X-Ray Experiments in Solid State Physics: Bragg Diffraction and Planck's Constant

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ABSTRACT

The primary objective of this experiment is examine two major contributions to solid state physics and emulate the experiment results originally determined by W.H. Bragg and son. This experiment is subdivided into two major portions for each experiment conducted, 1)Bragg Diffraction - to determine the distance between layers of atoms in a crystalline structure & 2)Planck constant - to independently find Planck's constant with an appreciably high degree of accuracy from our measurements. Most notably in the the second portion of this experiment Planck's constant is found to a fairly high degree of accuracy.

Bragg Diffraction and Planck's Constant Experiments

1 Introduction to Bragg Diffraction & Planck's Constant

1.1 Bragg Diffraction

The principle of the first experiment dates back to the 1915 Nobel Prize that awarded to Lawrence Bragg and his father William Henry Bragg for their work using X-Ray Diffraction to determine crystal structures of Sodium Chloride (NaCl), Zinc Sulfide (ZnS), and Diamond. They established that there must be a mathematical and physical condition for the accuracy of finding the distance d between two layers of atoms in crystals. Matter, at the molecular level is constructed of crystalline structures that can be categorically differentiated according to the organization of atoms in a unit cell [1]. There are various forms of crystalline structure that include Simple Cubic (SC), Face-Centered Cubic (FCC) & Body-Centered Cubic (BCC), normally analyzed in momentum space. For example, NaCl crystal has face-centered cubic (FCC) structure, which consists of an atom at each cube corner and an atom in the center of each cube face. There are variations of each type of structure, however for the purposes of this laboratory, the focus will be restricted to the three listed[1] (Refer to Figure 1).
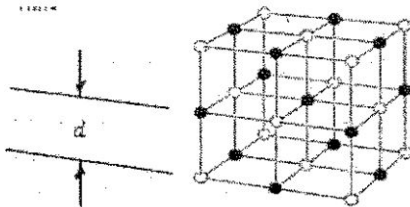

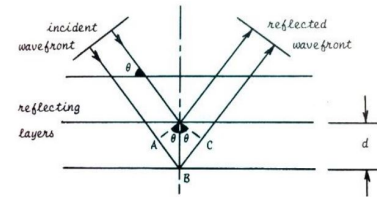**Figure 1.** Face Centered Cubic (FCC)Structure

Figure 2. Bragg Diffraction Wave Diagram

Equation 1 below shows the relationship between the separation distance and molecules per unit volume. Where d is the separation between layers of atoms for a certain crystal, N is Avogadro's number, M is the molecular weight & ρ is the specified crystal density [2]. For example, NaCl is a diatomic, thus the number of atoms per unit volume should be 2ρ. The equation below is the most convenient form for this laboratory:

$$d^3 = \frac{1}{\rho \frac{N}{M}} \implies \boxed{d = \sqrt[3]{\frac{M}{\rho \cdot N}}} \tag{1}$$

A mathematical reiteration of the Bragg condition can easily be expressed in terms of θ [3] as a condition of

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[1] basic building block of a crystal, that contains a single lattice point

[2] please note that the density change dependent on the identity of the crystal

[3] where θ is the incident scattering angle of an incoming wavefront

angular equivalence of incident and reflective wave fronts & constructive interference of light reflections of several layers. This experiment the crystalline structure is timed by the blue motor to move at approximately 0.5 the speed of the detector to satisfy the first. Mathematically,:

$$n\lambda = 2dsin(\theta) \tag{2}$$

Where n is the nth peak, λ is the wavelength of the incident wave in this case of X-Ray, and θ is the scattering angle of diffraction. The incident wave front can scatter into two different paths, one can be a reflection off of the first layer of the crystal, while the other will permeate the first layer and bounce form the second as a reflection (Refer to Figure 2). Bragg's condition ensures that these two reflected waves constructively interfere, this is essentially how a diffraction pattern is formed. A diffraction patern is observed at an angle of 2θ[2].

1.2 Planck's Constant

In 1900, Max Planck presented the constant through his derived formula for the distribution of Blackbody Radiation[4]. X-rays emission can also be generated by colliding high energy electrons with an atom. When the collision happens, the high energy electron removes one of the atom's (copper atom particularly) inner core electrons. This excited electron gains enough energy to become a free particle. To minimum energy, the empty state of the positive ion is filled by the transition of an electron from higher occupied energy state. The X-ray emission from this step helps to conserve the energy.

