FINDING AND COMPARING RELATIVE INTENSITY OF XRD PATTERNS OF NANOPARTICLES USING MATLAB

Project Report

Submitted by

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ERNAKULAM
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ST. TERESA'S COLLEGE

(AUTONOMOUS)

B SC. PHYSICS

PROJECT REPORT

This is to certify that the project report entitled "**FINDING AND COMPARING OF RELATIVE INTENSITY OF XRD PATTERNS OF NANOPARTICLES USING MATLAB**" is an authentic work done by **NIMITHA MARY T.J.**

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EXAMINERS :

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ST. TERESA'S COLLEGE (AUTONOMOUS)

ERNAKULAM

CERTIFICATE

This is to certify that the project report entitled **"FINDING AND COMPARING OF RELATIVE INTENSITY OF XRD PATTERNS OF NANOPARTICLES USING MATLAB"**is an authentic work done by **NIMITHA MARY T.J**, St Teresa's College, Ernakulam, under my supervision at Department of Physics, St. Teresa's college , Ernakulam, for the partial requirements for the award of Degree of Bachelor of Science in Physics during the academic year 2022-23.The work presented in this dissertation has not been submitted for any other degree in this or any other university.

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Place: ERNAKULAM
Date: 18-4-23

DECLARATION

I **NIMITHA MARY T.J**, final year B.Sc Physics students. Department of Physics St. Teresa's College, Ernakulam do hereby declare that the project work entitled "**FINDING AND COMPARING OF RELATIVE INTENSITY OF XRD PATTERNS OF NANOPARTICLES USING MATLAB** " has been originally carried out under the guidance and supervision of **Dr. MARY VINAYA,** Assistant Profession Department of Physics, St. Teresa's College, Ernakulam, in partial fulfilment for the award of the Degree of Bachelore of Physics, I further declare that this project is not partially or wholly submitted for any other purpose and the data included in the project is collected from various sources and are true to the best of my knowledge.

Place : Ernakulam

Date : 18-4-23

NIMITHA MARY T.J

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ABSTRACT

The project gives one a method to easily understand the basic concepts by giving the input parameters and see how XRD pattern will appear through a MATLAB program of an element of a certain crystal type under certain conditions such as when given x-ray source and lattice parameter very efficiently. Saving one from lack of time and confusion and helping them to readily understand the results of ones research with lesser errors.

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CHAPTER-1

INTRODUCTION

CHAPTER -1

INTRODUCTION

INTRODUCTION

Chapter 1 introduces the idea of crystal structure and its classification and different types with examples. Within this framework, concepts of crystallinity and non crystallinity are introduced. It mainly focusing on the classification of crystal structure that is hexagonal close packed structure(hcp), face centered cubic structure(fcc), body centred cubic structure(bcc) ,simple cubic structure(sc). This chapter also includes basic information about the matlab program.

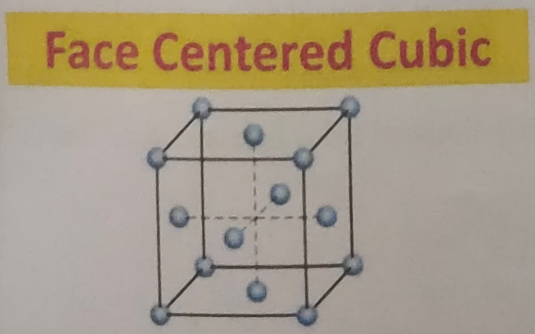
1.0 Basic crystal structures

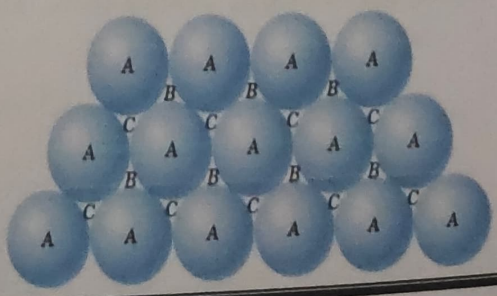
Crystal are 3-dimensional structures. A crystal is obtained by stacking different atomic planes one over the other. Different methods of stacking give rise to different crystal structures. Crystal structure are classified as close packed structure and loose packed structure. Close packed structure be again classified as hexagonal close packed structure(hcp) and face centered cubic structure(fcc). Loose packed structure be again divided as body centered cubic structure(bcc) and simple cubic structure(sc).

1.1 Closed packed structures

They are mostly found in monoatomic crystals having nondirectional bonding such as metallic bonding. In order to describe close packed structures, define a parameter called packing fraction. Packing fraction is defined as the ratio of volume actually occupied by the atoms in the unit cell to the total volume of the unit cell. For close packed structures like hcp and fcc, packing fraction is found to be 0.74.

1.2 Face centred cubic crystal structure

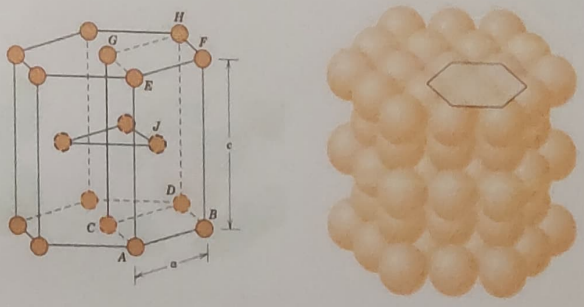




The crystal structure found for many metals has a unit cell of cubic geometry, with atoms located at each of the corners and the center of all the cube faces. Such cubic structure is called as face centered cubic crystal structure (FCC). Some of the metals having this crystal structure are copper, silver, aluminum and gold. Each corner atom in the FCC crystal structure is shared by eight-unit cells, as opposed to just two for a face centered atom. As a result, each of the eight corner atoms is made up of one-eighth and each of the six face atoms is made up of one-half. A unit cell may contain up to four whole atoms. Two other factors of crystal structure are the coordination number and atomic packing factor (APF).

For FCC, the coordination number is 12. And the atomic packing factor is 0.74.

1.3 Hexagonal close packed crystal structure

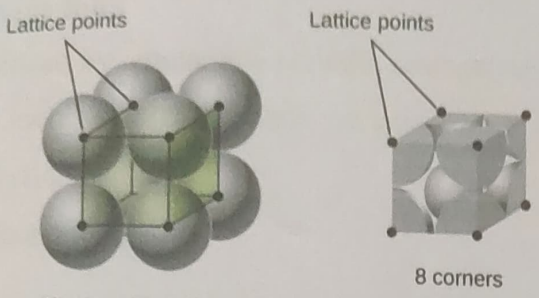


The name corresponding to the shape of the conventional unit cell which is hexagonal. Such crystal structure is called as hexagonal close packed crystal structure. In HCP, the equivalent of six atoms is contained in each unit cell; one-sixth of each of the 12 top and bottom face corner atoms, one-half of each of the 2 center face atoms, and all 3 midplane interior atoms. For HCP, the coordination number is 12 and atomic packing factor is 0.74.

1.4 Loose packed structures

Loose packed structure is that in which the coordinate number of an atom is less than 12 and its packing fraction is below 0.74. Two common loose packed structures are simple cubic (SC) and body centered cubic structure (BCC).

1.5 Simple cubic structure



Simple cubic lattice cell

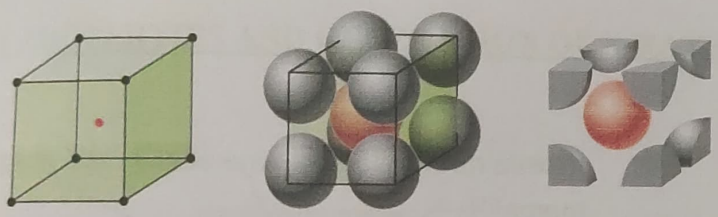
The conventional unit cell is primitive with a basis of one atom.

Atomic packing factor= 52%

Coordination number= 6

Number of atoms per unit cell= 1

1.6 Body centered cubic structure



Body-centered cubic structure

A BCC unit cell has atoms at each corner of the cube and an atom at the centre of the structure. Examples of BCC metals are sodium, potassium, Lithium, chromium. For BCC, coordination number is 8 and atomic packing factor is 68%.

2.0 Crystal and their structures

Some characteristics of crystalline solids are influenced by the arrangement of atoms, ions, and molecules in the materials crystal structure. There are countless distinct crystal formations, all of which have long-range atomic order, which ranges from comparatively simple structures for metals to incredibly complex. Several of the ceramic and polymeric materials exhibit complex ones. Atoms (or ions) are seen as solid spheres with well- defined diameters when describing crystalline structures. It is named as atomic hard-sphere Solid is one of the states of matter. In solids, the atoms are attached to each other with strong forces of attraction. Solid have definite size, shape, and they occupy a definite volume. They can be

broadly classified into crystalline and non-crystalline solids depending on the arrangement of atoms in them.

2.1 Crystalline solid

It is characterized by regular and periodic arrangement of atoms. They have long range order. It has sharp melting point. Crystals are anisotropic. The physical properties are different in different directions.

Examples: diamond, quartz.

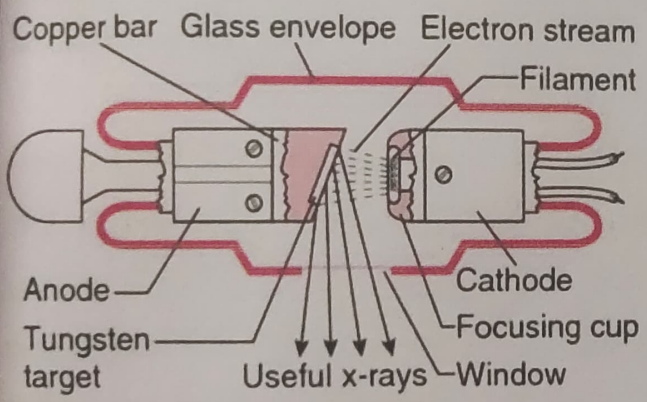
2.2 Non-crystalline solid

It has completely random arrangement of atoms. It exhibits short- range order. Amorphous solids do not sharp melting point. They are isotropic.

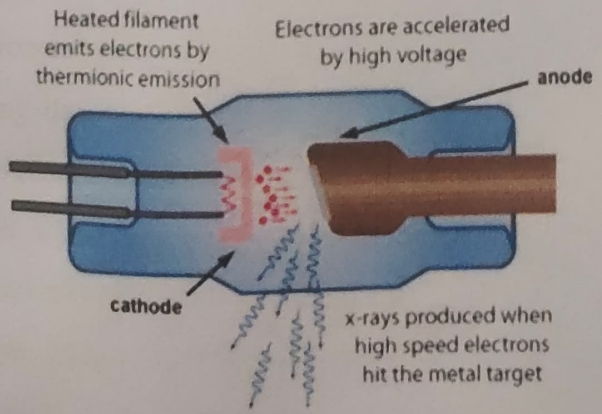
Examples: glass, graphite, rubber, plastic.

3.0 X-RAY DIFFRACTION

3.1 PROPERTIES AND GENERATION OF X-RAYS



Typical X-ray tube operation



X-rays are a form of electromagnetic radiation with wavelengths ranging from 0.01 to 10 nanometers. In the setting of diagnostic radiology, X-rays have long enjoyed use in the imaging of body tissues and aid in the diagnosis of disease. Simply understood, the generation of X-rays occurs when electrons are accelerated under a potential difference and turned into electromagnetic radiation.An X-ray tube, with its respective components placed in a vacuum, and a generator, make up the basic components of X-ray production. Essential components of an X-ray tube include a cathode, and an anode separated a short distance from each other, a vacuum enclosure, and high voltage cables forming the X-ray generator attached to the cathode and anode components. In the generation of X-ray production, a cathode filament machined in a cathode cup is activated, causing intense heating of the cathode filament.The heating of the filament leads to the release of electrons in a process called thermionic emission. The released electrons form in an electron cloud at the filament surface, and repulsion forces prevent the ejection of electrons from this negatively charged cloud. Upon application of a high voltage by an X-ray generator to the cathode as well as the anode, there is an acceleration of electrons ejected to an electrically positive anode. The filament and the focusing cup determine this path of acceleration. The number of electrons is measured in the form of milliampere (mA) units, where 1 milliampere is equal to 6.24 x 10^15 electrons/s. Electron kinetic energy (measured in keV) is related to the applied voltage. The tube voltage, tube current, and exposure duration (measured in seconds) are adjustable by the user.

Once the high kinetic energy electrons finally reach the anode target, this initiates the process of X-ray production. Tungsten is often the usual anode target, although other material targets are also employed. Electrons come extremely close to the nucleus of the target, causing a deceleration and change in direction, converting the kinetic energy to electromagnetic radiation in a process known as “breaking radiation” or bremsstrahlung.The output is a spectrum of X-ray energies. Incident electrons can also result in ionization, whereby the approaching electron can remove a second electron belonging to an atom of the anode target, losing its energy through ionization or excitation. This process leads to an emission of a photon as the electron orbit vacancy gets filled by an orbital shell electron from a further out shell. Considering orbital energies and their differences are unique in atoms, this leads to a “characteristic X-ray” with energies that can serve as a fingerprint unique to each anode target. Bremsstrahlung X-rays, however, constitute the majority of X-rays produced in this process.

Before understanding the final production of an X-ray image, it is essential to understand the interaction of X-rays with individuals exposed to X-rays. There are three important types of interactions that occur between X-rays and the tissues of our body. The "classical" or "coherent" interaction occurs when an X-ray strikes an orbital electron and subsequently bounces off and changes direction.These X-rays are low energy and do not cause ionization and only add a small dose amount to a patient. In "Compton" scattering, X-rays of higher energy strike an outer shell electron and are strong enough to remove it from the shell, causing ionization of an atom. This phenomenon contributes to dose and also contributes to scatter. Photoelectric interactions occur when an incoming X-ray strikes an inner shell electron, removing it from the shell and causing a downward cascade of outer shell electrons filling inner orbit vacancies, further releasing secondary X-rays. This type of interaction contributes to image contrast. Finally, the differential absorption of X-rays within the tissues of the body subsequently contributes to the production of the final image. Attenuation of X-rays ultimately depends on the effective atomic number in tissue, X-ray beam energy, and tissue density.

Image detectors come in the form of digital and analog film detectors. One limitation of analog systems is the limited range of exposure intensities that it can accurately detect; this lends itself to multiple images taken for an adequate and interpretable study, and therefore subsequently leads to increased radiation exposure to a patient. Digital systems allow a user to fix contrast and brightness and provide greater post image processing options.

3.2 WHAT IS X-RAY POWDER DIFFRACTION (XRD)

An analytical method known as x-ray powder diffraction (XRD) is quick and is primarily used to determine the phase of crystalline materials. It can also reveal information about unit cell dimensions. The material under analysis is finely powdered, homogenized, and the bulk composition is calculated on average.

