Powder Pattern Simulation

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COMPUTATIONAL DOCUMENT

The written instructions for the operations in this document are contained in the file cub2ins.mcd. You may obtain a copy from your instructor or the WWW site url he gave you.

DESCRIPTION OF THE STRUCTURE

You see below the description of a structure of Na metal which is simple (Primitive) cubic with one atom in the asymmetric unit at the origin of the unit cell. For this arrangement natom=1 and symno=1 The ASYM matrix describes the number of electrons and the position for the sodium atom.

natoms := 1 symno := 4

$$ASYM := \begin{bmatrix} 11 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The value of natoms must be the same as the number of columns in the ASYM matrix. The possible symno values are 1, 2, and 4.

We also enter the wavelength of the X-rays λ and the unit cell dimension 'a' both in Angstoms. B is a measure of the amplitude of atom vibration in the lattice.

λ := 1.5418 a := 4.000 B := 3.0

The matrices below are used to compute the atoms symmetrically related to the atoms in ASYM. The complete list of atoms is called ATOMS.

$$SYMP := \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad SYMI := \begin{bmatrix} 0 & 0 \\ 0 & .5 \\ 0 & .5 \\ 0 & .5 \end{bmatrix} \qquad SYMF := \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & .5 & .5 \\ 0 & .5 & 0 & .5 \\ 0 & .5 & .5 & 0 \end{bmatrix}$$

nn := 1 .. natoms

$$S := \begin{cases} SYMF & \text{if symno} = 4 \\ SYMI & \text{if symno} = 2 \\ SYMP & \text{if symno} = 1 \\ SYMP & \text{otherwise} \end{cases}$$

Note: the origin for matrices has been set to 1. The default in Mathcad is 0. Resetting is done through the Math drop down menu Built in Variables selection.

$mm := 1 .. symno$

$ATOMS^{\langle symno \cdot (nn - 1) + mm \rangle} := ASYM^{\langle nn \rangle} + S^{\langle mm \rangle}$

$$ATOMS = \begin{bmatrix} 11 & 11 & 11 & 11 \\ 0 & 0 & 0.5 & 0.5 \\ 0 & 0.5 & 0 & 0.5 \\ 0 & 0.5 & 0.5 & 0 \end{bmatrix}$$

Explain to your partner or group what is happening here.

We finally accumulate the numbers of electrons, x values, y values, and z values in column matrices.

$Noele := \left(ATOMS^{T}\right)^{\langle 1 \rangle}$

Note: the superscripts here denote the column number of the transpose of matrix ATOMS

$x := \left(ATOMS^{T}\right)^{\langle 2 \rangle}$ $y := \left(ATOMS^{T}\right)^{\langle 3 \rangle}$ $z := \left(ATOMS^{T}\right)^{\langle 4 \rangle}$

COMPUTER READS DATA FROM FILES

A list of the first 63 possible hkl reflections for a cubic lattice are stored on your disk in a file called HKLPM.PRN. For each reflection the file contains h, k, l, Q, and M. The Q value is the multiplicity or the number of possible hkl reflections which diffract at this same angle. The computer reads this file and assigns the first column (number 1) to h, etc. The Q values tell the computer how many reflections will diffract at this same θ value. The value of M is also included.

$hkl := READPRN(HKLPM)$

$nref := rows(hkl)$ $nref = 63$ $h := hkl^{<1>}$ $k := hkl^{<2>}$ $l := hkl^{<3>}$

$Q := hkl^{<4>}$ $M := hkl^{<5>}$ h k l Q M

$hkl =$

	1	2	3	4	5
1	1	0	0	6	1
2	1	1	0	12	2
3	1	1	1	8	3
4	2	0	0	6	4
5	2	1	0	24	5
6	2	1	1	24	6
7	2	2	0	12	8
8	2	2	1	30	9
9	3	1	0	24	10
10	3	1	1	24	11
11	2	2	2	8	12
12	3	2	0	24	13
13	3	2	1	48	14

Next the computer calculates the values of $\sin^2\theta$, $\sin\theta$, and θ and puts them into arrays. Only those values are included for which $\sin^2\theta < 1$.

