SOUL - Physics Simulations Project using Apps on Physics

Bragg Formulation of X-ray Diffraction by a Crystal – Bragg's Reflection

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ABSTRACT

The experiment determines the **path difference in accordance with Bragg's law**. X-ray diffraction provides fundamental understanding of how crystalline structures interact with incident x-rays leading to constructive interference. Interatomic distance in a solid are of the order of an angstrom and therefore, whatever probe (i.e., electromagnetic wave) must have a wavelength on the order of interatomic distance, characteristic to x-rays.

In crystalline materials, for certain wavelengths and incident directions, intense peaks of scattered radiation (Bragg peaks) were observed. According to Bragg's law, in order for the observed peaks to form, the x-rays reflected by the lattice planes must interfere constructively, which happens when the path difference between rays specularly reflected (angle of incidence equals the angle of reflection) from adjoining planes is an integer number of wavelengths.

The required experiment is provided in **Apps on Physics**, under solid state physics.

The **Bragg's law equation** (given below) is used for calculations, yielding the path difference.

$$\Delta s = 2\, d \sin\theta = k\,\lambda$$

Δs = path difference (for neighbouring rays)
d = interplanar distance
θ = glancing angle (between ray and lattice plane)
k = order of diffraction (1, 2, 3, ...)
λ = wavelength

A given unknown crystal has many planes of atoms in its structure, therefore the collections of reflections of all the planes can be used to uniquely identify an unknown crystal.

AIM OF THE EXPERIMENT

To determine path difference and verify Bragg's Law using the App, Bragg Reflection.

INTRODUCTION

A crystalline solid consists of identical molecules located at regular intervals along three dimensions. Light is an electromagnetic field propagating through space, mathematically described by a sinusoidal wave. X-rays which lie the EM spectrum, between ultraviolet and gamma rays, has a wavelength (λ) between 0.1 and 100 angstroms. Interatomic distance in a solid are of the order of an angstrom and therefore, whatever probe (i.e., electromagnetic wave) must have a wavelength on the order of interatomic distance, characteristic to x-rays.

In 1912, two scientists, W.H. Bragg and W.L. Bragg, discovered that crystalline substances produced unique patterns of reflected X-rays, distinct from those observed in liquids. They formulated this principle as Bragg's Law, using it to analyse crystal structures through X-ray diffraction. They found that the distribution of x-rays scattered by a rigid periodic array of ions reveals the locations of the ions within that structure.

When an X-ray beam interacts with a crystal, it is scattered in all directions by the crystal's structure. In some directions, the scattered waves undergo destructive interference (reflected waves are out of phase), resulting in intensity minima; while in others, constructive interference (reflected waves are in phase) leading to intensity maxima (later referred as Bragg peaks). Consequently, the intensity maxima are observed in directions where the x-rays appear to be reflected by a family of parallel reflecting planes that extend through the atoms within the crystal.

Bragg peaks form under specific conditions: the X-rays must be specularly reflected by the ions in a single plane, and the reflected rays from consecutive planes must interfere constructively. For the rays to interfere constructively, the path difference must be an integral number of wavelengths, leading to Braggs condition. In specular reflection, the angle of incidence equals the angle of reflection.

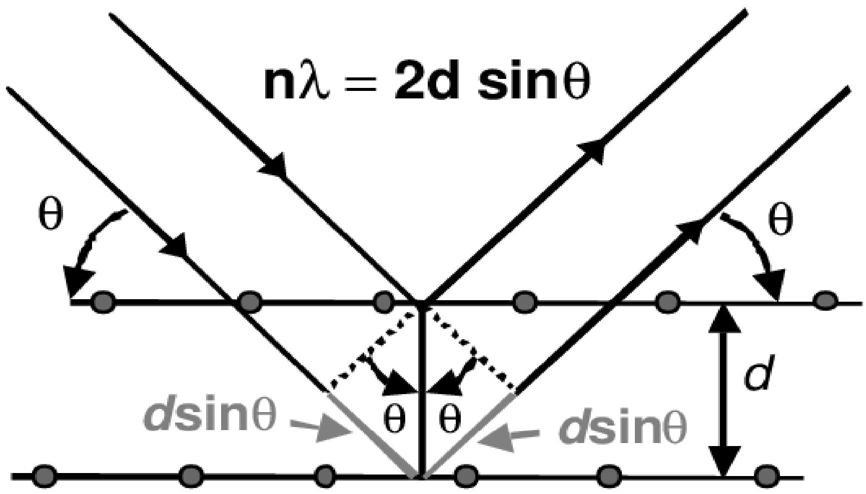

Figure 1-Schematic diagram of constructive x-ray interference by Bragg reflection

To illustrate Braggs reflection (Figure 1), consider a crystal lattice with X-rays incident on it. The rays arrive at the crystal in phase and are reflected while remaining in phase. The ray striking the second parallel plane travels an additional distance known as the path difference. For these rays to be in phase and constructively interfere, the path length difference must be an integer multiple of the wavelength of the x-rays. The general relationship between the wavelength of the incident X-rays, angle of incidence and spacing between the crystal lattice planes of atoms is known as Braggs law, expressed as:

$$\Delta s = 2\, d \sin\theta = k\, \lambda$$

Δs = path difference (for neighbouring rays)
d = interplanar distance
θ = glancing angle (between ray and lattice plane)
k = order of diffraction (1, 2, 3, ...)
λ = wavelength

Bragg Reflection app shows a virtual interface of lattice planes and incident x-rays. The interface also provides a green panel with start/pause and reset buttons, and boxes to enter variable values within certain limits such as the interplanar distance, wavelength, glancing angle and, number of lattice planes. Once the values are entered, we press start and the output, the diagram and the path difference, is produced on the yellow panel. There is also a slow-motion checkbox, which on clicking slows down the graphics.

