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Project	NCNR Instrument Project		Revision ☐	
Originator	NCNR Project Participants	If revision, provide the following:		
Date	November 12, 2003	Previous Submittal	038-xxxx	
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Scope

Submittal of updated top level specification for MACS

Purpose

Submit updated "MACS list of requirements" Revision D under configuration management.

Description

This document is the top level specification for the MACS spectrometer. The document has the following release history:

1998 : Development of top level specification
July 27 1999 : First signed release
December 14, 2001 : Revision A
April 14, 2003 : Revision B Changes in Rev. C relative to this version are red
June 21, 2003 : Revision C Changes in Rev. D relative to this version are highlighted
Earlier releases are available at http://www.pha.jhu.edu/~broholm/MACS/archive.htm

Filing

When filed as a submittal, this form and the information attached to it transforms into a released document when it is signed by all parties named in it. The form with attachments is kept on file in the office of the NIST chief engineer. When attachments are electronic in nature (such as electronic CAD data) that information and its hierarchical position in the project design tree shall be identified in or under this submittal. Information Requests, Submittals and Releases are numbered separately, yet sequentially.

Change Process

Anyone can propose a change to documentation that is released under this form. To such end an Engineering Change Request (ECR) is filed. A priori, the change board is composed of the individuals that signed the submittal against which the ECR is drawn. Approval of the ECR turns it into an Engineering Change Notice (ECN), which gives authority to prepare a new submittal. The new submittal covers at least the fully executed ECN. Approval of the new submittal signifies close-out (full implementation) of the ECN.

Endorsements (list composition is part of release and determines Change Board for ECR/N's)

Submitted		Reviewed		S 038-0009
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List of Requirements for MACS [(1)]

This document defines the top-level specification for **M**ulti **A**xis **C**rystal **S**pectrometer, MACS, at NG0 of the NIST reactor (NBSR). The document becomes effective only if all parties whose names appear below have signed it. Changes to the signed document can be initiated by each of those parties, or their replacements, at which time a new document including the proposed revision is prepared. Changes become effective only after all parties sign the new document. Newly modified sections shall be marked as such. The old document remains part of the record.

Changes in Rev. D relative to Rev. C are highlighted.
Changes in Rev. C relative to Rev. B are marked in **red**.

1. Beam extraction system

1.1 Beam tube dimensions

The aperture at L_a=1654 mm from the source shall be left open. The beam tube opening following this aperture shall be minimized while ensuring that the $w_m \times h_m$ = 441 mm x 357 mm monochromator when in monochromatic focusing geometry is illuminated as much as possible throughout the range of incident energies considering the afore mentioned aperture. For this optimization, the active part of the source shall be taken to be the geometrical optical image on the source of a 20 mm wide by 40 mm tall sample located on the sample table.
Bore diameter @ 1654 mm = 181.8 mm, Divergence Angle 3.200 degrees

1.2 Beam line shielding and atmosphere

From source to sample beam path segments shall be evacuated or filled with helium wherever feasible when the path length, L, exceeds $840\times t$, where t is the combined beam path length through aluminum windows associated with the containment. All space which is not part of the active beam tube as specified by 1.1, shall to the extent feasible, be filled with neutron shielding material. There are two exceptions to this: Shielding around the monochromator that can be viewed from the sample position shall be recessed so that the reactor beam does not illuminate it. Furthermore, the location and characteristics of the main beam dump shall be chosen to minimize its contribution to the detector count rate.

1.3 Shutter

The main beam shutter shall be outside the biological reactor shielding and have a total active length of 700 mm. The main shutter must reduce radiation on the sample to less than 5 mR/hr when closed. It must be possible to reduce radiation incident on the monochromator sufficiently to allow extraction of it for repairs while the reactor is operating. If this cannot be accomplished with the main shutter, then a suitable secondary shutter mechanism shall be implemented. The time to open or close the main shutter shall be less than 15 sec. Beam shutter controls and beam status annunciation shall be consistent with NIST specifications.

