Concept Presentation

MACS
Multi-Axis Crystal Spectrometer
Scientific Program and Requirements

- What type of Spectrometer is MACS?
- Which experiments is it good for?
- Specifications to MACS-imize science output
Goals in Neutron Spectroscopy

• A central tool in condensed matter physics
  – Unique information about dynamic correlations
  – Model independent access to interaction strength
  – Access microscopic structure of dynamic systems

• Limited scope on current instruments
  – Need cm$^3$ sized crystals
  – Need weeks of beam time
  – Need to be neutron scattering expert

• Increased sensitivity will broaden impact
  – Smaller samples earlier in new materials cycle
  – Impact in a wider range of science
  – Parametric studies
  – Comprehensive surveys for tests of theory
MACS – a New High Intensity Cold Neutron Spectrometer at NIST

- $Q$ and $E$ resolved spectroscopy requires
  \[ \Delta E \approx 0.1 J \quad \Delta Q \approx 0.1 a^{-1} \]
- Energy scale $J$ varies more than length scale $a$

<table>
<thead>
<tr>
<th>Lattice</th>
<th>Compound</th>
<th>$J$ (meV)</th>
<th>$a$ (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D Cubic S=5/2</td>
<td>$\La_{0.7}\Pb_{0.3}\MnO_3$</td>
<td>8.8</td>
<td>3.9</td>
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<tr>
<td>2D Square S=1/2</td>
<td>$\La_2\CuO_4$</td>
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<tr>
<td>2D Kagomé S=3/2</td>
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</table>

- To probe solids with low energy scales
  - Reduce $\Delta E$ by cooling neutrons
  - Increase angular divergence to match $\Delta Q$
Comparing TOF to TAS

TAS like
- Can focus neutrons with Bragg optics
- Freely select range of energy transfer
- Can use reactor CW flux

TOF like
- Large detector solid angle is possible
- E-scan without moving parts
- Can use spallation source peak flux
Holes in a Quantum Spin Liquid

Y$_3^+$

Ni

Ca$_2^+$

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TOF Data from MAPS/ISIS

TAS Data from NIST

September 24, 2002
Collin L. Broholm
Timothy D. Pike
Elements of Scientific Program for MACS

- Expand the scope for Inelastic scattering from crystals:
  - 0.5 mm³ samples
  - Impurities at the 1% level
  - Complete surveys to reveal spin-wave-conduction electron interactions
  - Extreme environments: pressure and field

- Probing short range order
  - Solid ionic conductors, spin glasses, quasi-one-dimensional charge and spin polarons, quantum magnets

- Excitations in artificially structured solids
  - Spin waves in magnetic super-lattices
  - Magnetic fluctuations in nano-structured materials

- Weak broken symmetry phases
  - Incommensurate charge, lattice, and spin systems
Overall Requirements for MACS

➢ Maximize sensitivity
  – Maximize flux on sample $\delta E \approx 0.2$ meV, $\delta Q \approx 0.1$ Å$^{-1}$
  – Maximize detection solid angle at fixed $E_f$
  – Minimize background

➢ Optimize performance for users
  – Robust and reliable soft- and hard-ware
  – Standardized dynamic “finger prints” of sample
  – Versatility cannot compromise basic mode
  – Streamline experimental process

➢ Start Commissioning in 3 years from now
MACS – a New High Intensity Cold Neutron Spectrometer at NIST

Top Level Specification

Requirements for MACS

1. Room-extraction system
   a. From sample-detectors through filter exchanger

   b. From monochromator to sample shall be a converging super-mirror guide with the
   x by hm energies considering the afore mentioned aperture. For this optimization, the
   penetration of the local beam direction back to the center of the source.

2. Monochromator
   a. As close as possible and no more than 1100 mm from the center of rotation of the
   single crystal monochromator assemblies. Exchange shall take less than 1 minute.

3. Sample table
   a. 5.2 Automated alignment.
      b. 5.3 Permanent electrical wiring.
      c. 5.5 Radiation Safety Exclusion zone.

4. Detection system
   a. 4.1.4 Background and integrated flux shall vary by less than 10% from channel to channel.
   b. The average background over the full width of the detection channel shall be less than
   30 counts per hour per channel in the second detector over the full energy range.
   c. "Channels" which view the sample with a relative offset in scattering angle that
   shall be available to position in front of any of the detection channels for
   orientation of the PG filters shall be reproducible to within 0.1 degrees.

5. Sample
   a. 4.2.8 Most filters shall be alumina.
   b. 4.3 Neutron shielding material. There are two exceptions to this: Shielding around the
   monochromator for repairs while the reactor is operating. It must also reduce
   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.