Using Apps on Physics, we now solve numerical problems from standard textbooks to enhance our understanding of Bragg's Reflection.

We solve the pre-written problem available in the standard textbook, Fundamentals of Physics (with changes to the range).

Numerical Problem - *An x-ray beam of wavelengths from 120 to 200 pm is incident at $\theta = 45.0°$ to a family of reflecting planes with spacing $d = 275$ pm. What are the longest wavelength λ and associated order number m and the shortest λ and associated m of the intensity maxima in the diffraction of the beam?*

CALCULATIONS

The fundamental formula to use is Bragg's Law (provided below). If an unknown variable is presented in the question, solve for it using Bragg's Law, and then input the values into the app.

$$\Delta s = 2\, d \sin\theta = k\, \lambda$$

The given values as per the question are-

Angle of incidence, θ=45.0°

Interplanar distance, d=275pm

Range of the x-ray wavelength, λ= 120 pm to 200 pm

To calculate the longest and shortest wavelength permissible within the given range, we use Braggs formula, 2d sin θ = kλ

$$k\,\lambda = 2 * 275\ pm * \sin(45) = 389\ pm$$

Now, for k=1, λ=389 pm

for k=2, λ=194 pm;

for k=3, λ=130 pm;

for k=4, λ=97.2 pm

Within the range of X-rays from 120pm to 200pm; the longest wavelength is 194 pm and its associated order is 2, the shortest wavelength is 130 pm and its associated order is 3.

Using the app, we can now verify our results, indicating the fulfilment of Bragg's Law.

PROCEDURE

1. Open Apps on Physics. Select Bragg Reflection, under Solid State Physics. We see a panel with reset button, start/pause button. There are boxes to enter values of interplanar distance, wavelength, glancing angle, and number of lattice planes, as shown in figure 2.

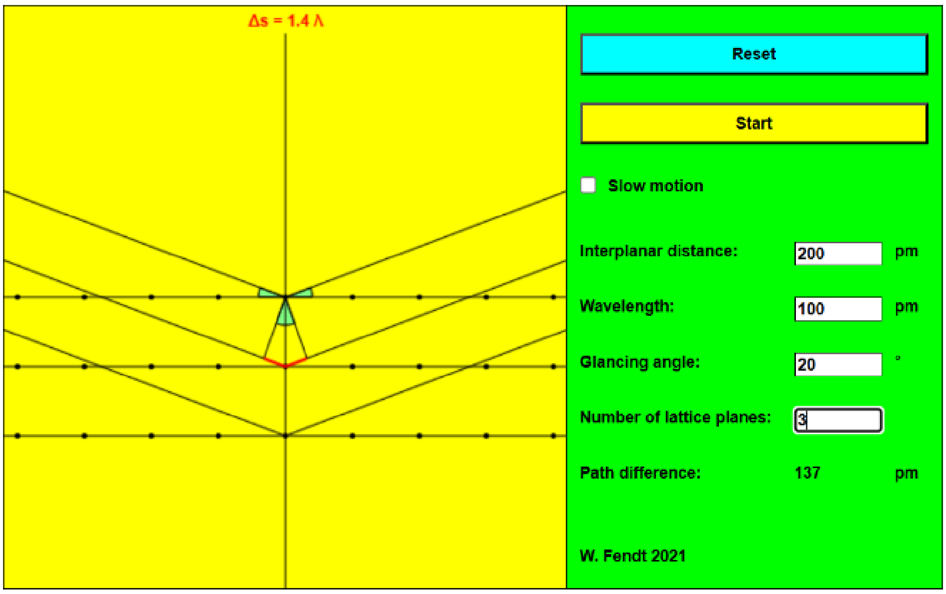

Figure 2

2. Solve the given question for the unknown variable, i.e., the wavelength. Upon yielding the longest and shortest wavelength, we enter these values into the App.
3. Enter the values- the interplanar distance(d), wavelength (λ), glancing angle(θ), and the number of lattice planes as given in the question. We enter the wavelength as 200 pm first, and obtain its diagram (as shown in figure 3).