Max. Operations req'd:	100-cycles/day ≈	20k cycles/yr ≈	400k cycles/life
Specified Operations:	25-cycles/day ≈	5k cycles/yr ≈	100k cycles/life
Nom. operations req'd:	10-cycles/day ≈	2k-cycles/yr ≈	40k cycles/life

1.4 Pre monochromator filters

There shall be a 3-position filter exchanger immediately following or part of the shutter mechanism. All filters shall be large enough in their transverse dimensions to accommodate the full beam as specified in 1.1. Shielding material shall surround each filter such that neutrons either pass through the filters or are absorbed in the surrounding shielding. All filters shall be cooled to liquid nitrogen temperatures or colder. T-type thermocouples should be mounted in a way to provide temperature readings representative of the filter material. Filter changes shall be effectuated from the instrument control computer. The filter exchange mechanism shall be built to ensure that at least one filter is in the beam at all times. Ordered along the direction of the neutron beam the filter options shall be the following filter options:

1.4.1 Fast neutron filter to enable operation with incident energies above 15 meV. The tentative choice is single crystalline sapphire grade B4 or better from Crystal Systems Inc. or equivalent, with a beam path length of **150** mm. The orientation of the single crystalline material must be uniform throughout the filter to within 10 degrees. However, the average crystal orientation with respect to the beam direction is unimportant and can be chosen to minimize cost. (Density = 3.98 gm/cm^3). The minimum diameter for this filter satisfying 1.4 is **300** mm in the current MACS layout.

1.4.2 Beryllium grade I-220-H from Brush Wellman, or equivalent, with a beam path length of 100 mm. The minimum diameter satisfying 1.4 is **307** mm in the current MACS layout. (Density = 1.85gm/cm^3)

1.4.3 Pyrolytic Graphite **with a maximum of 5^o Full Width at Half Maximum mosaic and a total beam path length of 100 mm**. The minimum diameter satisfying 1.4 is **313** mm in the current MACS layout. The c-axis shall be oriented to within 2 degrees of the local beam direction back to the center of the source. (Density = 2.2**6** gm/cm^3)

2. Monochromating system

2.1 General Principle

The monochromator design is based on a system in which the crystal slides along the white beam, while it rotates simultaneously. At the same time, a shielding drum holding a converging super-mirror guide rotates around an axis that is located on the line connecting the sample rotation axis and the current monochromator rotation axis. The sample position axis is permanently attached to this drum. The drum shall be tightly sandwiched in the beam line shielding, yet be free to rotate. We denote the location of the monochromator at $2\theta_M = 90^0$ as the reference position. The distance from the reference position to the source and to the center of the drum shall be minimized while maintaining all other specifications. The distance from the center of the drum to the sample shall be chosen to maximize the average flux on the sample.

2.2 Pre-monochromator collimators

2.2.1 Immediately following the filter exchanger shall be a variable radial collimation system. Changes in collimation shall be effectuated from the control computer. It shall take less than 30 sec. to change between any two collimation settings. The collimation system shall be embedded in neutron shielding material so that neutrons either pass through the active window of the collimation system or are absorbed. This shielding shall have high Boron content.

2.2.2 Four different collimation options shall be achieved by introducing longitudinal segments of a radial collimator in the beam. There will be two segments, which we denote by A and B. The following combinations of these segments in the beam shall be possible: none, A, B, or A+B. The focal point shall be the source. The window of the collimator shall match the size of the beam as specified in 1.1. The spacing between blades shall be given by

$$d = \alpha\ell \frac{L_{0r}}{L_{0r} - L_{cr}},$$

where L_{cr} is the distance from the center of the monochromator at its reference position to the down stream and broadest end of the collimator. L_{0r} is the distance from monochromator reference position to the source. The length, ℓ, of the collimator blades for segments A and B shall be 14 cm and 21 cm respectively. The thickness of the blades shall be 0.1 mm or less. The effective local beam divergence at the monochromator, α, shall be 40' when only the longest segment B is in the beam. The blades in segment A shall match those in segment B in location and orientation. The short segment A shall be closest to the source.
Collimation: A only: 60’ B only: 40’ A & B: 24’

2.2.3 The focal point of the collimator shall coincide with the brightest part of the source to within 100 mm in the longitudinal direction. A line parallel to the central blade of the collimator shall coincide with the centerline of the CTW beam port to within 5 mm throughout the length of the instrument. The blades in the two segments of the collimator shall be parallel to each other to within $\pm 0.05^{o}$ and they shall be aligned in the transverse direction to within $\pm$0.05 mm. The distance from the end of a blade in one segment to the beginning of the corresponding blade in the second segment shall be minimized and shall not exceed 1 cm.

