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Xrd reference patterns database

Qualitative powder diffraction involves the identification of a phase or phases in a specimen by comparison with single-phase X-ray powder diffraction patterns compiled in a database called the Powder Diffraction File (PDF-2). Information obtained from this database include: interplanar spacings (d), relative intensities (I/Io), Miller indices, cell data, physical properties and references to sources of information. The latest version contains 163,835 entries of inorganic and organic phases. It is maintained and continually upgraded by the International Centre for Diffraction Data (ICDD). PDF-2 is incorporated with XRD processing software such as Evaluation (DIFFRACplus EVA V. 9.0). To process a trace a Peak Search is undertaken initially to assign d-values for each reflection. A Search Match routine is then carried out which gives the user a list of possible minerals or phases in a specimen. For each phase a good match is one where relative intensites and positions of 3 strongest lines and minor lines (the greater the number of lines that match the better) of unknown and standard pattern from database coincide. Logical choices of possible phases in the specimen are made by the user based on information he has about the sample (results from other analyses, environment of formation eg., geological specimen, and information from previous works/ literature). Some steps for performing qualitative analysis of an XRD sample are as follows: Peak identification. The first part of data evaluation is to identify diffraction peaks. This involves several steps: Kα2-stripping: most diffractometers use bichromatic radiation that corresponds to the Kα1/Kα2-doublett of the anode material. This is reflected by a splitting of peaks. To prevent an accidental counting of α2-peaks, these contributions are automatically stripped off. Background subtraction: powder diffractograms contain a significant amount of background due to air scattering and the presence of amorphous phases. The background is fitted with a mathematical polynomial and then subtracted. This way it does not interfere with the data evaluation. Smoothing: most diffraction patterns contain a considerable amount of noise. This may hamper the discrimination of peaks from random noise. A step of smoothing is often employed to reduce the random noise. Peak search: smoothing is followed by the actual identification of peaks. With good patterns (high signal to noise ratio, narrow peaks) this can be done automatically. Otherwise it is necessary to insert peaks by hand and refine them. Profile fit: whether found automatically or by hand, peak positions and intensities are not well determined by the previous step. A profile fit refines peak positions and intensities. Phase identification. In powder diffraction the term phase is often used as a synonym for substance. Using the powder diffraction file: Every single substance has a characteristic powder pattern at a given wavelength in terms of peak position and peak intensity. This pattern can be used as a fingerprint to identify this substance in a powder pattern. For this purpose, the International Centre of Diffraction Data has collected known powder patterns found in the Powder Diffraction File (PDF) to help identify various substances. As of 2006 the PDF contains 186,107 entries. Identification of peaks: the next step is to assign the peaks in the experimental pattern to the correct phase. Once all peaks have been identified with the correct phase, the powder pattern can be considered solved. Limit the database: it is useful to limit the database in a reasonable way. The first thing to examine is the preparation method. Let's say the present sample was made from calcium fluoride, phosphoric acid and calcium carbonate. After precipitation, the raw product was filtered off and calcined in an alumina crucible. The following elements can possibly be found in your sample: Calcium, phosphorus, oxygen, fluorine, carbon, hydrogen and aluminium (don't dismiss the crucible material in a high temperature reaction!). Oxygen will have to be present at any rate, due to the reaction conditions. Calcium, phosphorus and fluorine are at least present in one phase each, and carbon, aluminium and hydrogen are optional. The powder diffraction file contains deleted and doubtful entries. These are also to be dismissed. After dismissing these two entries, the database is to reduce to only 702 choices. Automatic search: an automated search procedure can be performed. The best matches will be displayed first and the database patterns can be overlaid into the experimental one. In the case of the example pattern, all peaks can be explained with substance only. If unexplained peaks remain, these residual peaks should be saved separately and the procedure repeated with the residual peaks until all are explained. Thus a qualitative analysis of the powder pattern is obtained. Quantitative powder diffraction Quantitative powder diffraction leads to determination of the lattice parameters and can also identify the fraction of each phase in a sample. Reitveld methods of analysis of powder diffraction patterns enables structure refinement. Reciprocal space methods and real space methods can be used to obtain structure solutions from powder diffraction data. Peak analysis gives us information on crystallite size distribution, microstrain analysis and extended defect concentration. In