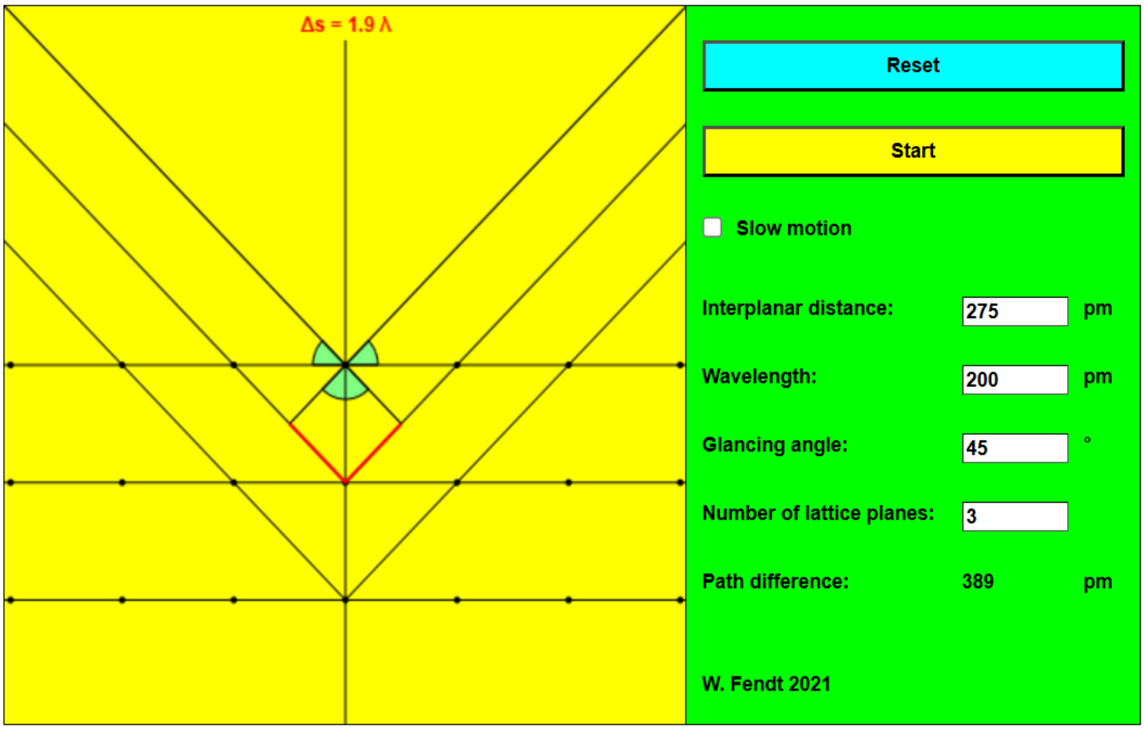

Figure 3

On pressing start, the rays start moving as shown in figure 4.

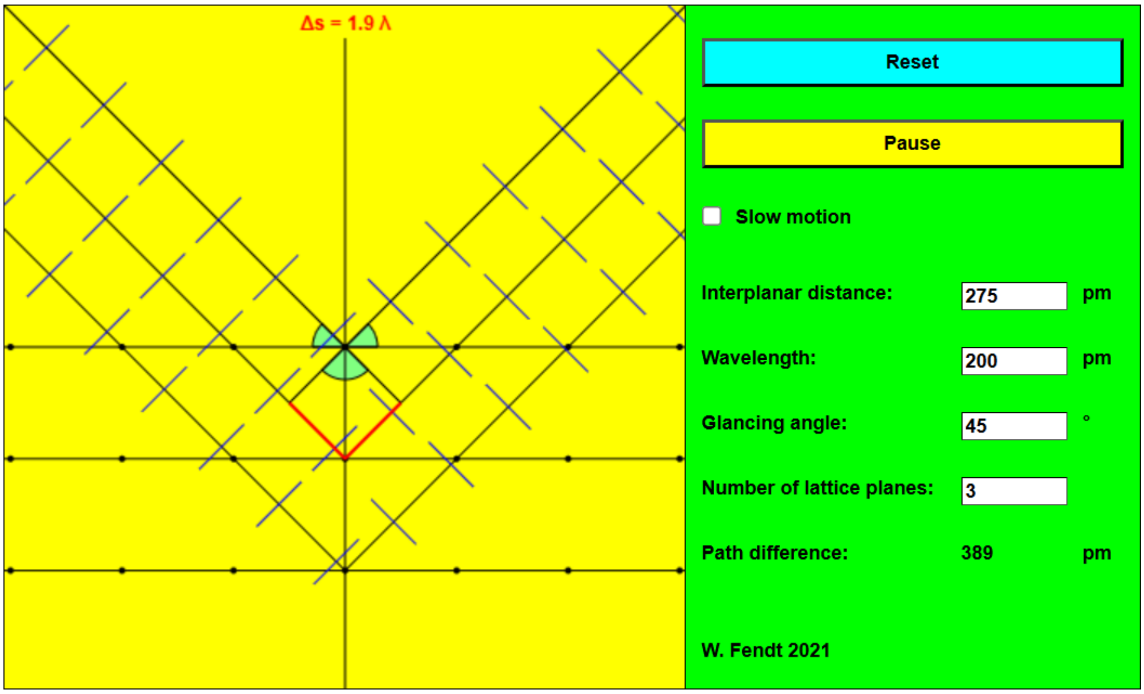

Figure 4

Here, the lines marked red represents the path difference. Path difference is the difference in the distance travelled by two rays to a given point from their source.