3.3 FUNDAMENTAL PRINCIPLES OF X-RAY POWDER DIFFRACTION(XRD)

In 1912, Max von Laue made the discovery that crystalline materials behave for X-ray wavelengths like the spacing of planes in a crystal lattice, acting as three-dimensional diffraction gratings. Today, the study of crystal structures and atomic spacing is frequently conducted using X-ray diffraction.

X-ray diffraction is based on constructive interference of monochromatic X-rays and a crystalline sample. These X-rays are generated by a cathode ray tube, filtered to produce monochromatic radiation, collimated to concentrate, and directed toward the sample. The interaction of the incident rays with the sample produces constructive interference (and a diffracted ray) when conditions satisfy Bragg's Law ($n\lambda=2d \sin \theta$). This law relates the wavelength of electromagnetic radiation to the diffraction angle and the lattice spacing in a crystalline sample. These diffracted X-rays are then detected, processed and counted. By scanning the sample through a range of 2θangles, all possible diffraction directions of the lattice should be attained due to the random orientation of the powdered material.

3.4 XRD INSTRUMENTATION-HOW IT WORKS?

X-ray diffractometers consist of three basic elements: an X-ray tube, a sample holder, and an X-ray detector.



X-rays are generated in a cathode ray tube by heating a filament to produce electrons, accelerating the electrons toward a target by applying a voltage, and bombarding the target material with electrons. When electrons have sufficient energy to dislodge inner shell

electrons of the target material, characteristic X-ray spectra are produced. These spectra consist of several components, the most common being K_α and K_β. K_α consists, in part, of $K_{\alpha 1}$ and $K_{\alpha 2}$. $K_{\alpha 1}$ has a slightly shorter wavelength and twice the intensity as $K_{\alpha 2}$. The specific wavelengths are characteristic of the target material (Cu, Fe, Mo, Cr). Filtering, by foils or crystal monochromators, is required to produce monochromatic X-rays needed for diffraction. $K_{\alpha 1}$and $K_{\alpha 2}$ are sufficiently close in wavelength such that a weighted average of the two is used. Copper is the most common target material for single-crystal diffraction, with CuK_α radiation = 1.5418Å. These X-rays are collimated and directed onto the sample. As the sample and detector are rotated, the intensity of the reflected.

X-rays is recorded. When the geometry of the incident X-rays impinging the sample satisfies the Bragg Equation, constructive interference occurs and a peak in intensity occurs. A detector records and processes this X-ray signal and converts the signal to a count rate which is then output to a device such as a printer or computer monitor. The geometry of an X-ray diffractometer is such that the sample rotates in the path of the collimated X-ray beam at an angle θ while the X-ray detector is mounted on an arm to collect the diffracted X-rays and rotates at an angle of 2θ. The instrument used to maintain the angle and rotate the sample is termed a *goniometer*. For typical powder patterns, data is collected at 2θ from ~5° to 70°, angles that are pre-set in the X-ray scan.

4.0 MATLAB

4.1 What is MATLAB?

Mathematical software with programming, graphical, and numerical capabilities is called MATLAB. It has both procedural and object-oriented programming constructs, as well as an integrated development environment.

4.2. How to access MATLAB?

After login in, one can typically use the system command MATLAB to access MATLAB and the command quit or exit to leave MATLAB. Your local installation, however, might let you access MATLAB through a menu or by clicking an icon.

4.3 Statements, Expressions and Variables

When you type an expression into MATLAB, it is interpreted and evaluated. Most MATLAB Expressions take the form .

variable=expression or simply expression

Typically operator, functions and variables names make up expression. The matrix created by the expressions evaluation is displayed on the screen and allocated to the variable to use later. With a carriage return, a statement is finished. However a statement can be confused to the next line with three or more periods followed by a carriage return. However if they are separated by colons or semicolons, multiple Statements can be positioned on a single line.MATLAB is case sensitive in the names of commands, functions and variables.

4.4 Saving a Session

All variables when one logs out or quits the program. However all variables are written to a deskfile name matlab.mat which is non-human readable such that the command load will restore to its original statement when one reenters MATLAB.

4.5 MATLAB Building Functions

Convenient matric building functions are

1) eye - identity matrix
2) zeroes – matrix of zeroes
3) ones- matrix of ones
4) diag- create or extract diagonals
5) triu-upper triangular part of matrix
6) tril- lower triangular part of matrix
7) rand- randomly generated matrix
8) hilb- Hilbert matrix
9) magic- magic square

4.6 For, while, if- and relations

In their basic forms ,MATLAB flow control statements operate like those in most computer Languages.

4.7 For

The for statement permits any matrix to be used except 1:n. The variable consecutively just assumes the value of each column of the matrix.

4.8 While

The general form of a whole loop is

while relation

statement

end

For as long as the relation is true, the sentence will be repeatedly executed.

4.9 If

The general form is

if relation

statement

end

The statement will be executed only of the relation is true.

5.0 Relations

The relation operators in MATLAB are

1)>-greater than

2)<-less than

3)>=-greater than or equal to

4)<=-less than or equal to

5)==-equal

6)~=-not equal

5.1 Scalar Functions

Some MATLAB functions primarily operate on scalars but behave elementally when applied to a matrix.

5.2 Vector functions

MATLAB functions operate essentially on a vector but act on an m×n matrix (m>=2) in a column by column fashion to produce a row vector containing the result of their applications to each column.

5.3 Matrix Functions

Much of MATLAB's power comes from its matrix functions.

5.4 Command line Editing and Recall

The command line in MATLAB can be easily edited. The cursor can be positioned with left/right arrows and the backpace key used to delete the character to the left of the cursor.

5.5 Submatrices and Colon Notation

Vectors and submatices are often used in MATLAB to achieve fairly complex data manipulation effects. Colon notation which is usually used to generate Vectors and subscription by integral Vectors are key to efficient manipulation to these objects.

5.6 M-files

MATLAB can execute sequence of statements stored in diskfiles. Such files are called M-Files because they must have the file type ".m" as the last part of there filename.

There are two types of M-Files

1)Script files

2)Functions files

5.7 Script Files

A script file consists of a sequence of normal MATLAB statements. Script files maybe used to enter data into a large matrix in such a file entry errors can be easily corrected.

5.8 Function Files

Function file provide extensibility to MATLAB. You can create new function specifics to your problems which will then have the same status as other MATLAB functions.

5.9 Graphics

MATLAB can produce planar plots of curves,3D mesh surface plots and 3D faceted surface plots. The primary commands for these facilities are plot,plot3,mesh and surf respectively.

CHAPTER-2

THEORY

THEORY

Intensity of Diffraction: the Structure Factor Equation

The concepts of Ewald sphere and reciprocal lattice or Bragg's law predict when diffraction will occur but give no indication of the intensity of a given diffraction event.

If we start with the scattering formula as seen earlier:

$$F(\mathbf{S}) = \sum_{n} f_n e^{2\pi i \, \mathbf{S}.\mathbf{r}_n}$$

We describe the position, **r**, of atoms by the use of fractional coordinates (x, y, z) of the repeat units **a**, **b**, **c** of the crystal, i.e.

$$\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$$

and substituting this gives:

$$F(\mathbf{S}) = \sum_{n} f_n e^{2\pi i \, \mathbf{S}.(x\mathbf{a} + y\mathbf{b} + z\mathbf{c})} = \sum_{n} f_n e^{2\pi i \, (\mathbf{S}.a x + \mathbf{S}.b y + \mathbf{S}.c z)}$$

But we know that for a large number, N, of repeats the 3 von Laue conditions will apply. So writing these ($\mathbf{S}.\mathbf{a} = h$, $\mathbf{S}.\mathbf{b} = k$, $\mathbf{S}.\mathbf{c} = l$) into the above equation gives:

$$F(\mathbf{S}) = \sum_{n} f_n e^{2\pi i \, (hx + ky + lz)}$$

This effectively is the final answer required except to note that sometimes the summation is written in the form:

$$F(\mathbf{S}) = \sum_{x} \sum_{y} \sum_{z} f_n e^{2\pi i \, (hx + ky + lz)}$$

thus recognising that to sum over all space (x, y, z) within a unit cell is equivalent in diffraction terms to summing over all atoms (n) within the unit cell.

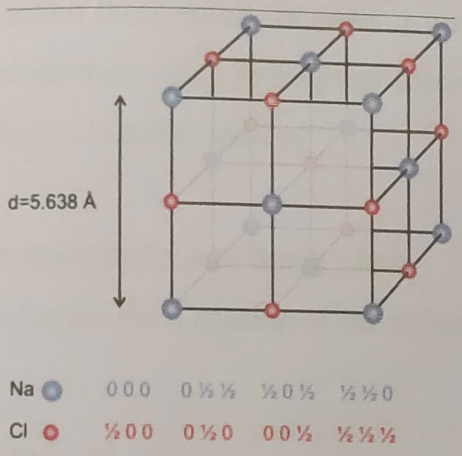
If Bragg's equation is the most well-known equation, then the structure factor equation must be the second most well-known. As much of crystallography is involved with determining atomic structure from the intensity of diffraction spots/peaks, then this equation acts as the basic computational link between the two.

Calculating the Intensity of Diffraction Using the Structure Factor Equation

First we take the example of NaCl for understanding the calculations:-

Sodium chloride (NaCl) is a face centred cubic structure (below figure) with a unit cell *d* spacing of 5.638 Å and fractional coordinates for the 4 Na and 4 Cl ions as follows:

Na 0,0,0;	0, ½, ½	½ ,0, ½	½, ½, 0
Cl: ½, 0,0	0, ½,0	0,0, ½	½,½,½



We start with the fundamental structure factor equation:

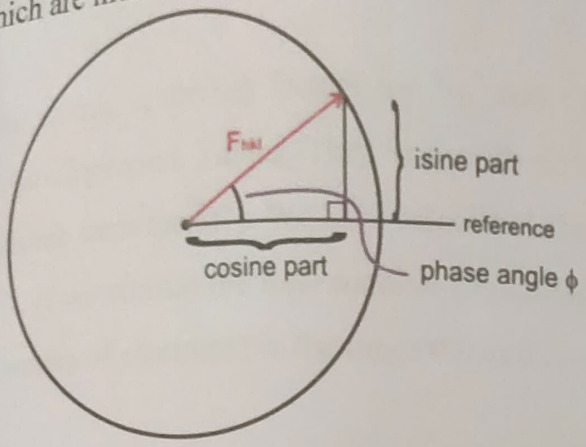
$$F(S) = \sum_{n} f_n e^{2\pi i (hx + ky + lz)}$$

This complex form is used to represent the fact that the diffracted wave has an amplitude and a phase. The equation is really a notational way of saying there are two parts: a sine part and a cosine part,

$$F(S) = \sum_{n} f_n \cos\{2\pi (hx + ky + lz)\} + i \sum_{n} f_n \sin\{2\pi (hx + ky + lz)\} \text{ (in radians)}$$

$$F(S) = \sum_{n} f_n \cos\{360 (hx + ky + lz)\} + i \sum_{n} f_n \sin\{360 (hx + ky + lz)\} \text{ (in degrees),}$$

which are illustrated in the following diagram:



The amplitude is represented as the radius of the circle and the phase as the angle made to a reference direction (horizontal). In general we calculate the cosine and sine parts separately and then combine them using Pythagoras' theorem to get the final amplitude.

Calculation for (111) miller indices

(1) Using Crystallography and Bragg's law

We need to calculate the *d* spacing of the reflection involved. The formula for *d* for cubic crystals is:

$$d_{hkl} = a / \sqrt{(h^2 + k^2 + l^2)}$$

For hkl=111we have

$$d_{111} = 5.638 / \sqrt{(1^2 + 1^2 + 1^2)} = 5.638 / \sqrt{3} = 3.255 \text{ Å}$$

From Bragg's law

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

So

$$\sin\theta / \lambda = 1 / 2d = 1 / (2 \times 3.255) = 0.154 \text{ Å}^{-1}$$

(2) Working out what atomic scattering factors (f_n) we will need

The atomic scattering factors for Na^+ and Cl^- ions can be obtained from the *International Crystallographic Tables*. They vary with $\sin\theta / \lambda$ for reasons that were explained earlier (the "atomic form factor"). We have calculated above that for the 111 reflection, $\sin\theta / \lambda = 0.154$ $Å^{-1}$. If we consult the *International Crystallographic Tables* we get the following *f* values (in numbers of electrons) in the range 0.0 to 0.2:

(3) Working out the cosine part of F_{111}

We will perform this part in degrees and the next in radians, so that you can see how to calculate the values by either convention. The cosine part for F has 8 terms corresponding to the 8 atoms involved. Inserting the appropriate *f* values, coordinates and *hkl* = 111 gives:

$$\sum_n f_n \cos\{360\,(hx + ky + lz)\} = 8.98 \cos\{360\,(1\times0 + 1\times0 + 1\times0)\}$$

$$+ 8.98 \cos\{360\,(1\times0 + 1\times1/2 + 1\times1/2)\}$$
$$+ 8.98 \cos\{360\,(1\times1/2 + 1\times0 + 1\times1/2)\}$$
$$+ 8.98 \cos\{360\,(1\times1/2 + 1\times1/2 + 1\times0)\}$$
$$+ 13.97 \cos\{360\,(1\times1/2 + 1\times0 + 1\times0)\}$$
$$+ 13.97 \cos\{360\,(1\times0 + 1\times1/2 + 1\times0)\}$$
$$+ 13.97 \cos\{360\,(1\times0 + 1\times0 + 1\times1/2)\}$$
$$+ 13.97 \cos\{360\,(1\times1/2 + 1\times1/2 + 1\times1/2)\}$$
$$= 8.98 \cos 0 + 8.98 \cos 360 + 8.98 \cos 360 + 8.98 \cos 360$$
$$+ 13.97 \cos 180 + 13.97 \cos 180 + 13.97 \cos 180 + 13.97 \cos 540$$
$$= 8.98 + 8.98 + 8.98 + 8.98 - 13.97 - 13.97 - 13.97 - 13.97$$
$$= -19.96$$

(4) Working out the sine part of F_{111}

We will perform this part in radians. Again inserting the appropriate values gives:

$$\sum_n f_n \sin\{2\pi(hx + ky + lz)\} = 8.98 \sin\{2\pi(1 \times 0 + 1 \times 0 + 1 \times 0)\}$$

$$+ 8.98 \sin\{2\pi(1 \times 0 + 1 \times 1/2 + 1 \times 1/2)\}$$
$$+ 8.98 \sin\{2\pi(1 \times 1/2 + 1 \times 0 + 1 \times 1/2)\}$$
$$+ 8.98 \sin\{2\pi(1 \times 1/2 + 1 \times 1/2 + 1 \times 0)\}$$
$$+ 13.98 \sin\{2\pi(1 \times 1/2 + 1 \times 0 + 1 \times 0)\}$$
$$+ 13.97 \sin\{2\pi(1 \times 0 + 1 \times 1/2 + 1 \times 0)\}$$
$$+ 13.97 \sin\{2\pi(1 \times 0 + 1 \times 0 + 1 \times 1/2)\}$$
$$+ 13.97 \sin\{2\pi(1 \times 1/2 + 1 \times 1/2 + 1 \times 1/2)\}$$
$$= 8.98 \sin 0 + 8.98 \sin 2\pi + 8.98 \sin 2\pi + 8.98 \sin 2\pi$$
$$+ 13.97 \sin \pi + 13.97 \sin \pi + 13.97 \sin \pi + 13.97 \sin 3\pi$$
$$= 0 + 0 + 0 + 0 + 0 + 0 + 0 + 0$$
$$= 0$$

(5) Combining the cosine and sine parts of F_{111}

Mathematically we would present this as a complex number result:

$$F_{111} = -19.96 + i \times 0$$

But non-mathematical students might find it easier to visualise the previous figure showing a right angled triangle with F_{hkl} on the hypotenuse,

so

$$F_{hkl}^2 = \{\text{cosine part}\}^2 + \{\text{sine part}\}^2$$
$$F_{hkl}^2 = (-19.96)^2 + 0^2 = 398$$

There will be no need to take the square root of F_{hkl}^2

(6) The intensity I_{111}

Since the diffraction experiment measures the squares of the amplitudes (but not phase information) assuming we have kinematic diffraction, then a very crude value for the peak intensity, which makes no allowance for any correction factors, might simply be given as:

$$I_{111} = F_{111}^2 = 398 \text{ units}$$

From Structure Factor to measured intensities

For an ideal Crystal we can take the above equation. But in reality the actual experimentally measured intensity will be yet different again since a number of additional experimental effects need to be taken into account, the main ones being:

1) multiplicity, j
2) the polarisation factor, P
3) the Lorentz factor, L
4) X-ray absorption, A
5) Temperature

The first four are often referred to as "corrections". It is true that the fifth factor, temperature, also refers ultimately to the experimental conditions but the effect of temperature is so intimately tied into the structure that we think of it rather in those terms.

