Crystallography using Scilab

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Abstract: This project is aimed at providing a visual representation, using computer simulation, of the different planes in a cubic crystal of different types, their corresponding reciprocal lattice points and the Laue back diffraction spots that they produce. This is achieved using the open-source programming software SCILAB. This project is intended to provide a deeper insight into the rather abstract ideas in crystallography with a hands-on approach to the topic for students taking introductory solid-state physics.

I. INTRODUCTION

Crystal structures form basis to almost every day-to-day object we observe, ranging from wooden tables to little sugar cubes, these crystal structures are what gives the macroscopic objects their properties. Solid state physics is the subject where one learns these unique structures and how they contribute to properties of various things.

While going through varies textbooks on this topic, one may come across the idea of ***reciprocal lattice***. Reciprocal lattice plays an important role in defining these properties and also extends its applications in the realms of quantum mechanics and thermodynamics. The concept of reciprocal lattice is rather abstract and tends to baffle students of introductory solid-state physics. In this paper, using methods of simulation with the help of open-source software, we provide an insight towards what ***families of planes*** and their ***reciprocal lattice vectors*** look in a 3-D space and how diffraction patterns are produced. Diffraction patterns of crystals give us vital information about a crystal structure.

The present work proposes a methodology of generating reciprocal lattice from the direct or ***real lattice*** graphically and plotting the points using SCILAB.

Our work here presents 2×2×2 cubic structures in real space. Simple cubic, face-centered cubic and body centered cubic structures along with their families of planes and reciprocal lattices.

II REAL SPACE AND FAMILY OF PLANES

II.I REAL SPACE

To set the plot of the basic comprehension of reciprocal space and phenomenon of diffraction, one must know what Real space is meant in a lattice.

Real space lattice consists of the real-world lattice points which represent the positions where atoms or group of atoms are found. These lattice points form the Real Space. In other words, the lattice points where a base atom is found in a crystal structure is what is known as the Real space lattice point and altogether comprises the Real space.

Figure 1 shows the 2x2x2 real space lattice of SCC, FCC and BCC, with the **dark blue spots** representing the corner lattice points while the **light blue spots** are made to represent face and body centered points.

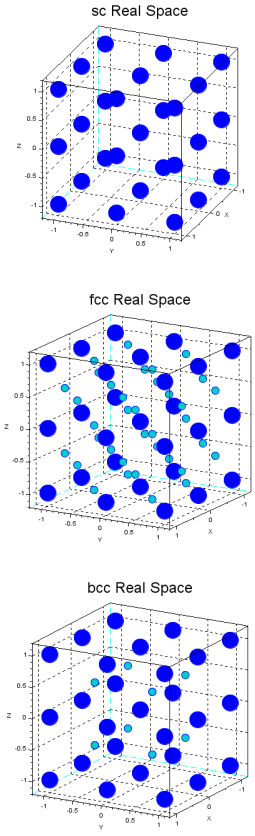

Figure 1: SCC, FCC, and BCC structures in real space

II.II FAMILY OF PLANES

A plane, in general mathematical sense, is the area enclosed by the lines joining intercepts (or any three points) on x- , y- and z- axes respectively. The given lattice can be then viewed as families or stacks of parallel planes. These families of parallel planes are described using Miller Indices (for e.g., (1 2 1), (2 2 2) etc. Each family of parallel planes can be identified by two parameters, firstly the specific orientation with respect to the origin (the direction normal to the planes) and secondly the inter-planar distance between any two adjacent planes. Since all planes in each family are equivalent, hence an entire family of parallel planes may be represented by only one plane which is closest to the origin i.e., has the smallest perpendicular distance from the origin. For e.g., in a 5 x 5 x 5 cubic lattice, the family of plane (1 1 1) contains planes (1 1 1), (2 2 2), ..., (5 5 5). So, in a 2 x 2 x 2 lattice as in our case, all families of planes can be represented by one plane each. Figure 2 here shows different planes that can exist in different 2x2x2 cubic lattice.

Now, the length of perpendicular drawn from origin to the plane represents the ***planar distance*** given as d_{hkl}.
The inverse of this planar distance is known as the ***reciprocal distance*** and the point which it represents in the 3D space is known as the ***reciprocal point*** of that plane. It's not just the inverse which plays an important role, but when this reciprocal distance is multiplied by the factor 2π, *it* represents a wave space or k-space, which holds significance in the study of diffraction pattern.