6. Environment
   a. 4.4.4 The third position shall be an auxillary slot that can hold a plate with a thickness
   between 1 mm and 10 mm, width 40 mm and height 50 mm. When selected by
   2.2 Pre-monochromator collimators
   a. 2.8.2 Immediately following the filter exchanger shall be a 4-position
   b. The third position shall be an auxillary slot that can hold a plate with a thickness
   between 1 mm and 10 mm, width 40 mm and height 50 mm. When selected by
   2.1.2 General Principle (modified)
   a. 2.1.2.1 G enerally, the monochromator shall be a slit capable of closing the reactor beam from the
   center of the drum, and to the sample shall be minimized while maintaining all
   the constraints that it is not illuminated by the reactor beam. Furthermore, the location and
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Part I

Engineering Project Structure
Scientific Context Dissemination

• Input
  - Publication(s)
  - White Paper(s)
  - Colloquium(s)

• Output
  - Funding commitments
Top Level Specification/ List of Requirements

• Input
  Scientific Concept

• Output
  Functional Requirements
  Scope definition
  Release
Project execution plan

• **Input**
  
  Top Level Specification/List of Requirements

• **Output**
  
  Major Milestones
  Proposed Cost
  Management Model
  Configuration Management Plan
  Critical technology R&D projects (e.g. DFM)
Concept Review (Today)

• Input (Science)
  Present Problem (Top Level Specs)

• Output (Engineering)
  Rephrase Problem
  Propose Problem Solution Strategy
    Physical Solution
    or: Specification thereof
    or: Path thereto

• Review
  Is the Problem well stated by engineering?
  Does Solution Strategy Adequately Address Problem?
Part II

Design Philosophy
Part II
Design Philosophy

• Scientific Specification vs. Engineering Specification

• Instrument Dimensions: Units of Measure

• Prototyping vs. Single Deliverable Unit

• Shielding & Safety

• Mechanical vs. Software
**Scientific Specification vs. Engineering Specification**

- **Scientific**
  - What the Instrument Does

- **Engineering**
  - How the Instrument Does it

- **Scientific**
  - Sample & Stimuli Produces Data

- **Engineering**
  - Engineering Design Produces Instrument
Instrument Dimensions:
Units of Measure

• Metric
  MKS or CGS depending on Part size.

• Inch References
  Inch Units Referenced on Design Documentation.

• Precision Hardware
  Metric Goniometers, Stages, Bearings & etc.

• Specification
  MACS Specification Developed in Metric units.

• Scientific Standard
  Metric Units: Standard within the Scientific Community
Prototyping vs. Single Deliverable Unit

• Proof of Concept

• Production Quantities
  Common Design Elements, Multiple Usage.

• Sub element Refinement
  Critical Designs Require Iterations

• Fabricated & Purchased
  Verification of Compatibility between Systems.

• Well Integrated Assembly
  Design, Assemble, Test.
  Repeat.
Shielding & Safety

• Radiation
  World’s Most Intense Monochromatic Cold Beam.

• Shielding is Critical
  Biological & Background Shields.

• Initial Calculations
  Basis for Existing Development.

• Refined Calculations
  Refinement for Specific Machine Elements.

• Simulations
  Verification to Reduce Risk.
Mechanical vs. Software

• Optimized Blend
  Mechanical Devices, Electronic Monitoring, S/W Control

• Physical Limits
  Positive Stops for Safe Operation

• Mechanical Interlocks
  Prevent Access to Physical & Radiation Hazards

• Not Just Software
  Safe Operation Isn’t Just in the Software

• Safe Operation - Only
  Safe for Operators, Safe for Spectators, Safe for Maintenance Personnel
Part III

Incident Beam Line
Strategy and Components for Incident Beam line

- Goals for incident beam line
- Active beam line components
- Projected Performance
Goals for Incident beam line

• Maximize monochromatic ($\delta E=0.2$ meV) flux on sample
• Minimize fast neutrons leaving enclosure
• Decouple energy and wave vector resolution
• Rapid and accurate setting of $E_1$
• Robust design, no need to realign.
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Increase brightness at fixed neutron production

\[ \varphi = 4.8 \times 10^{13} \text{ n/cm}^2 / s \]

\[ T_{\text{eff}} = 45 \text{ K} \]

New cold source installed in 2002 has increased flux by 1.8
Symmetric horizontal focusing

Focal point for monochromator \( \tau \)-distribution is on its bisector (symmetric reflection geometry)
Space constraints require $L_0 \approx 3L_1$

$L_0 = 5400 \text{ mm}$

$L_1 = 1475 \text{ mm}$
Solutions to asymmetry problem

- Create virtual source point with super-mirror guide
  - Can close fast neutron aperture
  - E-dependent angular divergence limited to $m\theta_c \approx 2^0$
  - Loss of efficiency when guide cannot get close to source

- Use focusing monochromator for $L_0 \neq L_1$
  - Can use full solid angle view of source at all $E$
  - Can vary energy and angular distribution independently
  - Greater aperture for fast neutrons
Asymmetric horizontal focusing

Focal point for monochromator $\tau$-distribution is not on bisector (Miscut geometry)
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- Rotate full device to satisfy tangency condition
- Rotate individual blades to achieve focusing
- Neutrons that go through the cracks do so to satisfy Liouville

Top view
Other Venetian blind monochromator configurations

resolution function can be manipulated through choice of $\phi$

- $\phi$: tangent to Rowland circle
  - Good energy resolution
  - Coarser transverse Q-resolution

- $\phi = 2\theta \Rightarrow$
  - Coarse energy resolution
  - Good transverse Q-resolution