4. Now, reset and enter the values, only changing the wavelength to 194 pm (since we are considering the longest possible wavelength) as shown in figure 5.

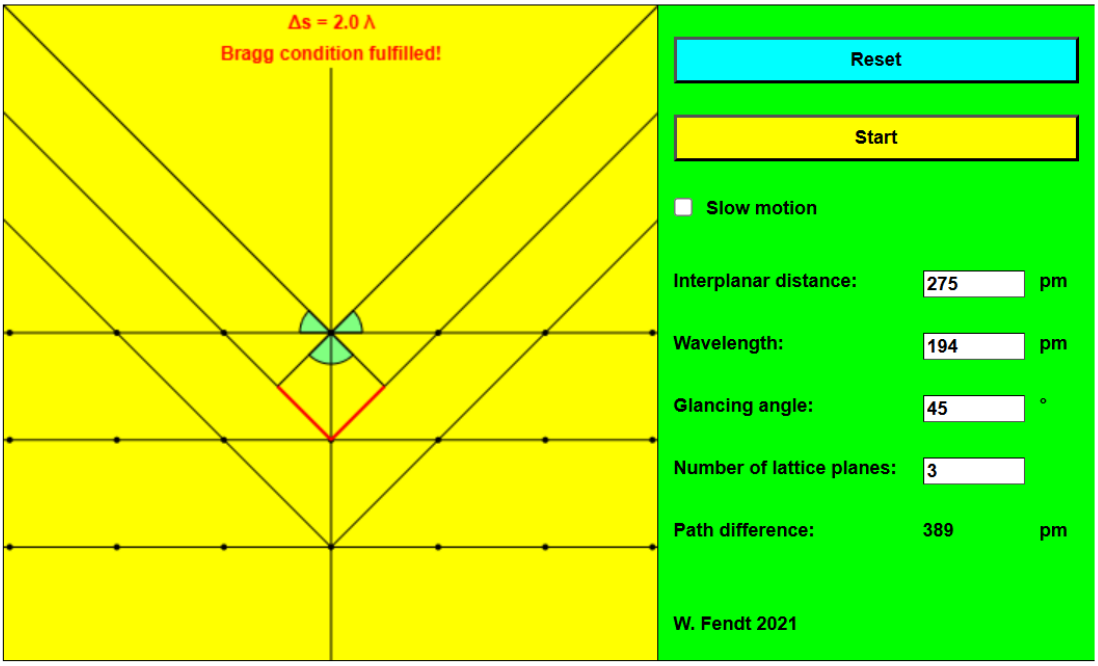

Figure 5

5. Select the start button. The rays now start moving. Select the 'slow motion' button to slow down the rays (as shown in figure 6).

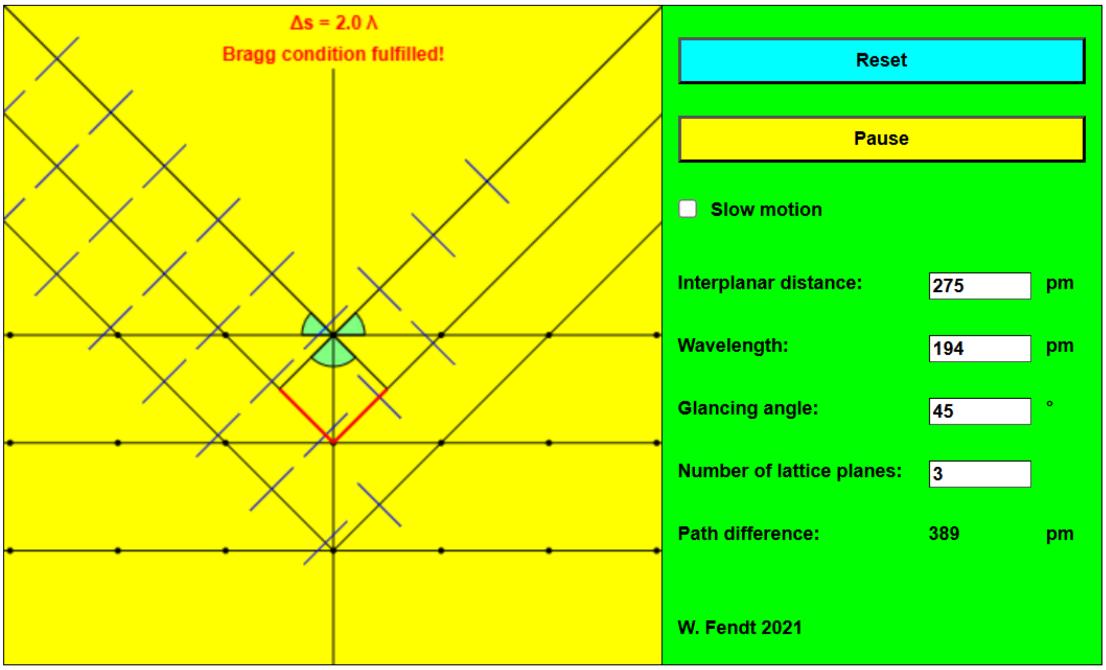

Figure 6

6. Now, reset and change the wavelength to 130 pm (since we are considering the shortest possible wavelength) as shown in figure 7.