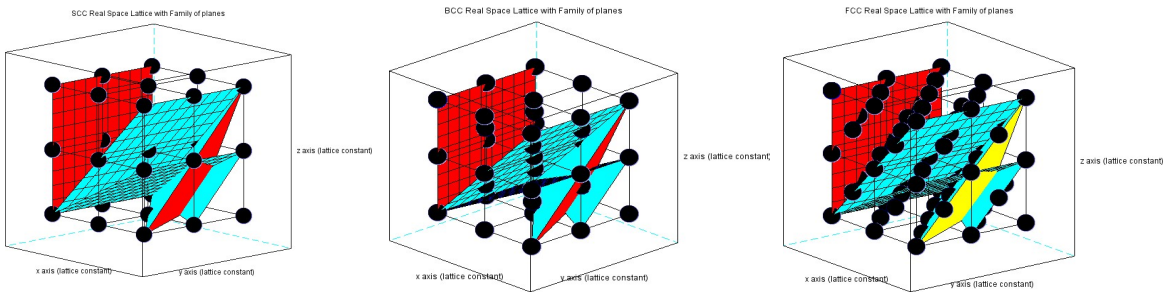

Figure 2: Shows the different families of planes that can exist in a 2 ×2 ×2 SCC, BCC and FCC lattice

III. RECIPROCAL SPACE AND DIFFRACTION PATTERN

III.I RECIPROCAL SPACE

In the same way we can plot the plane (222) as shown in figure 3 as explained in Graphical Pedagogy of Teaching Reciprocal Space, by Dr. Adarsh Singh and Mitushi Gupta [1]. Also, each of these planes can be then converted into one reciprocal point. In fact, all the planes (111), (222), (333), and so on, result in a linear array of lattice points. This forms a

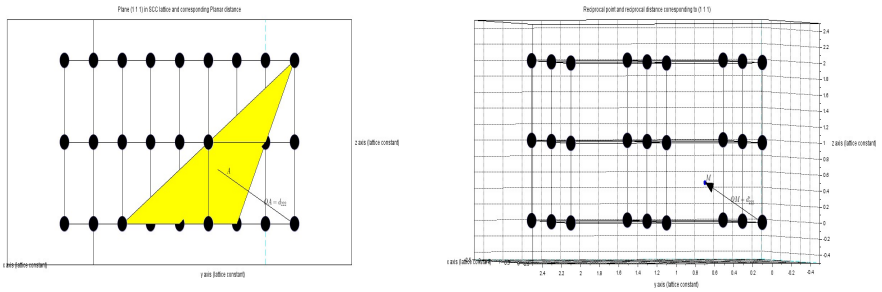

Figure 3: Shows plane (222) corresponding planar distance (top) and its corresponding reciprocal point (bottom) in SCC

family of planes and we can consider other Miller indices to form a complete 3D reciprocal lattice.

Reciprocal Lattices of simple cubic, face centered cubic and body centered cubic structures are as shown here in figure 4:

III.II DIFFRACTION PATTERNS

With the discovery of X-Rays in the early 1900s, wavelengths of light comparable to the atomic spacing could be produced. When these rays interact with atoms in a crystal, they produce diffraction patterns which contain information about the families of planes which exist in an atomic structure. These are vital to the understanding of crystal structures and their properties. This gave rise to an entirely new field of study called crystallography. In 1912 van Laue explained the formation of such patterns using interference of light.

III.II.I LAUE BACK REFLECTION METHOD

Bragg's condition for constructive interference between two rays of wavelength λ incident at an angle θ on a crystal array of spacing d is given as

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

$$n = 1,2,...$$

n defines the order of the corresponding maxima.

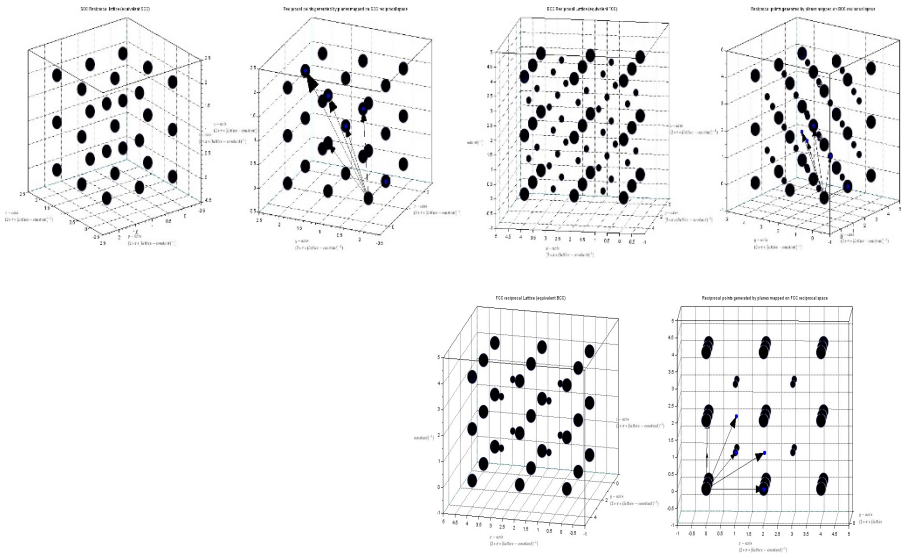

Figure 4: This shows the mathematically obtained reciprocal lattice of SCC, BCC and FCC respectively on left and on right are the points obtained by all the families of planes that can exist (in blue dots)

