INDIAN INSTITUTE OF TECHNOLOGY BOMBAY

MATERIALS MANAGEMENT DIVISION

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Ref. No. 1000052302 **RFx No. 6100002680**

Technical Specifications for Multipurpose Automated X-Ray Diffractometer

S.N.	Specifications	Technical Compliance (Yes/No)
1.	Multipurpose Automated X-ray Diffractometer: Floor mounted X-ray diffractometer with following application capabilities- a) Powder X-ray diffraction measurements in Bragg Brentano reflectiongeometry with automatic measurement capability with minimal, to nil, user intervention. b) Polycrystalline and Epitaxial Thin film analysis in different modes - GIXRD, XRR, RSM, and Rocking curve measurements. c) Future upgradability to Low temperature sample stage for powder X-ray diffraction study at 12 K or lower	
2.	X-ray generator: a) 3 KW (or higher) capable of using silver, molybdenum, copper, cobalt X-ray targets. b) Efficiency should be $\geq$ 85 %. c) Stability: $\leq$ 0.005% for voltage/current selected in the generator. d) Safety devices: The instrument should trip upon overload, over voltage, over current, interruption of water flow, failure of warning lamps, XRD door open. Must follow all the international and Indian safety norms.	
3.	X-ray Source: a) X-ray Tube $\geq$ 1.8 kW Cu target long fine focus and Ceramic Insulated body. b) The offered X-Ray tube should have a line focus and point focus windows. Line focus must not be attenuated to achieve point focus. c) The changeover from line focus to point focus should be possible to do by the user without detachment of HV or water connections	

4.	Goniometer: a) Two-circle, vertical goniometer with θ-θ geometry. b) The minimum step size: 0.0001° 2 θ or lower. c) Angular reproducibility ≤ + 0.0005° 2 θ or better. d) 2 θ Angular range: -90°<2 θ < +165° or better e) Goniometer diameter: 460 mm or higher.	
5.	Optics: a) Suitable incidence optics consisting of I. Motorized Programmable Divergence slit and II. Motorized graded parallel beam Multi-layered Mirror Optics (for Cu) with beam divergence of 0.02 deg. or better. III. The incident optics should be able to switch between Bragg Brentano geometry and Parallel beam geometry automatically (with software). IV. The instrument should facilitate easy alignment free, software-controlled changeover of the optics from parallel beam multilayered Mirror to slits and vice versa. V. The powder and polycrystalline thin film measurement optics should be completely automated and software controlled b) Suitable High-resolution Optics: I. For High resolution RSM and XRD of epitaxial thin films, a parallel beam mirror with 2-bounce monochromator, low beam divergence (<22 arcseconds) and high intensity should be offered. II. The instrument should facilitate easy alignment free, software-controlled/ assisted changeover of the optics from slit to parabolic mirror to 2-bounce monochromator and vice versa. c) Suitable diffracted beam optical module consisting of I. motorized, programmable anti-scatter slit and suitable long Soller collimators for high intensity and high resolution. II. The instrument should facilitate easy, alignment-free changeover of the optics from Soller collimator to slits and vice versa by the user without any manual intervention. III. Diffraction optics should be completely automated, and software controlled and should work in sync with the incident optics via software, with no manual intervention from User.	

6.	Detector: You should offer two detectors as below. The first detector should be capable of working efficiently in 0D, 1D, & 2D mode which can handle all the required applications such as powder, thin film analysis, pole figures, and RSM measurements etc. 1. Latest Fast Solid-State Detector or equivalent with minimum specifications - a) Detector should be capable of working with different X ray emission lines (Cu, Cr and Co radiation) with an efficiency of 95% or more. b) Active area: ≥ 14 mm x 14 mm or larger. c) Angular coverage: ~ 3.0° or more at 450 mm dia. d) Number of strip/ pixels in any one direction: 190 or more. e) The Detector (Pixel/Strip) Spatial resolution should be ≤ 75 µm. f) Detectors should be capable of working in 0D, 1D and 2D mode. g) The detector offered should be capable of generating a global count rate of 100 million CPS or more. 2. In addition to the above, a second (0D) detector, preferably a scintillator or silicon strip detector should be offered for high resolution measurements with minimum specifications as follows a) 0D Detector should be capable of working with all high energy X-ray emission lines i.e. (Cu, Mo, Ag). b) Count Rate: 1 million cps or higher c) Should not require cooling via water or air compressor.	
7.	Ambient Sample Stage: 1. For Powder, thin films, GIXRD, XRR and RSM measurement a necessary Eulerian Cradle with motorized Chi, Phi &Z movement should be quoted with minimum below specifications or better. Phi range: 0 to 360 deg. Chi range: minus -3 to +90 deg. Z range: 0 to 2 mm. 2. For above stage Minimum 20 number of sample holders should be quoted as following: a. Minimum 8 sample holders for transmission measurement b. Minimum 1 low or zero background sample holders for low	