For the Tel-X ometer in the lab, the electrons undergo sequential glancing collisions with particles of matter, undergo a loss of energy and increase the average energy of the targeted particle. Collisions in rapid succession expel energy in the form of heat, causing the crystal to become hot to the touch. When the electrons decelerate, they give some of their kinetic energy to the target particle as well as some in the form of electromagnetic radiation. However, because the depth of these collisions is specific, this causes the radiation to break and a continuous spread of wavelengths. Equation 3 below shows how minimum wavelength (or maximum energy) can be determined, where V is the voltage of the tube and β is a constant integer.

$$V\lambda_{min} = \beta \tag{3}$$

Besides, Einstein's theory of the photoelectric effect holds true for both radiation's emission and absorption, thus the energy of each photon can be calculated by utilizing Equation 4 shown below, where ω is the energy associated with each photon, ν is the frequency of radiation, and h is Planck's constant.

$$\omega = h\nu \tag{4}$$

Furthermore, total kinetic energy of the electron can be converted into maximum energy of a photon (electron Voltage/ eV) by using Equation 5. Where λ is the minimum wavelength, h is Planck's constant, and c is the speed of light:

$$V_e = \frac{hc}{\lambda} \tag{5}$$

2 Experimental Setup

By using the Tel-X ometer and Tel-X Driver Program for X-ray diffraction, Bragg's and Plank's constant can be determined with Sodium Chloride (NaCl) and Lithium Fluoride (LiF) crystal samples. Figure 3 displays the X-Ray Diffractor and Computer setup station.

2.1 Bragg Diffraction

The experiment begins with the Tel-X Ometer off, this is crucial step to note. Then, open the lead glass cover and mount the NaCl crystal sample in the crystal post. Figure **??** below shows the "Primary Beam Collimator" with 1mm vertical slot, and Figure [insert] displays the "Geiger - Muller tube" as well as 1 mm and 3 mm slide collimators. Mount the 3 mm slide collimator at slide slot 13 and the 1 mm at slide slot 18 (Refer to Figure 5. Next, mount the "Geiger - Muller tube" at its holder, slot 26. After that, remove the "TEL-X Driver 2590" (blue box), there is a switch to adjust the voltage that goes across the anode and cathode (Refer to Figure 6). This switch can be set to 20kV or 30kV for automated scanning, in this case set the switch to 30 kV.

