

Specification for a High Resolution X-ray Diffractometer Goniometer System

The Naval Research Laboratory (NRL) has a requirement for a high resolution x-ray diffractometer (XRD) goniometer system for materials and thin film research. Thin films consist of epitaxially grown single crystal semiconductors, metals, metal oxides, carbides and nitrides, superconductors, polymers and liquid crystals. This goniometer system will be mated to the right port of an existing Rigaku UltraX 18kW rotating anode x-ray generator currently at NRL. NRL requires a stable and horizontal high resolution goniometer equipped with an encoder. The goniometer must consist of the following components and must meet or exceed the following minimum specifications:

A. GENERAL SPECIFICATIONS:

1. Independent driving omega (ω) and 2θ axes with goniometer alignment base.
2. ω rotation range = -100° to 190° , resolution = 0.0001° /step.
3. ω encoder with 0.0001° readout, absolute precision 2 arc sec or less.
4. 2θ rotation range = -3° to 165° , resolution = 0.0002° /step.
5. 2θ encoder with 0.0001° readout, absolute precision 2 arc sec or less.
6. Goniometer base translation range = -5 to 20mm, resolution = 0.002mm/step.
7. Goniometer controller providing stepper motor control for the following 14 axes:
 - a. Channel-cut crystal rotations ω_1 , ω_2 , and second slit translation (S).
 - b. Goniometer ω , 2θ , and goniometer base translation (T).
 - c. Open Eulerian cradle sample stage X, Y, Z, phi (ϕ), and chi (χ).
 - d. Attenuator exchange (A), analyzer crystal rotation ω_A , detector translation (D).

B. INCIDENT BEAM OPTICAL SYSTEM:

The computer-controlled incident beam optical system must consist of a slit block and a 4-bounce monochromator. The first slit is located between the x-ray source and the 4-bounce monochromator. The second slit is located at the exit position of the 4-bounce monochromator. The 1st slit, 2nd slit, and monochromator must meet or exceed the following minimum specifications:

1. 1st Slit: One slit for width and one slit for height must be included:
 - Width slit: 0.05, 0.1, 0.2, 0.5, 1.0, 2.0mm; 6 kinds.
 - Height slit: 0.5, 1.0, 2.0, 5.0, 10mm; 5 kinds.
2. 2nd Slit: One slit for width and one slit for height must be included. The

second slit must be set up so that parallel movement at right angles to the x-ray beam can be moved from -2 to 15mm, and the stepper motor driven at 0.001mm/step. Specifications for the width slit and the height slip are as follows:

- Width slit: 0.05, 0.1, 0.2, 0.5, 1.0, 2.0mm; 6 kinds.
- Height slit: 0.5, 1.0, 2.0, 5.0, 10mm; 5 kinds.

3. Monochromator:

- Ge (220)/(440) channel-cut crystals.
- Crystal rotation: 2 axes: ω_1 , ω_2 , stepper motor driven.
- Rotation range: $\omega_1 = 0^\circ$ to 90° ; $\omega_2 = -90^\circ$ to 90° .
- Resolution: $\Delta\omega_1 = 0.0001^\circ/\text{step}$, $\Delta\omega_2 = 0.0001^\circ/\text{step}$.

4. Optical System Changeover:

- Computer-controlled and software selectable.
- User-selectable among slit collimation only, slits and 2-bounce channel-cut monochromator, or slits and 4-bounce monochromator.
- Changeover must be completed without any manual intervention or removing of optical components.

C. PARABOLIC MULTILAYER MIRROR

A parabolic multilayer mirror must be included. This mirror must be integrated seamlessly with NRL's existing Rigaku UltraX 18 rotating anode x-ray generator.