quantitative powder diffraction, analysis of the peaks in the diffractogram gives information on crystallite size distribution, microstrain analysis and extended defect concentration. Some simple steps for performing quantitative analysis of an XRD sample are as follows, but note that quantitative analysis is largely beyond the scope of this online module: Using sophisticated Rietveld software such as Fullprof or Topas, there can be further analysis of powder diffraction data. A quantitative analysis of all crystalline components can be obtained from the integrated intensities. This can also include a refinement of the crystal structure. The exact lattice parameters of each crystalline component are refined from the peak positions. The profile shape can be used to extract micro-structural information on the phases present such as crystallite size and strain for each phase. Summary of analysis cues Peak positions show: Crystal system Space group symmetry Translational symmetry Unit cell dimensions Qualitative phase information Peak intensities show: Unit cell contents Point symmetry Quantitative phase fractions Peak shapes and widths show: Crystallite size Non-uniform microstrain Extended defects (stacking faults, antiphase boundaries etc) Step-by-step procedures ▶ Barbara L Dutrow, Louisiana State University , Christine M. Clark, Eastern Michigan University What is X-ray Powder Diffraction (XRD)X-ray powder diffraction (XRD) is a rapid analytical technique primarily used for phase identification of a crystalline material and can provide information on unit cell dimensions. The analyzed material is finely ground, homogenized, and average bulk composition is determined. Fundamental Principles of X-ray Powder Diffraction (XRD)Max von Laue, in 1912, discovered that crystalline substances act as three-dimensional diffraction gratings for X-ray wavelengths similar to the spacing of planes in a crystal lattice. X-ray diffraction is now a common technique for the study of crystal structures and atomic spacing. 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 (nλ=2d sin θ). 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. Conversion of the diffraction peaks to d-spacings allows identification of the mineral because each mineral has a set of unique d-spacings. Typically, this is achieved by comparison of d-spacings with standard reference patterns. All diffraction methods are based on generation of X-rays in an X-ray tube. These X-rays are directed at the sample, and the diffracted rays are collected. A key component of all diffraction is the angle between the incident and diffracted rays. Powder and single crystal diffraction vary in instrumentation beyond this. X-ray Powder Diffraction (XRD) Instrumentation - How Does It Work?X-ray diffractometers consist of three basic elements: an X-ray tube, a sample holder, and an X-ray detector. Bruker's X-ray Diffraction D8-Discover instrument. Details 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 Kα and Kβ. Kα consists, in part, of Kα1 and Kα2. Kα1 has a slightly shorter wavelength and twice the intensity as Kα2. The specific wavelengths are characteristic of the target material (Cu, Fe, Mo, Cr). Filtering, by foils or crystal monochrometers, is required to produce monochromatic X-rays needed for diffraction. Kα1and Kα2 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 CuKα 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. HideX-ray powder diffractogram. 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 preset in the X-ray scan. Applications X-ray powder diffraction is most widely used for the identification of unknown crystalline materials (e.g. minerals, inorganic compounds). Determination of unknown solids is critical to studies in geology, environmental science, material science, engineering and biology. Other applications include: characterization of crystalline materials identification of fine-grained minerals such as clays and mixed layer clays that are difficult to determine optically determination of unit cell dimensions measurement of sample purity With specialized techniques, XRD can be used to: determine crystal structures using Rietveld refinement determine of modal amounts of minerals (quantitative analysis) characterize thin films samples by: determining lattice mismatch between film and substrate and to inferring stress and strain determining dislocation density and quality of the film by rocking curve measurements measuring superlattices in multilayered epitaxial structures determining the thickness, roughness and density of the film using glancing incidence X-ray reflectivity measurements make textural measurements, such as the orientation of grains, in a polycrystalline sample Strengths and Limitations of X-ray Powder Diffraction (XRD)? Strengths Powerful and rapid (< 20 min) technique for identification of an unknown mineral In most cases, it provides an unambiguous mineral determination Minimal sample preparation is required XRD units are widely available Data interpretation is relatively straight forward Limitations Homogeneous and single phase material is best for identification of an unknown Must have access to a standard reference file of inorganic compounds (d-spacings, hkls) Requires tenths of a gram of material which must be ground into a powder For mixed materials, detection limit is ~ 2% of sample For unit cell determinations, indexing of patterns for non-isometric crystal systems is complicated Peak overlay may occur and worsens