We can write down a very simple equation to accommodate the first four factors:

$I_{hkl} = c\, jPLA\, F_{hkl}^2$

in which c can be considered to contain all the remaining factors.

From this we can calculate predicted intensities from a known structure.

PROGRAM

xrd-simulate

MATLAB Code to Simulate XRD Patterns

Getting Started

This collection of MATLAB scripts is designed to simulate relative-intensity XRD patterns using the basic theory of x-ray interaction with atoms in a bulk material. The calculations are based off of information that can be found in Structure of Materials: An Introduction to Crystallography, Diffraction, and Symmetry by Marc De Gaef and Michael E. McHenry.

If the user is unfamiliar with the basics mathematics behind XRD, a brief background math section is provided below. If the user is unfamiliar with crystallography the McHenry text or another basic text is strongly suggested.

Installing

The script **XRD_Intensity_Simulation.m** controls the entirity of the simulation. To begin the program simply run this script with the following functions and files in the same directory:

- dialogue.m
- dspace.m
- theta_s_calc.m
- scatterfactor.m
- scatterfactorcalc.m
- Scatteringdata.xlsx
- structurefactor.m
- intensitycalc.m
- lorentz.m
- compareintensity.m

Simulating XRD Patterns

In its current form, this script is designed to simulate a crystalline substance's XRD pattern the user-defined parameters:

1. Type of X-Ray source (Cu, Co, Mo, Cr, Fe)
2. Crystal Structure (BCC, FCC, SC, CsCl, HCP, Diamond)
3. Elemental Components
4. Lattice Spacing

The curvature of the XRD peaks plotted are provided for visualization's sake and do not represent expected FWHM. Modifying the compareintensity.m code can easily configure the plotting characteristics. Likewise, mixtures of components can be achieved by using rule of mixtures for the atomic scattering factors of various components - though caution should be taken at the validity of the results.

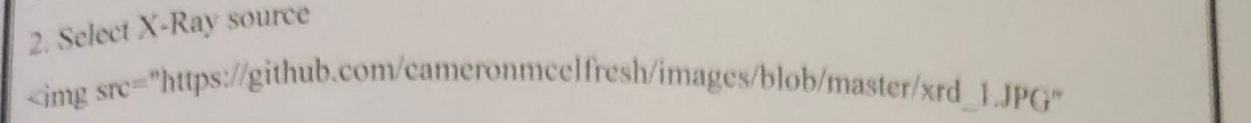
Input

No parameters need to be pre-defined unless the user requires a rule of mixtures component. In this case, the user should edit Scatteringdata.xlsx and add the desired component to the end of the sheet.

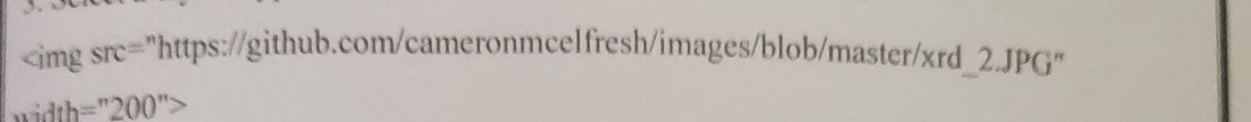
To operate the program, use the following procedure:

1. Run XRD_Intensity_Simulation.m

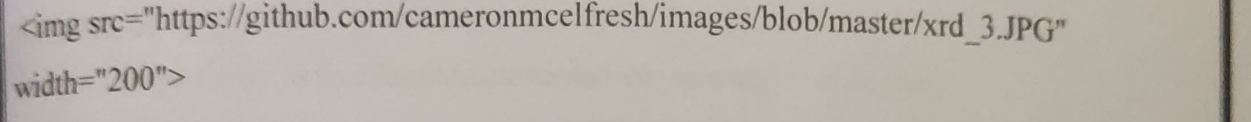
2. Select X-Ray source



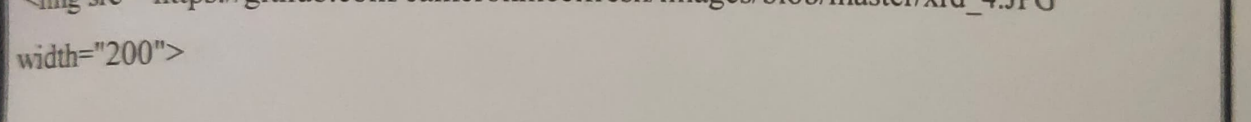
3. Select a crystal type



4. Select atom type

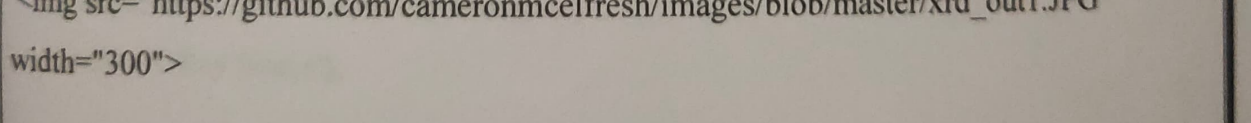


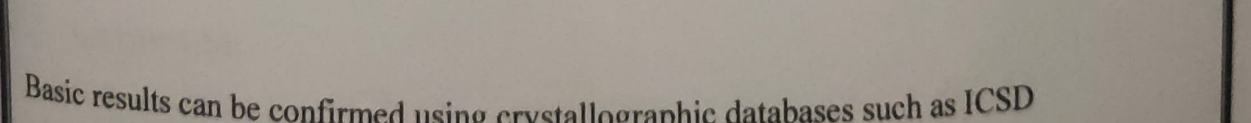
5. Enter the lattice parameter (angstroms)



Output

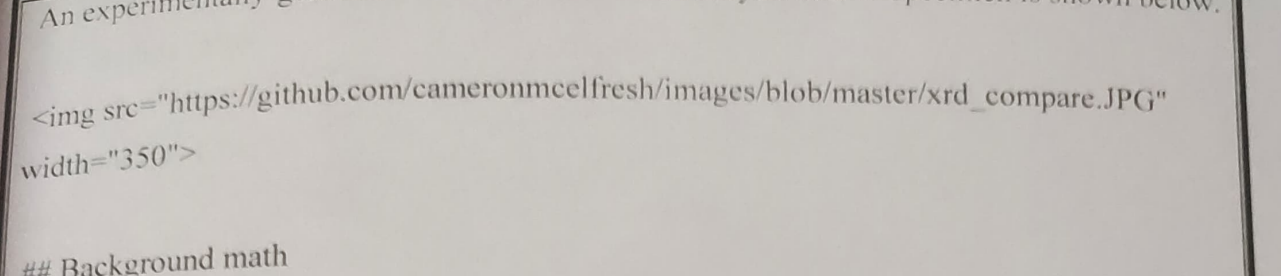
Following the input of the above information (Source: Cu K Alpha, Crystal: BCC, Atom: W, Lattice Parameter: 3.165), the program will output:



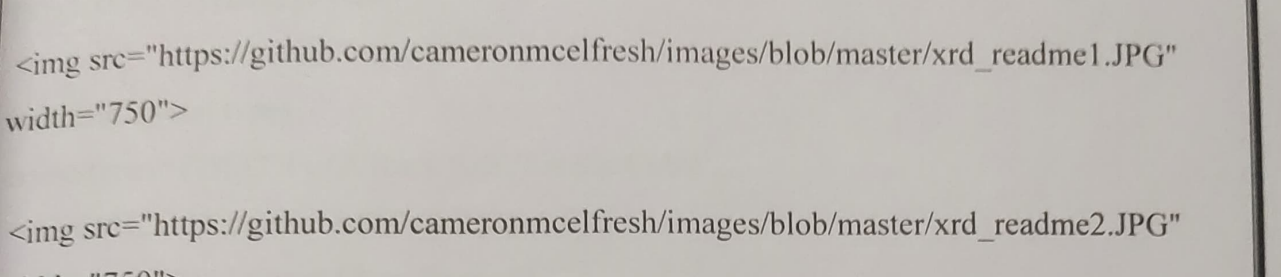


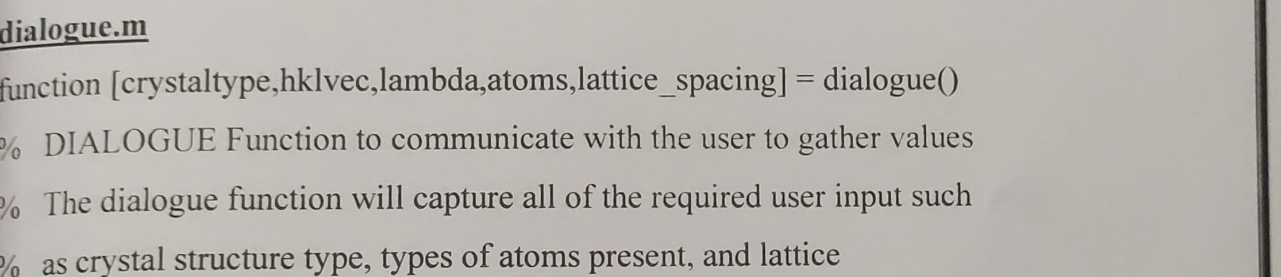
Basic results can be confirmed using crystallographic databases such as ICSD (https://www.fiz-karlsruhe.de/en/produkte-und-dienstleistungen/inorganic-crystal-structure-database-icsd)

An experimentally-generated XRD spectrum from analysis of a W specimen is shown below.



Background math





dialogue.m

```
function [crystaltype,hklvec,lambda,atoms,lattice_spacing] = dialogue()
%  DIALOGUE Function to communicate with the user to gather values
%  The dialogue function will capture all of the required user input such
%  as crystal structure type, types of atoms present, and lattice
%  parameter(s)

%% Extract X-Ray Source data

%Define x-ray sources
xraytypes = {'Cu K alpha','Co K alpha', 'Mo K alpha', 'Cr K alpha', 'Fe K alpha'};
xray_index = listdlg('ListString', xraytypes, 'SelectionMode', 'single', ...
   'PromptString', 'Select a X-Ray Source',...
   'Name', 'X-Ray Souce');

switch xray_index %In Angstroms
   case 1
      lambda=1.54;
   case 2
      lambda=1.79;
   case 3
      lambda=0.71;
```

```
    case 4
        lambda=2.29;
    case 5
        lambda=1.94;
end

%% Extract crystal type data

%Define crystal types
crystaltypes={'BCC','FCC','Rock Salt','Simple Cubic',...
    'CsCl/BCC Diatomic  A(0,0,0) B(0,0.5,0)',...
    'Diamond','Hexagonal Close Packed'};

%Prompt user to select the crystal type
crystaltype = listdlg('ListString', crystaltypes, 'SelectionMode', 'single', ...
    'PromptString', 'Select a crystal Type',...
    'Name', 'Crystal Type');

switch crystaltype
    case 1 %BCC
        hklvec={[1,1,0],[2,0,0],[2,1,1],[2,2,0],[3,1,0],[2,2,2]};
    case 2 %FCC
        hklvec={[1,1,1],[2,0,0],[2,2,0],[3,1,1],[2,2,2],[4,0,0]};
    case 3 %Rock Salt aka Diatomic FCC
        hklvec={[1,1,1],[2,0,0],[2,2,0],[3,1,1],[2,2,2],[4,0,0]};
    case 4 %Simple Cubic
        hklvec={[1,0,0],[1,1,0],[1,1,1],[2,0,0],[2,1,0],[2,1,1]};
    case 5 %Diatomic BCC aka CsCl
        hklvec={[1,0,0],[1,1,0],[1,1,1],[2,0,0],[2,1,0],[2,1,1]};
    case 6 %Diamond
        hklvec={[1,1,1],[2,2,0],[3,1,1],[4,0,0],[3,3,1],[4,2,2]};
    case 7 %Hexagonal
        hklvec={[1,0,0],[0,0,2],[1,0,1],[1,0,2],[1,1,0],[1,0,3]};
end
```

```
%% Extract element name data
elementdata = importdata('Scatteringdata.xlsx');
elements = elementdata.textdata;

atoms =[];
if crystaltype == 1 || crystaltype == 2 || crystaltype ==  4 || crystaltype ==6 || crystaltype==7

   atom_index = listdlg('ListString', elements, 'SelectionMode', 'single',...
      'PromptString', 'Select atom type',...
      'Name', 'Elements');
   atoms = (elements(atom_index));
end


if crystaltype == 3 || crystaltype == 5

   atom_index = [];

   [~,sizeVal] = size(atom_index);

   %Continue selection until 2 atom types are selected
   while sizeVal ~= 2

      atom_index = listdlg('ListString', elements, 'SelectionMode', 'multiple',...
         'PromptString', 'Select the two atom types',...

         'Name', 'Elements');

      [~,sizeVal] = size(atom_index);

   end

   atoms = [elements(atom_index(1)); elements(atom_index(2))];
```

```
end

%% Retrieve the lattice spacing

lattice_spacing = [];

if crystaltype == 7
    a = nan;
    c = nan;

    while not(not(isnan(str2double(a))) && not(isnan(str2double(c))))

        inputs = {'Enter the "a" lattice parameter (Angstroms)','Enter the "c" lattice parameter
(Angstroms)'};

        spacing_vals = inputdlg(inputs, 'Lattice Spacing',[1 45], {'0.00','0.00'});
        a = spacing_vals{1};
        c = spacing_vals{2};

    end

    lattice_spacing = [str2double(a);str2double(c)];

else
    a = nan;

    while isnan(str2double(a))
        a = inputdlg('Enter the lattice parameter (Angstroms)', 'Lattice Spacing',1,{'0.00'});
    end

    lattice_spacing = [str2double(a)];

end
```

