# Specification for X-Ray Powder Diffraction System

## Description

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

The requirements for this instrument are not defined solely by scientific metrics, they are based on maintainability, usability and risk management to include simplified transition from one configuration to another. The instrument is not a specialty item to be used by one highly skilled operator. Instead, this instrument will serve multiple sections and possibly other divisions. As such, in a single week, multiple operators will use this instrument for multiple purposes. These users will have a variety of experience in XRD; some will have decades of familiarity with XRD, while others will have very limited experience. These requirements, especially in regards to reconfiguring the instrument for different types of measurements, are designed to eliminate potential operator errors. Thus, whenever possible, either no-realignment or auto-realignment is preferred over other more user dependent modes of reconfiguring the instrument.

Requirements:

### 1. Safety

1. Threshold Requirement: System must comply with all national radiation safety regulations. Objective Requirement: Additional consideration will be given for any documentation or other evidence of enhanced/improved radiation safety devices or protective capabilities.

### 2. Goniometer

1. Accurate performance over the entire 2 Theta Range. Threshold Requirement is an accuracy of 0.05 degrees. Objective Requirement is 0.02 degrees of accuracy or better.
2. Collision or component conflict detection. Threshold requirement is either an alarm or computer notice when an operator attempts to perform a measurement that would either cause a collision between instrument components or when an improper measurement is attempted with a previous instrument configuration from a prior user.
3. Large angular range of motion. Preference will be given for the largest range of motion.
4. Accurate angle position detection across the entire 2-Theta Range.
5. Highly accurate 2-Theta movements. Threshold requirement is for 0.001 degrees 2-Theta. Objective Requirement is for better than (smaller than) 0.001 degrees 2-Theta.

6. High angular speed across the entire 2-Theta Range. Threshold requirement is for 5 degrees 2-Theta per second. Objective Requirement is for 10 degrees 2-Theta per second or higher.

**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. If the x-ray tube needs to be replaced preference is given for a system which either does not require realignment, or performs an auto-realignment.

**4. Optics**

1. Optics must include both Bragg Brentano and Goebel Mirror geometries. Threshold requirement is for a system to be able to switch between these configurations without realignment, or with automated realignment. Objective requirement is that alternate geometries are computer controlled without the need for realignment or with automated realignment.
2. Slit controls. The requirement is that slits be computer controlled.
3. Changes to the optics. Threshold requirement is that the optics be simple to change for alternate applications or upgrades. The objective requirement is that this change be accomplished without the need for realignment, or with automated realignment.

**5. Sample Stages**

1. A high temperature stage is required that:
   A. Can reach, at a minimum, a temperature of 1000 C.
   B. Must be a variable atmosphere system capable of working with oxygen, inert gases or reforming gas.
2. The system must include a multiple sample holder that automatically changes samples when an experiment is completed. The minimum requirement is that the sample holder holds 6 samples. The objective requirement is that the sample holder holds 8 or more samples.
3. Must include enough powder holders sufficient to fill the sample changer.
4. Changing from the multiple sample holder to a different sample holder should be as easy as possible. Threshold requirement is that this be accomplished either without the need for realignment or with automated realignment.

**6. Detector**

1. Detector must be a high resolution detector allowing for the ability to rapidly (10 minutes or less for polycrystalline samples) collect a diffraction pattern.

**7. Software**

1. All system operation and data evaluation software must be included.
2. System must be able to be operated remotely by users.
3. Library Search software and database for phase identification must be included.
4. ICDD PDF2 library must be included.
5. Provide auto-indexing capability and structure determination.
6. 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. Threshold Requirement: Vendor must provide system training for one (1) person.
2. Objective Requirement: Vendor should also provide an advanced operator training for at least one person 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.