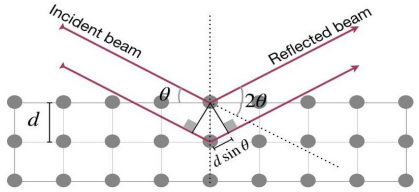

Figure 5: Bragg's condition for interference

The diffraction patterns are produced using computer simulation of ***Laue back reflection method***. The experimental procedure from Bailey 2016 [3] is simulated using SCILAB to obtain diffraction patterns as one would expect from an actual experiment. Laue back reflection is a method of obtaining the diffraction pattern of crystal structures where X-Rays are incident on a crystal from a particular direction and a spot is produced by some λ for each plane in the crystal which is formed for a particular angle θ and for a plane spacing d for a given n in accordance with Bragg's condition. That is, a ***Laue spot*** is produced in a direction making an angle 2θ with the incident X-ray beam. Different spots due to Laue back reflection are shown in figure 6.
Because d and θ are fixed, all orders of interference of n, for a given crystal plane are superimposed onto each other, making the spot brighter. These overlapping beams in one spot are all the members of one family of planes.

As one might expect, orientation of the crystal with respect to the incident x-ray is important as it determines the symmetry observed in the diffraction pattern. If a crystal is oriented along an axis having high symmetry, it becomes easy to identify the spots.

For example, in *NaCl* as shown in figure 7 below with incoming x-ray aligned with (110) plane perpendicular to incident x-ray beam, the Laue spots lie on lines passing through the point where the x-ray beam crosses the photographic film [4]. Each of the lines that can be identified in the pattern is a called a *zone* which contains the spots that correspond to the reflections from planes that have a common axis.
Every zone may be represented as [*uvw*] which contains all the planes (*hkl*) that satisfy

$$hu+kv+lw=0$$

For example, we see that in figure, 6 we have the zone [001] and all the planes are aligned with the z-axis. The spots which belong to any zone that is perpendicular to the x-ray axis lie on a straight line. All other reflections which are

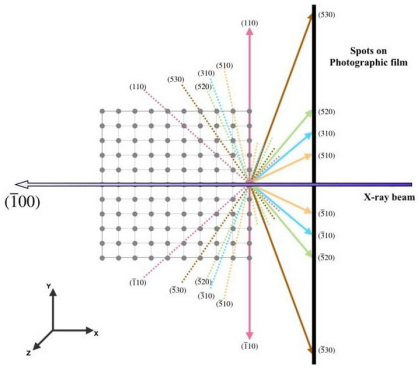

Figure 6: Laue back reflection on a photographic film showing the [001] zone planes and their spots on the film

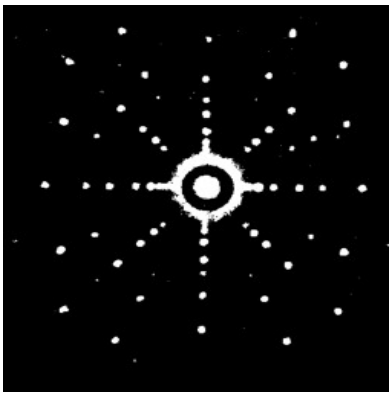

Figure 7: NaCl diffraction pattern showing the zones present

not perpendicular to the beam form the shape of a ***hyperbola*** as shown in the figure (taken from [3]) below.

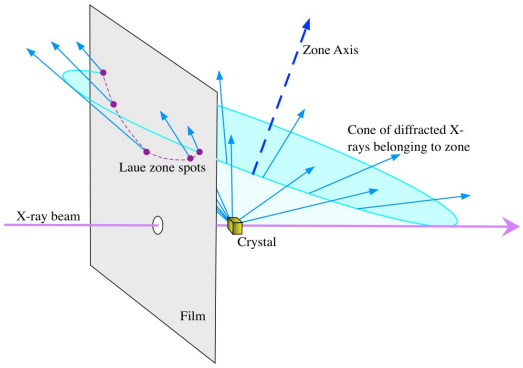

Figure 8: Cone of reflections for a zone axis

III.II.II Position of Spots from Miller indices

If we consider the x-ray beam incoming along the x-axis, then the spots lie on the photographic plate in the y-z plane. If the intersection of the x-ray is taken to be the origin, then the formula relating the y-z position of a spot to its hkl

