Simulation of X-ray diffraction and determination of the crystal structure

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Overview

- X-ray diffraction is one of the most common ways to study the structure of a crystal
- the diffraction peaks are characteristic of the crystal and can be used to identify the crystal
- It is important to develop a simulation tool that can be used to emulate the experimental results of X-ray diffraction and analyze the crystal structure
- We will also describe the approach we had in coding the modules, and explain the calculations involved in the code.
- Additionally, we present the results of our simulation, including visualizations of the lattice structure, reciprocal space, and the resulting diffraction pattern for a face-centered cubic (FCC) lattice as a demonstration

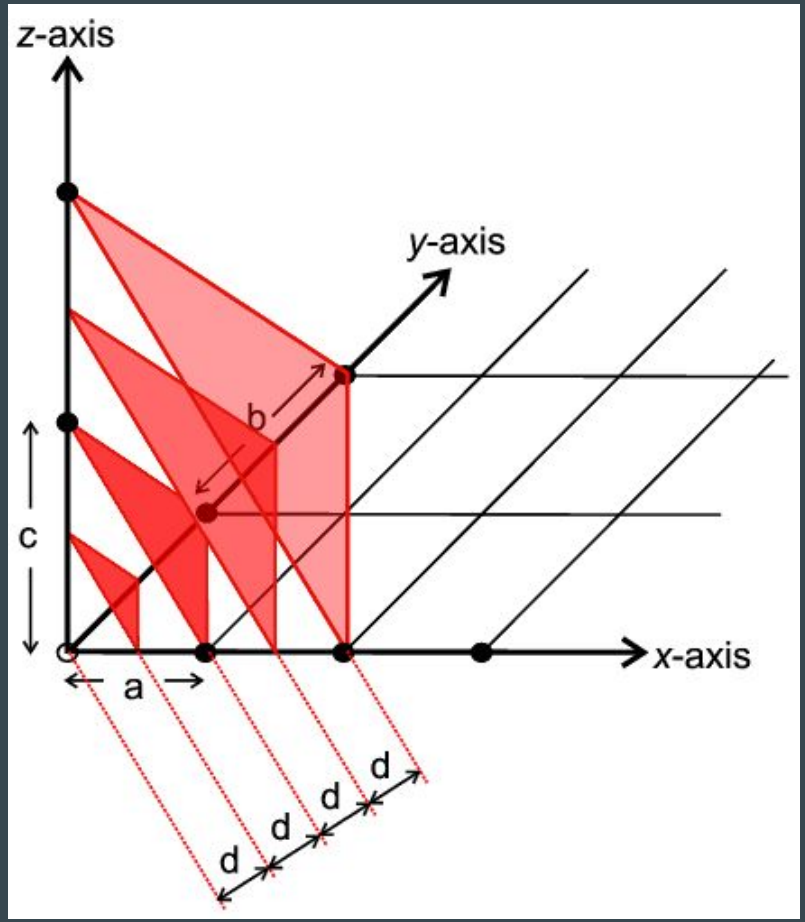
Theoretical Background

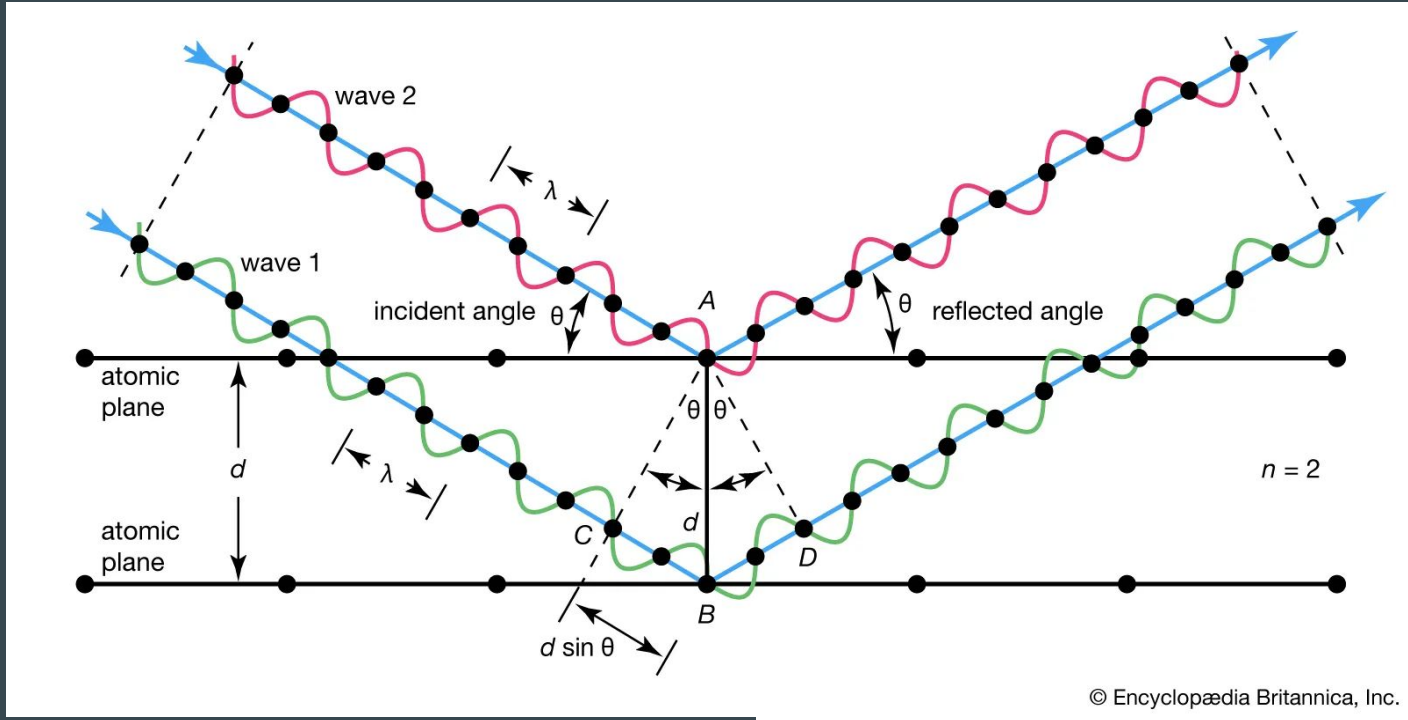
- By transitioning into reciprocal space and examining the points where diffraction peaks occur, we can determine many valuable properties of the crystal.
- The diffraction peaks are characteristic of the crystal and can be used for its identification.

Theoretical Background