dspace.m

```
function [ dspacing ] = dspace(hklvec,crystaltype, lattice_spacing)
%This function calculates the dspacing of an FCC or BCC crystal given
%the lattice parameter and hkl values. Input is given as
%dspace(latticeparameter,h,k,l). Units in Angstroms

dspacing=zeros(1,6);

if crystaltype==7

   lattice_parametera=lattice_spacing(1);
   lattice_parameterc=lattice_spacing(2);

    for i=1:6
      dspacing(i)=...
        ((4/3)*((hklvec{i}(1)^2 + hklvec{i}(1)*hklvec{i}(2) +
hklvec{i}(2)^2)/lattice_parametera^2)+...
        hklvec{i}(3)^2/lattice_parameterc^2)^-0.5;
   end

else
   lattice_parameter=lattice_spacing;

   for i=1:6

dspacing(i)=(lattice_parameter/(sqrt((hklvec{i}(1)^2)+(hklvec{i}(2)^2)+(hklvec{i}(3)^2))));
   end
end

 end
```

theta_s_calc.m

```
function [ thetavec,svalvec ] = theta_s_calc(lambda,dspacing)
%This function recieves a lambda and d spacing and returns a theta of
```

```
%reflection and an s value.
thetavec=zeros(1,6);
svalvec=zeros(1,6);

for i=1:6

   thetavec(i) = asind(lambda/(2*dspacing(i)));

   svalvec(i)=(1/(2*dspacing(i)));

end
end
```

scatterfactor.m

```
function [scatterfactors] = scatterfactor(svec, crystaltype, atoms)
%This function calculates the scattering factor of individual atoms in hkl
%planes based on their respective Z,a, and b values. The output of this
%fucntion is a matrix organized row-wise for s-values (input argument) and
%column-wise by atom entered.


%Return a cell array that holds the atom title, atomic number, and then
%scattering parameters. The output is organizaed as;
% {'Abbreviation',Z,a1,b1,a2,b2,a3,b3,a4,b4}

if crystaltype == 1 || crystaltype == 2 || crystaltype ==  4 || crystaltype ==6 || crystaltype==7
   numatoms=1;
end

if crystaltype == 3 || crystaltype == 5
   numatoms=2;
end

scatterdata=importdata('Scatteringdata.xlsx');
```

```
for i=1:length(atoms)

  row=1;
  while strcmp(scatterdata.textdata(row),atoms(i))==0
    row=row+1;
  end

  atoms{i,2}=scatterdata.data(row,1);
  atoms{i,3}=scatterdata.data(row,2);
  atoms{i,4}=scatterdata.data(row,3);
  atoms{i,5}=scatterdata.data(row,4);
  atoms{i,6}=scatterdata.data(row,5);
  atoms{i,7}=scatterdata.data(row,6);
  atoms{i,8}=scatterdata.data(row,7);
  atoms{i,9}=scatterdata.data(row,8);
  atoms{i,10}=scatterdata.data(row,9);
end

%%
%Calculate the scattering factor for each atom AND in each plane. Output
%vector will be in the form of rows organized by hkl reflection planes, and
%columns ordered by atoms scattering factor in that respective plane. Atoms
%are ordered by how they are entered.
scatterfactors=[];

for plane=1:length(svec)

  atomfactors=[];
    for i=1:numatoms

      sctrfctr=scatterfactorcalc(atoms{i,2},svec(plane),atoms{i,3},atoms{i,4},atoms{i,5},...
        atoms{i,6},atoms{i,7},atoms{i,8},atoms{i,9},atoms{i,10});
```

```
        atomfactors=[atomfactors,sctrfctr];
    end
    scatterfactors=[scatterfactors;atomfactors];
end
end
```

scatterfactor(2).m

```
%This function calculates the scattering factor of individual atoms in hkl
%planes based on their respective Z,a, and b values. The output of this
%fucntion is a matrix organized row-wise for s-values (input argument) and
%column-wise by atom entered.

%Return a cell array that holds the atom title, atomic number, and then
%scattering parameters. The output is organizaed as;
% {'Abbreviation',Z,a1,b1,a2,b2,a3,b3,a4,b4}

if crystaltype == 1 || crystaltype == 2 || crystaltype ==  4 || crystaltype ==6 || crystaltype==7
    numatoms=1;
end

if crystaltype == 3 || crystaltype == 5
    numatoms=2;
end

scatterdata=importdata('Scatteringdata.xlsx');

for i=1:length(atoms)
    row=1;
    while strcmp(scatterdata.textdata(row),atoms(i))==0
        row=row+1;
    end

    atoms{i,2}=scatterdata.data(row,1);
    atoms{i,3}=scatterdata.data(row,2);
```

```
    atoms{i,4}=scatterdata.data(row,3);
    atoms{i,5}=scatterdata.data(row,4);
    atoms{i,6}=scatterdata.data(row,5);
    atoms{i,7}=scatterdata.data(row,6);
    atoms{i,8}=scatterdata.data(row,7);
    atoms{i,9}=scatterdata.data(row,8);
    atoms{i,10}=scatterdata.data(row,9);
  end

  %%
  %Calculate the scattering factor for each atom AND in each plane. Output
  %vector will be in the form of rows organized by hkl reflection planes, and
  %columns ordered by atoms scattering factor in that respective plane. Atoms
  %are ordered by how they are entered.
  scatterfactors=[];

  for plane=1:length(svec)

    atomfactors=[];
      for i=1:numatoms

        sctrfctr=scatterfactorcalc(atoms{i,2},svec(plane),atoms{i,3},atoms{i,4},atoms{i,5},...
          atoms{i,6},atoms{i,7},atoms{i,8},atoms{i,9},atoms{i,10});


        atomfactors=[atomfactors,sctrfctr];
      end
    scatterfactors=[scatterfactors;atomfactors];
  end

  end
```

scatterfactorcalc.m

```
function [scatteringfactor] = scatterfactorcalc(Z,s,a1,b1,a2,b2,a3,b3,a4,b4)
%This function calcualtes the scattering factor of an atom given the Z
%value (atomic number), s value, and corresponding a(i) and b(i) values.
%Input is given as scaterfactor(Z,s,a1,b1,a2,b2,a3,b3)

scatteringfactor=Z-41.78214*(s^2)*[a1*exp(-b1*s^2)+a2*exp(-b2*s^2)+...
  a3*exp(-b3*s^2)+a4*exp(-b4*s^2)];

end
```

structurefactor.m

```
function [structurevec] = structurefactor(scattervec,crystaltype)
%This function calculates the structure factor given the scattering factors
%of the atoms present.

structurevec=zeros(6,1);
switch crystaltype

   case 1 %BCC
      structurevec(1)=2*sum(scattervec(1,:));
      structurevec(2)=2*sum(scattervec(2,:));
      structurevec(3)=2*sum(scattervec(3,:));
      structurevec(4)=2*sum(scattervec(4,:));
      structurevec(5)=2*sum(scattervec(5,:));
      structurevec(6)=2*sum(scattervec(6,:));

   case 2 %FCC
      structurevec(1)=4*sum(scattervec(1,:));
      structurevec(2)=4*sum(scattervec(2,:));
      structurevec(3)=4*sum(scattervec(3,:));
      structurevec(4)=4*sum(scattervec(4,:));
      structurevec(5)=4*sum(scattervec(5,:));
```

```
    structurevec(6)=4*sum(scattervec(6,:));

case 3 %Rock Salt
    structurevec(1)=4*(scattervec(1,1)-scattervec(1,2));
    structurevec(2)=4*(scattervec(2,1)+scattervec(2,2));
    structurevec(3)=4*(scattervec(3,1)+scattervec(3,2));
    structurevec(4)=4*(scattervec(4,1)-scattervec(4,2));
    structurevec(5)=4*(scattervec(5,1)+scattervec(5,2));
    structurevec(6)=4*(scattervec(6,1)-scattervec(6,2));

case 4 %Simple Cubic
    structurevec(1)=sum(scattervec(1,:));
    structurevec(2)=sum(scattervec(2,:));
    structurevec(3)=sum(scattervec(3,:));
    structurevec(4)=sum(scattervec(4,:));
    structurevec(5)=sum(scattervec(5,:));
    structurevec(6)=sum(scattervec(6,:));

case 5 %CsCl structure aka Diatomic BCC
    structurevec(1)=(scattervec(1,1)-scattervec(1,2));
    structurevec(2)=(scattervec(2,1)+scattervec(2,2));
    structurevec(3)=(scattervec(3,1)+scattervec(3,2));
    structurevec(4)=(scattervec(4,1)-scattervec(4,2));
    structurevec(5)=(scattervec(5,1)+scattervec(5,2));
    structurevec(6)=(scattervec(6,1)-scattervec(6,2));

case 6%Diamond
    structurevec(1)=(32^0.5)*sum(scattervec(1,:));
    structurevec(2)=8*sum(scattervec(2,:));
    structurevec(3)=(32^0.5)*sum(scattervec(3,:));
    structurevec(4)=8*sum(scattervec(4,:));
    structurevec(5)=(32^0.5)*sum(scattervec(5,:));
    structurevec(6)=8*sum(scattervec(6,:));
```

```
 case 7 %HCP
    structurevec(1)=(scattervec(1,1));
    structurevec(2)=(scattervec(2,1));
    structurevec(3)=(3^0.5)*(scattervec(3,1));
    structurevec(4)=(scattervec(4,1));
    structurevec(5)=2*(scattervec(5,1));
    structurevec(6)=(3^0.5)*(scattervec(6,1));


end
```

intensitycalc.m

```
function [ intensityvec ] = intensitycalc(structurevec,crystaltype,thetavec)
%This function calculates intensity based on strucuture factor, Lorentz
%polarization factor, and multiplicity.
%Create multiplicity values
m=zeros(6,1);
switch crystaltype
  case 1 %BCC
     m(1)=12;
     m(2)=6;
     m(3)=24;
     m(4)=12;
     m(5)=24;
     m(6)=8;


  case 2 %FCC
     m(1)=8;
     m(2)=6;
     m(3)=12;
     m(4)=24;
     m(5)=8;
     m(6)=6;


  case 3 %Rock Salt
```

```
    m(1)=8;
m(2)=6;
    m(3)=12;
    m(4)=24;
    m(5)=8;
    m(6)=6;

  case 4 %Simple Cubic
    m(1)=6;
    m(2)=12;
    m(3)=8;
    m(4)=6;
    m(5)=24;
    m(6)=24;

  case 5 %CsCl aka Diatomic BCC
    m(1)=6;
    m(2)=12;
    m(3)=8;
    m(4)=6;
    m(5)=24;
    m(6)=24;

  case 6 %Diamond
    m(1)=8;
    m(2)=12;
    m(3)=24;
    m(4)=6;
    m(5)=24;
    m(6)=24;

  case 7 %HCP
    m(1)=3;
    m(2)=4;
```

```
    m(3)=6;
    m(4)=5.5;
    m(5)=2.5;
    m(6)=5.25;


end

%Create Lorentz Polarization values
lf=zeros(6,1);

for i=1:6
  lf(i)=lorentz(thetavec(i));
end

%Create final vector of intensities
intensityvec=zeros(6,1);
for i=1:6
  intensityvec(i)=(structurevec(i)^2)*m(i)*lf(i);


end
```

Lorentz.m

```
function [ lorentzfactor ] = lorentz(theta)
%This function uses a theta value to calculate the lorentz polarization
lorentzfactor= (1+cosd(2*theta)^2)/((sind(theta)^2)*cosd(theta));
end
```

compareintensity.m

```
function compareintensity(intensityvec,hklvec,thetavec,crystaltype,atoms,lattice_spacing)
%This function recieves the intensity data and outputs a formatted result.

relintensity=intensityvec/max(intensityvec);

switch crystaltype
  case 1
```

```
    type='BCC';
  case 2
    type='FCC';
  case 3
    type='Rock Salt';
  case 4
    type='Simple Cubic';
  case 5
    type='CsCl/Diatomic BCC';
  case 6
    type='Diamond';
  case 7
    type='Hexagonal Close Packed';
end

fprintf('\n')
fprintf('--------------------------------\n--------------------------------\n')
fprintf('Crystal Type: %s\n',type)
fprintf('Element(s): ')

for i=1:length(atoms)
  fprintf('%s ', atoms{i})
end

fprintf('\n')

if length(lattice_spacing)==1
  fprintf('Lattice Parameter: %3.3f A\n',lattice_spacing)
end

if length(lattice_spacing)==2
  fprintf('Lattice Parameter (a): %3.3f A\n',lattice_spacing(1))
  fprintf('Lattice Parameter (c): %3.3f A\n',lattice_spacing(2))
end
```

```
fprintf('2 Theta    (hkl)   Relative Intensity')

for i=1:6
   fprintf('\n  %-6.2f    %i%i%i
%0.2f',thetavec(i)*2,hklvec{i}(1),hklvec{i}(2),hklvec{i}(3))
   fprintf('%f ',relintensity(i))
end

fprintf('\n---------------------------------- \n----------------------------------')
fprintf('\n')


%Plot the values with 2 Theta vs. Relativy Intensity
%Plot curvature/FWHM is arbitrarily set - can be removed or set to a straight line
figure
for i=1:6
   c=0.25;
   xval=linspace(thetavec(i)*2-5,thetavec(i)*2+5,100);
   yval=relintensity(i)*exp(-((xval-thetavec(i)*2).^2)/(2*c^2));
   plot(xval,yval,'k')
   hold on
end
xlabel('2\Theta')
ylabel('Relative Intensity')
axis([0 thetavec(end)*2+5 0 1.1])

%Add annotations
for i = 1:length(hklvec)
   ann_string = string(hklvec{i}(1)) + string(hklvec{i}(2)) + string(hklvec{i}(3));
   text(thetavec(i)*2, relintensity(i)+0.02, ann_string, 'HorizontalAlignment', 'center');
end
end
```

CHAPTER-3

OBSERVATION &

RESULT

OBSERVATION

The mathlab program was run and the following results where obtained for 9 nanoparticles. This result is compared between the results obtained from various research papers(from search engine GOOGLE) where through experimental methods XRD Pattern was obtained. The. XRD Pattern of 9 such nanoparticles where taken from various number of research papers . The various parameters available for running the program and before attaining the result is the X-ray source is to be selected from the options, next we are given the option of selecting the crystal type , after which we select the element we used there are various options of elements according to the sample we took and then we type in the lattice parameter(it is the length between two points of corners of a unit cell)in Angstrom.

