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 ➢ **GIXRD for Polycrystalline Thin Film analysis** ➢ 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.

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Data acquisition by the XRD equipment

S. No.	Service Description (Operational features)	**Price (INR) For** Internal Students (UG, PG & Ph.D. students)/ Internal Faculty / Staff	**Price (INR) For** Students/staff of other academic Institution / Funded Projects of Institute	**Price (INR) For** Industries / R&D Laboratories
1	**Routine Sample Phase Analysis** Applied to all samples, which requires sample preparation from NIT Raipur for XRD analysis.	100/- per sample	500/- per sample	1500/- Per Sample
2.	**Thin Film Phase Analysis** Applied to thin coatings, electroplated materials, semiconductor devices	250/- per sample	1600/- per sample	4000/- per sample.
3.	**XRD – Small angle X-ray Scattering (SAXS) analysis** 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	400/- per sample	2000/- per sample	5000/- per sample.

Note: GST as applicable will be Extra

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Analysis of XRD patterns

S.No.	Service Description (Analytical features)	**Price (INR) For** Internal Students (UG, PG & Ph.D. students) **Internal Faculty / Staff**	**Price (INR) For** Students/staff of other academic Institution / Funded Projects of Institute	**Price (INR) For** Industries / R&D Laboratories
1.	**Phase Identification-1** *Applies to*: phases with intensity of strongest peak height with intensity [I/I_{100}] >50%	200/- per sample	1000/- per sample	2000/- per sample
2.	**Phase Identification-2** *Applies to*: phases with intensity of strongest peak height with intensity 50% > [I/I_{100}] > 30%	250/- per sample	1000/- per sample	3000/- per sample
3.	**Quantitative Phase Analysis by Rietveld Method-1** *Applies to*: 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)	300/- per sample	2000/- per sample	4000/- per sample
4.	**Crystallite size determination using Scherrer spherical crystal approximation**	200/- per sample	1000/- per sample	2000/- per sample
5	**XRD – Small angle X-ray Scattering (SAXS) analysis**	200/- per sample	1000/- per sample	2000/- per sample

Note: GST as applicable will be Extra

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Practical Information's

- The external user who would like to avail the facility must pay in advance by **online Banking /Demand draft drawn in favor of "Director, 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.
- Students from Department of Metallurgical Engineering would not be charged any testing charges.
- ***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***.