Inside a crystal, there are periodic arrangements of atoms that create hollow areas acting like slits for incident X-rays. These hollow areas correspond to the spacings between different periodic planes within the crystal. Each set of periodic planes is assigned unique Miller indices (h,k,l), which serve as labels for these planes

- This image demonstrates the concept of Miller indices in crystallography, showing lattice planes intersecting the axes at specific points





- This image illustrates the principle of Bragg's Law and the constructive interference of X-rays reflecting from crystallographic planes.

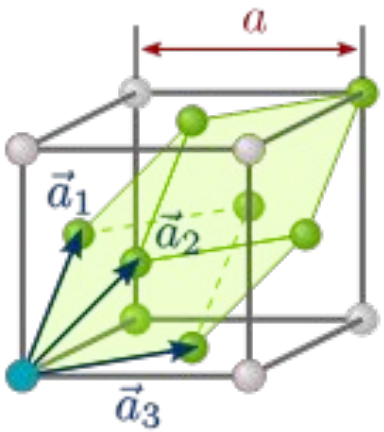
$$n\lambda = 2d_{hkl}\sin\theta$$

- Each set of planes with Miller indices (h,k,l) has a fixed spacing d_hkl between them and follows Bragg's law for diffraction
- The diffraction pattern in real space is complex, making it challenging to identify which set of planes contributes to each diffraction peak. To address this, we transition to reciprocal space.
- In reciprocal space, each point is represented by a reciprocal lattice vector G defined as:

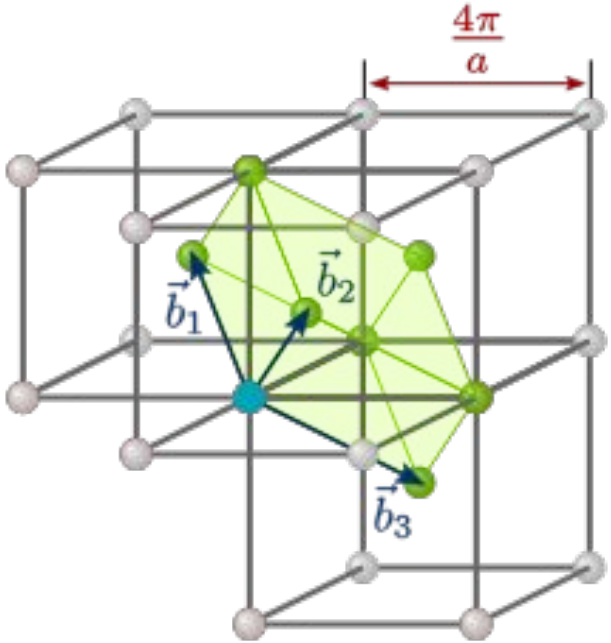
$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