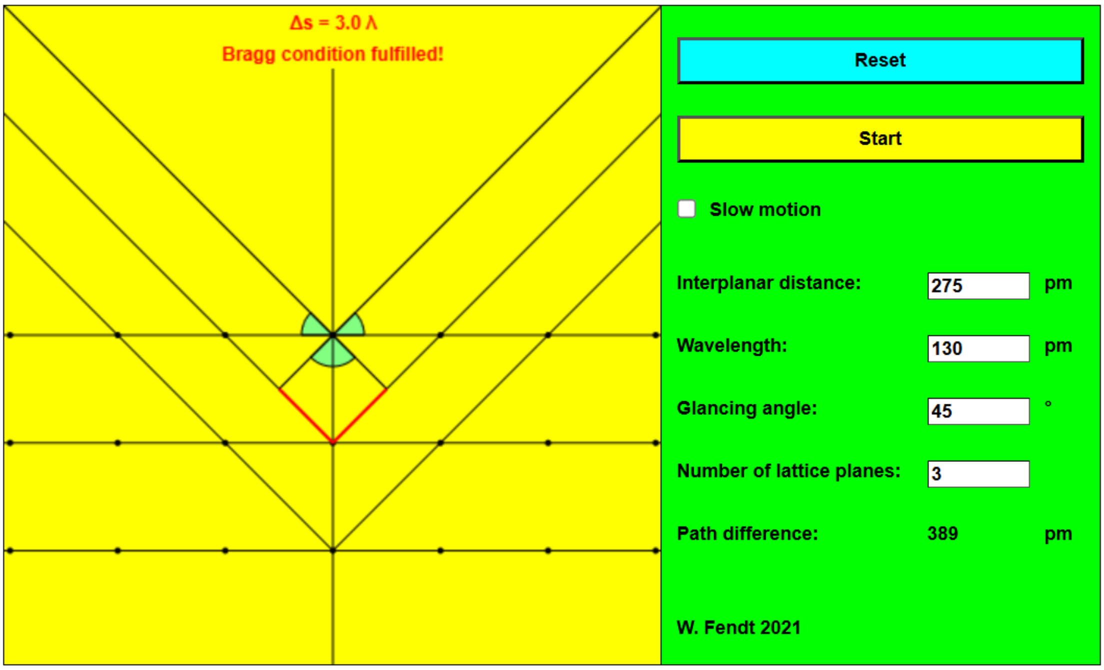

Figure 7

7. Select the start button. The rays now start moving. Select the 'slow motion' button to slow down the rays (as shown in figure 8).

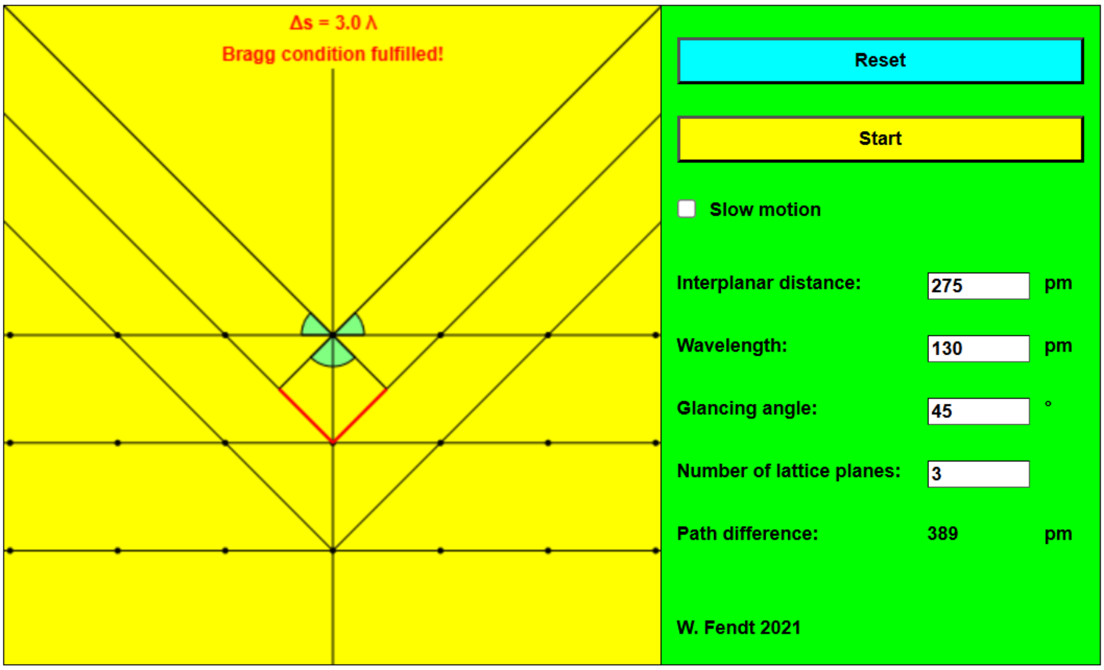

Figure 8

8. Observe the following-
    a. the path difference in terms of picometre (pm) is shown in the green panel at the bottom
    b. the path difference in terms of wavelength, λ, is shown in the yellow panel at the top
    c. A statement, Bragg Condition fulfilled!, also appears on the yellow panel at the top. This helps us deduce that Bragg condition, i.e., for the x-rays to constructively interfere and be in phase, the path difference must be an integral multiple of X-rays, has been met.