SILVER NANOPARTICLES

The results obtained from running the program where the X-ray source was given CuK-alpha, the crystal type as Face Centered Cubic(a single atom at each lattice point on the cube's corners and faces),next the element was given which is Silver in this case and then the lattice parameter was typed in. The program is then run and 2 Theta(Theta is the angle between incident ray and scatter plane)values, the miller indices(used to specify directions and planes) and relative intensity of absolute intensity of every peak by the absolute intensity of the most Intense peak).

Program

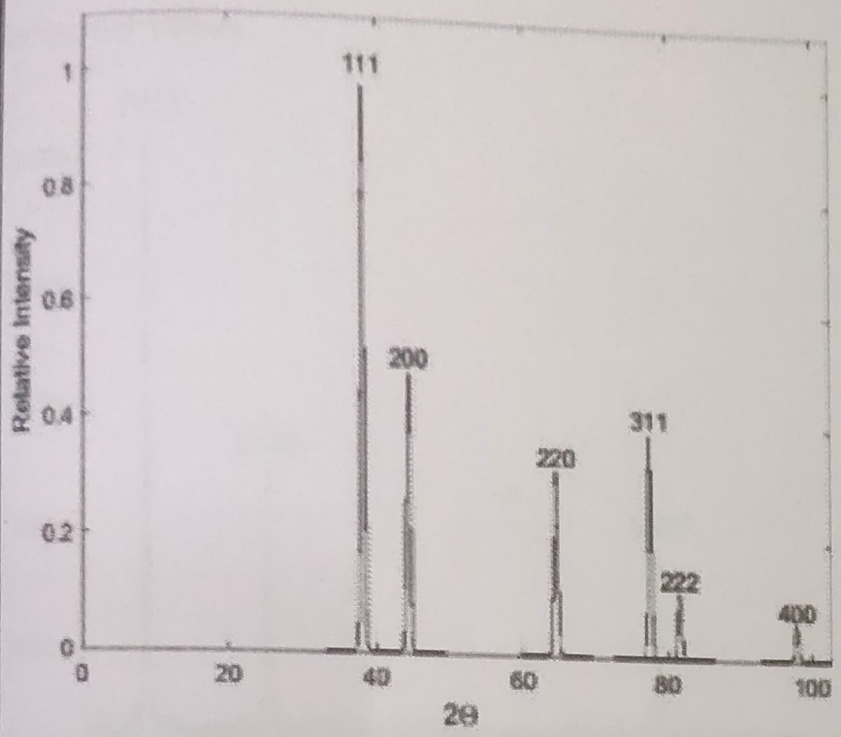
Crystal Type: FCC

Element(s): Ag

Lattice Parameter: 4.090 A

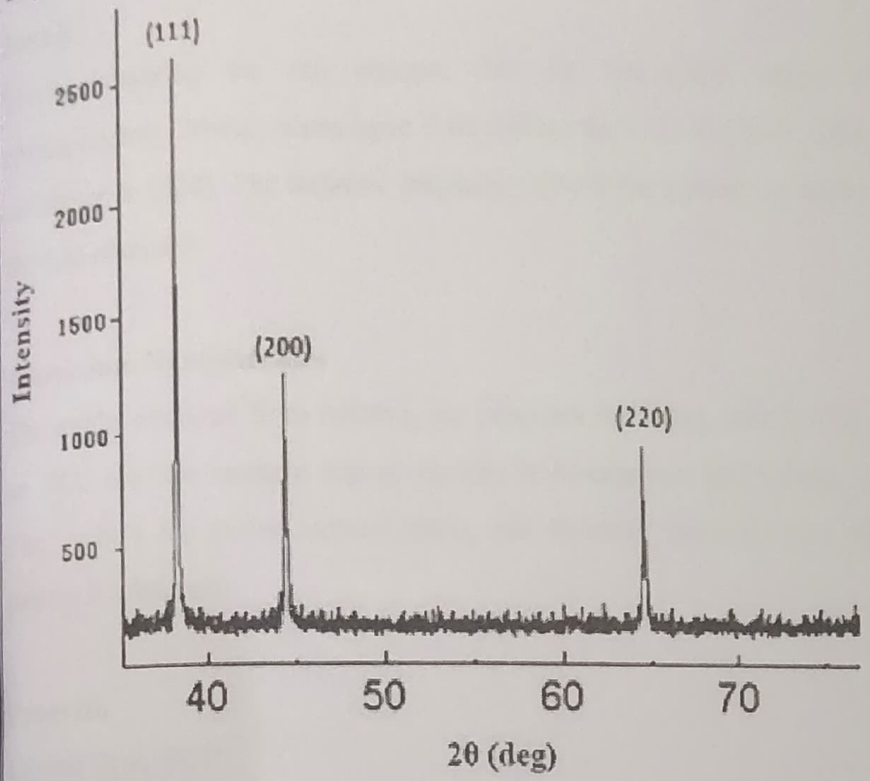
OBSERVATION

Silver Nanoparticles



2 Theta	(hkl)	Relative intensity
38.06	111	1.000000
44.23	200	0.481454
64.34	220	0.296681
77.27	311	0.346108
81.40	222	0.101049
97.70	400	0.054866

Experimental Values



From the research paper "The effect of silver nanoparticles on composite shear bond strength to dentin with different adhesion protocols" we get the experimental values for miller indices,2theta and intensity from the corresponding graph.

2 Theta	(hkl)	Intensity	Relative intensity
38.00	111	2600	1.000000
44.20	200	1250	0.48
64.30	220	750	0.29

Substitution: 1250÷2600= 0.48

X-ray diffraction (XRD) pattern of silver nanoparticles . Peaks are assigned to diffraction from the (111), (200) and (220) planes of silver. Silver has an fcc crystal structure with a basis of one silver atom. The lattice parameter, a, is 0.409 nm.

Result

From comparing we can observe that for the (hkl) values (111),(200) and (220) corresponding 2theta values have 0.06 difference in (111),0.03 difference in (200),and 0.04 difference in (220). The Relative Intensity of both the values are approximately same for both the data obtained.

Aluminium Nanoparticles

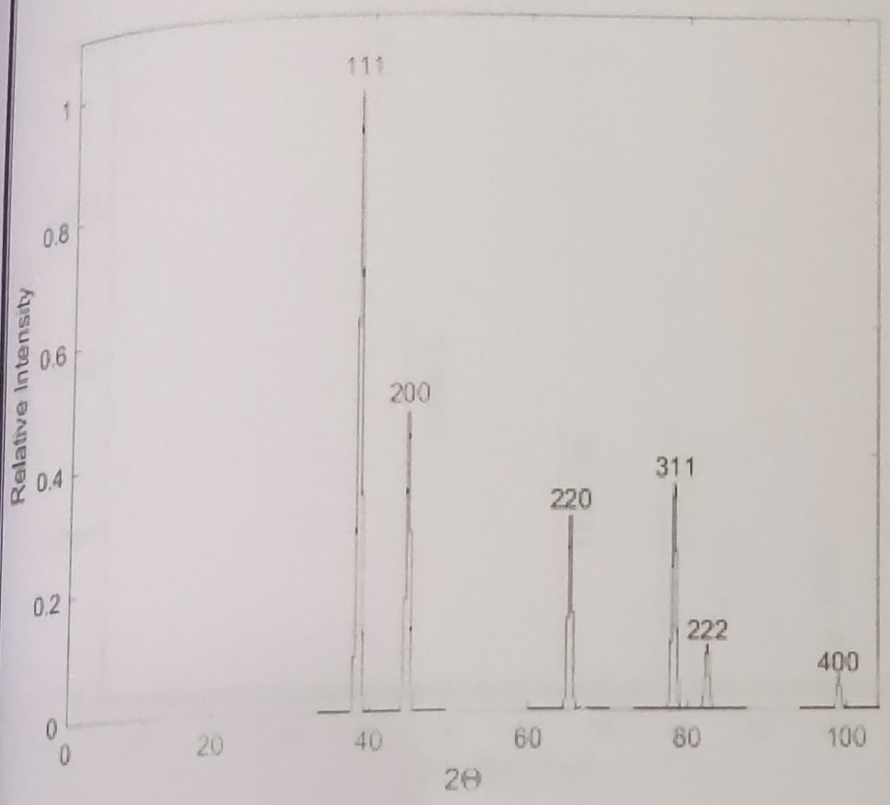
The results obtained from running the program for X-ray source CuK-alpha ,the crystal type as FCC next the element was given that is Aluminium and Lattice Parameter was typed in. The values for miller indices,2theta and Relative intensity and the corresponding XRD pattern is obtained.

Program

Crystal Type: FCC

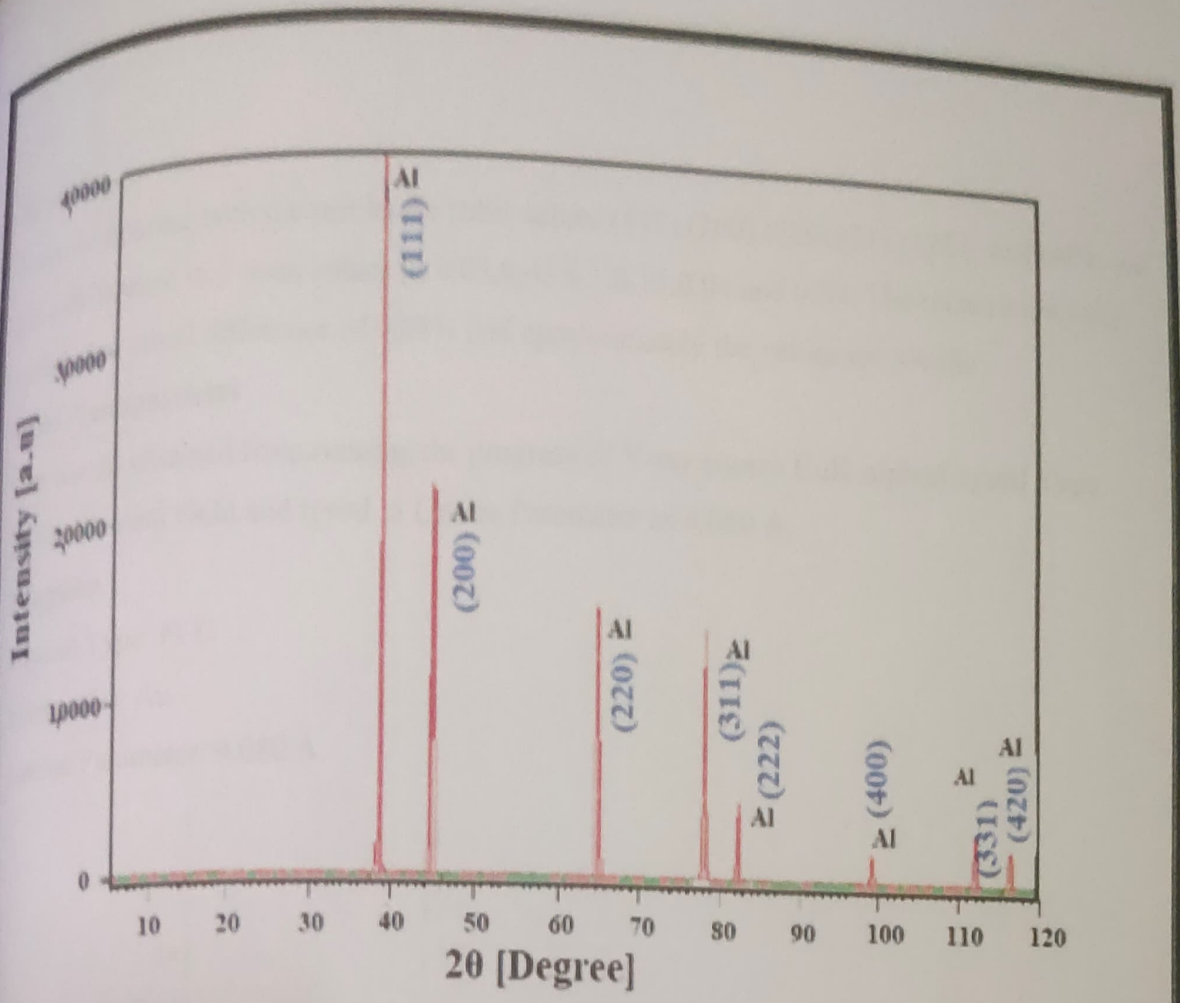
Element(s): Al

Lattice Parameter: 4.048 A



2Theta	(hkl)	Relative intensity
38.47	111	1.000000
44.72	200	0.481351
65.10	220	0.310441
78.23	311	0.363044
82.44	222	0.105137
99.09	400	0.053734

Experimental Values



The experimental XRD Pattern for Aluminium nanoparticles are extracted from the research paper "Experimental Analysis and Characterization of High-Purity Aluminum Nanoparticles (Al-NPs) by Electromagnetic Levitation Gas Condensation (ELGC)". From the experimentally extracted XRD Pattern from research paper the 2theta,(hkl) and relative intensity values are

2Theta	(hkl)	Intensity	Relative intensity
38.50	111	40000	1.0000
44.70	200	20500	0.5125
65.00	220	13000	0.325
78.10	311	12500	0.3125
82.40	222	4000	0.10
99.00	400	2000	0.05

Result

From comparing both the results for (hkl) values (111),(200),(220),(311),(222) and (400) we get a difference in 2 theta values as 0.03,0.02,0.1,0.13,0.04 and 0.09. The relative intensity values has small difference of 0.05% and approximately the values are similar.

Gold Nanoparticles

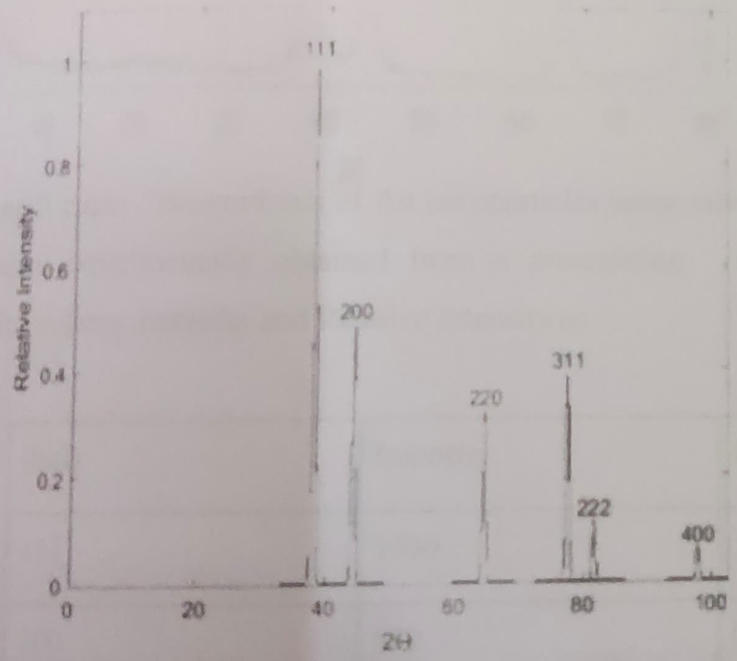
The results obtained from running the program of X-ray source CuK-alpha,Crystal Type FCC, Element Gold and typed in Lattice Parameter as 4.080 A.

