

Spreadsheet Applications for Materials Science

Introduction to X-ray Powder Diffraction

Introduction

X-ray powder diffraction is a powerful analytical technique that is widely used in many fields of science and in many industries. Applications range from basic research to routine quality control and includes determining the structure of new materials, identifying unknown materials in based on their crystal structures, detecting the presence of impurities or strain, measuring the size of the crystals, and other fine-scale structural defects. The basis of all of these techniques is the phenomenon of constructive interference where when conditions are just right a sample that had been illuminated with a strong beam will emit a strong beam. The wide variety of analysis techniques are based on clever uses of secondary factors.

This tutorial focuses on how a basic analysis of the diffraction data is done. It begins by describing a typical diffractometer and how the data are collected, then it reviews Bragg's law, the important first criterion for diffraction, and finally the reflection rules, simple but handy rules that tell us something about the intensity of the diffracted beam, at least for simple structures. The exercises include importing, plotting, and analyzing the data and using this data to identify unknown materials.

A Typical X-ray Powder Diffraction System

In many respects all powder diffractometers are alike. They all utilize an x-ray source that is aimed at the sample, a detector that is also pointing at the sample, and these components move so that a range of diffraction angles (2θ) is scanned. Figure 1 shows a modern computer-controlled diffractometer where the x-ray source (left, moves), detector (right, moves), and a specimen holder (center, does not move), are all enclosed in a cabinet that protects the operator from exposure to x-

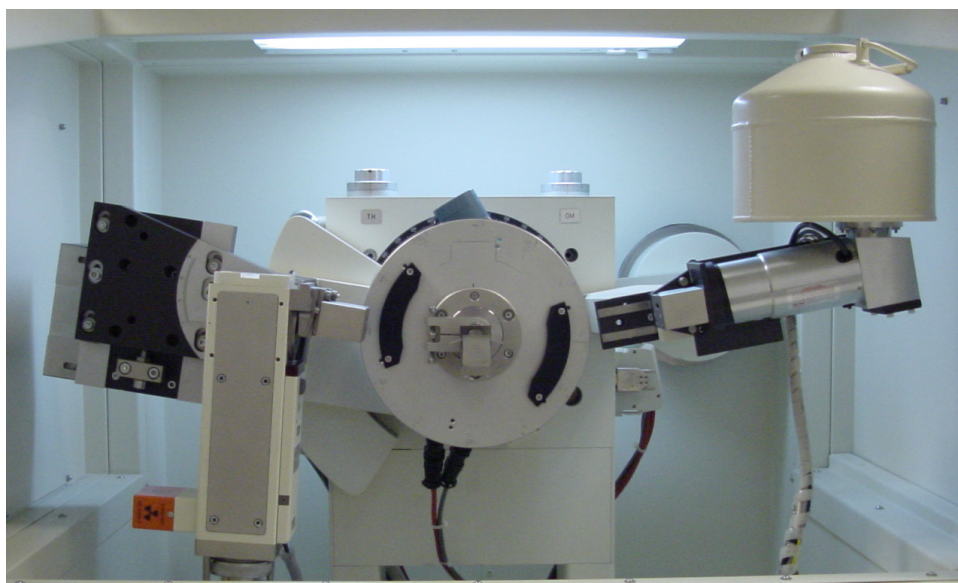


Figure 1 A modern x-ray diffractometer. The x-ray source with its warning lights is located on the left, the detector and its liquid nitrogen dewar are on the right, and the sample holder is in the center.

rays. The top of figure 2 shows the source in more detail, including the warning lights, the β -filter that blocks unwanted x-rays, and a pair of slits that control the divergence of the incident beam. The second image in figure 2 shows a liquid nitrogen cooled x-ray detector which also has a pair of slits (under the cover) that limits the angles from which x-ray can enter the detector. The third image shows a sample in the center of the goniometer. The x-ray source can be seen in the background, aimed at the sample.

The principal dimensions and angles for this system are shown in the bottom image in figure 2. In this system the source and detector are located 250 mm from the center of the goniometer (diffractometer circle). The angle between the source and the horizontal is called ω and in this figure is shown at 10 degrees. The detector is also positioned at $\theta=10$ degrees during an experiment both the source and detector can scan angles from 2 to 70 degrees. The sample is located in the center of this circle. Care is taken to ensure that the sample is as close as possible to this center, that it is not tilted, and that it is smooth and flat.

A Typical X-ray Diffraction Analysis

During a typical experiment using the system shown in the figures above, the sample position is fixed while the angles of the source and detector scan a specified range of angles, typically 20 to 90 degrees 2θ for the routine analysis of metals and simple compounds, and 10 to 60 degrees 2θ for many minerals. In this system the source and detector angles are always equal, $\omega=\theta$, $2\theta=\omega+\theta$.

