Powder X-Ray Diffraction Unit

Introduction

Powder X-ray diffraction diagrams are routinely used, mainly for identification and structure evaluation of materials. Powdered samples of practically any material are suitable for examination, provided that the samples are air stable. The method is of key importance in materials synthesis and development.

Facilities & Infrastructure

Hardware Equipment

The powder XRD unit is located in the Physics Department, University of Ioannina and is available for use from scientists of the Departments of Physics, Chemistry and Materials Science and Technology.

The unit was purchased from BRUKER axs (D8 ADVANCE), is equipped with a Cu X-ray tube (Fe tube is also available) and works in θ-θ geometry (Figs. 1, 2). A variable divergence slit is located after the Soller slit of the divergence beam. The slit width is computer controlled, permitting the illuminated area of the sample to be from 1 to 20 mm. As illustrated in Fig. 3, the diffracted beam passes through the antiscatter and detector slits and through a Ni filter, before being monochromatized by a secondary monochromator (for Cu radiation). The system is capable of collecting data in the 1-180° 2θ range, for powder and oriented film samples.

The system is completely controlled by a PC, which is connected to the unit and serves for experimental setup control, data collection and analysis. The PDF-4 (Release 2009) database from the International Center for Diffraction Data is available on the same personal computer.

Figure 1: General view of the powder X-ray diffractometer.

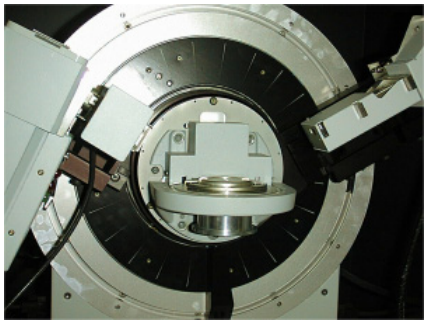

Figure 2: Close view of the powder X-ray diffractometer.

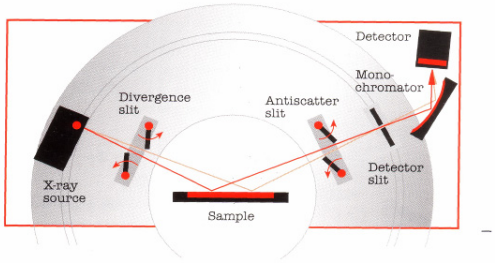

Figure 3: The typical geometry of X-rays diffraction from a flat sample.

Software available

The following software has been installed on the computer.

1. **DIFFRAC ^{plus} Basic, data acquisition**
   This is the basic software for operating the diffractometer and provides:
   - ❑ Control of the diffractometer
   - ❑ Alignment of the goniometer
   - ❑ Adjustment of the measurement electronics
   - ❑ On-line display of measured data
2. **DIFFRAC ^{plus} Basic, data evaluation software EVA**
   This is an extensive graphics program for data evaluation and presentation, with the following features:
   - ❑ Peak search and creation d/I – files
   - ❑ Background subtraction
   - ❑ Data smoothing
   - ❑ Ka_2 stripping
   - ❑ Calculation of line position, center of gravity, integrated area and half width.
   - ❑ Overlay of several diagrams
   - ❑ 3-dimensional presentation

3. **DIFFRAC ^{plus} RIETVELD**
   This software performs Rietveld analysis on powder diffraction diagrams.
4. **DIFFRAC ^{plus} SEARCH**
   This software permits full search in the PDF database.

Staff & Contact Information

A Scientific/ Administrative Committee, made up of staff personnel of the University of Ioannina is responsible for the X-ray powder Diffraction Unit. Information concerning the Unit may be obtained from Prof. T. Bakas (tbakas@cc.uoi.gr).

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Representative Publications

1. Origin of ferromagnetism in ^{57}Fe-doped NiO
   Douvalis A., Jankovic L., Bakas T.
   J. Phys. Cond. Matt., 19, 436203, (2007)
2. Structural and biological studies of organotin(IV) derivatives with 2-mercapto-benzoic acid and 2-mercapto-4-methyl-pyrimidine
   Xanthopoulou M.N., Kourkoumelis N., Hadjikakou S.K., Hadjiliadis N., Kubicki M., Karkabounas S., Bakas T.
   *Polyhedron, **27**, 3318, (2008)*
3. Novel Nanohybrids Derived from the Attachment of FePt Nanoparticles on Carbon Nanotubes
   Tsoufis T., Tomou A., Gournis D., Douvalis A.P., Panagiotopoulos I., Kooi B., Georgakilas V., Arfaoui I., Bakas T.
   *J. Nanosc- Nanotech. **8**, 5942, (2008)*