Program

Crystal Type: FCC

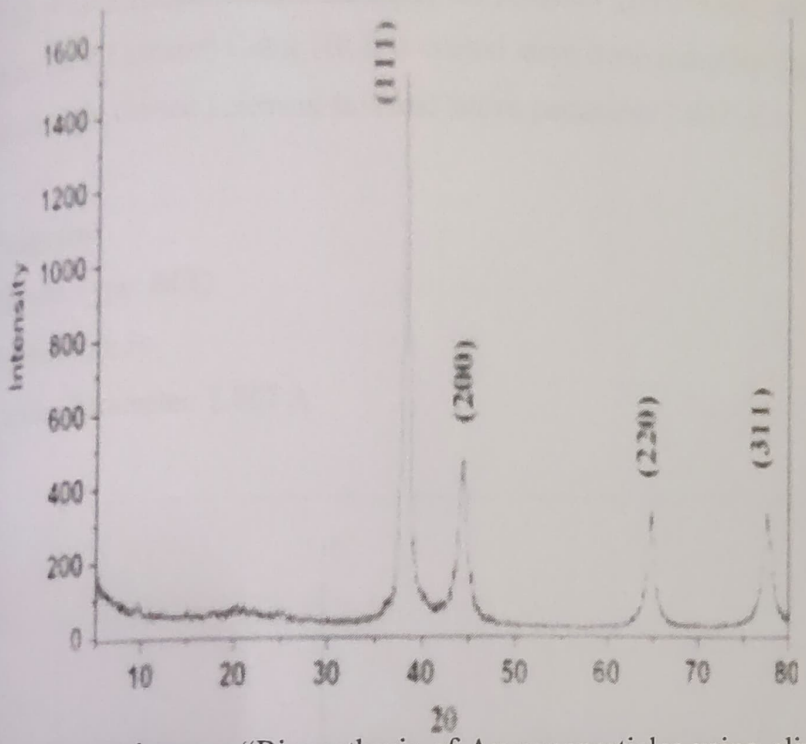
Element(s): Au

Lattice Parameter: 4.080 A



2 Theta	(hkl)	Relative intensity
38.16	111	1.000000
44.35	200	0.493888
64.52	220	0.328174
77.50	311	0.396597
81.65	222	0.116917
98.03	400	0.065613

Experimental values



From research paper "Biosynthesis of Au nanoparticles using olive leaf extract." we get the XRD Pattern experimentally obtained from a pre-existing research paper taking the 2theta,miller indices ,Intensity and Relative Intensity as

2 Theta	(hkl)	Intensity	Relative intensity
38.10	111	1500	1.0000
44.30	200	570	0.3933
64.50	220	400	0.2666
77.50	311	400	0.2666

Substitution:570÷1500=0.3933

Result

We can observe that for the (hkl) values (111),(200),(220) and (311) we get difference of 2theta

0.06,0.05.0.02 and 0 and the relative intensity value difference are 0.1005%,0.0615% and

0.1299%.

Iron Nanoparticles

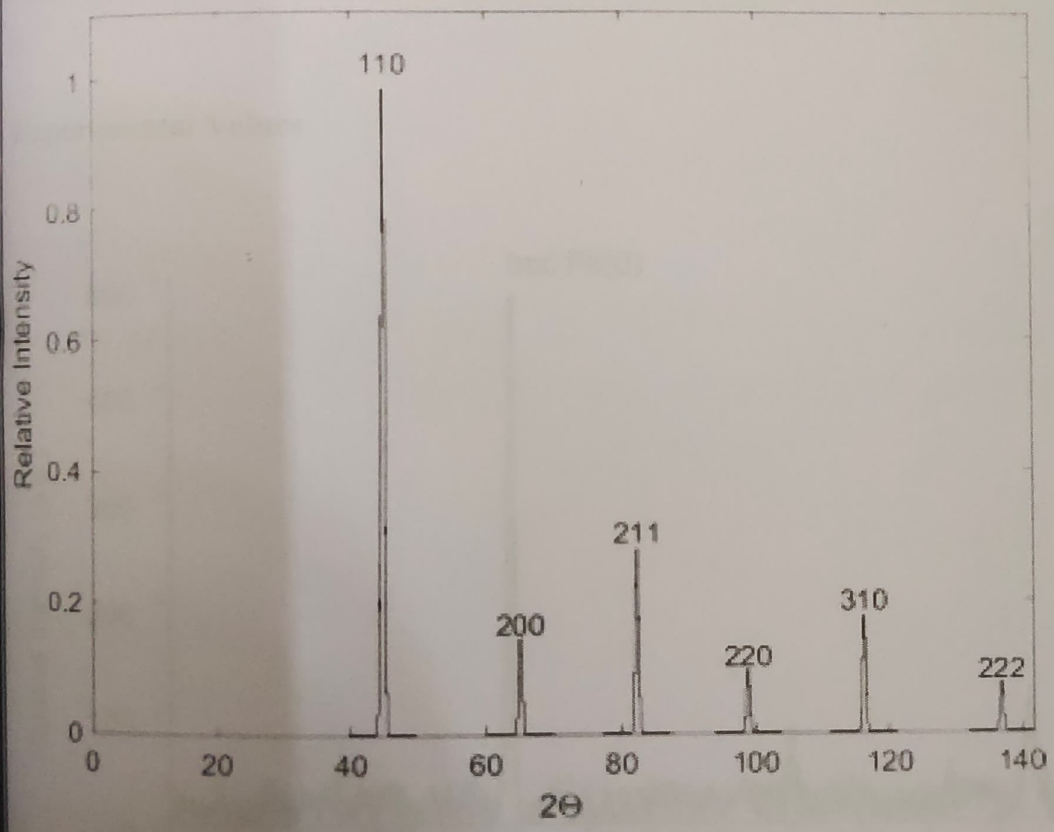
The results we obtain from running the program given X-ray source as CuK-alpha, Crystal type Base Centered Cubic (BCC-a central atom surrounded by eight atoms which are located at all eight corners),element Iron and lattice parameter 2.867 A.

Program

Crystal Type: BCC

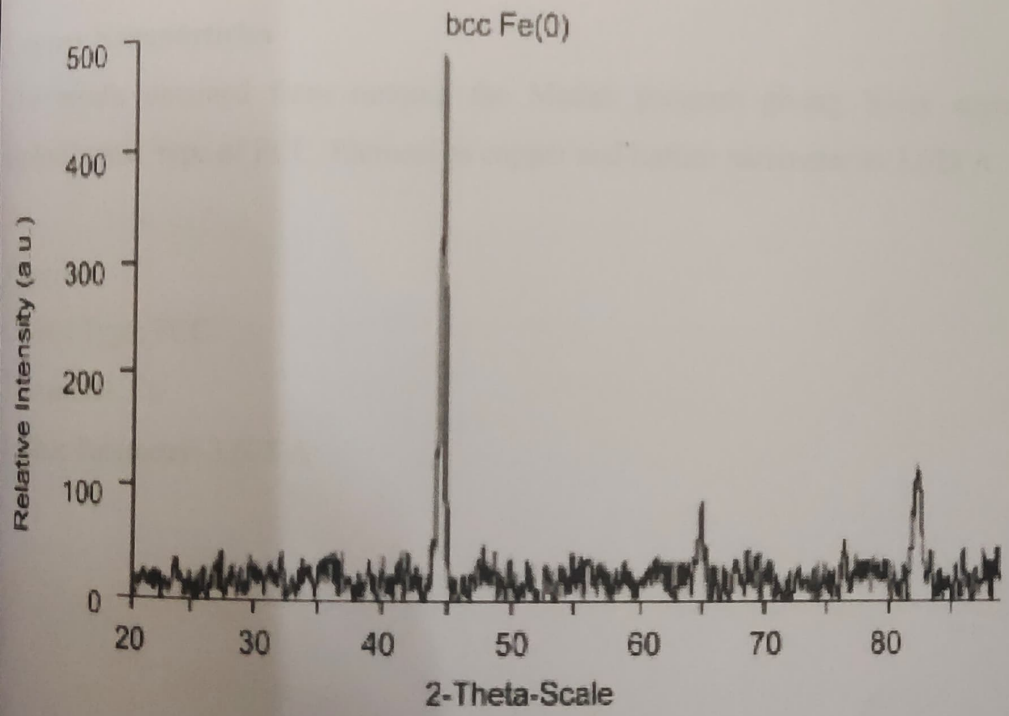
Element(s): Fe

Lattice Parameter: 2.867 A



2 Theta	(hkl)	Relative intensity
44.65	110	1.000000
64.99	200	0.146920
82.29	211	0.284774
98.89	220	0.097406
116.30	310	0.180918
137.03	222	0.077277

Experimental Values



From Research paper "Remediation of Malathion Contaminated Soil Using Zero Valent Iron Nano-Particles" we get the XRD Pattern of experimental values of miller indices (110),(200) and (211) of Iron nanoparticles we get 2theta and Relative intensity values as

2 Theta	(hkl)	Intensity	Relative intensity
44.60	110	500	1.000
64.99	200	100	0.2
83.00	211	150	0.3

Substitution:100÷500=0.2

Result

Comparing the two results we can observe that for the miller indices the have a 2theta value difference of 0.05 ,0 and 0.71 and the Relative intensities of both different by 0.1%.

Copper Nanoparticles

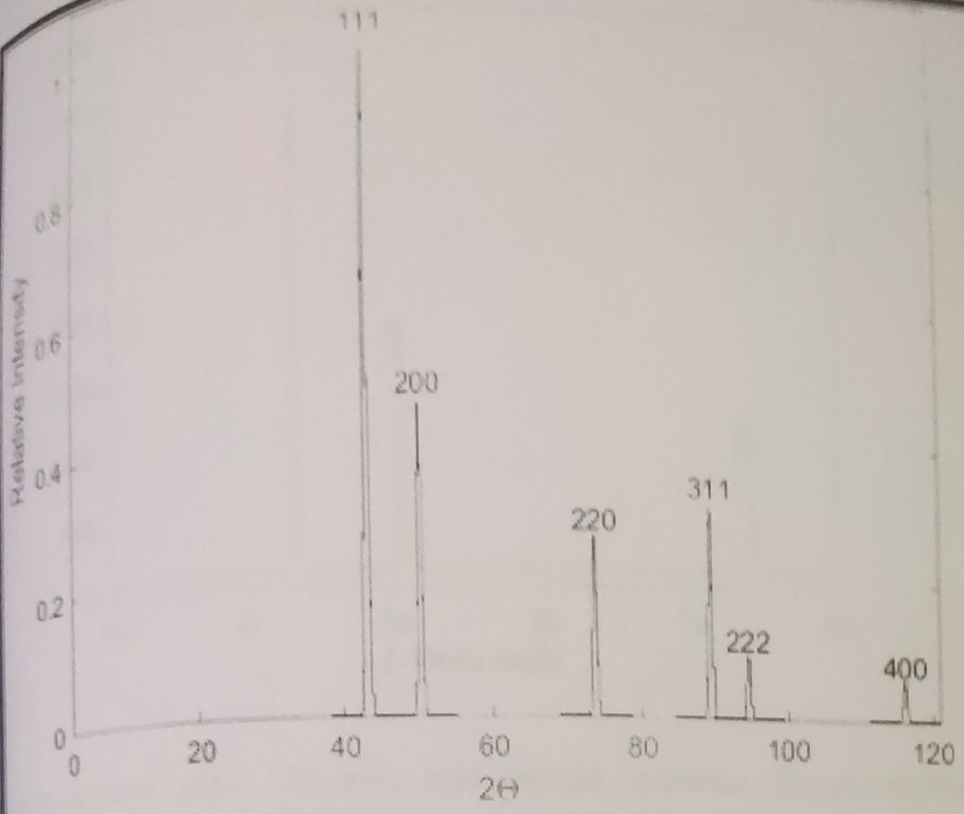
The results obtained from running the Matlab program giving X-ray source as CuK-alpha,Crystal type of FCC, Element as copper and Lattice parameter as 3.628 A.

Program

Crystal Type: FCC

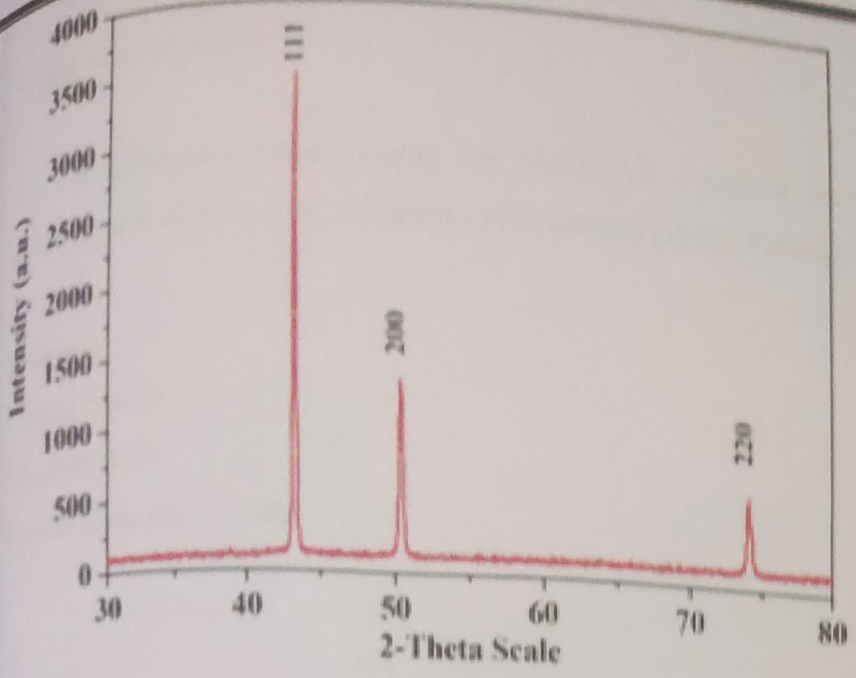
Element(s): Cu

Lattice Parameter: 3.628 A



2 Theta	(hkl)	Relative intensity
43.14	111	1.000000
50.24	200	0.466854
73.78	220	0.267527
89.48	311	0.318315
94.65	222	0.095212
116.20	400	0.062065

Experimental Values



From research paper "Ascorbic acid assisted synthesis, characterization and catalytic application of copper nanoparticles" we get access to Research papers where experimentally extracted XRD Pattern can be found. From the XRD Pattern we will get 2theta and Relative intensity values for miller indices (111),(200) and (220) as

2 Theta	(hkl)	intensity	Relative intensity
43.10	111	3500	1.000000
52.20	200	1450	0.41
73.70	220	800	0.22

Substitution:1450÷3500= 0.41

Result

Comparing the XRD Pattern from the program and the existing experimental values we see that for the miller indices (111),(200) and (220) we get that 2theta values have a difference of 0.04 and 0.08 and relative intensities differ by 0.05 % and 0.04%.