   Hence, the path difference is determined, which is the aim of the App. We also confirm the theoretical value of path difference(=389pm) and that obtained from the App(=389pm).
9. Bragg's law verified using the App, Bragg Reflection.
10. Similarly, we can vary the values of interplanar distance, wavelength, and the glancing angle to observe the variation of path difference. This way, we check the fulfilment of Bragg's law condition.
11. In the App, enter the value of interplanar distance as default, i.e., 200. Press start and observe the change in the path difference as the interplanar distance is varied. Then, press reset to change its value. The wavelength and glancing angle remains constant at 100 pm and 20°. Refer figure 9.
    The minimum allowed value of interplanar distance in the App is 100 pm and maximum is 1000 pm.

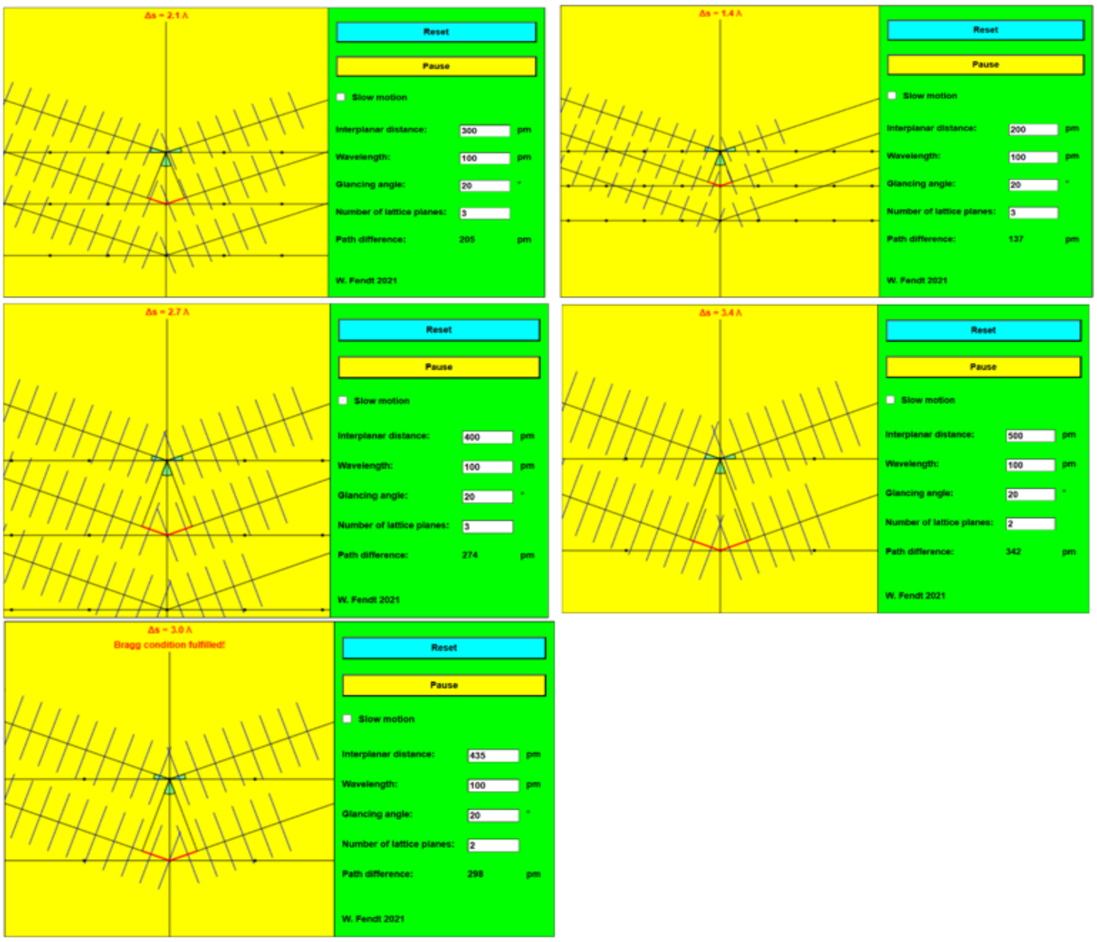

Figure 9

12. In the App, enter the value of wavelength as default, i.e., 100. Press start and observe the change in the path difference as the wavelength is varied. Then, press reset to change its value. The interplanar distance and glancing angle remains constant at 200 pm and 20°. Refer figure 10.
    The minimum allowed value of wavelength distance in the App is 100 pm and maximum is 1000 pm.