2.3 Variable Reactor Beam aperture

As close as possible and no more than 1500 mm from the center of rotation of the monochromator in the reference position shall be a neutron aperture. The aperture width and height shall be independently variable under computer control from closed to a setting that accommodates the full beam specified in 1.1. The aperture shall not be within line of sight of the sample in normal operation. The aperture shall be 100 mm thick and made from materials that effectively moderate and absorb the reactor beam with minimal secondary radiation. The aperture shall be centered with respect to the line connecting the monochromator rotation axis to the center of the source to within 2 mm.

2.4 Monochromating assembly

The monochromator is based on PG and the mechanical assembly is specified separately. It shall be possible to extract the monochromating assembly from the instrument for service or exchange while the reactor is operating. A camera with appropriate lighting shall enable remote viewing of the monochromator for diagnostic purposes when it is driven to a specific position along the translation stage. The image shall be accessible from the instrument control computer.

2.5 Monochromator shield

2.5.1 Range of scattering angles shall be 35° to 130°**.** It shall take less than 1 min. to change the scattering angle from one extreme to the other. The monochromator translation stage and the drum rotation shall provide a setting accuracy of 0.03^{o} for the monochromator scattering angle.

2.5.2 The total thickness of shielding materials between the reactor beam and the MACS sample table and detection system shall not be less than 600 mm. Allowable radiation dose rate, and background, outside of monochromatic beam: ALARA.

2.6 Monochromator to sample super-mirror guide.

From monochromator to sample shall be a converging super-mirror guide with the largest practical critical angle of order $3\theta^{Ni}_{c}$. The guide shall extend from as close to the monochromator as possible until 250 mm before the sample. The inside height of the guide as a function of the distance, *x*, from the sample shall be given by

$$h(x) = h_s + \left(h_m - h_s\right)\left(1 - \frac{x}{L_{1r}}\right),$$

where h_s=40 mm is the sample height, h_m=357 mm is the monochromator height, and L_{1r} is the monochromator to sample distance at the $2\theta_M$=90^o reference position. The sample end of the guide shall have an inside width of 18 mm and be centered with respect to the reference line that connects the sample rotation axis to the monochromator rotation axis to within 0.5 mm. The angle between the guide sides and the reference line shall be independently variable under computer control from 0 to 2.5^o with an accuracy of 0.03^o. The guide shall be mounted on shielding material that functions as a beam defining apertures. The surface layer of this shielding shall have a high neutron absorption cross section. On the sample end of the guide this shielding shall extend until the end of the guide and on the monochromator side it shall be as long as possible. The incoherent scattering cross section of materials that are illuminated by the monochromator and visible from the sample shall be minimized to avoid diffuse and non-monochromatic contributions to the neutron flux on sample.

2.7 Beam optics between super mirror guide and sample

The following items shall be permanently mounted just after the super mirror guide. Their total thickness shall be less than 50 mm.

2.7.1 A neutron monitor that shall have a sensitivity of approximately 10^{-5} at 5 meV. The sensitivity shall be proportional to wavelength.

2.7.2 An attenuation exchanger with four positions shall be capable of introducing three different planar objects into the beam under computer control. Two of the positions shall provide 10 times and 100 times attenuation respectively at 3.7 meV. These attenuators shall be permanently installed in the exchanger. The third position shall be an auxiliary slot that can hold a plate with a thickness between 1 mm and 5 mm, width 30 mm and height 50 mm. When selected by the attenuation exchanger the plate shall be held in the center of the beam to within 1 mm. The attenuation exchanger shall be controlled from the main instrument control computer.

2.7.3 A computer controlled thermal neutron aperture with variable opening from closed to the full width and height of the beam. The aperture shall be centered in the beam to within 0.5 mm and its degrees of freedom shall only be the width and height of the opening. The positioning accuracy shall be better than 0.5 mm. The neutron absorbing blade material ordered in the direction of the neutron beam shall be Lithoflex followed by sintered B_4C. The thickness of each layer shall be approximately 1 mm or as determined by available materials. To avoid contamination, the Lithoflex shall be fully contained. In the direction towards the monochromator the containment material shall be a thin aluminum plate. In other directions the containment can be aluminum or B_4C as most convenient from a design standpoint.