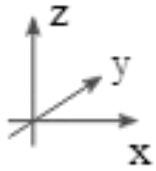
- where h, k, and l are Miller indices, and b1, b2, b3 are the reciprocal lattice vectors

direct lattice:
fcc with edge length a

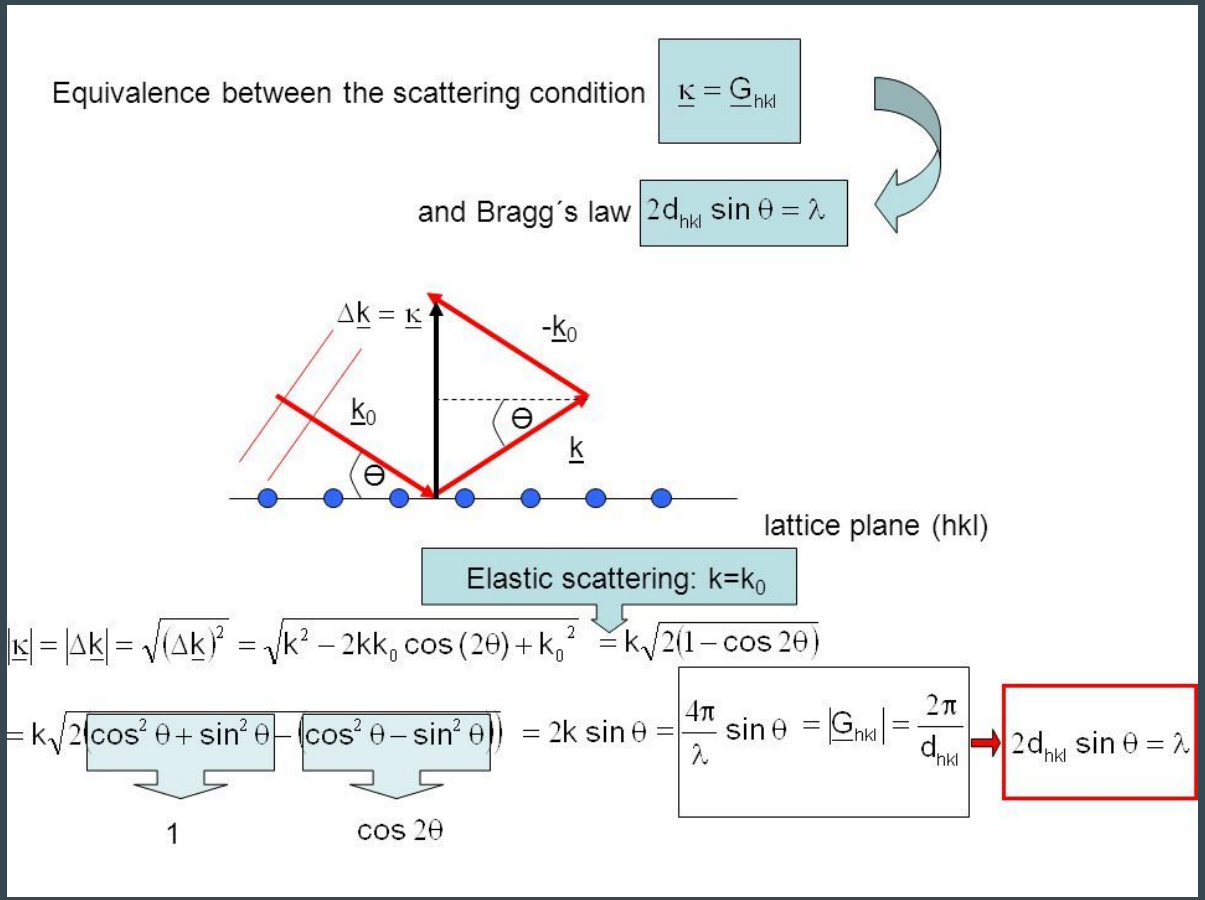


reciprocal lattice:
bcc with edge length 4π/a

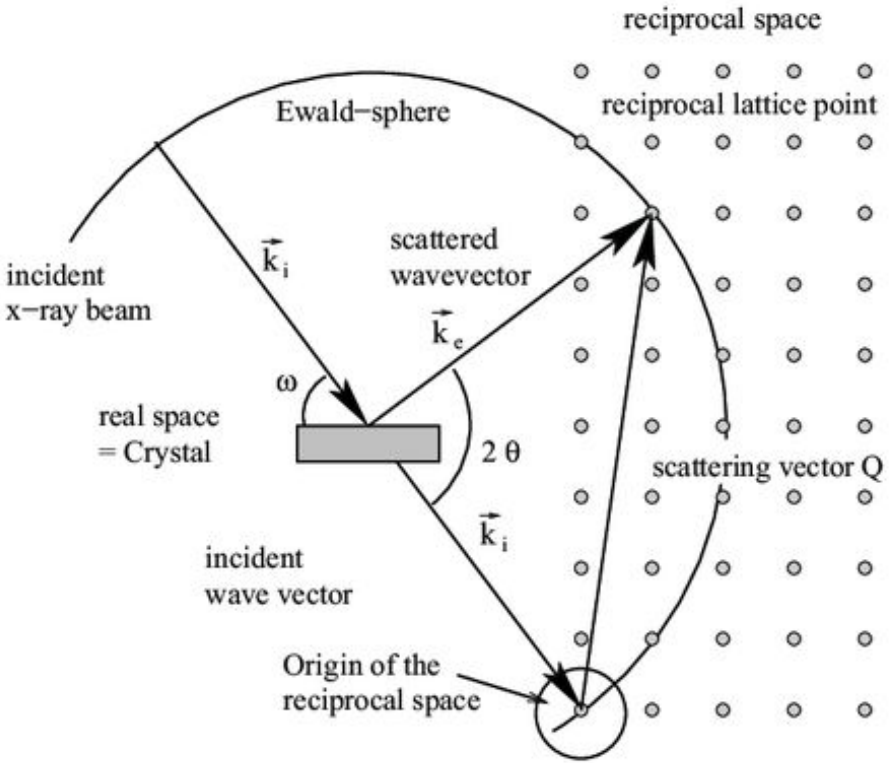




- This figure connects elastic scattering, wavevector changes, and Bragg's Law. It shows that $2d_{hkl} \sin\theta = \lambda$ can be derived from the wavevector relationships



- Assuming no energy loss during diffraction (elastic scattering), the magnitudes of ki and kf are equal. The Ewald sphere construction is a valuable tool for visualizing the diffraction process in reciprocal space.
- The Ewald sphere construction in reciprocal space. It relates ki, kf, and reciprocal lattice points. Intersection of reciprocal lattice points with the Ewald sphere indicates possible diffraction conditions.



- Each peak represents a plane with specific Miller indices, and the set of peaks is characteristic of the material. By examining the peaks in reciprocal space and their corresponding Miller indices, we can identify the lattice structure and the identity of the material

The diffraction condition in reciprocal space follows the Laue condition:

$$\mathbf{k}_f - \mathbf{k}_i = \mathbf{G} \tag{3}$$

where $\mathbf{k}_i$ is the incident wavevector and $\mathbf{k}_f$ is the scattered wavevector. This condition implies that the scattering vector $\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i$ must coincide with a reciprocal lattice vector $\mathbf{G}$. Therefore, for every diffraction peak, there exists a combination of (h, k, l) corresponding to a set of planes in the crystal.

The Modules

- implemented in Python, utilizing libraries such as NumPy for numerical computations,Matplotlib for plotting, and SciPy for advanced mathematical functions.

Visualising the lattice

This module provides a 3D visualization of the crystal lattice, illustrating how atoms are arranged in real space. By representing the primitive lattice vectors and basis atoms, users can gain an intuitive understanding of the crystal's geometric structure.

Visualising the Diff. peaks

This module transitions the real-space lattice into reciprocal space, plotting the diffraction peaks that satisfy the Laue condition. By visualizing reciprocal lattice vectors, users can identify the positions and intensities of potential diffraction peaks.