The scan rate, the rate at which 2θ changes, is chosen to provide the desired quality of results, slower scans providing higher quality results than faster, more economical, scans. A quick preliminary scan may take only 5 minutes but the peaks may not be well defined and small peaks may be difficult to distinguish from the background signal. The higher quality scans required for detailed analyses may require 1 or more hours depending on the size and type of sample being analyzed. The reason for these differences is that during slow scans more x-rays

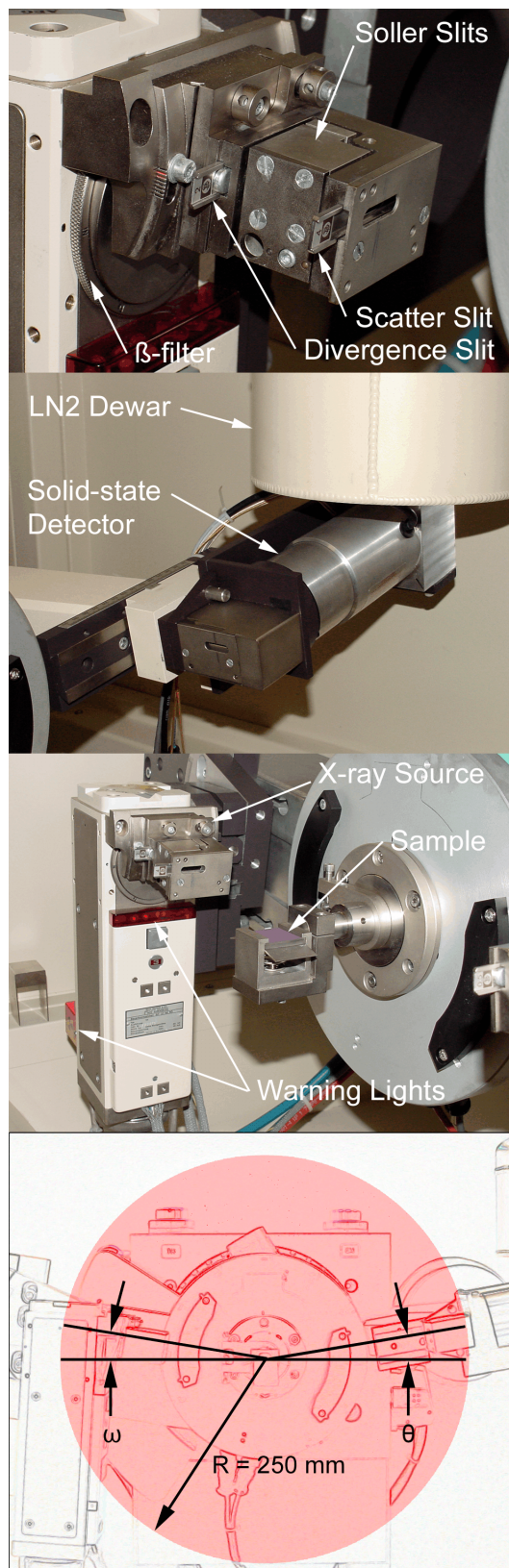


Figure 2 A close-up look at an x-ray diffractometer. Top – soller slits, divergence and scatter slits and β -filter, Second – solid-state detector, Third – sample and x-ray tube, Bottom – angles and dimensions.