3. Sample table

3.1 Location

The distance from the sample rotation axis to the monochromator rotation axis shall be chosen to maximize intensity on the sample position. When the spectrometer is in its $2\theta_M$=90° reference position this distance shall be 1675 mm.

3.2 Non-magnetic materials shall be employed wherever possible in and adjacent to the sample area for all positions of the instrument. Within 750 mm of the sample position there shall be no ferromagnetic materials.

3.3 Degrees of freedom provided

3.3.1 Rotation of sample 0-360° with accuracy of 0.005°. (ω)

3.3.2 Tilt of sample table +/- 12° about two mutually perpendicular horizontal axis. Accuracy better than 0.1° for loads in the range specified in 3.3. The effective rotation axes shall lie within 20 mm of beam height. (α, β)

3.3.3 Elevator +/- 20 mm about beam center. Accuracy better than 1 mm. (z)

3.3.4 Horizontal translation shall be +/- 15 mm along two mutually perpendicular horizontal directions. Accuracy better than 0.5 mm. Translation shall occur along the sample tilt axes. (x, y)

Summary:

Rotation:	(ω)	0-360° ± 0.005°
Pitch & Yaw:	(α, β)	± 12° ± 0.1°
Translation	(z)	± 20mm ± 1mm
Translation	(x, y)	± 15mm ± 0.5mm

3.4 Dimensions and load capacity.

The mounting surface shall lie at least 152 mm below the beam center. Load capacity shall be 400 kg on axis. Max horizontal torque shall be 4×10^2 Nm and shall result in less than a 0.1° tilt of the sample rotation axis from the vertical.

4. Detection system

4.1 Specification for detector bank as a whole:

The detection system **shall consist of 20** identical and equidistant detection "channels" which view the sample with a relative offset in scattering angle that shall be minimized and shall not exceed 8°.

4.1.1 The bank of detectors must be able to rotate as a whole around the sample through a range of 17° for all settings of the instrument. The setting accuracy shall be better than 0.01°.

4.1.2 The effective scattering angle detected by each channel shall be within 0.03° of the nominal value

4.1.3 It shall take less than 1 minute to rotate the detector bank between its extreme positions.

4.1.4 The direct beam will always be incident on a part of the detector bank. Therefore, there must be a primary beam stop between the sample and the detector bank. The beam stop shall be as close to the detector bank as possible so it cannot scatter neutrons into active detection channels. The illuminated beam stop shall produce as little neutron and hard gamma radiation as possible. The width of the beam stop shall be minimized.

4.1.5 A video camera with scintillating plate and image intensifier shall be available to position in front of any of the detection channels for radiography of the sample region or viewing Bragg reflected beams from the sample. The sensitivity shall allow real time imaging of 10,000-500,000 neutrons per second or integrated imaging of 1000 counts per second. The thickness of the camera at beam height shall be minimized. The images shall be available to the main computer for analysis and printing.

4.2 Specification of individual detection channel:

Each detection channel shall view a 20 mm wide by 40 mm tall sample with a horizontal divergence of at least 2 degrees and a vertical divergence of 8°. While the filters and collimator need not be independently selectable, the final energy setting of each channel must be. Each channel shall consist of the following items:

4.2.1 Computer controlled selection of one of three different filters. All filters shall be cooled to a temperature of 77 K or less. Absorbing spacers shall prevent horizontal thermal neutron propagation by more than a channel width perpendicular to the beam. Filter options shall be 150 mm Thermalox 995 BeO machining stock from Brush Wellman, or equivalent. 100 mm Be with BW specification I220H Rev A type I from Brush Wellman, or equivalent. 50 mm Pyrolytic Graphite grade ZYH from Advanced Ceramics (PG), or equivalent. When in position each filter shall completely block the beam paths for all detection channels. Positioning of the filters with respect to each of the channels shall be reproducible to within 1 mm in all directions. PG filters must be oriented so that their crystallographic c-direction is within 1 degree of the average beam direction for the corresponding channel. The orientation of the PG filters shall be reproducible to within 0.1 degrees.

4.2.2 Four different collimation options shall be available by introducing segments of parallel beam collimators into the scattered beam path. All channels of the detection system shall have common collimation settings at all times. Each channel shall have two collimator segments, A and B, with active lengths 60 mm and 90 mm respectively and ordered in that sequence away from the sample.