$m := 1 .. nref$

$$ssq\theta_m := until\left(1 - \frac{\lambda^2}{4 \cdot a^2} \cdot M_m, \frac{\lambda^2}{4 \cdot a^2} \cdot M_m\right)$$

$nr := last(ssq\theta)$ $nr = 24$

$m := 1 .. nr$

$$\sin\theta_m := \sqrt{ssq\theta_m} \qquad \theta_m := \frac{180}{\pi} \cdot asin\left(\sin\theta_m\right)$$

$ssq\theta =$

	1
1	0.037
2	0.074
3	0.111
4	0.149
5	0.186
6	0.223
7	0.297

Using the complete list of atoms in the ATOMS matrix above we proceed with the calculation of the scattering amplitudes F_{hkl}. The calculation is made over the nr reflections for which $\sin^2\theta < 1$

$m := 1 .. nr \qquad nr = 24$

$$Fcalc_m := \sum_{n=1}^{(natoms \cdot symno)} \left[(Noele)_n \cdot \exp\left(-B \cdot \frac{ssq\theta_m}{\lambda^2} \right) \right] \cdot \exp\left[2 \cdot \pi \cdot i \cdot \left(h_m \cdot x_n + k_m \cdot y_n + l_m \cdot z_n \right) \right]$$

Note that the F_{calc}'s are complex numbers. The intensity of the diffraction line is calculated by taking the intensity ($F \cdot F^*$) times the multiplicity MULT. For complex waves the intensity is equal to the product of F times its complex conjugate F*. MULT is the number of times this intensity is superimposed at the same value of θ.

$$I_m := Q_m \cdot \left(Fcalc_m \right) \cdot \overline{\left(Fcalc_m \right)}$$

We wish to display the diffraction peaks as error bars, so in MATHCAD we need to tell the program that the bottom of each error bar is zero.

$$J_m := 0$$

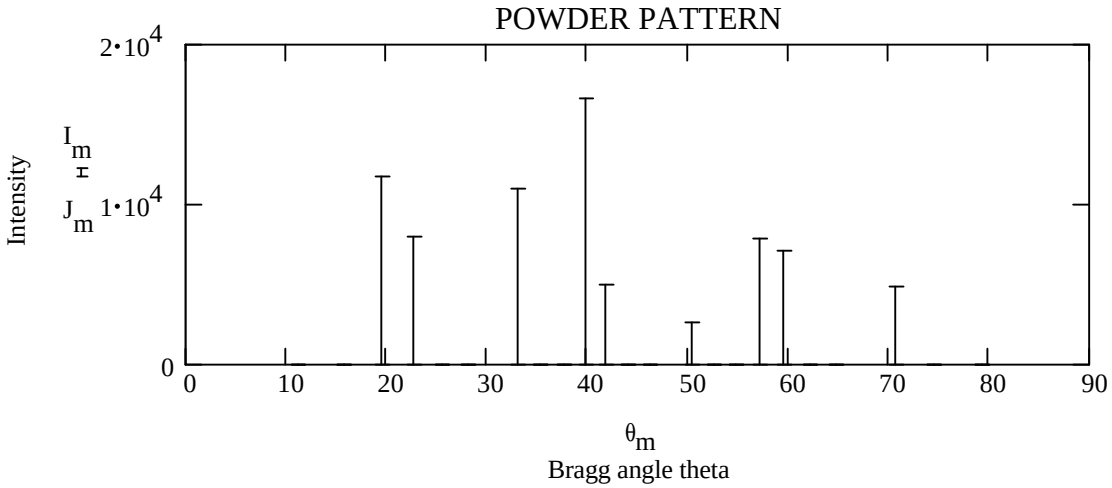
Finally the powder pattern appears below.

MATHCAD HELP: It may be necessary to change the y axis to an appropriate scale. To do this click on the graph and change the range value in the upper left corner. To print this page click on the print button above, select 'current page' and then 'print.'

Standard values a=4.00 λ=1.5418 B=3.0 natoms = 1 symno=1

COMPOUND FOR THIS PATTERN: Na simple cubic

Write a label here for your graph!



To see the numerical results of the powder pattern we define a matrix F

$F^{<1>} := h \quad F^{<2>} := k \quad F^{<3>} := l \quad F^{<4>} := M$

$F^{<5>} := Q \qquad F^{<6>} := ssq\theta \quad F^{<7>} := Fcalc \quad F^{<8>} := I$

h k l M Q ssθ F QFF*

F =

	1	2	3	4	5	6	7	8
1	1	0	0	1	6	0.04	$2.57\cdot10^{-15}i$	0
2	1	1	0	2	12	0.07	0	0
3	1	1	1	3	8	0.11	38.23	$1.17\cdot10^{4}$
4	2	0	0	4	6	0.15	36.48	$7.98\cdot10^{3}$
5	2	1	0	5	24	0.19	$2.13\cdot10^{-15}i$	0
6	2	1	1	6	24	0.22	$4.07\cdot10^{-15}i$	0
7	2	2	0	8	12	0.3	30.24	$1.1\cdot10^{4}$
8	2	2	1	9	30	0.33	$1.77\cdot10^{-15}i$	0
9	3	1	0	10	24	0.37	0	0
10	3	1	1	11	24	0.41	26.27	$1.66\cdot10^{4}$