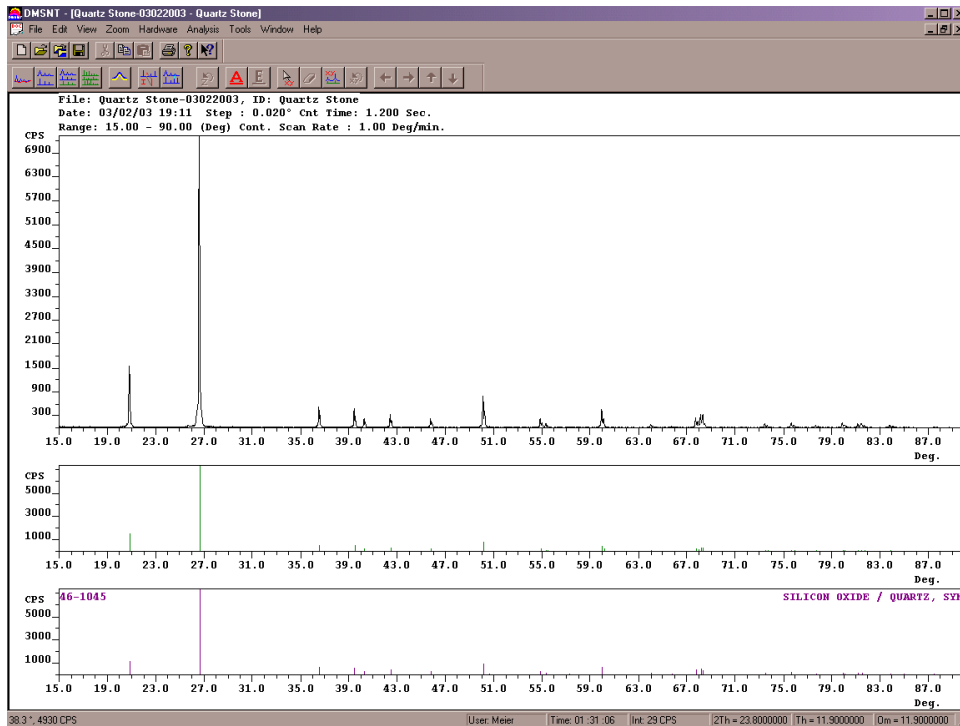


Figure 3 Screen shot of Scintag's DMSNT software. The top graph shows the raw data, the center graph shows plots of the peaks found by the software, and the bottom graph shows the results of the search-match procedure which found the pattern for quartz best matched the data.

photos are counted and this reduces the uncertainty in the measurements. A slow scan will produce relatively smooth lines in the diffraction pattern while faster scans will produce patterns that look like the signal contains a lot of noise.

Typical results from an x-ray diffraction analysis are shown in figure 3. The top graph shows the raw data, plotted as the intensity of the diffracted x-ray beam as a function of the diffraction angle 2θ . The peaks indicate angles at which all of the conditions for x-ray diffraction have been met. The middle graph shows which peaks the software found while the bottom graph shows a plot of a pattern from a database of diffraction data for over 100,000 elements, alloys, and compounds. The software searched this database in only a few seconds, comparing the positions and intensities of the peaks in the measured pattern to those in the database, and found several matches. The pattern which was the closest match was quartz.

This analysis illustrates a common application of x-ray diffraction, identifying a substance in terms of its crystalline structure. Many other types of analyses are also possible. Slight shifts of the peaks may indicate the presence of impurities or stress. The shapes of the peaks may be able to tell us about the size of the crystals and the intensities of the peaks can tell us about the concentration of this material if it were a mixture.

Geometry of Diffraction

Two criteria must be met before a peak in the diffraction pattern can be obtained. The first involves

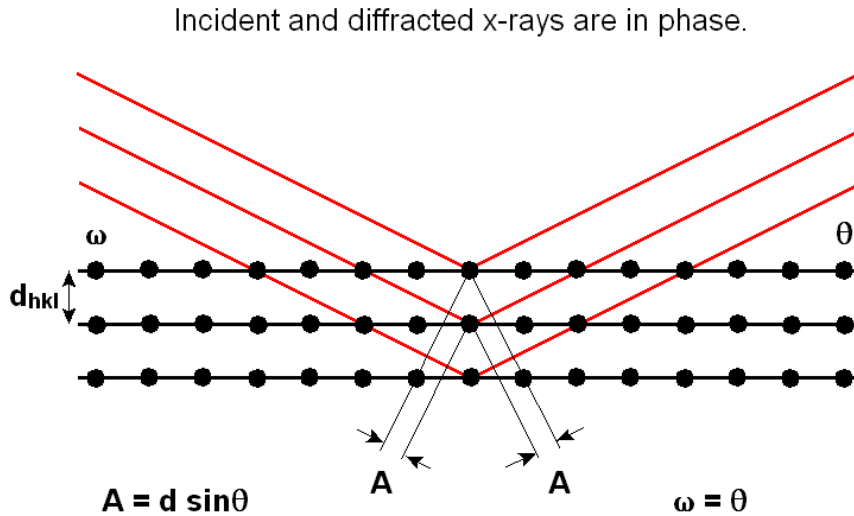


Figure 4 An illustration of the reflection analogy of diffraction.

the geometry of diffraction where the combination of the wavelength of the incident x-ray, the angle between the incident beam and the diffracting plane, and the inter-planar spacing must satisfy conditions that will produce constructive interference, or at least not totally destructive interference, of the diffracted beam. Figure 4 illustrates the reflection analogy that is often used to represent this criterion. Rays of the incident beam are in phase when they reach the sample. Some rays “reflect” off the first plane, others off the second and other parallel planes, and these will reemerge from the sample if they are in phase. This will only happen when the incident angle and inter-planar spacing are such that the path differences $2A$ traveled by each ray are equal to integral values of the wavelength. It is these in-phase beams that form the diffracted beam.

The geometric requirements of diffraction are summed up in Bragg’s law,

$$n\lambda = 2d\sin(\theta) \tag{1}$$

where n is the order of diffraction, λ is the wavelength of the x-ray, d is the interplanar spacing and θ is the incident/diffracted angle. In these types of analyses the value of n is assumed to be 1.

