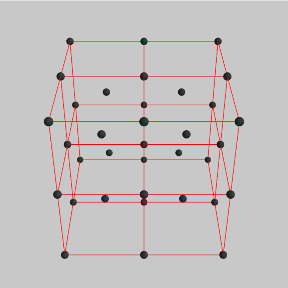


Figure 14: A crystal lattice with body centered cubic unit cells

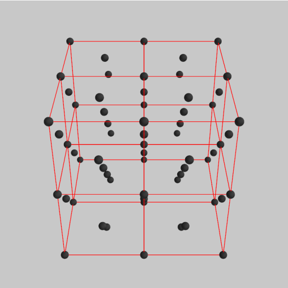


Figure 15: A crystal lattice with body centered cubic unit cells

Bragg's Law

Bragg's Law allows us to deduce the angle a light beam needs to strike the surface of a crystall latice at, in order to produce constructive interference.

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

Figure 16: An equation describing braggs

- n is any integer
- λ is the wavelength of the incident light
- d is the distance between layers of atoms
- θ is the angle of the incident light

Bragg's Law Example

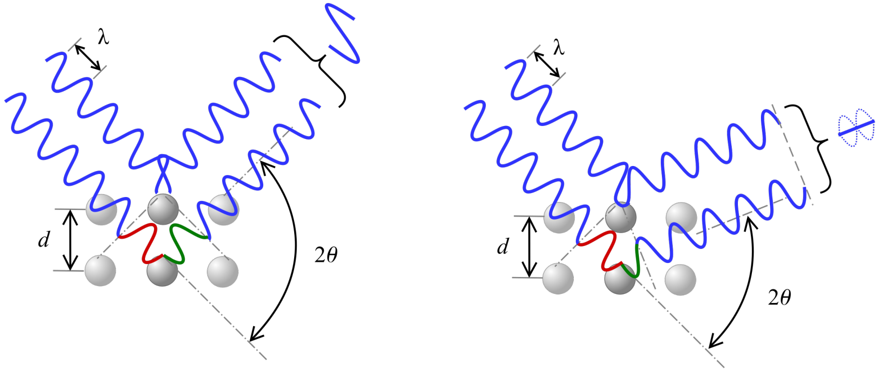


Figure 17: An example of braggs diffraction

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