

## Specifications of An XRD System (Revised per Amendment 0001)

The Chemistry Division at the Naval Research Laboratory (NRL) intends to purchase an X-ray diffractometer (XRD) with accessories and with potential to upgrade. The instrument is intended for analysis of a range of materials, including crystalline powders, semi-amorphous powders, irregularly shaped solids, liquid-based colloid systems, and thin films. High resolution is essential for the analysis of particles that are on the order of 2.5 nm in diameter and thin film analysis. The recovery of valuable samples after analysis is also critical, so it must be possible to mount powder samples without binders. An autosampler is also required for expedient sample analysis.

The equipment must be highly versatile, user friendly, and able to manage a large workload with low maintenance. No part of the goniometer or optics may be a prototype and all components must have proven sales, ownership, and service track records in the USA.

The component specifications for the desired XRD unit must meet or exceed the following specifications:

**Goniometer:** A vertical theta/theta goniometer is required. The goniometer must be able to function with independently controlled (decoupled) axes. The goniometer must meet the following minimum specifications: precision =  $\pm 0.0001^\circ$ ; resolution =  $\pm 0.0005^\circ$ ; setting reproducibility =  $\pm 0.0005^\circ$ ; minimum step width =  $0.001^\circ 2\theta$ ; accuracy  $\pm 0.0025$ .

**Anode and X-ray generator:** A Cu anode with a maximum output power rating of 3.0 kW with an operating current and voltage to 60 kV and 60 mA is required. A long-line focus, Cu anode must be housed in such a way as to ensure long life and low maintenance.

**Optics:** A system with parallel-beam optics and a parabolic (e.g., Göbel) mirror is required. Variable computer-controlled divergent and anti-scatter slits are also essential. The equipment should have a diffracted beam secondary monochromator for both powder diffraction and parallel beam applications, plus include other optics required to optimize the signal from the parabolic mirror.

**Detector:** A scintillation detector (or equivalent) is required with digital counting linearity to  $5 \times 10^5$  counts per second. The electronics and software for detector control must be included.

**Sample holder/stage for powder analysis:** A rotating sample stage must be included with an automatic sample changer for 5 to 15 samples. The appropriate

electronics and software for automation of the sample stage must also be included. At least 30 sample holders must be provided.

**Thin-film analysis (Optics/Sample stage/capability):** The equipment must come with a stage, optics, and software for thin-film reflectivity measurements. A thin-film attachment with soller slits is required. The common user should be able to exchange the reflectivity and powder sample stages within a short period of time (e.g., < 20 min).

**Computer and software:** The XRD must be operated with a computer having Windows-NT, -98, or -2000 software. The computer must be fully operational with all necessary components (i.e. color monitor, keyboard, mouse, color ink-jet printer) and have modern features (minimum of a Pentium III processor, 96 MB RAM, 10 GB hard disk, and CD-ROM drive). The software must be capable of fully controlling the equipment, such as the goniometer position, width of the optics slits, and automated sample analysis. The XRD software must include a license to a full reference database of materials diffraction data, complete with crystallographic system information and Miller indices, as is included in the ICDD-JCPDS PDF-2 database. This database must be integrated with the data analysis software and have capabilities for search/match, database to data comparison, and reference card display. The XRD software must also include capabilities for background correction, data file export to ASCII format, peak finding, and graphic manipulation. Other software features must include capabilities for thin film reflectivity measurements and interpretation and other features as necessary for complete operation of the XRD unit.

**Instrument console/Radiation enclosure:** The XRD unit (goniometer, sample stage and optics) must be fully housed in a locking cabinet. The cabinet must also house the X-ray generator unit, microprocessor control unit(s) and provide space for accessory control electronics. When closed, the cabinet must provide full radiation protection. The unit must include safety interlocks so that the Cu anode shutter closes automatically when the main housing is opened and the user is not exposed to direct or scattered X-rays.

**Heat exchanger/chiller:** A mechanically refrigerated heat exchanger with a cooling capacity must be included with the XRD unit. The chiller should be located inside of the XRD console to conserve space. Chiller must be capable of fully cooling XRD unit during operation.

**Installation:** The price of the system must include contractor's full on-site installation of the XRD unit. Installation will be deemed complete when the XRD unit is fully operational. The contractor shall provide the tools (e.g., allen wrenches, etc.) necessary for changing detectors and for performing routine maintenance. Installation must be performed within 30 days of receipt of the equipment at NRL.

**Warranty:** The contractor shall provide the Government with at least the same warranty terms, including offers of extended warranties, offered to the general public in customary commercial practice. Technical support must be available by telephone during working hours (e.g. Mon-Fri 10 to 5 PM EST) and by e-mail. The warranty terms must be included in the system price.

**Training:** The contractor must provide on-site training for three (3) individuals designated by the Technical Manager in the operation, alignment, maintenance, and troubleshooting of the XRD System. The duration of the training shall be for two (2) days. The contractor shall provide one copy of all written documentation customarily provided to the public for commercial items.

**System upgrade:** A separate contract may be issued for upgrade of the system at a later date. The XRD System must be upgradeable with the following attachments: a temperature stage with operating capabilities to 1200 °C; a temperature-controlled humidity chamber with operating ranges from 25 to 50 °C and 5 to 95% relative humidity; capillary analysis; and an open Eulerian cradle.