Intensity of Diffraction

Bragg’s law tells us when the geometric requirements are such that diffraction can occur, but it does not say anything about the actual intensity of this beam. There are a number of factors that determine this.

The Structure Factor

The structure factor determines if a diffracted beam of any intensity at all will result. It is basically a sum of the contributions of each atom in the lattice to the diffracted beam. It turns out that the value of the structure factor is 0 for all but a relatively few cases, and this means that it is very possible that even if Bragg’s conditions are met diffraction may still not take place.

One interesting thing about the structure factor is that it is independent of the size of the lattice. The structure factor will be the same for all fcc materials, for example, even though their lattice parameters are different.

The Reflection Rules

The structure factors for simple, high symmetry (i.e., cubic) structures can be reduced to a few simple rules that can be used to identify a structure by looking at a list of peaks from a diffraction pattern. These rules are summarized in the table below.

Table 1. A summary of the reflection rules for cubic structures.

Structure	Reflection Rule	Examples
Simple Cubic (sc)	All hkl's	(100), (110), (111), (200)
Body-centered Cubic (bcc)	h + k + l must be an even number	(110), (200), (220), (310)
Face-centered Cubic (fcc)	All indices must be either all even or all odd	(111), (200), (220), (311)

Other Factors

The structure factor, which gives us the reflection rules, is a key factor in determining the intensity of the diffracted beam, and especially whether or not a diffracted beam will even be produced. But there are still several other factors that influence the final intensity of the beam to consider.

- Multiplicity factor** Some families of planes have more members than others, and all things being equal, the families with more members will produce stronger diffracted beams. The {100} family in a cubic structure, for example, has 6 members while the {111} family has 8. If the intensity of x-rays diffracted by a (100) and (111) plane are the same, then the {111} peak in the diffraction pattern will be 25% stronger than that of the {100} peak.
- Polarization** Polarization is a result of the way the x-ray beam interacts with the electrons orbiting the atomic nuclei in the sample. Basically, polarization is not the same in all directions, and its effect on the diffraction pattern is to make the peaks at low and very high angles (near 0 and 180° 2θ) stronger than peaks nearer the middle. This is one reason why low-angle peaks tend to be stronger than peaks near 90° 2θ.
- Lorentz Factor** This factor accounts for geometric characteristics of the diffractometer that creates a situation where x-rays diffracted at low and high angles are more concentrated (spread out over a smaller area) than at angles near 90° 2θ. The effect on the diffraction pattern is similar to that of polarization.
- Absorption** A portion of the incident beam will penetrate into and be absorbed by the sample. The magnitude of this effect is different for each material, as figure 5 shows. One result of this is that it can be very difficult to obtain good strong peaks when analyzing highly absorbing materials.

Temperature

Most diffraction work is done at room temperature so this is not normally much of a concern. But at high temperatures the greater thermal oscillation of the atoms means they spend more time farther from their ideal lattice position. This results in smaller and broader diffraction peaks.

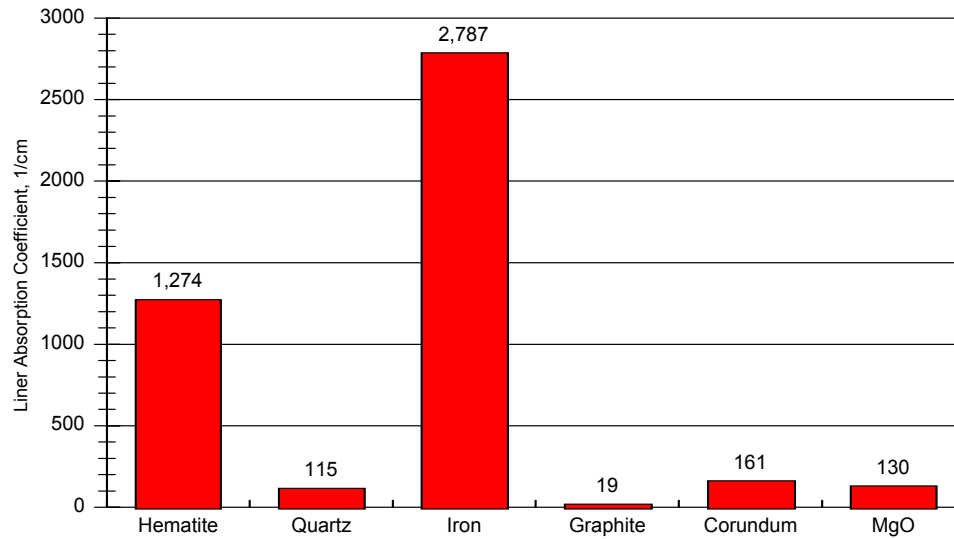


Figure 5 Linear absorption coefficients for selected materials and for Cu- k_{α} x-rays. Note the very high absorption coefficients for iron and iron oxide.