The open collimating channel width between blades shall be 1.32 mm. The blade thickness shall be minimized and shall not exceed 0.075 mm. It shall be possible to introduce A, B, A+B, or no collimator into the detection channels, corresponding to 75', 50', 30', and 120' FWHM beam divergence respectively. Clearance space between collimators A and B, before collimator A, and after collimator B shall be minimized with a target of less than 5 mm. When both collimators are engaged, the blades of the collimators for a single detection channel shall be parallel to within $\pm 0.05^{\circ}$ and shall be in transverse alignment to within ± 0.04 mm.

The collimator frame shall be made from non-magnetic steel or ^{10}B:Aluminum. The volume between collimators shall be filled with material with similar B/H ratio as 30% boron-loaded polyethylene. The collimator opening shall be minimized while allowing view of a 20 mm wide by 40 mm tall sample with a horizontal divergence of 1.25° and a vertical divergence of 8°. When a collimator is disengaged, the transverse dimensions of the open channel segment at beam height shall be minimized while allowing view of a 20 mm wide by 40 mm tall sample with a horizontal divergence of 2° and a vertical divergence of 8°.

4.2.3 Double crystal PG(002) analyzer system covering the range of scattering angles from 40° to 140°. The width of the blades shall be 60 mm. **The mosaic of the crystals making up the analyzer blades shall be 1.4 times greater than for the monochromator and the thickness shall be 2 mm. The analyzer crystal that is in direct view of the sample shall deflect neutrons towards the right as viewed along the direction of travel. This is the opposite sense of scattering compared to the monochromator.** Both analyzers shall have fixed vertical focusing with a radius of curvature of 500 mm and their height shall be 180 mm. The axis of rotation for each analyzer shall pass through the center of mass of the crystals to within 1 mm. The direction of translation for the first analyzer crystal shall coincide with the nominal centerline for the corresponding detection channel to within 0.03° and 0.5 mm. The detailed specification for the double crystal analyzer system shall be provided separately.

4.2.4 There shall be two cylindrical ^{3}He detectors associated with each channel. One detector shall immediately follow the first crystal and view the sample through the collimator, and one detector shall follow the second crystal. Both detectors shall have a partial ^{3}He pressure and thickness to achieve 90% detection efficiency for 15 meV neutrons over the full width of the detection channel. The height of the detectors shall be minimized under the constraint that they shall be tall enough to yield an eight-degree vertical acceptance taking into account the fixed vertical focusing of the crystals.

4.2.5 Shielding shall be sufficient to yield a fast neutron background of no more than 30 counts per hour per channel in the second detector over the full range of incident energies and configurations of the monochromating and analyzing system. The background in the first detector shall be less than 240 counts per hour under similar conditions.

4.2.6 The energy resolution, integrated intensity, and fast neutron background shall vary by less than 10% from channel to channel. Background and integrated intensity shall vary less than 5% and mean energy less than 5 % of FWHM resolution following continuous use of the instrument for one month.

5 System Wide Requirements.

5.1 Low friction motion of the MACS detection system shall be enabled by the NCNR air-pad and dance floor system. The dance floor shall extend from the MACS beam line shielding to the BT7 instrument and will be contiguous for the two instruments. The MACS sample table can either be cantilevered from the super mirror drum or supported by air-pads on the same dance floor. The distance from the dance floor surface to beam height remains to be specified.

5.2 **Hard and soft limits.** All degrees of freedom shall be equipped with soft and/or hardware limits that prevent any collisions but allow the full range of angles physically achievable. Sample rotation is a special case where hardware limits must be variable because of the different constraints associated with different sample environments.

5.3 **Automated alignment.** The need for periodic re-alignment of the MACS instrument shall be minimized and preferably eliminated. For any degrees of freedom that require alignment on a regular basis there shall be an automated computer assisted procedure.

5.4 **Permanent electrical wiring.** All wiring shall be permanently installed and comply with applicable NIST specifications and national electrical code standards

5.5 The instrument will require a dedicated and integrated **software package** to plan, execute, and analyze data to take optimal advantage of the doubly focusing monochromator and the multi-channel analyzing system. Details are to be specified separately.

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(1) Through the entire document metric units were used. Where standard stock sizes of materials differ from the metric unit system, the value to the nearest 0.001-inch will apply.