

Specification for X-Ray Powder Diffraction System

Description

The specifications are for an X-Ray Powder Diffraction System to be delivered by the contractor to the Naval Research Laboratory (NRL), Washington, DC.

The system must consist of the following components and shall meet or exceed the following minimum-specifications.

X-Ray Powder Diffraction System – CLIN 0001

1. Enclosure and Radiation Safety

1. Must follow “Good Diffraction Practice” for safety and ergonomics.
2. Must comply with the highest national and international safety regulations regarding radiation, mechanical, and electrical safety.

2. Goniometer

1. Guaranteed performance for peak position accuracy, NIST SRM 1976a Al₂O₃ standard to within 0.01° across the entire 2-Theta range.
2. An optical bench mounting base that allows true plug and play quickness and tool free optics exchange without re-alignment.
3. Sample stage and detector exchange must be made without a re-alignment or re-alignment check.
4. Real time, fail-safe automatic component recognition system including all source, incident and diffracted beam, sample stage and detector components. Real-time component conflict detection.
5. Maximum usable angular range must be at least $-110^\circ < 2\text{-Theta} \leq 168^\circ$.
6. Angle positioning Stepper motors with optical encoders.
7. Smallest addressable increment 0.0001°.
8. Maximum angular speed 20°/s.

3. X-ray generator and Tube

1. Must include an x-ray generator of at least 3.0 kW.
2. Must include a Cu fine focus x-ray tube.
3. Ability to change X-ray tube between line and point focus without the need to disconnect water and electrical lines, remove the x-ray tube from housing, or re-align the X-ray tube.

4. Optics

1. Optics should be a fully automated system providing motorized switching between optimized Bragg Brentano and Goebel Mirror geometries. Incident

beam switch is between variable slits and Goebel mirror beam paths and diffracted beam switching is between variable slits and soller slits. All switching must be under full computer control. Must not require any manual intervention.

2. Optics must be prealigned in a permanently aligned mounting system based on an optical bench. This means that the optics and the primary beam side are not permanently mounted to the x-ray tube housing which means that the optics may be removed and exchanged with other upgradable optics, such as a polycapillary or other primary beam monochromators, without the need to re-align or do an automatic alignment. Optics requiring manual or automated re-alignment is not acceptable.
3. Tool free and alignment free component change. True plug and play component installation functionality.
4. An air scatter screen must be included on the incident beam.

5. Sample Stages

1. High temperature, variable atmosphere heated stage capable of heating to 1200 C. Must be equipped with a spinner and motorized alignment. Temperature stage must be automatically recognized by the instrument.
2. A minimum of 9 position sample changer must be provided and it must include the capability of both reflection and transmission measurement. Stage must be automatically recognized by the instrument.
3. Bayonet stage mounting system for sample stages, no realignment required.
4. Must include low background holder, both well and flat design, along with powder holders sufficient to fill the sample changer.

6. Detector

1. Detector must be a high resolution 1D gas proportional detector, capable of measuring at least 10° 2-Theta. The detector must use a permanent gas without requiring refilling or replacing gas. Detector must be capable of operating in fixed and scanning modes and have a fluorescent resolution capability of at least 20%.
2. Detector must be radiation hardened and have no dead channels.
3. Detector must be automatically recognized by the system, by containing component recognition technology.

7. Software

1. All system operation and data evaluation software must be included.
2. System must include an on-board system diagnostics that monitors in real-time all aspects of the system. This on-board diagnostics monitoring system must be fully accessible to the users without the need to contact the vendor to de-code fault messages. System must also work remotely so that vendor technical support may access on-board diagnostics and control the system.
3. System must be able to be operated remotely by users.
4. Library Search software and database for phase identification must be included.

5. ICDD PDF2 library must be included.
6. Provide auto-indexing capability and structure determination of novel polycrystalline materials such as ceramics, alloys, intermetallic compounds, and organometallic compounds.
7. The system must include a computer for system operation. Computer must allow remote access for on-board diagnostics and system control.

8. Water Cooling

1. A water to water chiller must be provided.

Training – CLIN 0002

1. Vendor must provide system training for one (1) person within 3 days of acceptance of CLIN 0001.
2. Vendor must provide factory based operator training for at least one person at vendor's site within one year of installation.

Documentation – CLIN 0003

1. One (1) complete set of manuals for system operation/maintenance must be delivered with CLIN 0001.

Maintenance/Support – CLIN 0004

1. Vendor must provide standard Telephone Technical Support staffed by a dedicated team of technicians available during business hours.
2. Support must be available for service and applications.

Delivery – CLIN 0005

1. Delivery of CLIN 0001 and CLIN 0003 shall be no later than 120 days from date of award.

Installation – CLIN 0006

1. Contractor shall install equipment within 30 days of delivery of CLIN 0001.

Warranty – CLIN 0007

1. The system must include a 1-year warranty that covers all parts, labor, and travel expenses for on-site support of the equipment. The 1-year warranty will become effective after acceptance of CLIN 0001.