Spreadsheet Exercises

The following exercises employ a number of the concepts described above and provide opportunities to explore them more. The spreadsheets themselves will be useful in the project-scale exercises given later in this document.

The following guidelines should help in completing these exercises and producing a spreadsheet that is easy to use and easy to read and understand.

- Set up a spreadsheet using the recommended format, including the header, a description of what the spreadsheet does, and sections for physical constants and conversion factors, as appropriate.
- Create a section where the name of the material, experimental conditions, sample form and dimensions, and similar details that are relevant in the calculations or otherwise important to note are listed. All key parameters should be defined before the real work begins.
- The main calculations should be done in tables that include proper headings. Using well-organized tables will help keep the work itself organized and the result will be much easier for the reader to understand what you did. In many cases these tables can even be copied directly into reports.
- All of these exercises can be done in one multi-sheet notebook. (A notebook contains many spreadsheets.)

1. Diffraction Angle - d-spacing Conversions

Powder diffraction data is usually published as the intensity of peaks for specific d-spacings, rather than the diffraction angle 2θ . The reason for this is that not everyone uses the same x-ray source, so reporting the d-spacings is more universal. Use a spreadsheet to convert the d-spacings given in published sources to the 2θ positions that can be expected to be seen in a diffraction pattern.

Note – The figure 6 shows a screen shot of the spreadsheet created for this exercise. Note how it was laid out so that it is easy to use and easy for someone else to understand how the calculations were done.

- Set up the spreadsheet using the guidelines given above.
- Enter a wavelength for an x-ray source (see appendix 1), then set up a table to receive the diffraction data: peak numbers, Miller indices, d-spacings, and relative intensities. This table should be able to hold information for at least 21 peaks.
- Enter the diffraction data for zinc. See appendix 3.
- Add one more column to this table and calculate 2θ .
- This spreadsheet provides a good foundation for performing additional useful calculations, such as the value of $s = \sin(\theta)/\lambda$ that is widely used in x-ray diffraction calculations. (This

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Exercise 1:046

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Spreadsheet Applications for Materials Science - X-ray Diffraction Basics

Exercise 1. Diffraction Angles - d-spacing Conversions

Materials and Source Parameters

Material: Zinc
 Structure: hexagonal
 Wavelength: 0.154056 nm

Table 1. Diffraction Angles and s-values from PDF-type Data

Peak #	Miller Indices	d-spacing, nm	Relative Intensity	Diffraction Angle, 2θ	sinθ/λ, nm ⁻¹
1	(002)	0.24730	53	36.296	2.022
2	(100)	0.23080	40	38.992	2.166
3	(101)	0.20910	100	43.231	2.391
4	(102)	0.16870	28	54.336	2.964
5	(103)	0.13420	25	70.056	3.726
6	(110)	0.13320	21	70.660	3.754
7	(004)	0.12370	2	77.027	4.042
8	(112)	0.11729	23	82.102	4.263
9	(200)	0.11538	5	83.765	4.334
10	(201)	0.11236	17	86.557	4.450
11	(104)	0.10901	3	89.920	4.587
12	(202)	0.10456	5	94.900	4.782
13	(203)	0.09454	8	109.129	5.289
14	(105)	0.09093	6	115.798	5.499
15	(114)	0.09064	11	116.385	5.516
16	(210)	0.08722	5	124.048	5.733
17	(211)	0.08589	9	127.487	5.821
18	(204)	0.08437	2	131.841	5.926
19	(006)	0.08245	1	138.211	6.064
20	(212)	0.08225	9	138.947	6.079
21				ERR	ERR

Figure 6 This screen shot of exercise 1 shows the typical layout that will work for all of the exercises in this module.

calculation is optional.)

- Experiment with different wavelengths and diffraction patterns. How much does changing the wavelength change the positions of the peaks? If you were planning to perform diffraction measurements on similar types of materials, what range of angles would you need to scan? It was noted earlier that scans of metals and alloys usually range from 20 to 90° 2θ, while for clays these angles were somewhat lower. Why?

2. Interplanar Spacings

The positions of diffraction peaks is a function of the d-spacings in the structure and the wavelength of the incident x-ray. Build a spreadsheet that calculates these d-spacings for any (hkl).

Start a new spreadsheet (new sheet in the current notebook) and do these calculations for the cubic structure. Assume a lattice parameter of $a=0.3$ nm. (The relationship between the d-spacing and lattice parameter for several crystal systems are given in appendix 2.) Do these calculations for at least 10 planes, and perform the intermediate calculation of $h^2+k^2+l^2$ in its own column.

Experiment with the lattice parameters and indices. Try using the lattice parameters and indices listed in appendix 3.