Start the TEL-X Driver program in the computer, the window program will appear (Refer to Figure 4). There are several editable dialogue box that can be changed accordingly for different setup. First of all, set the "Counting
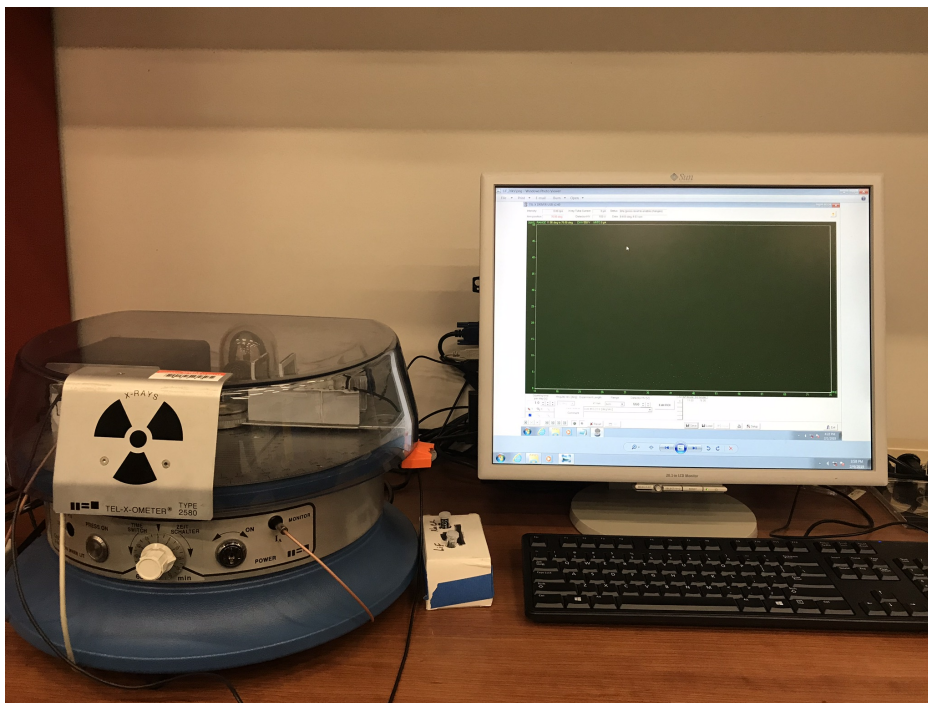
Figure 3. X-Ray Diffractor (left) and Tel-X Driver Computer Program (right)
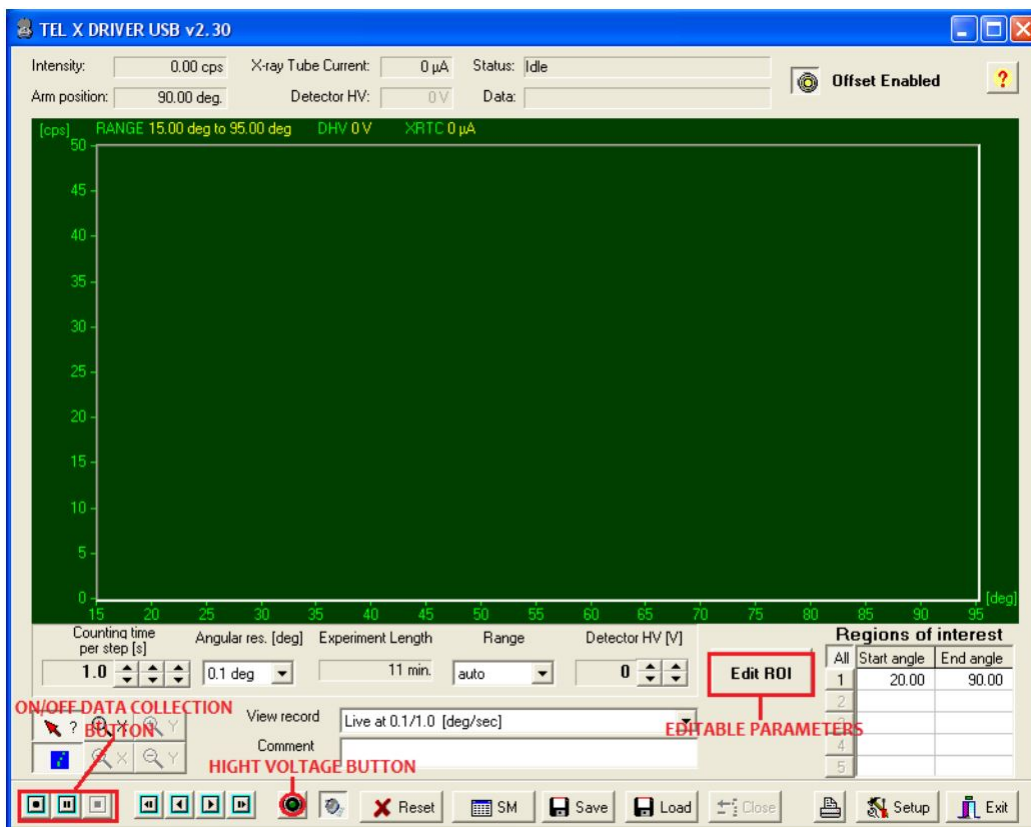

