Crystallography : Reciprocal X-Ray Lattice Simulations

--TEAM MEMBERS--
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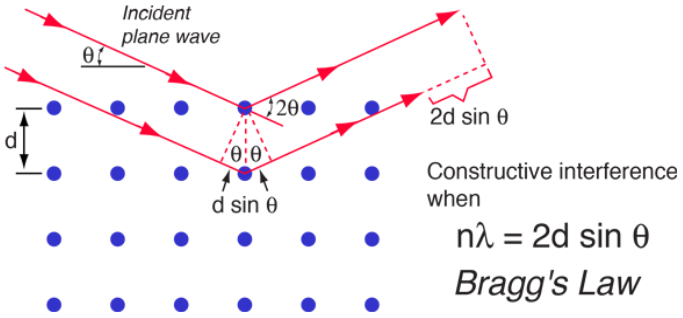
ABSTRACT

X-ray Crystallography (XRC) is a method of determining the structure of any crystal using diffraction phenomenon. Crystallography is the best fit method to discretize the structure that appears almost similar in other methods.



The intensities of these reflections may be recorded with the photographic film, an area detector (such as a pixel detector) or with a charge coupled device (CCD) image sensor.

After taking the diffraction pattern, if the inverse discrete space fourier transform is applied, it gives a 2D structure of the surface plane.

Here, we have generated the input by transforming it into Reciprocal
Space. It is an end-to-end matching code, which verifies the proof of the concept.
Along with this , the code can generate the Reciprocal lattice vectors for the given set of inputs.
All algorithmic functions in the code are self written and are upto the mark with the inbuilt functions.

1. INTRODUCTION

1.1 Why did we choose this topic?

- Reciprocal space is a mathematical tool which is used in many other applications. E.g. Crystallography,Hamiltonian oscillations, phonons measurement etc.
- This encouraged us to gain knowledge about it. Succedently , implement it in this Project.
- Simulating this phenomenon to solve the real life problems of perfect crystal formation.

1.2 What tools of signals and systems would be utilized here?

- Discrete space fourier transform in two dimensions (2D)
- Inverse discrete space fourier transform in 2D.
- Reciprocal space inversion.

1.3 What is our PROBLEM STATEMENT?

- Getting proteins to form crystals can be hard
- In the crystallographer market, X-ray diffractometer costs in the millions.
- If we simulate exact thing, it could make the study easily accessible and efficient
- Finding the perfect crystals without any defects is difficult practice.
- Diffractometer ranges with errors of 8-10 % .
- These apparatus are usually built just for a specific range of X-ray frequencies.
- For X-rays, which are electromagnetic radiation of a shorter wavelength (typically between 2 and 200 wavelengths), the refractive index of X-rays in different materials is equal and close to unity. No refractive lenses can be constructed for these rays.

2. Crystallography using Fourier Analysis

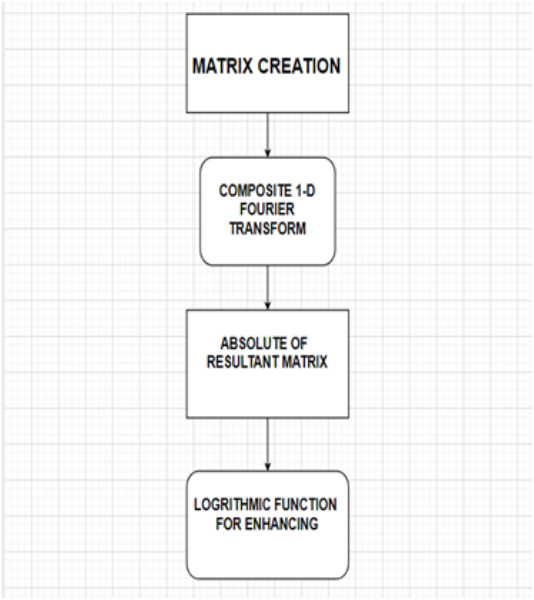
2.1 Real Space to Reciprocal Space

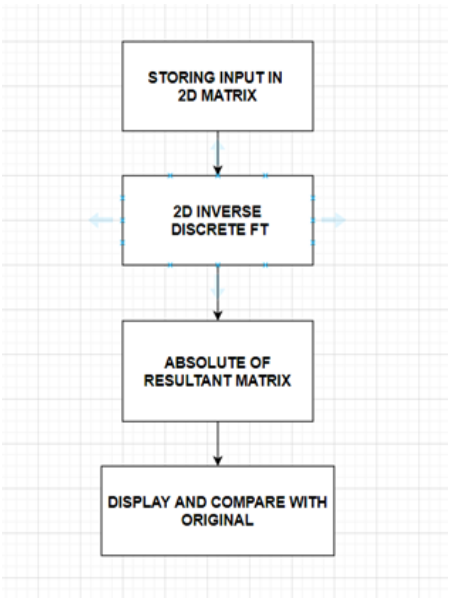
Step **1:** Creating a matrix with respect to ideal (or real) crystal structure.
Step **2** : Simulating the x ray diffraction pattern on a Roentgen absorbent screen.
Step **3** : Applying the 1-D discrete fourier transform on each row from top to bottom.
Step **4** : Combining the result from step 3 and once again apply 1-D discrete fourier transform.
Step **5** : Using the Logarithmic function to enhance the reciprocal lattice
Step **6** : Displaying the absolute of the resultant matrix by inbuilt matlab function.

2.2 X-ray Crystallography : Reciprocal Space to Real Space

Suppose now if the crystallographer needs to predict the Crystal structure along with the input of Reciprocal lattice structure

Step 1: Taking the input of Reciprocal Vectors and storing in 2D Matrix.
Step 2: Applying the 2D inverse discrete fourier transform.
Step 3: Taking the magnitude of the complex matrix .
Step 4: Simply Displaying the so-called predicted structure.
Step 5: Rechecking with the original structure.