Analyzing the peaks

This module analyzes the diffraction peaks obtained in reciprocal space. By matching the pattern of peaks and their corresponding Miller indices with known reference patterns, the module can determine the crystal structure and identify the material

For the First Module: Visualization of the Lattice Structure

- The lattice vectors are determined based on the provided lattice parameters and angles. The unit cell is then replicated along each axis to create a larger crystal structure for visualization.

The lattice vectors **a**, **b**, and **c** are calculated using the lattice parameters a, b, c and the angles α, β, γ between them:

$$\mathbf{a} = \begin{bmatrix} a \\ 0 \\ 0 \end{bmatrix} \tag{4}$$

$$\mathbf{b} = \begin{bmatrix} b\cos\gamma \\ b\sin\gamma \\ 0 \end{bmatrix} \tag{5}$$

$$\mathbf{c} = \begin{bmatrix} c\cos\beta \\ c\left(\frac{\cos\alpha - \cos\beta\cos\gamma}{\sin\gamma}\right) \\ c\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}/\sin\gamma \end{bmatrix} \tag{6}$$

For the Second Module: Visualization of Diffraction Peaks

- The reciprocal lattice vectors a*, b*, and c* are computed using the following relations →
- By applying the Laue condition, the module identifies reciprocal lattice points that correspond to possible diffraction peaks. These points are then plotted in reciprocal space, providing a visual representation of where diffraction events are likely to occur based on the crystal structure.

$$\mathbf{a}^* = \frac{2\pi \mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}$$

$$\mathbf{b}^* = \frac{2\pi \mathbf{c} \times \mathbf{a}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}$$

$$\mathbf{c}^* = \frac{2\pi \mathbf{a} \times \mathbf{b}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}$$

For the Third Module: Analysis of Diffraction Peaks

- It calculates the structure factors for each allowed (h,k,l) reflection, considering atomic form factors and multiplicities based on the crystal system's selection rules.
- The sum runs over all atoms in the unit cell, fj is the atomic form factor of the j-th atom, and (u,v,w) are the fractional coordinates of the atom.
- The intensity Ihkl of each reflection is proportional to |Fhkl|^2. By comparing the simulated diffraction pattern with known reference patterns, the module identifies the crystal structure and the corresponding material.

$$F_{hkl} = \sum_j f_j e^{2\pi i(hu+kv+lw)}$$

Results

To demonstrate the functionality of our simulation tool, we present the results for a face-centered cubic (FCC) lattice, specifically modeling copper (Cu) as an example.

3D Visualization of the Lattice

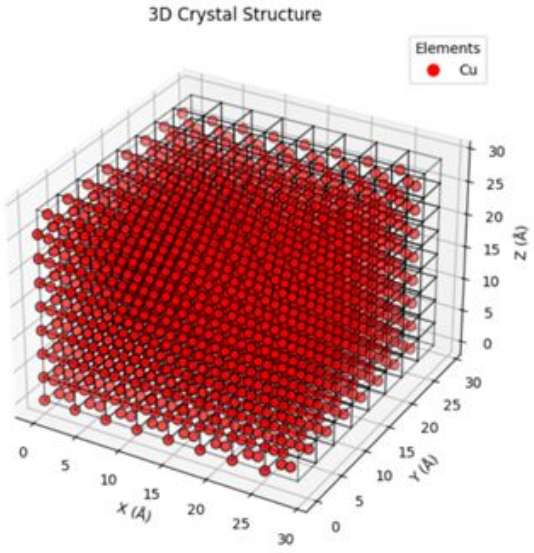


Figure 6: 3D visualization of the FCC lattice structure for copper (Cu). Atoms are represented by colored spheres, and the unit cell edges are depicted in black lines.