3. Bragg Diffraction Angles

Bragg's law provides a simple relationship between the wavelength of the x-ray, the d-spacing, and the diffraction angle. A typical diffraction pattern will contain peaks for many planes and even for different x-rays when the source radiation is not adequately filtered. Built upon the spreadsheet from the previous exercise to add the calculation of the diffraction angle 2θ . Place the wavelengths in a column so that different wavelengths can be used in each 2θ calculation. Use any of the λ_{Cu} wavelengths listed in appendix 1.

Experiment with the effect of the wavelengths on the diffraction angles. For instance, chromium characteristic radiation is used in systems designed to measure residual stresses in steels. How do the angles for low and high indices ($h^2+k^2+l^2$) planes change when compared to systems that use copper x-ray sources?

Experiment with the Miller indices to see how the diffraction angles change. For example, are the diffraction angles for the (100), (010) and (001) planes the same? Is the diffraction angle for the (400) plane four times larger than that for the (100) plane?

Suggestion – try using your spreadsheet's string-handling functions to generate a string of the form (hkl) where h, k and l are values in the cells of your spreadsheet.

4. Reflection Rule

The reflection rules are useful when interpreting the diffraction patterns of simple structures. Having a table that lists which planes can be expected to produce a diffracted beam for different structures can be very handy.

Start a new spreadsheet and in it set up a table that lists the peak number, the three Miller indices, and calculates $h^2+k^2+l^2$. Enter indices for $h^2+k^2+l^2$ from 1 to 64. Set up two more columns and label them BCC, and FCC. In these columns enter formulas that will return a result indicating whether or not diffraction could occur.

Hint – To do this you will need to use your spreadsheet's even and odd functions, boolean logical functions, and possibly the equals sign in a logical test context. For example, the formula

$$=IsOdd(5)=IsEven(8)$$

will return a 1 since both conditions are true.

Suggestion – If your spreadsheet program supports custom formatting of cells then see if you can get it to display a symbol such as +, -, ●, ✓, ✗, ◆ instead of a number to indicate whether or not a diffraction could be expected.

Spreadsheet Projects

The above exercises explored a few basic aspects of x-ray powder diffraction and produced spreadsheets that hopefully will be useful to you in the future. The following projects take these to the next level by plotting and examining real diffraction data and identifying an unknown substance based only on its diffraction pattern.

1. Examine a Diffraction Pattern

What does a diffraction pattern actually look like? To find out, import the Silicon.txt data file into a spreadsheet and plot it. Determine the maximum intensity in the pattern and scale the data so that the highest peak is the 100% relative intensity peak, then plot this as 2θ versus relative intensity.

Locate each peak and note their relative intensities and 2θ positions. Compile this data in a table and compare it to the peak positions listed in silicon's powder file (appendix 3). Look at the trends in peak intensities to see if they follow the trend described in the introduction. Are there cases where pairs of peaks are located very close to each other? How would this pattern compare to the pattern for diamond?

Hint – It is very difficult to filter x-rays to the extent that the $k_{\alpha 2}$ peak can be eliminated. The k_{β} peak is usually filtered well, but in systems that use an older x-ray tube the $W-L_{\alpha}$ x-ray may become strong enough to produce peaks in your pattern.

2. Identify and Unknown from a Peak File

A common application of x-ray diffraction is identifying materials in terms of their crystalline structure. The method usually employed is to list the positions and relative intensities of all peaks in the pattern and then have a computer search a database looking for a match. For simpler cases, and especially when one has a pretty good idea what the material is, manually pulling one of the files from this database and seeing if there is a match may be sufficient. If these fail, and the pattern is a simple one, the Miller indices of each peak can be determined manually and these can be interpreted in terms of the reflection rules to figure out what the crystal structure is. If the substance is a pure element, then the atomic radius can be calculated from the lattice parameter. A match can then be obtained by comparing these results to the types of data usually listed in the periodic table of the elements.

Analyze the peak files provided to find out what the substances are. Use whichever method above that works best. If a match is found with one of the sets of data in appendix 3, make sure to include an analysis of how good the match is. If the manual indexing method is used then include an analysis of how good the lattice parameter determination was and how close the results are to the reference data. Optionally, calculate the density of the sample from the diffraction data and compare

that to the density listed in references.

Note – while x-ray diffraction is very good at providing accurate measurements of the d-spacings, the peak intensities can differ significantly from that in the reference data. This is due to a number of issues usually related to sample preparation and the nature of the sample itself. Differences in intensity of around 1 percent would be considered excellent, but larger differences are normal in routine analyses. Nevertheless, the general trend in the intensities should be similar.