Nickel Nanoparticles

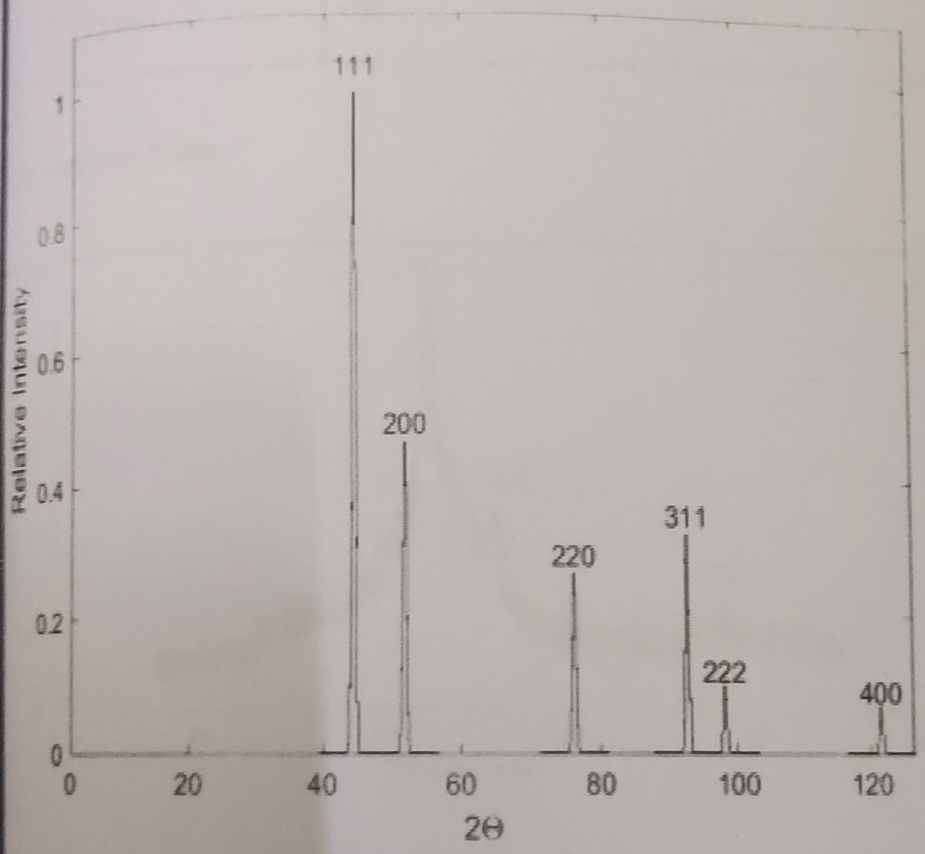
The results obtained from running the MATLAB Program giving X-ray source as CuK-alpha, Crystal type as FCC, Element as Nickel and Lattice Parameter as 3.530 A.

Program

Crystal type:FCC

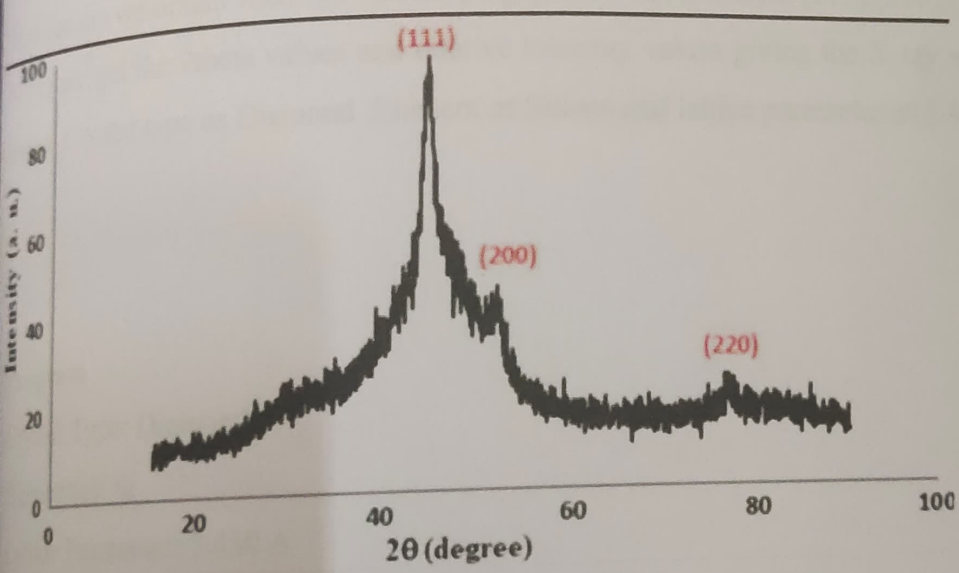
Element(s):Ni

Lattice parameter:3.530A



2theta	(hkl)	Relative intensity
44.40	111	1.000000
51.74	200	0.463999
76.20	220	0.266827
92.70	311	0.327201
98.18	222	0.099379
121.53	400	0.070721

Experimental Values



From Research paper "Synthesis of nickel nanoparticles by a green and convenient method as a magnetic mirror with antibacterial activities"we obtain the experimental values for nickel nanoparticles my existing research papers the 2theta and Relative intensity values for corresponding miller indices (111),(200), and (220) are

2 Theta	(hkl)	Intensity	Relative intensity
44.30	111	90	1.0000
51.70	200	43	0.4777
76.25	220	25	0.2777

Result

We difference of 2theta values observe from comparing both the results we see for the miller indices (111),(200) and (220) the is 0.1,0.04 and 0.05 and relative intensity values difference is 0.01% each.

Silicon nanoparticles

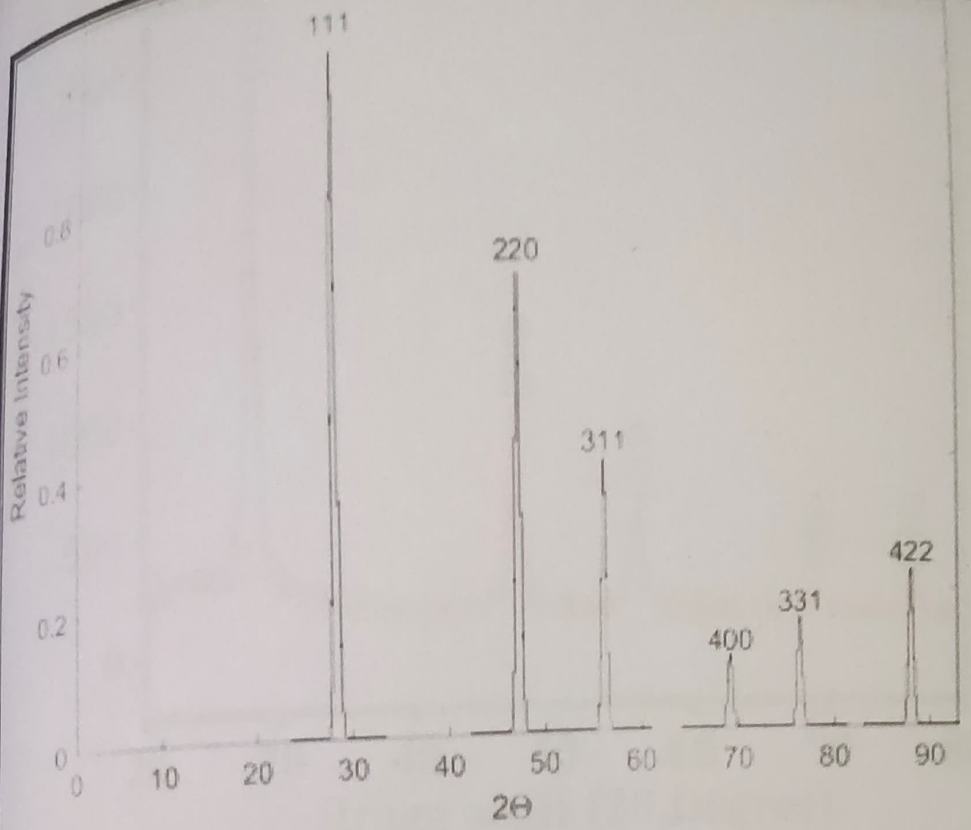
The results we obtain when we run the program for miller indices (111),(220),(311),(400) and (331) we get the 2theta values and relative intensity values giving the X-ray source as CuK-alpha, Crystal type as Diamond ,Element as Silicon and lattice parameter as 5.430A.

Program

Crystal Type: Diamond

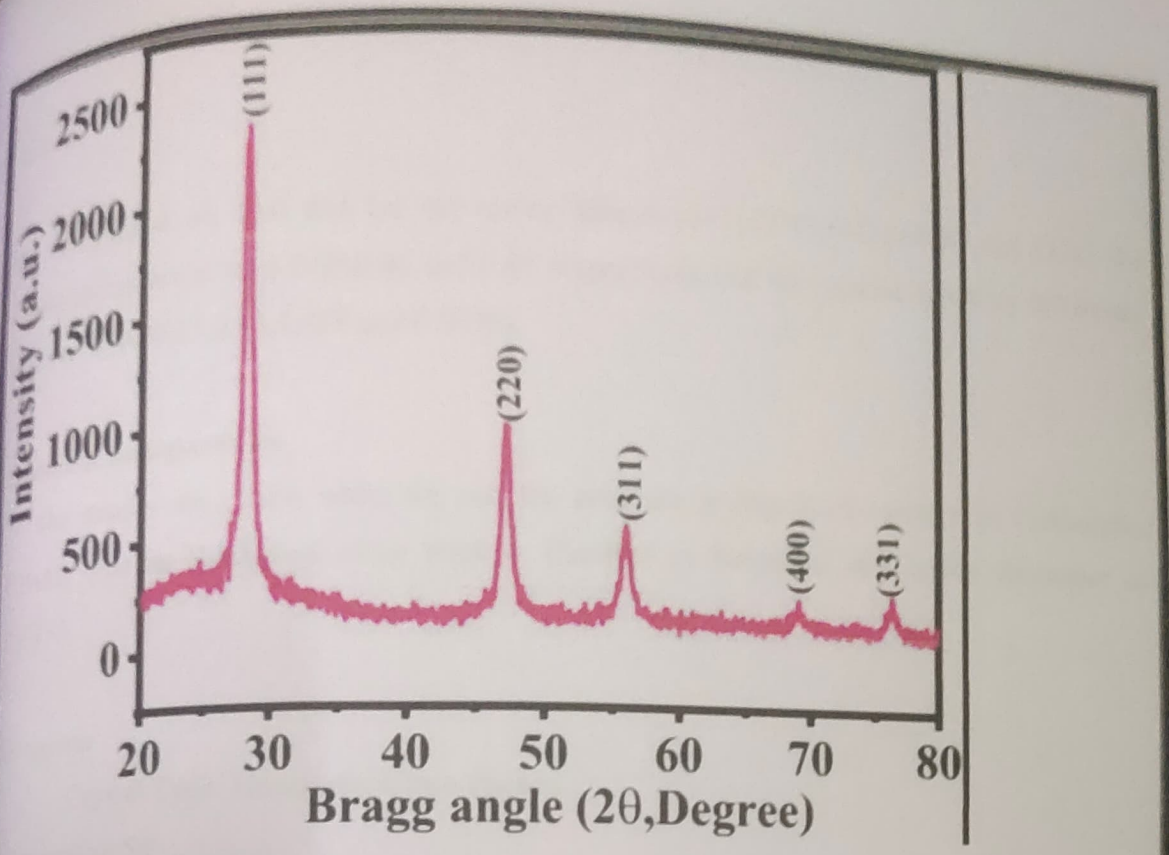
Element(s): Si

Lattice Parameter: 5.430 A



2 theta	(hkl)	Relative intensity
28.44	111	1.000000
47.29	220	0.666634
56.11	311	0.395966
69.11	400	0.107142
76.36	331	0.163383
88.01	422	0.234812

Experimental Values



From research paper "Silicon nanoparticles: a new and enhanced operational material for nitrophenol sensing" we get the experimentally extracted XRD Pattern from pre-existing research papers from which we obtain the 2theta and intensity values for (111),(220),(311),(400) and (331).

2 theta	(hkl)	Intensity	Relative intensity
28.40	111	2400	1.0000
47.20	220	1000	0.4166
56.10	311	600	0.25
69.10	400	300	0.125
76.30	331	400	0.166

Result

On comparison we find that for the miller indices (111),(220),(311),(400) and (331) the 2theta difference is 0.04,0.09,0.06 and 0.01 respectively and the relative intensity difference is found to be 0.24,0.14,0.018 and 0.003%.