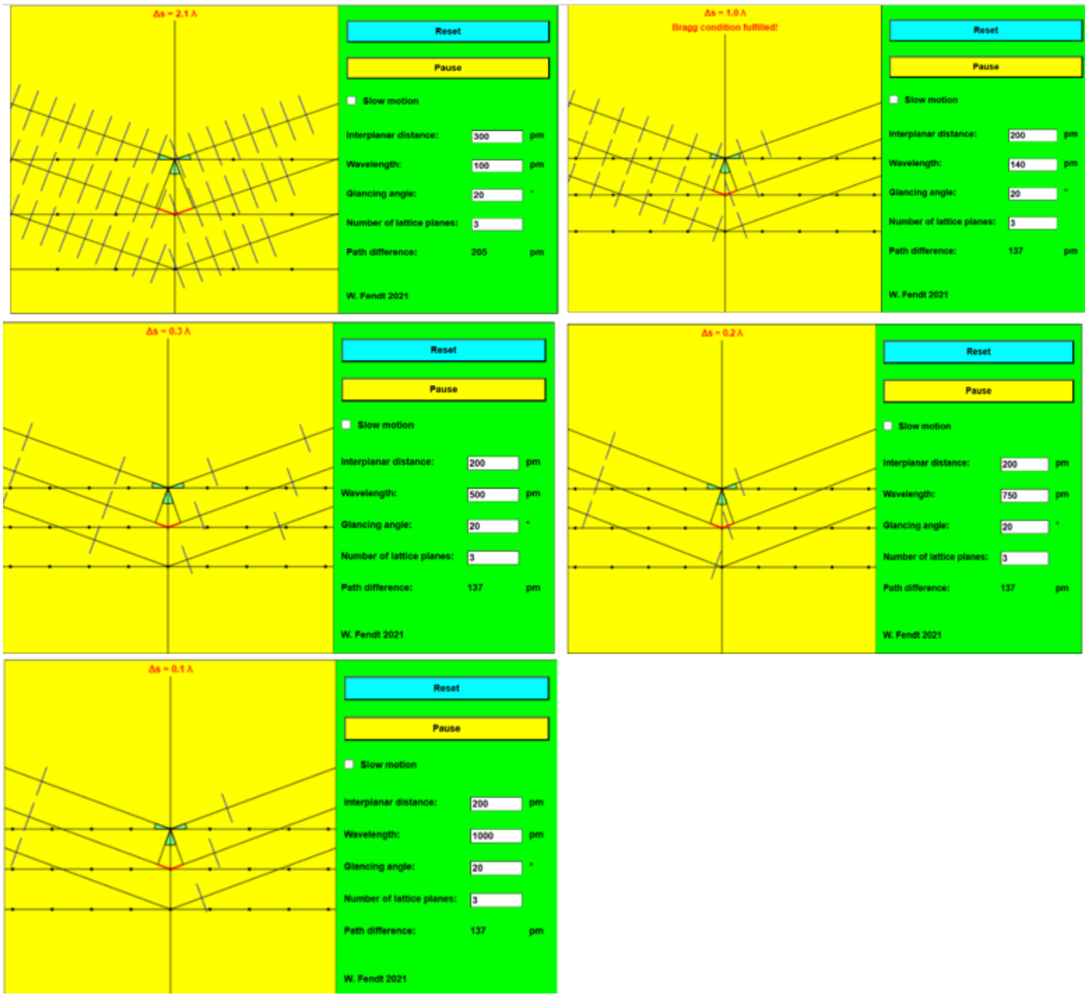

Figure 10

13. In the App, enter the value of glancing angle as default, i.e., 20. Press start and observe the change in the path difference as the glancing angle is varied. Then, press reset to change its value. The interplanar distance and wavelength remains constant at 200 pm and 100 pm. Refer figure 11.
    The minimum allowed value of glancing angle in the App is 1° and maximum is 89°.