3. Identify an Unknown from a Diffraction Pattern

Modern diffractometers usually include software that will plot the data, automatically find the peaks, and even match the pattern to those in a database. The peak-finding routines can be very sophisticated and can provide a lot of information about each peak, things like the position, height, area under the peak, shape, symmetry, and much more. All of this can be invaluable when you need to estimate the concentration of minerals present, the size of nano-scale particles, residual stress, etc. For a routine phase identification analysis, however, all that is needed are accurate measurements of the peak positions and decent measurements of the peak intensities, and these can be obtained using a spreadsheet.

Data files for several unknown materials are provided. Import, plot, and analyze them to find out what the samples are.

4. X-ray Diffraction of Non-crystalline Materials

Everything in this module so far has dealt with crystalline materials. But what do the diffraction patterns for non-crystalline materials look like? Do they have sharply defined peaks like the patterns for crystalline materials do? Are there no peaks at all since there are no clearly defined planes of atoms, and therefore no characteristic inter-planar spacings? Import and plot the file GC.txt to find the answer.

Appendix 1. Characteristic Wavelengths of Common X-ray Sources

Source: B.D.Cullity, Elements of X-ray Diffraction, Addison-Wesley, Reading, Massachusetts, pp.464-465, 1963.

Element	Wavelength, nm				
	Weighted Average K_{α}	$K_{\alpha 1}$ (strongest)	$K_{\alpha 2}$ (strong)	K_{β} (weak)	L_{α}
Chromium	0.229092	0.228962	0.229351	0.208480	-
Cobalt	0.179021	0.178892	0.179278	0.162075	-
Copper	0.154178	0.154051	0.154433	0.139217	1.3357
Iron	0.193728	0.193597	0.193991	0.175653	-
Manganese	-	0.210175	0.210568	0.191015	-
Molybdenum	0.071069	0.070926	0.0713543	0.0632253	0.540625
Nickel	-	0.165784	0.166169	0.150010	-
Tungsten ¹	-	0.0208992	0.0213813	0.0184363	0.147635
Zinc	-	0.143511	1.43894	0.129522	1.2282

¹ Tungsten is not a typical x-ray target, but rather is used as the filament in an x-ray tube. Over time tungsten will be deposited on the target and as a result tungsten x-rays will be emitted along with the target material's x-rays.

Appendix 2. Useful Equations

Planar spacings

Cubic system:

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \quad (2)$$

Tetragonal System:

$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2} \quad (3)$$

Hexagonal System:

$$\frac{1}{d^2} = \frac{4}{3} \frac{h^2 + hk + k^2}{a^2} + \frac{l^2}{c^2} \quad (4)$$

Appendix 3. Diffraction Data from Selected PDF Files

The International Centre for Diffraction Data has been collecting, evaluating, and publishing data from powder diffraction measurements for over 40 years. The database they have put together, called the Powder Diffraction File (PDF), currently contains over 120,000 entries for elements, metals, ceramics, polymers, pharmaceuticals, minerals, virtually every known crystalline material, natural and synthetic. Most entries are from diffraction experiments but recently it has also included calculated patterns.

The data offered in this appendix are from several of ICDD's PDF files. Only peaks whose relative intensity is 1% or greater and a total of up to 18 peaks are listed. The lattice parameters and density are also listed.

PDF # 04-0831								
Name: Zinc								
Crystal System: Hexagonal								
Lattice Parameters:			a=0.2665 nm	b=	c=0.4947 nm			
			α =	β =	γ =			
Density:			7.136 g/cm ³					
Diffraction Data								
d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)
0.2473	53	(002)	0.11729	23	(112)	0.09064	11	(114)
0.2308	40	(100)	0.11538	5	(200)	0.08722	5	(210)
0.2091	100	(101)	0.11236	17	(201)	0.08589	9	(211)
0.1687	28	(102)	0.10901	3	(104)	0.08437	2	(204)
0.13420	25	(103)	0.10456	5	(202)	0.08245	1	(006)
0.13320	21	(110)	0.09454	8	(203)	0.08225	9	(212)
0.12370	2	(004)	0.09093	6	(105)			

PDF # 44-1294

Name: Titanium

Crystal System: Hexagonal

Lattice Parameters: a=0.29505 nm b= c=0.46826 nm
 α = β = γ =

Density: 4.506 g/cm³

d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)
0.2555	25	(100)	0.12776	1	(200)	0.09886	2	(203)
0.2341	30	(002)	0.12481	9	(112)	0.09658	1	(210)
0.2243	100	(101)	0.12324	6	(201)	0.09459	4	(211)
0.17262	13	(102)	0.11707	1	(004)	0.09170	3	(114)
0.14753	11	(110)	0.11215	1	(202)	0.08928	1	(212)
0.13320	11	(103)	0.10643	1	(104)			