Selenium nanoparticles

The results we obtain when we run the program giving X-ray source as CuK-alpha, Crystal type as Hexagonal close packed, Element as Selenium and lattice parameter as 2.373A

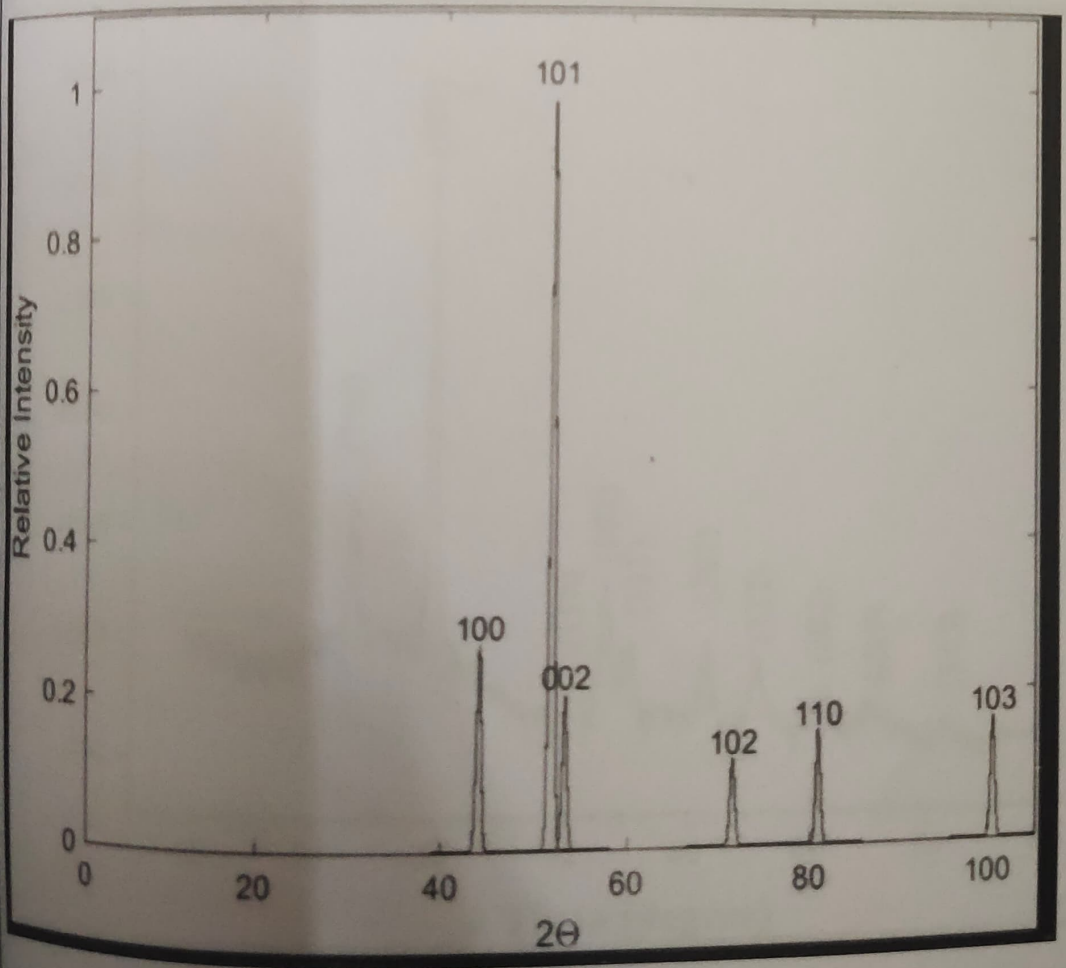
Program

Crystal Type: Hexagonal Close Packed

Element(s): Se

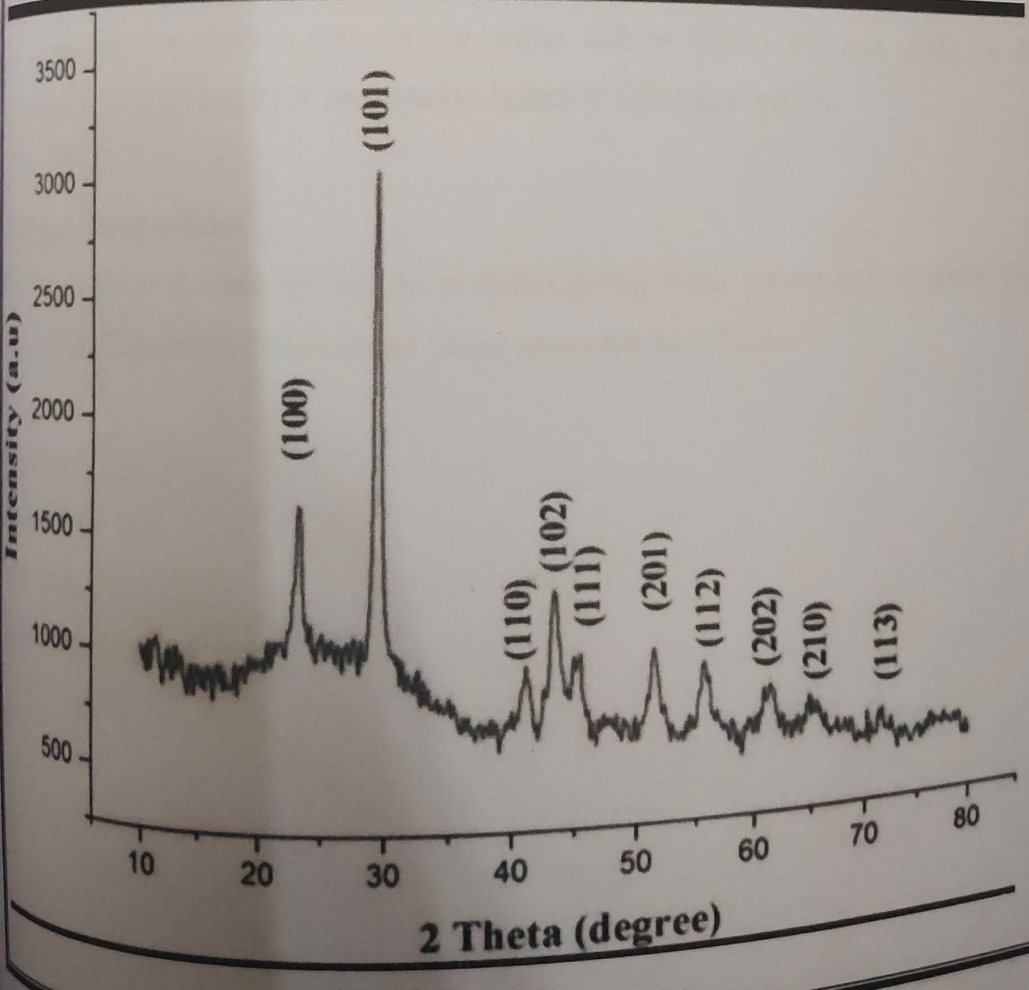
Lattice Parameter (a): 2.373 A

Lattice Parameter (c): 3.436 A



2 theta	(hkl)	Relative intensity
44.01	100	0.270897
53.26	002	0.203928
51.77	101	1.000000
71.49	102	0.115559
80.93	110	0.151220
100.65	103	0.164700

Experimental Values



From Research paper " Diospyros montana leaf extract-mediated synthesis of selenium nanoparticles and their biological applications"we get the experimental XRD Pattern of selenium nanoparticles from pre-existing research papers for the miller indices (100),(101) and

(102). From the XRD Pattern we get the 2theta and Relative intensity values.

2 Theta	(hkl)	Intensity	Relative intensity
24.00	100	1550	0.51
29.00	101	3025	1.0000
44.00	102	1125	0.371

Result

On comparison we observe that for the miller indices (100),(101) and (102) the 2theta difference is 20 ,22.7 and 27.4 and relative intensity difference is 0.2%.

Platinum Nanoparticles

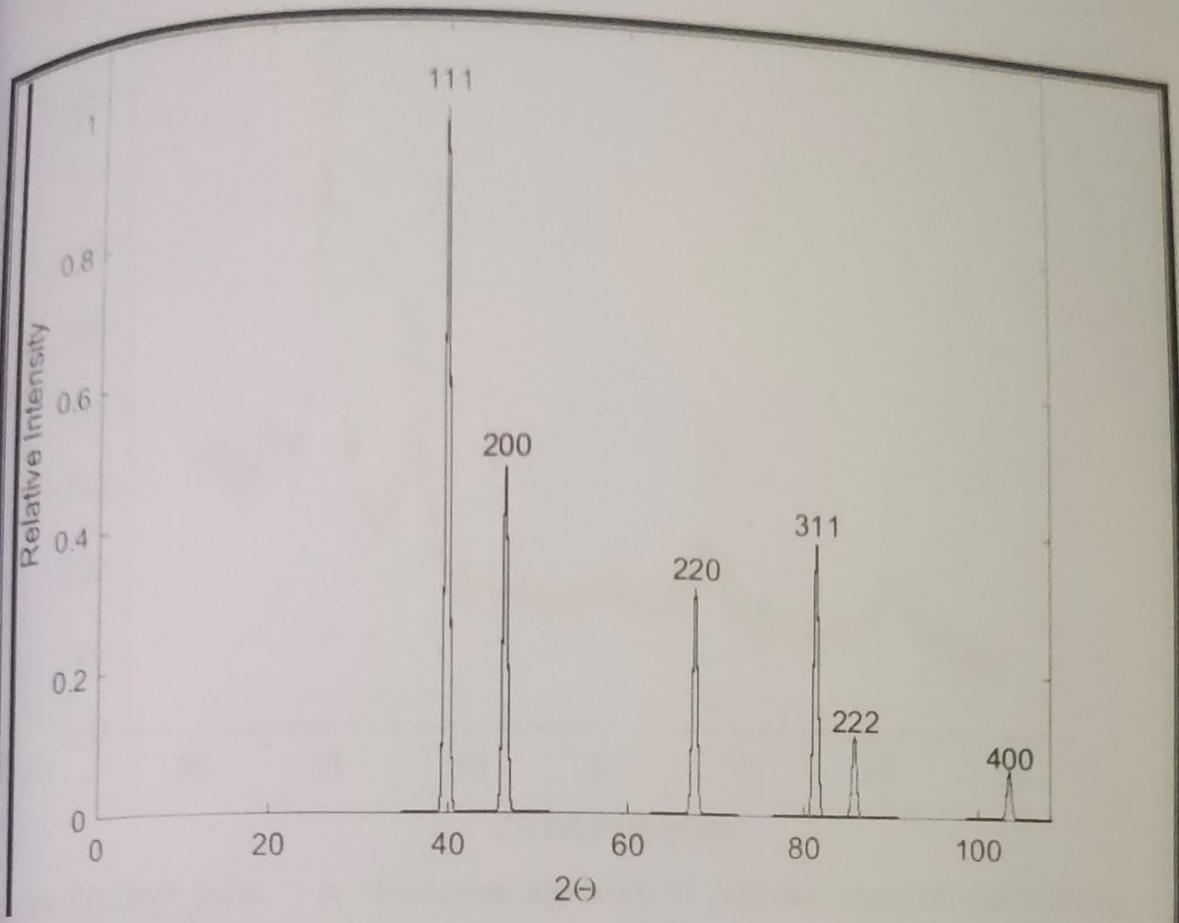
The results obtained when we run the program giving X-ray source as CuK-alpha, Crystal type as FCC, Element as Platinum and lattice parameter as 3.920A.

Program

Crystal Type: FCC

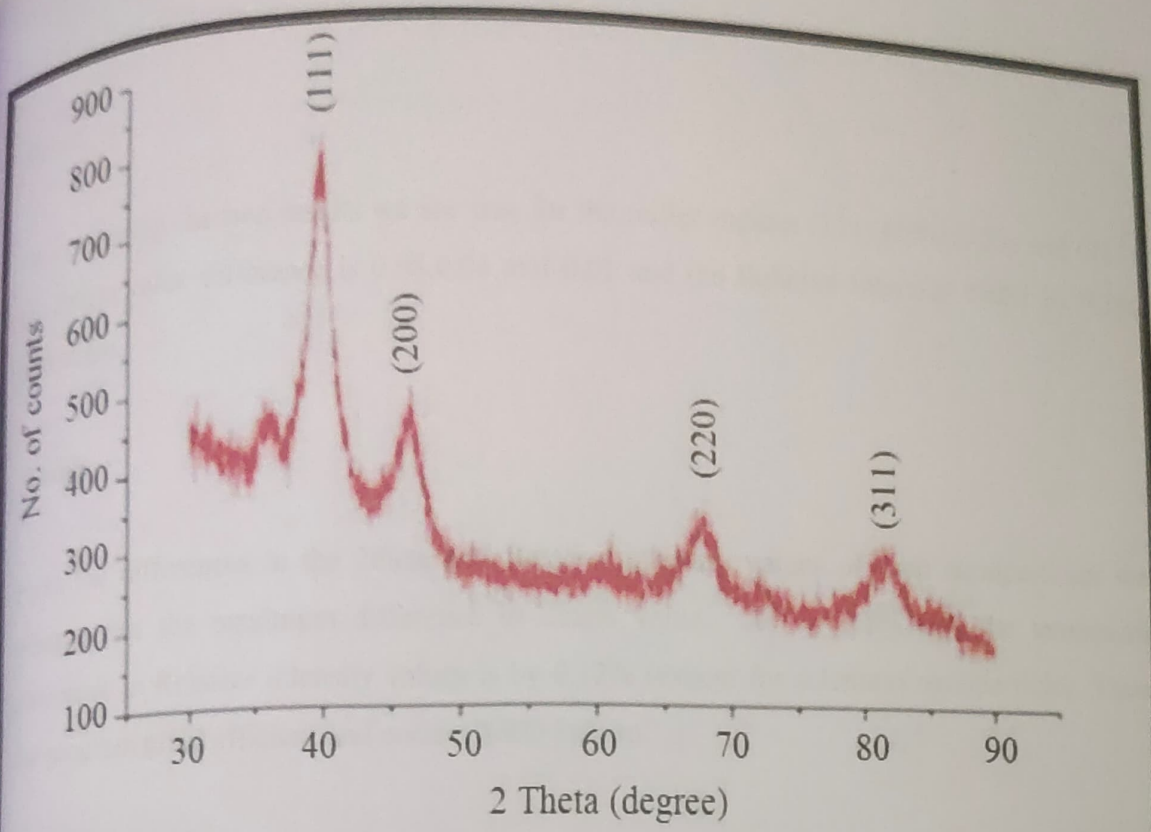
Element(s): Pt

Lattice Parameter: 3.920 A



2 theta	(hkl)	Relative intensity
39.78	111	1.000000
46.26	200	0.491091
67.50	220	0.322503
81.31	311	0.390801
85.76	222	0.115978
103.57	400	0.69299

Experimental Values



From Research paper " A clean-green synthesis of platinum nanoparticles utilizing a pernicious weed lantana (Lantana camara)"we get the experimental XRD Pattern for the miller indices (111),(200),(220) and (311). From which we take the 2theta and Relative intensity values.

2theta	Hkl	intensity	Relative intensity
39.70	111	820	1.0000
46.20	200	490	0.5975
67.50	220	290	0.3536
81.30	311	270	0.3292

Result

On comparing the two results we see that for the miller indices (111),(200),(220) and (311) the 2theta value difference is 0.08,0.06 and 0.01 and the Relative Intensity differ by 0.1% maximum.

Result

From the differences in the 2theta and Relative intensity values of each nanoparticles we observe that the maximum difference in 2theta value. is by 0.7% and the maximum difference in Relative intensity values is by 0.12% (except for selenium nanoparticle). Thus the program gives efficient and correct XRD Pattern.

CHAPTER-4

APPLICATIONS

CONCLUSION

REFERENCE

Applications

The major applications of X-ray diffraction are

- characterization of crystalline materials.
- identification of fine-grained minerals.
- determination of unit cell dimensions.
- measurement of sample purity.

MATLAB as we know has a range of applications in Industry and academia including deep learning and machine learning, signal processing and communications, image and video processing, control systems ,test and measurement, computational finance, and computational biology.

The MATLAB program for obtaining the XRD Pattern is thus applicable for various purposes such as it's helps to test and measure the values obtained from experimental results and check the accuracy and for calculation of other parameters.

Conclusion

This program is very useful and efficient in obtaining the required results in minimum amount of time. The program will help the user to reach an efficient comparison for the results they may experimentally obtained or will act as a guide to get the best possible useful results. It aids our understanding and reasoning capabilities in a more effective and efficient manner at a low cost.

References

Links

http://pd.chem.ucl.ac.uk/pdnn/pdindex.htm#diff2

https://www.researchgate.net/

https://www.ncbi.nlm.nih.gov/books/NBK537046/#:~:text=Simply%20understood%2C%20the%20generation%20of,components%20of%20X%2Dray%20production

Books

1)Unit cell XRD Book

2)Structure of materials-An introduction to Crystallography, Diffraction and Symmetry by Marc De Graef and Michael E McHenry