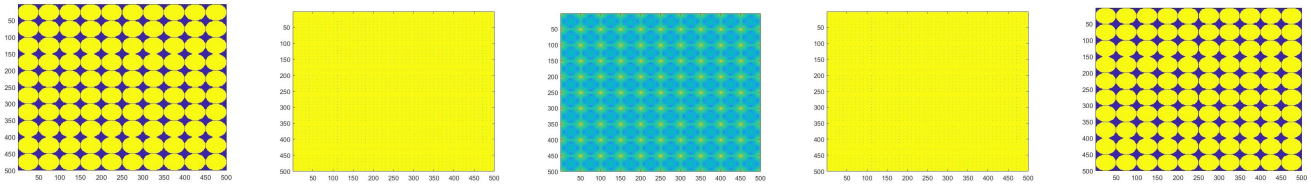
3 Results and Observations:

3.1 Simulation.

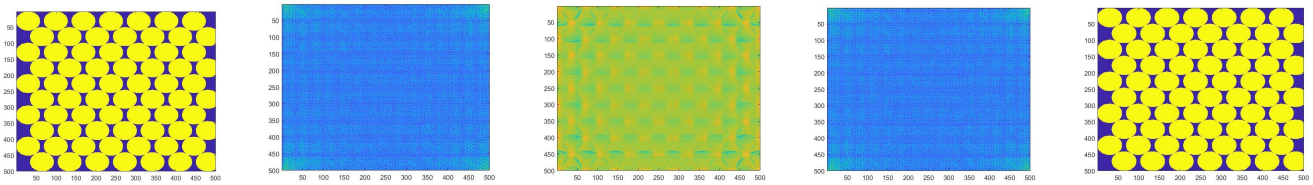
With loop and image stacking, we successfully demonstrated the simulation of this phenomena.

Attached herewith are the Results performed on :

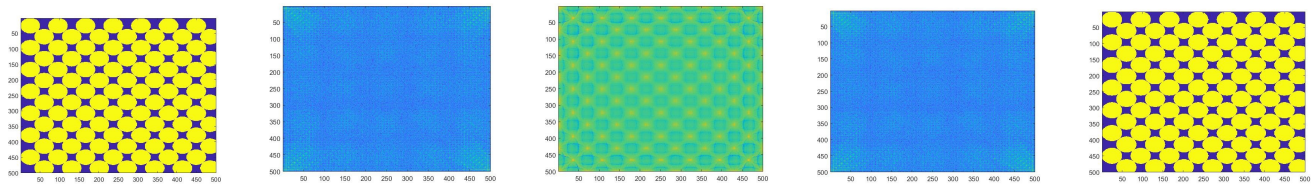
3.1.1Simple Cubic Bravais Lattice



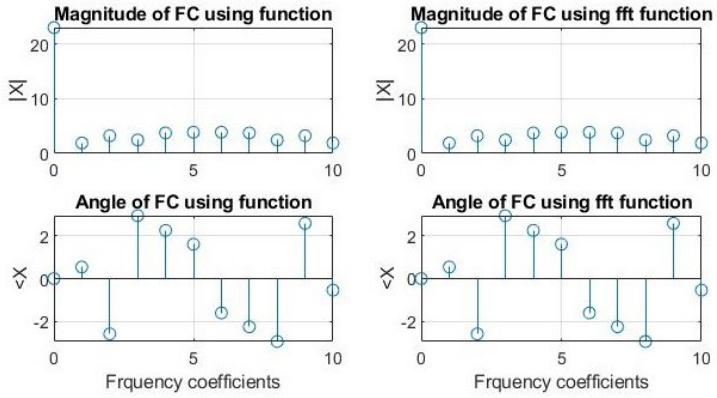
3.1.2 Body Centered Cubic Unit Cell



3.1.3 Face Centered Cubic Unit Cell.



PS: The comparison with inbuilt function is below.



4 CONCLUSIONS & LIMITATIONS

4.1 Conclusions :

- We observed that symmetrical behaviour in reciprocal space leads to crucial information of its electron density structure.
- Irregularities in the diffraction pattern shows the defects in crystals such as interstitial sightings, unoccupied space, exceptional bonding etc.
- Diffraction of X-ray along the edges of the unit cell shows high diffraction grating. This phenomenon was seen in the fourier transform of the Fcc lattice with radius of atom set to scale of 135.
- The Ewald Sphere in reciprocal lattice showed the characteristics of atom movements, along with Heisenberg's uncertainty principle.

4.2 Limitations:

- The code takes an input of the matrix which is periodic. But in real structure it is never accurately periodic. Hence it is a disadvantage that the results are filled with errors.
- In the practical apparatus, the absorbent screen on which the X-ray falls after diffraction,Is highly resolutive. Resolution ranges in 2^16 parts per picture. This depth is hard to simulate in code, hence we have ranged in possible scale.
- To predict the exact structure in 3Dimensions , thousands of inputs are needed at each bravias angle of the surface plane. Processing all these and then generating results is what the apparatus do. But in simulation we have restricted to the front normal plane, this might be considered as a limitation of code.

- This simulation just shows the result of the input matrix and changes according to the input.
  Given a crystal substance without knowing its structure, the reciprocal lattice is not shown by simulation because it's not actually using any X-rays digitally.

4.3 Future scope:

- This project can later be expanded for non periodic lattices e.g. DNA structure, AMINO-group lattices etc.
- Our result can also be used to predict which atoms can fit into the interstitial voids to Find new combinations based on their stability.
- We can also display the structures from all possible directions as it is only displaying the front view in our work.
- Furthermore, It could also be used to study the structure of new elements having atomic mass greater than 118.

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