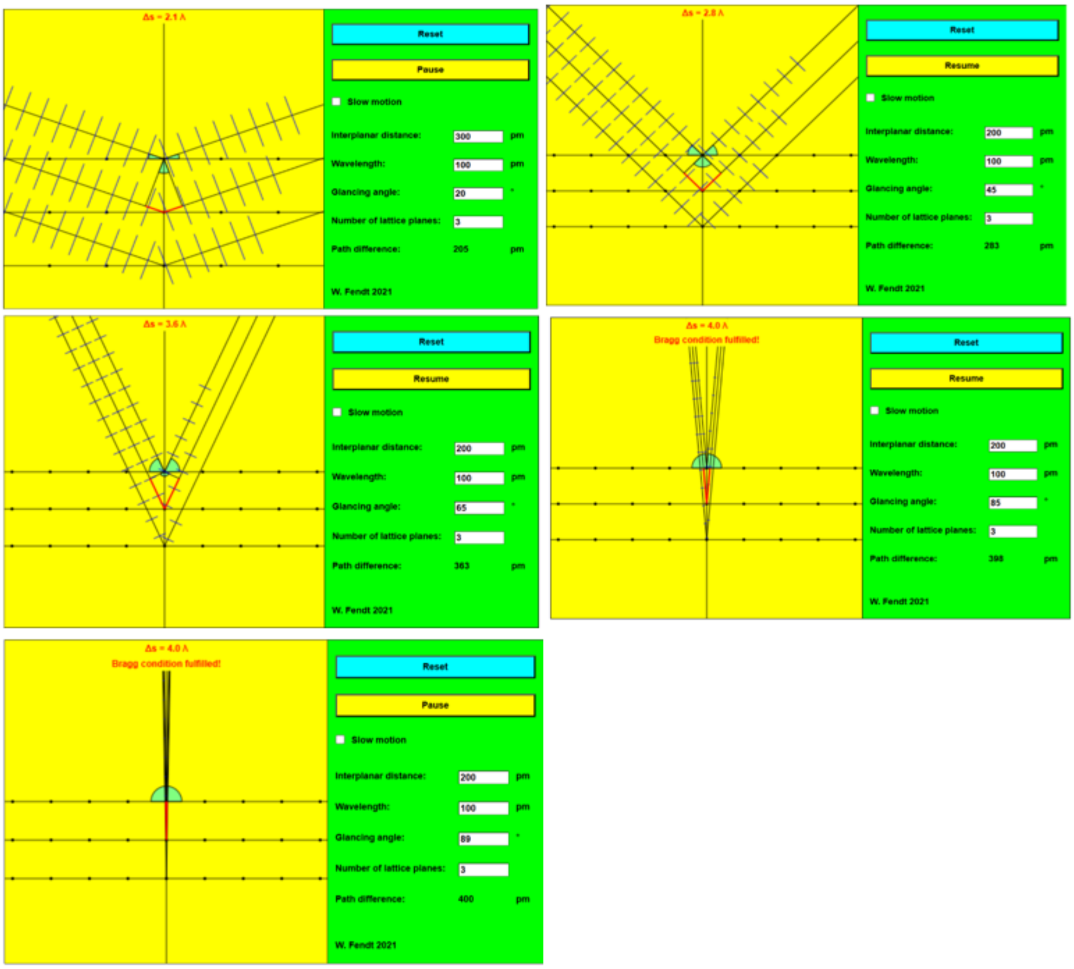

Figure 11

14. Steps 9-11 are done and the condition of Bragg Reflection is checked.

RESULTS

Result to the numerical problem- *the longest wavelength is 194 pm and its associated order is 2, the shortest wavelength is 130 pm and its associated order is 3.*

We solved the numerical problem and verified Bragg's Law using the App. A text, 'Bragg Condition Fulfilled' appeared in red, which only appears when the path difference is an integral multiple of the wavelength of the X-ray.

By varying the values of wavelength, interplanar distance, and glancing angle, we observed the change in path difference. The values were chosen at random (ref. steps 9-12 in procedure).

Table 1 – Varying the value of Interplanar distance

Interplanar distance (in pm)	*Path difference, Δs (in pm)*	*Order of diffraction, k*
200	137	1.4
300	205	2.1
400	274	2.7
435	298	3.0
500	342	3.4

The table above depicts that, as the interplanar distance increases, the path difference increases. Bragg condition is fulfilled when the interplanar distance is 400 pm.

Table 2 – Varying the value of Wavelength

Wavelength (in pm)	*Path difference, Δs (in pm)*	*Order of diffraction, k*
100	137	1.4
140	137	1.0
500	137	0.3
750	137	0.2
1000	137	0.1

The table above depicts that, as the wavelength increases, the path difference remains the same but the order of diffraction changes. Bragg condition is fulfilled when the wavelength is 140 pm.

Table 3 – Varying the value of Glancing angle

Glancing angle	*Path difference, Δs (in pm)*	*Order of diffraction, k*
20	137	1.4
45	283	2.8
65	363	3.6
85	398	4.0
89	400	4.0

The table above depicts that, as the glancing angle increases, the path difference increases. Bragg condition is fulfilled when the glancing angle is 85° and 89°.

CONCLUSION

Bragg's law is essential in understanding interactions between electromagnetic waves and matter. It is the fundamental principle used in the field of X-ray diffraction and crystallography. By observing Bragg peaks, we deduce the crystalline structure.

While the diffraction of X-rays by atoms is complicated, the App simplifies it providing a simpler interface. The path difference provided in the App can be used to solve numerical problems, albeit within limits. It is a very useful tool to familiarize oneself with the complexity of diffraction and interference.

REFERENCES

1. Apps on Physics- www.walter-fendt.de/html5/phen/braggreflection_en.htm

2. N. W. Ashcroft and N. D. Mermin, *Solid State Physics*. Holt, Rinehart and Winston, 1976

3. Halliday and R. Resnick, *Fundamentals of Physics*, 10th ed. Wiley, 2014

4. G. N. Eby, *Principles of Environmental Geochemistry*. Brooks/Cole-Thomson Learning, 2004, pp. 212-2

5. Figure 1 - Huxtable, Scott. (2002). Heat transport in superlattices and nanowire arrays