Plot of the Reciprocal Space

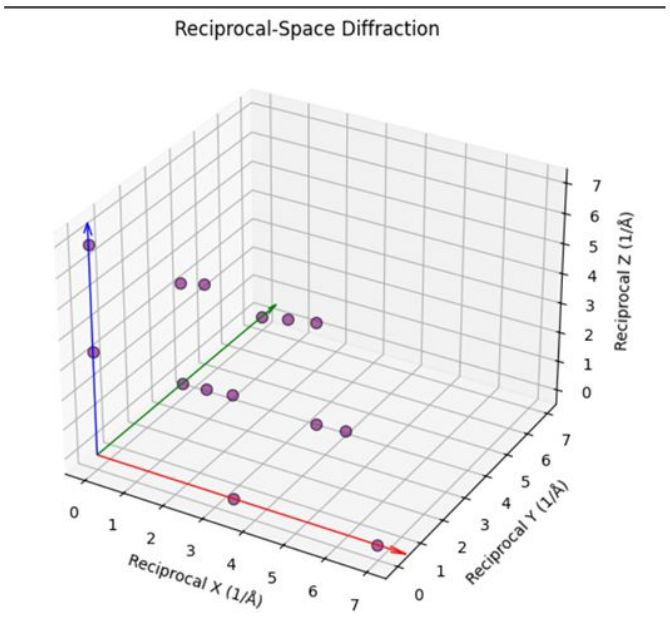


Figure 7: 3D reciprocal-space diffraction pattern for the FCC single lattice of copper (Cu). Reciprocal lattice vectors are shown as purple points. The red, green, and blue arrows represent the reciprocal lattice axes $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$, respectively.

Diffraction Peaks and Powder Diffraction Pattern

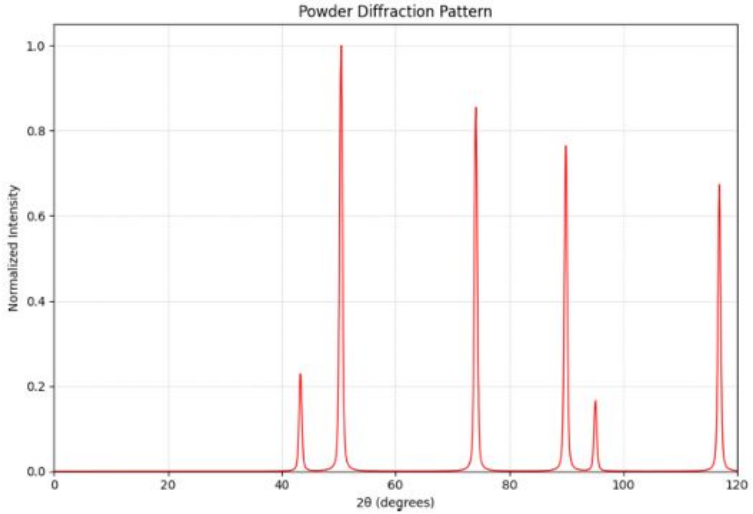


Figure 8: Simulated powder diffraction pattern for the FCC lattice of copper (Cu). Peaks correspond to allowed (h, k, l) reflections, with intensities normalized to the maximum peak.

Explanation

- Using the first module, we generated a 3D visualization of the FCC lattice structure. The unit cell of FCC consists of atoms at the corners and centers of each face of the cube. By replicating the unit cell along each axis, we created an extended crystal structure, allowing for a clear and comprehensive visualization of the periodic arrangement of atoms.
- The second module was utilized to plot the reciprocal lattice of the FCC structure. The reciprocal lattice of an FCC crystal is body-centered cubic (BCC). In reciprocal space, each reciprocal lattice point corresponds to a set of Miller indices that satisfy the Laue condition for diffraction.

Explanation

- The third module analyzed the diffraction peaks and generated a powder diffraction pattern for the FCC lattice. The simulation calculated the structure factors for allowed reflections based on FCC selection rules, considering the multiplicity of each reflection. Theresulting powder diffraction pattern displays peaks at specific 2θ angles corresponding to the interplanar spacings of the FCC structure

Discussion

- The 3D Visualization of the FCC lattice (Figure 6) clearly shows the periodic arrangement of copper atoms within the unit cells. The reciprocal-space plot (Figure 7) accurately represents the BCC reciprocal lattice, indicating that our simulation correctly transitions from real space to reciprocal space
- The powder diffraction pattern (Figure 8) exhibits distinct peaks at angles corresponding to the FCC reflections, such as (1,1,1), (2,0,0), (2,2,0), etc. The positions and intensities of these peaks match the theoretical predictions based on Bragg's law and the structure factor calculations, validating the accuracy of our simulation tool.

Conclusion

- The simulation tool presented in this paper is a valuable asset for researchers and educators in materials science and crystallography.
- By providing modules for visualizing the crystal lattice in real and reciprocal spaces and analyzing diffraction peaks, the tool bridges theoretical concepts with practical applications.
- The detailed theoretical background and the implemented algorithms enable users to understand the underlying principles of X-ray diffraction and apply them to real-world scenarios.

Thank you