	sample quantity (less than 1 mg) c. Minimum 10 sample holders for powder samples in reflection geometry d. One sample holder for small thin films (5 mm or less) compatible with Eulerian cradle should be offered. The option to hold the sample via vacuum should be offered. e. A sample holder compatible with samples up to a minimum diameter of 80 mm should be offered. 3. A dedicated sample stage for powder samples should be offered with its dedicated 10 number of powder holders (metallic/PMMA type).	
8.	Display/ Computer/workstation: There should be minimum computer with > 16 GB RAM and > 1TB HDD and >= Intel i7processor to handle large volumes of data and 23 inch or larger LED screen.	
9.	Software: a) Software packages to control all instrument parameters, self-diagnosis, and provide best algorithms for controlling and collecting the data on the instrument. b) Analytical software/program suite for diffracted data processing and analysis for phase search/identification, qualitative, quantitative analysis which includes background Kα2 elimination, 2θ correction, auto/manual peak detection, auto file type detection, diffraction peak characterization including crystallite size estimate, smoothening functions, profile fitting assess to database. c)software should also be able to: i. Similarity analysis of scans (cluster analysis unlimited in no. of scans) ii. Preparing automated Rietveld analysis iii. Unit cell indexing iv. Whole powder pattern indexing. v. Unit cell refinement, Rietveld quantification vi. Space group testing and unit cell transformation vii. Structure reviewing, distances and angles calculations viii. Crystal size determination ix. Structure solution by charge-flipping (Superflip algorithm), Fourier series, flipping etc. x. Line profile analysis, microstructure analysis by profile and structure fits using Fundamental parameter method	

	xi. Mixed fits from structure-, HKL- and profile data xii. Bitmap image to data conversion facility to compare published data to observed data, xiii. Rietveld analysis based on Fundamental parameter method xiv. Preferred orientation correction. xv. Simulation of scan for other radiation. xvi. Extended scripting in standard Pascal and building custom graphical user interfaces xvii. Color coded patterns layout for comparison. xviii. Labeling peaks xix. Exportation of raw data and analyzed file in various format. xx. Analysis of various format raw datafile (other diffractometer outputs) xxi. Important to perform batch analysis for multiple samples at a time. Overnight usage of the system can be achieved with this feature. D. Software for analysis of Epitaxial thin film HR XRD, XRR and RSM data measurement must be quoted. E. Minimum 3 (three) dedicated individual licenses should be provided (server Licenses not acceptable) for all the software.	
10.	Chiller: The X-ray diffractometer system should overall be water cooled. A single chillerwith sufficient cooling capacity to support the X-ray tube is to be included in the quotation. Chiller should be Indian made for good service support	
11.	Branded UPS of 20 kVA with minimum 30 mins backup should be quoted.	
12.	Warranty: Comprehensive warranty for XRD system (including X-ray tube, detector and all the accessories), water chiller and UPS for 2 years with on-site installation.	
13.	Installation and user training: The system should be installed at IIT Bombay and necessary training to scientific staffs/faculty members on Operation, Maintenance, Calibration of the offered system and X-ray diffraction studies will have to be provided for minimum 3 working days after the installation of the system.	
14.	Minimum 30 Floor standing XRD system installations across India for the same model quoted is required.	