Figure 4. TELXDRIVER Program Window

time per step(s)" at 1.0. Then, edit the "Region of Interest (ROI)" so that the angle range is from 11 °to 76 °, and the arm position is at 15 °. Next, set the voltage of the "Detector" to 550V, count range to auto. Click the "Height Voltage Button" (Refer to Figure 4) to turn on the voltage. Click on "Run" to start scanning, and "Save" to save data as a ".text" file. Then, turn off the X-ray, and use the switch to change the voltage to 20 kV. Make sure the setting of "Counting time per step(S), "ROI", arm position, and the "Detector" are the same as the previous setting values. Turn on the voltage and start scanning. Save the collected data as ".text" file. Switch the NaCl crystal sample to LiF crystal sample, and repeat all of the steps above.
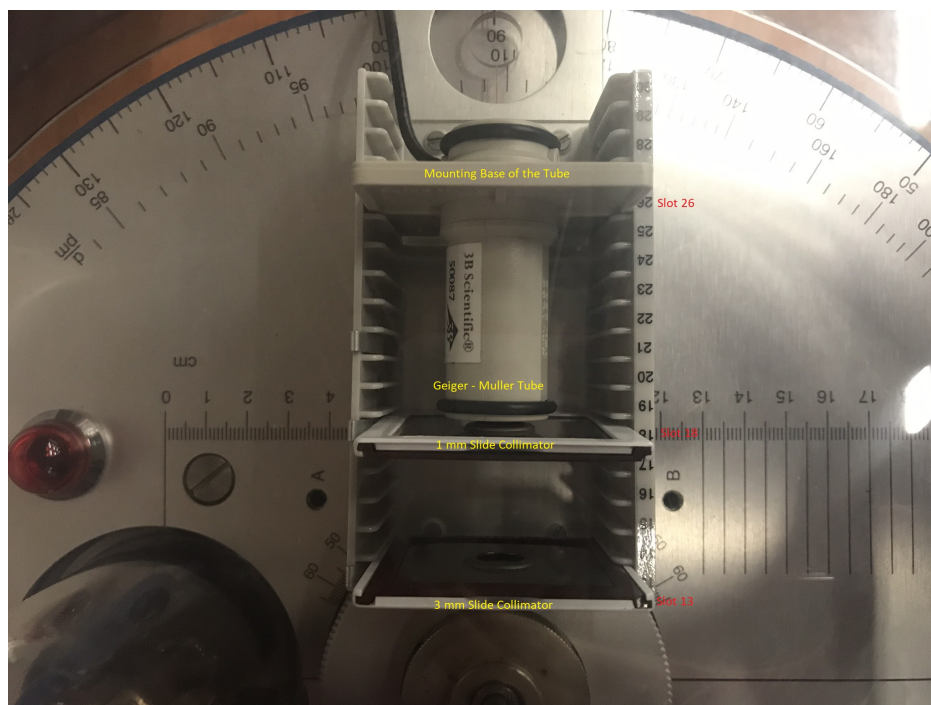

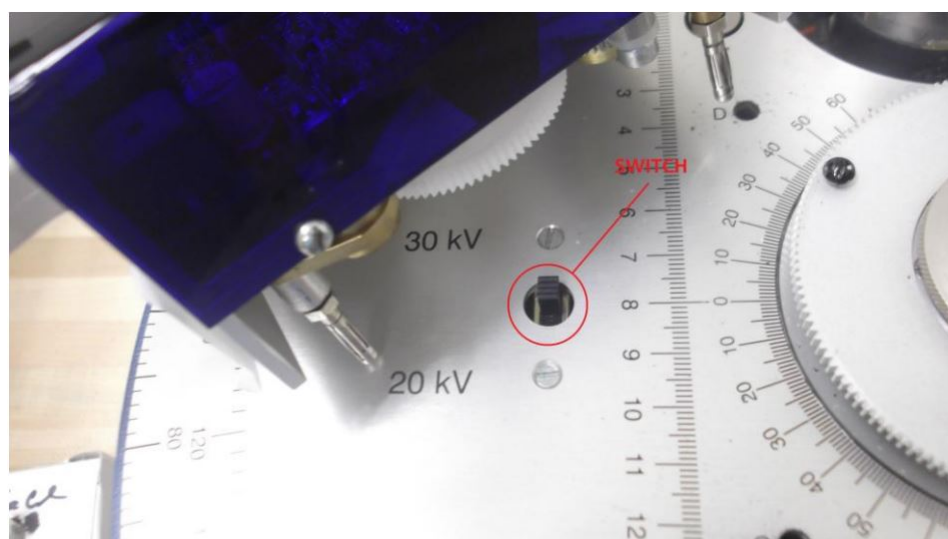**Figure 5.** Geiger-Muller Tube and Slide collimators Setup

Figure 6. Switch to Adjust the Voltage

2.2 Planck's Constant

To start the experiment, LiF crystal sample should be mounted in the crystal post as in the first experiment. Next, select the 30kV energy option and turn on the machine. Change the setting of the Tel-X Driver program in the computer, so that the "Detector HV" is set to 550V, "Counting time per step(s)" shows 30, "Angular res. (deg)" is adjusted to 0.5 deg, and the "Range" is changed to 200. Similar to the previous experiment, use "Edit ROI" to adjust the range of interested angles (from 11 ° to 75 °) as well as arm position (15 °). Turn on the voltage and start scanning. Save the collected data as ".text" file. Notice that