index is

$$y = \frac{2hkD}{h^2 - (k^2 + l^2)}$$

and

$$z = \frac{2hlD}{h^2 - (k^2 + l^2)}$$

For a spot with scattering angles $(2\theta,\varphi)$, the angles of the planes that produces it are (θ,φ). These angles can be related to the y-z positions using simple geometry to get

$$\theta = \tan^{-1}\frac{\sqrt{y^2 + z^2}}{D}$$

$$\phi = \tan^{-1}\frac{z}{y}$$

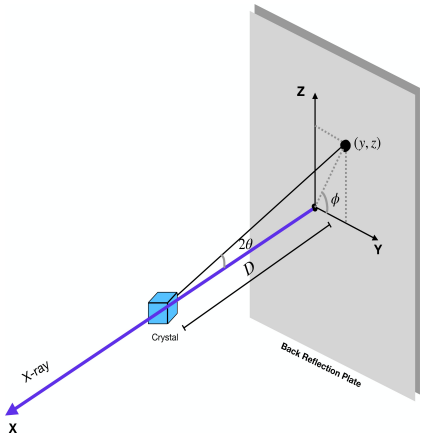

Figure 9: Position of diffraction spots due to Laue back reflection on a photographic film

In a cubic crystal, the observable planes are also constrained to

$$h^2 + k^2 + l^2 < \left(\frac{2a}{\lambda_{min}}\right)$$

where a is the lattice constant of the cubic crystal and λ_{min} is the minimum wavelength of the X-ray beam [3].

These formulae are taken from Bailey 2016 [3]. These are coded in SCILAB to get the y-z positions of the diffraction spots for an hkl plane using a scatter plot. But first, we must know the planes that exist and the intensity of their corresponding spots. These are calculated in the next subsection.

III.II.III Intensity of spots

For any given hkl plane, there exists a diffraction spot whose intensity is determined by the amount of X-Ray scattered by the plane. This adds a vital layer of information about any crystal structure as it indicates the density of atoms in the plane: greater the density, greater the scattering. In the program we vary the color of a spot to indicate the intensity. The formulae for the intensity of a particular spot are taken from Preuss 1974:27 [2]

$$I = \frac{(1+\cos^2 2\theta)F^2\left(\frac{\lambda}{\lambda_{min}}-1\right)}{\sin^2\theta} \cdot \frac{(\sin^2\theta-\cos^2\theta)^3}{\lambda^3} \qquad (1)$$

We run a loop over λ to select all the wavelengths that can produce diffraction spots in accordance with Bailey 2016: eq. (6) [3] and calculate their intensities.

Hence, the intensity varies with the angle a spot makes from the central spot as shown in figure 9.

F is known as the ***geometric structure factor*** and can take the value 0 or 1 to determine whether that spot exists in the pattern (This is a simplification for the value of F but works for our purposes here).

Equipped with this, we can now proceed to simulate diffraction patterns. We shall replicate the diffraction pattern of *NaCl* as seen in figure 7. *NaCl* has a lattice constant $a = 5.64$ and exhibits an FCC structure. For FCC structures, $F^2 = 1$ when h, k, l are all odd or all even and 0 otherwise.

We consider arbitrary but reasonable values for the wavelength λ of the X-Ray and distance D. Thus, we obtain the following diffraction pattern (left).

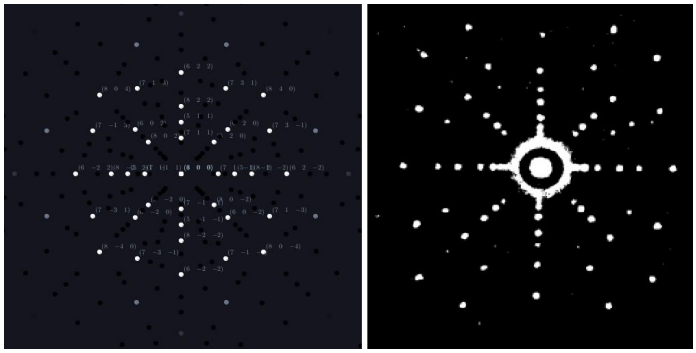

Figure 10: Comparison between simulated (left) and real (right) NaCl diffraction patterns

Each spot is labelled to indicate the plane which produces it. Overlapping miller indices seen in the simulated pattern indicate family of planes, all of which have a common diffraction spot. One can also see the four-fold symmetry in the diffraction pattern as one would expect.

This procedure can be extended to obtain many other diffraction patterns seen in nature.

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