D. SAMPLE STAGE:

The sample stage must be an open Eulerian cradle designed to hold and map a 4" wafer, allowing area map measurement of a rocking curve by X-Y translation as well as adjustment of ϕ and χ over a wide range. All five axes of the sample stage must be stepper motor driven with the following specifications:

1. X axis: translation range = $\pm 52\text{mm}$, resolution = 0.001mm/step.
2. Y axis: translation range = $\pm 52\text{mm}$, resolution = 0.001mm/step.
3. Z axis: translation range = 1 to -10mm , resolution = 0.0005mm/step.
4. ϕ axis: rotation range = -171° to 185° , resolution = 0.001 $^\circ$ /step.
5. χ axis: rotation range = -92° to 60° , resolution = 0.001 $^\circ$ /step.

E. DIFFRACTED BEAM OPTICAL SYSTEM:

The computer-controlled diffracted beam optical system must consist of a receiving slit, Ge (220) analyzer crystal, vertical halving slit, attenuator

exchanger, Ni filter, and a detector (see "X-ray Detector" section). The diffracted beam optical components must meet the following specifications:

1. Receiving slit: One slit for width and one slit for height must be included.
 - Width slit: 0.05, 0.1, 0.2, 0.5, 1, 2mm; 6 kinds.
 - Height slit: 0.5, 1, 2, 5, 10mm; 5 kinds.
2. Analyzer crystal:
 - Ge (220) channel-cut crystal.
 - 2-bounce standard. Optional 4-bounce capability must be available.
3. Halving Slit: Slit in front of receiving slit.
 - Vertical halving slit can be ON/OFF.
4. Attenuator Exchanger:
 - 5 Positions: 1/10, 1/100, 1/500 Attenuation, Ni filter, and Empty.
 - Analyzer crystal rotation ω_A range -1° to 70° , resolution = $0.0001^\circ/\text{step}$.
5. Optical System Changeover:
 - Computer-controlled and software selectable.
 - User-selectable receiving slit with or without Ge (220) 2-bounce reflection.
 - Changeover must be completed without any manual intervention or removing of optical components.

F. X-RAY DETECTOR & DETECTOR ELECTRONICS:

The detector provided with the x-ray system must be a scintillation counter (SC). Due to the high intensities gained from the rotating anode and reflectometry measurements, a SC linear to at least 750,000cps is required. The detector electronics must consist of a high voltage supply and a pulse height analyzer. Fitting with the automation model of this XRD system, the SC must be able to be translated from 0 to 13mm, depending on whether or not the Ge (220) analyzer crystal is used.

G. SOFTWARE:

- 1) X-ray Optical System Alignment Software
- 2) Data collection software with automatic crystal orientation software and crystal library.
- 3) Reciprocal Space Simulation & Analysis with 3D Reciprocal Lattice Map Display
- 4) Rocking Curve Simulation & Analysis
- 5) Reflectometry Software

H. CONTROLLING COMPUTER & PERIPHERALS

Intel Pentium PC, 2.x GHz, on-board video and sound, integrated network connection

256 MB DRAM

40 GB Hard Drive

3.5" 1.44 MB Diskette Drive

17" Color Monitor

Internal CD-R+W Drive

Keyboard, Mouse, and Pad

Microsoft Windows 2000 Operating System

HP DJ6122 Color Printer

Microsoft Office Professional

All Cabling & Power Cords

I. TRAINING

On-site training must be provided at NRL to be provided for a minimum of 2 days for 3 people. This training will be done after installation of the diffractometer. All travel and living expenses are the responsibility of the contractor.

J. INSTALLATION

Installation of the goniometer and integration with NRL's existing Rigaku UltraX 18 rotating anode must be included.

K. WARRANTY

The contractor shall offer the Government at least the same warranty terms, including offers of extended warranties, offered to the general public in customary commercial practice. These warranty terms must be included in the system price. The period of the warranty shall begin upon acceptance.

L. DOCUMENTATION

A full set of all written documentation customarily provided to the public with a commercial item shall be provided. This shall include users manual(s) or equivalent as well as copies of any software, and any manuals for the software included with the system, if customarily provided. This documentation must be received at NRL with the system hardware, unless other arrangements are agreed to by the authorized Government representative.