3 Results

3.1 Bragg Diffraction

Consider Equation (1) for NaCl crystal, the molecular weight (M) of NaCl is 58.46 x 10^{-3} $\frac{kg}{mole}$ and the crystal density of NaCl is 2.16 x 10^3 $\frac{kg}{m^3}$, substituting the known values:

$$d = \sqrt[3]{\frac{M}{2\rho \cdot N}} \implies d = \sqrt[3]{\frac{58.46 \cdot 10^{-3}}{2(2.16 \cdot 10^3)(6.02 \cdot 10^{23})}} = 2.82 \cdot 10^{-10} m = 0.282 nm$$
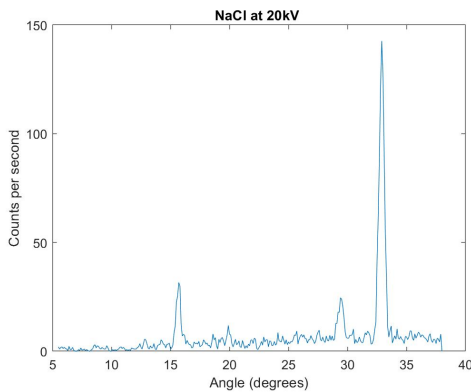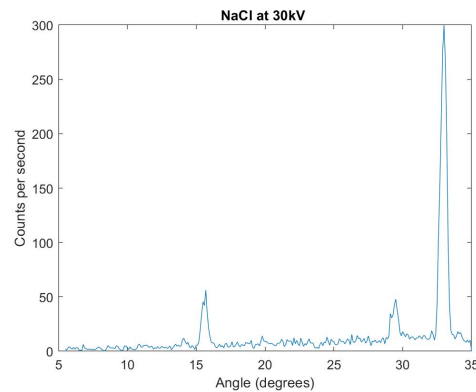

Figure 7. Sodium Chloride at 20 kV

Figure 8. Sodium Chloride Crystal at 30 kV

Figure 7 displays the peak angle for NaCl crystal with 20 kV, which can be used to determine the angle of diffraction. In addition, Figure 8 shows the peak angle for NaCl crystal at a different voltage of 30 kV. Since the orange automatic sliding angle guide reads 2 θ, calculations for the peak angle must be augmented by a factor of $\frac{1}{2}$. However, both figures are adjusted so that the peak angle is true value of θ, which is 33 °. Moreover, from Figure 7 and 8, it is determined that n = 2. By rearranging Equation 2, λ can be calculated:

$$n\lambda = 2d\sin(\theta) \implies \lambda = \frac{2d\sin(\theta)}{n} = \frac{2 \cdot 0.282(nm) \cdot \sin(33°)}{2} = 0.154 nm$$

Similarly, Equation 1 is considered for LiF crystal. Molecular weight (M) of LiF is 25.94 x 10^{-3} $\frac{kg}{mole}$, Avogadro's number (N) is 6.02 x 10^{23} $\frac{molecules}{mole}$, and crystal density is 2.64 x 10^3 $\frac{kg}{m^3}$, thus:

$$d = \sqrt[3]{\frac{M}{2\rho \cdot N}} \implies d = \sqrt[3]{\frac{25.94 \cdot 10^{-3}}{2(2.64 \cdot 10^3)(6.02 \cdot 10^{23})}} = 2.01 \cdot 10^{-10} m = 0.201 nm$$
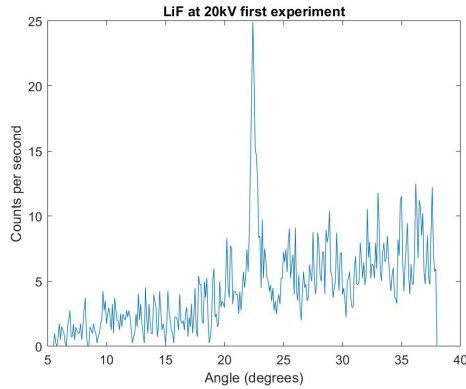
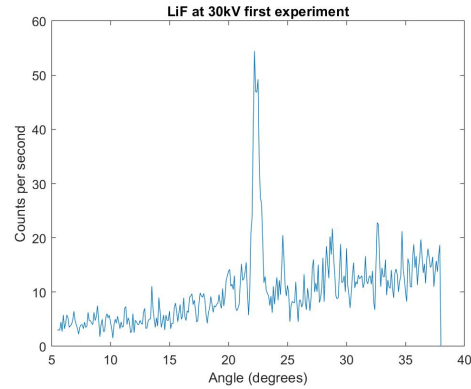**Figure 9.** Lithium Fluoride Crystal at 20 kV