PDF # 06-0696

Name: Iron

Crystal System: Cubic

Lattice Parameters: a=0.28664 nm b= c=
 α = β = γ =

Density: 7.875 g/cm³

d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)
0.20268	100	(110)	0.11702	30	(211)	0.09064	12	(310)
0.14332	20	(200)	0.10134	10	(220)	0.08275	6	(222)

PDF # 06-0675

Name: Carbon (Diamond)

Crystal System: Cubic

Lattice Parameters: a=0.35667 nm b= c=
 α = β = γ =

Density: 3.517 g/cm³

d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)
0.206	100	(111)	0.10754	16	(311)	0.08182	16	(331)
0.1261	25	(220)	0.08916	8	(400)			

PDF # 05-0628

Name: Sodium Chloride (NaCl, Halite)

Crystal System: Cubic

Lattice Parameters: a=0.56402 nm b= c=
 α = β = γ =

Density: 2.163 g/cm³

d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)
0.326	13	(111)	0.1294	1	(331)	0.09491	3	(600)
0.2821	100	(200)	0.1261	11	(420)	0.08917	4	(620)
0.1994	55	(220)	0.1151	7	(422)	0.08601	1	(533)
0.1701	2	(311)	0.1085	1	(511)	0.08503	3	(622)
0.1628	15	(222)	0.09969	2	(440)	0.08141	2	(444)
0.1410	6	(400)	0.09533	1	(531)			

PDF # 46-1045Name: Silicon Oxide (SiO₂, Quartz)

Crystal System: Hexagonal

Lattice Parameters: a=0.491344 nm b= c= 0.540524 nm
 α = β = γ =

Density: 2.649 g/cm³

d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)
0.42549	16	(100)	0.18179	13	(112)	0.13718	5	(301)
0.33434	100	(101)	0.16717	4	(202)	0.12879	2	(104)
0.24568	9	(110)	0.16591	2	(103)	0.12559	3	(302)
0.22814	8	(102)	0.15415	9	(211)	0.12283	1	(220)
0.22361	4	(111)	0.14528	2	(113)	0.11998	2	(213)
0.21277	6	(200)	0.13821	6	(212)	0.11839	2	(114)
0.19798	4	(201)	0.13749	7	(203)	0.11801	2	(310)

PDF # 46-1212Name: Aluminum Oxide (Al₂O₃, Corundum)

Crystal System: Rhombohedral

Lattice Parameters: a=0.47587 nm b= c=1.29929 nm
 α = β = γ =

Density: 3.987 g/cm³

d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)
0.34797	45	(012)	0.16015	89	(116)	0.12755	2	(208)
0.25508	100	(104)	0.15466	1	(211)	0.12391	29	(1 0 10)
0.23794	21	(110)	0.15150	2	(122)	0.12343	12	(119)
0.21654	2	(006)	0.15110	14	(016)	0.11931	1	(217)
0.20853	66	(113)	0.14045	23	(214)	0.11897	2	(220)
0.19643	1	(202)	0.13737	27	(300)	0.11600	1	(306)
0.17400	34	(024)	0.13359	1	(125)	0.11472	3	(223)

PDF # 21-1272Name: Titanium Oxide (TiO₂, Anatase)

Crystal System: Tetragonal

Lattice Parameters: a=0.37852 nm b= c= 0.95139 nm
 α = β = γ =

Density: 3.893 g/cm³

d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)
0.352	100	(101)	0.14930	4	(213)	0.11894	<2	(008)
0.2431	10	(103)	0.14808	14	(204)	0.11725	2	(303)
0.2378	20	(004)	0.13641	6	(116)	0.11664	6	(224)
0.2332	10	(112)	0.13378	6	(220)	0.11608	4	(312)
0.18920	35	(200)	0.12795	<2	(107)	0.10600	2	(217)
0.16999	20	(105)	0.12649	10	(215)	0.10517	4	(305)
0.16665	20	(211)	0.12509	4	(301)	0.10436	4	(321)

PDF # 21-1276Name: Titanium Oxide (TiO₂, Rutile)

Crystal System: Tetragonal

Lattice Parameters: a=0.45933 nm b= c=0.29592 nm
 α = β = γ =

Density: 4.250 g/cm³

d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)	d, nm	Relative Intensity	(hkl)
0.3247	100	(110)	0.14797	10	(002)	0.12006	2	(212)
0.2487	50	(101)	0.14528	10	(310)	0.11702	6	(321)
0.2297	8	(200)	0.14243	2	(221)	0.11483	4	(400)
0.2188	25	(111)	0.13598	20	(301)	0.11143	2	(410)
0.20540	10	(210)	0.13465	12	(112)	0.10936	8	(222)
0.16874	60	(211)	0.13041	2	(311)	0.10827	4	(330)
0.16237	20	(220)	0.12441	4	(202)	0.10425	6	(411)