for high angle 'reflections' User's Guide - Sample Collection and Preparation Determination of an unknown requires: the material, an instrument for grinding, and a sample holder. Obtain a few tenths of a gram (or more) of the material, as pure as possible Grind the sample to a fine powder, typically in a fluid to minimize inducing extra strain (surface energy) that can offset peak positions, and to randomize orientation. Powder less than ~10 μm(or 200-mesh) in size is preferred Place into a sample holder or onto the sample surface: Packing of fine powder into a sample holder. Details smear uniformly onto a glass slide, assuring a flat upper surface pack into a sample container sprinkle on double sticky tape Typically the substrate is amorphous to avoid interference Care must be taken to create a flat upper surface and to achieve a random distribution of lattice orientations unless creating an oriented smear. For analysis of clays which require a single orientation, specialized techniques for preparation of clay samples are given by USGS. For unit cell determinations, a small amount of a standard with known peak positions (that do not interfere with the sample) can be added and used to correct peak positions. Data Collection, Results and PresentationData Collection The intensity of diffracted X-rays is continuously recorded as the sample and detector rotate through their respective angles. A peak in intensity occurs when the mineral contains lattice planes with d-spacings appropriate to diffract X-rays at that value of θ. Although each peak consists of two separate reflections (Kα1 and Kα2), at small values of 2θ the peak locations overlap with Kα2 appearing as a hump on the side of Kα1. Greater separation occurs at higher values of θ. Typically these combined peaks are treated as one. The 2λ position of the diffraction peak is typically measured as the center of the peak at 80% peak height. Data Reduction Results are commonly presented as peak positions at 2θ and X-ray counts (intensity) in the form of a table or an x-y plot (shown above). Intensity (I) is either reported as peak height intensity, that intensity above background, or as integrated intensity, the area under the peak. The relative intensity is recorded as the ratio of the peak intensity to that of the most intense peak (relative intensity = I/I1 x 100). Determination of an Unknown The d-spacing of each peak is then obtained by solution of the Bragg equation for the appropriate value of λ. Once all d-spacings have been determined, automated search/match routines compare the ds of the unknown to those of known materials. Because each mineral has a unique set of d-spacings, matching these d-spacings provides an identification of the unknown sample. A systematic procedure is used by ordering the d-spacings in terms of their intensity beginning with the most intense peak. Files of d-spacings for hundreds of thousands of inorganic compounds are available from the International Centre for Diffraction Data as the Powder Diffraction File (PDF). Many other sites contain d-spacings of minerals such as the American Mineralogist Crystal Structure Database. Commonly this information is an integral portion of the software that comes with the instrumentation. Determination of Unit Cell Dimensions For determination of unit cell parameters, each reflection must be indexed to a specific hkl. LiteratureThe following literature can be used to further explore X-ray Powder Diffraction (XRD) Bish, DL and Post, JE, editors. 1989. Modern Powder Diffraction. Reviews in Mienralogy, v. 20. Mineralogical Society of America. Cullity, B. D. 1978. Elements of X-ray diffraction. 2nd ed. Addison-Wesley, Reading, Mass. Klug, H. P., and L. E. Alexander. 1974. X-ray diffraction procedures for polycrystalline and amorphous materials. 2nd ed. Wiley, New York. Moore, D. M. and R. C. Reynolds, Jr. 1997. X-Ray diffraction and the identification and analysis of clay minerals. 2nd Ed. Oxford University Press, New York. Related LinksFor more information about X-ray Powder Diffraction (XRD) follow the links below.Teaching Activities and ResourcesTeaching activities, labs, and resources pertaining to X-ray Powder Diffraction (XRD). X-ray techniques lab exercises from the SERC Teaching Mineralogy Collections Weathering of Igneous, Metamorphic, and Sedimentary Rocks in a Semi-Arid Climate - An Engineering Application of Petrology - This problem develops skills in X-ray diffraction analysis as applied to clay mineralogy, reinforces lecture material on the geochemistry of weathering, and demonstrates the role of petrologic characterization in site engineering. Teaching Guide to X-ray Diffraction at Cambridge A Powerpoint presentation on use of XRD in Soil Science (PowerPoint 1.6MB Sep7 07) by Melody Bergeron, Image and Chemical Analysis Laboratory at Montana State University. Brady, John B., and Boardman, Shelby J., 1995, Introducing Mineralogy Students to X-ray Diffraction Through Optical Diffraction Experiments Using Lasers. Jour. Geol. Education, v. 43 #5, 471-476. Brady, John B., Newton, Robert M., and Boardman, Shelby J., 1995, New Uses for Powder X-ray Diffraction Experiments in the Undergraduate Curriculum. Jour. Geol. Education, v. 43 #5, 466-470. Dutrow, Barb, 1997, Better Living Through Minerals X-ray Diffraction of Household Products, in: Brady, J., Mogk, D., and Perkins D. (eds.) Teaching Mineralogy, Mineralogical Society of America, p. 349-359. 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