

Department of Metallurgical Engineering, NIT Raipur
X-Ray Diffraction Laboratory

Equipment Detail:

X-ray diffraction (XRD) is a rapid analytical technique primarily used for phase identification of a crystalline material and can provide information on unit cell dimensions. X-ray diffraction is most widely used for the identification of unknown crystalline materials (e.g. metals, minerals, inorganic compounds). XRD measures the intensities of a reflected X-Ray beam from a small area. Atomic-level spacing within the crystal lattice of the specimen can be obtained by the results. This helps us in understanding details of the crystal structure for the substance. XRD helps in identifying different phases with identical compositions with finer details of the crystal structure, such as the state of atomic “order”. In addition, strain analysis and determination of the degree of crystallization can also be assessed. Due to this versatility XRD finds wide range of applications in geology, material science, environmental science, chemistry, forensic science, pharmaceutical industry and others.

The HRXRD facility at Department of Metallurgical Engineering , consists of a **PANalytical 3 kW X’pert Powder – Multifunctional**. This facility have following Specification:

X’pert Powder – Multifunctional XRD from PANalytical		
Components		Applications Capabilities
Main Unit	▪ X’pert Powder – Multifunctional XRD ▪ Cu LFF High Resolution X-ray tube (designed and manufactured by PANalytical) ▪ Flat Sample Stage for mounting powder samples with 25 holders. ▪ Zero back ground holder – 2No.	➤ Powder samples: ➤ In reflection mode ➤ In transmission mode ➤ Phase identification ➤ Phase quantification ➤ Rietveld quantification ➤ Structure refinement ➤ SAXS analysis ➤ Analysis of nano materials in transmission geometry for
Optics and slits	⇒ Programmable Divergent Slits ⇒ Programmable Anti-scatter Slit ⇒ SAXS slits ⇒ Parabolic mirror ⇒ Parallel plate collimeter for thin film analysis.	

Detector	➤ PIXcel – World’s most advanced linear detector developed by Medipix Technology in collaboration with CERN.	➤ Particle size determination ➤ Particle distribution analysis ➤ Particle surface area determination ➤ <u>GIXRD</u> <u>for Polycrystalline Thin Film analysis</u> ➤ Phase identification ➤ Phase quantification
Spinning Sample Stage	➤ Reflection cum Transmission Spinning Stage which remains in horizontal position in both modes also with controlled PHI (Φ) scan capability for THIN film analysis. ➤ Sample Holders for Reflection and Transmission geometry	
Software	➤ High Score Plus software ➤ Easy SAXS software – for nano materials analysis.	
Database	➤ ICSD Database ➤ PDF 4 Database	

The equipment used for the measurement is from PANalytical. Further information can be obtained from <http://www.panalytical.com/Home.htm>.

(Powder Diffraction Services Price List)

Data acquisition by the XRD Equipment

S.No.	Service Description (Operational features)	Price (INR) For Students of other academic Institution / Funded Projects of Institute	Price (INR) For Industries / R&D Laboratories
1	Routine Sample Phase Analysis - Only Data will be provided to the user	300 @ sample	750 @ sample
2.	Thin Film Phase Analysis - Applied to thin coatings, electroplated materials, semiconductor devices etc.	800 @ sample	2000 @ sample
3.	XRD - Small angle X-ray Scattering (SAXS) Measurements - Applied to determination of the microscale or nanoscale structure of particle systems in terms of parameters such as averaged particle sizes, shapes, distribution, and surface-to-volume ratio	1000 @ sample	3500@ sample

Analysis of XRD patterns

S.No.	Service Description (Analytical features)	Price (INR) For Students of other academic Institution / Funded Projects of Institute	Price (INR) For Industries / R&D Laboratories
1.	Phase Identification-1 <i>Applies to:</i> phases with intensity of strongest peak height with intensity $[I/I_{100}] > 50\%$	500 @ sample	1000 @ sample
2.	Phase Identification-2 <i>Applies to:</i> phases with intensity of strongest peak height with intensity $50\% > [I/I_{100}] > 30\%$	500 @ sample	1500 @ sample
3.	Quantitative Phase Analysis by Rietveld Method-1 <i>Applies to:</i> quantification of phases with known crystal structures and incorporated into ICSD or CCDC – unit cell, space group and coordinates of atoms or structural data supplied by customer in electronic format (e.g. CIF)	1000 @ sample	2500 @ sample
4.	Crystallite size determination using Scherrer spherical crystal approximation	500 @ sample	1000 @ sample
5.	XRD – Small angle X-ray Scattering (SAXS) analysis	500 @ sample	1000 @ sample

XRD Standard Report

S.No.	Description	Price (INR)
1.	Consulting <i>Applies to:</i> crystallography and powder diffraction <i>Includes:</i> phone and e-mail consultation	Rs. 1000 per hour basis
2	Data conversion customer-preferred formats recording on CD	Rs. 150/CD
3	Data conversion customer-preferred formats and transmission via e-mail	No charge
4	XRD Standard Report	No charge
5	Report, Interpretation, Presentation in customer-preferred format	Quoted on a project basis
6	Sample return to the customer	As per the charges of currier company /National Post Services

Terms and conditions (for Testing/consultancy):

- 1) Results will be available in the form of graphs and excel data.
- 2) Some sample types may require lengthy preparation and/or clean-up procedures. In such case, extra sample preparation charge will be applied.

Rush orders: We offer rush order services within 2-4 days or less from the day of the receipt of samples but additional 20% extra charges will be applied.

Practical Information's

- The external user who would like to avail the facility must pay in advance by Demand draft drawn in favor of "Registrar, National Institute of Technology Raipur".
- The sample providers in any case are not allowed to use the machine at their own under normal circumstances until special exceptions.
- In case of samples, which needs special precautions (contaminations, special handling procedures etc.), information must of provided by the sample provider to make sure the XRD operator can take account the measures.
- Particularly for the Powder Diffractions of finely grinded powder samples, sufficient quantity must be provided to the XRD Lab for good measurements.
- Departments/Centers may book time in advance for conducting regular UG/PG laboratory classes in advance for conducting regular laboratory classes if the X-RAY Diffractometer forms a part of the laboratory course curriculum. No payment need be made for such purposes. Concerned faculty members should contact the faculty in-charge, XRD laboratory for these purposes.
- Departments/Centers organizing short courses may book time in advance for visits /laboratory classes on payment of charges at par with the internal users.
- Head of the Departments/Centers/Principal Investigators of the sponsored/Consultancy Projects are required to sign the form before the work can be taken up. The charges will be transferred from the operating grant of the Department/Centers or from the Sponsored / Consultancy.