Figure 10. Lithium Fluoride Crystal at 30 kV

Figure 9 and 10 display the peak angle for LiF crystal with 20 kV and 30 kV accordingly, which can be used to determine the angle of diffraction. Similar to the result of NaCl crystal, both adjusted figures suggest that the peak angle is θ = 23 $^\circ$. From Figure 9 and 10, it is determined that n = 2. By rearranging Equation 2, λ can be calculated below:

$$n\lambda = 2dsin(\theta) \implies \lambda = \frac{2dsin(\theta)}{n} = \frac{2 \cdot 0.201(nm) \cdot sin(23^\circ)}{2} = 0.0401nm$$
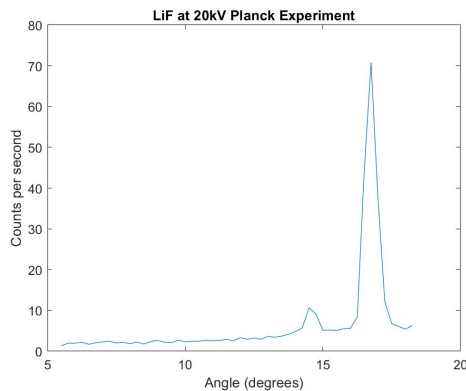
3.2 Planck's Constant

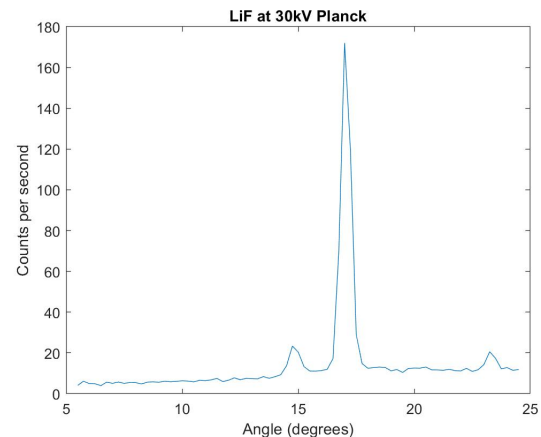**Figure 11.** LiF Crystal at 20 kV for Planck's Constant

Figure 12. LiF Crystal at 30 kV for Planck's Constant

From Figure 11 and 12, Planck's constant is resolved by using Equation 2 to find wavelength at the highest peak, where the highest peak is considered n=2. Once the wavelength is obtained from previous experiment, Equation 5 is use to determine for the experimental finding of Planck's constant.

Resulting Planck's constant for LiF at 30kV: 6.282 E-34 J·s
Resulting Planck's constant for LiF at 20kV: 6.194 E-34 J·s

Planck constants for 1st experiment results:
Nacl at 20kV: 1.636 E-33 J·s
NaCl at 30kV: 2.460 E-33 J·s

LiF at 20kV: 8.196 E-34 J·s
LiF at 30kV: 1.219 E-33 J·s

4 Conclusions

   All calculations of Planck's constant from the first experiment were significantly larger than the well-known Planck's constant of 6.626 E-34 J·s. The most accurate calculation was 6.282 E-34 J·s from the graph of LiF at 30kV in the second experiment with an accompanying margin of error of $\pm$ 5.2%. The primary source of error stems from the inability to take additional measurements to ensure the accuracy of results (unlike original experiments of 1900's) and graphs and to compare a range of voltages. The completeness of the experiment in the natural world depends on the ability to make a sufficient amount of repetitions, where the constant would essentially be verified. Another source of error lies within the restricted ability of the equipment to make extremely accurate measurements.

References

1. "What Is a Face-Centered Cubic? - Definition from Corrosionpedia." *Corrosionpedia*,
   www.corrosionpedia.com/definition/1592/faced-centered-cubic-fcc.

2. "X-Ray Scattering Techniques." *Wikipedia*, Wikimedia Foundation, 3 July 2018,
   en.wikipedia.org/wiki/X-ray_scattering_techniques

3. "Bragg's law" *Wikipedia*, Wikimedia Foundation, 3 December 2018,
   en.wikipedia.org/wiki/Bragg%27s_law#Bragg_condition

4. "Planck's Constant." *Encyclopaedia Britannica*, Encyclopaedia Britannica, Inc., 28 December 2018,
   www.britannica.com/science/Plancks-constant.