- other tradeoffs with values in between
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Two Radial Collimators that control energy resolution

Translating MACS Monochromator

Variable aperture that controls Q-resolution

Cooled Be, PG, and Al$_2$O$_3$

Beam Shutter

21 channel crystal analyzer

super mirror guide channel

Design by T. D. Pike and C. Brocker
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Incident beam filters

• PG filter (8 cm)
  – Order suppression at 13.7 meV and 14.7 meV
  – Fast neutron suppression E<15 meV

• Be filter (10 cm)
  – Order suppression E<5 meV
  – Fast neutron suppression E<5 meV

• Sapphire filter (8 cm)
  – Fast neutron suppression 15<E<20 meV
Collimators in series

\[ \alpha_A = \frac{d}{L_A} \]

\[ \alpha_B = \frac{d}{L_B} \]

\[ \alpha_{\text{eff}} \approx \frac{d}{L_B + L_B} = \frac{\alpha_A \alpha_B}{\alpha_A + \alpha_B} \]
MACS – a New High Intensity Cold Neutron Spectrometer at NIST

Y. Qiu (2002)
MACS – a New High Intensity Cold Neutron Spectrometer at NIST

Smee et al. (2002)

Focus Radius is 4 m
Target Diameter is 5 cm

5 cm
f=4 m

1428 cm² PG

MACS monochromator
Flux versus mosaic at fixed 0.2 meV energy resolution
Guide increases angular size of sample

![Graph showing the relationship between energy (E) and the ratio of \( \Phi_G / \Phi_{NG} \)]

- \( \Phi_G / \Phi_{NG} \) is plotted on the y-axis, ranging from 1.0 to 2.0.
- The x-axis represents energy (E) in meV, ranging from 0 to 20 meV.
- Symbols indicate different angular sizes: 20', 24', 40', and 60'.
Monte Carlo Simulation of MACS

Qiu and Broholm (2002)

Y. Qiu (2002)
Part III
Incident Beam Line

• Shielding Design of Incident Beam Portion of the Instrument: MACS General Layout, MACS Monte Carlo

• Beam Tube Design
• Shutter Design
• Cryo Filter Exchanger (CFX)

• In-Line Collimator Exchanger (ICX)
• Variable Beam Aperture (VBA)
• Super-mirror Guide (SMG)
Overall Design of Shielding for Incident Beam Portion of the Instrument

• Engineering Challenges
  Shielding, Shielding, Shielding

• Design Approach
  MCNP Values with AL₂O₃;
  Reduce Geometry to fn of Single Variable (SMG Dia.)

• Optimization
  Plan view, Kidney track, SMG
  Removable Insert segments for Large SMG openings
  25mm Clearance for Major elements at travel limits

• What’s Next?
  Additional MCNP studies, He/Vacuum Cask design
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MACS General Layout
v.1 Plan View
Drawing Courtesy of S. Smee

Fig. 3.1  Schematic of the Multi-Analyzer Crystal Spectrometer at the NIST Center for Neutron Research. The instrument views the cold source through the NG0 beam port.
MACS General Layout
v.2 Plan View
MACS General Layout

v.3 Plan View 1
MACS General Layout

v.3 Plan View 2
MACS General Layout

Optimization
MACS – a New High Intensity Cold Neutron Spectrometer at NIST

MACS Monte Carlo

Beam Optimization

2θ = 35°

2θ = 90°

2θ = 140°
MACS General Layout
C-100 Perspective 1
MACS General Layout
C-100 Perspective 2
MACS General Layout
MACS Perspective
Beam Tube Design

• Engineering Challenges
  Require Intense Illumination throughout DFM Travel
  Existing NG-0 Beam Tube Shell

• Design Approach
  Projection of Sample on source for 2θ = 35° & 105.56°

• Optimization
  L0 vs. L1 Curves (Rowland Circle & DFM ⊥ beam)
  Max angle 3.747, min angle 3.547
  Point of intersection picked @ -1146 ->
  1146 + 1654 = 2800
  Circular x-sect to Collimator & Variable Aperture

• What’s Next?
  Detail Drawings, Bidding, Vendor Selection
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Take-off Angle vs. $L_0/L_1$

- $L_0$ Ref = 5400
- $L_1$ Ref = 1475

$L_0, L_1, (\text{meters}); L_0/L_1$

Take-off Angle, Degrees
MACS Beam Tube
Top & Side Views
Shutter Design

• Engineering Challenges
  Reducing N & $\gamma$ to below 100mR/hr, Minimize Streaming, Rapid operation

• Design Approach
  Drum Design with convex & concave spherical faces
  (w/ center flats)

• Optimization
  Cross section source term from Dr. Williams MCNP
  Shielding Spreadsheet from Christoph Brocker

• What’s Next?
  Investigate efficacy of additional Shutter Openings, Drive & Registration Design, Scale Model, Vendor Search, Detail Drawings
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MACS Shutter
Plan View
MACS Shutter Calculation Results

Excel Spreadsheet Courtesy of C. Brocker

<table>
<thead>
<tr>
<th>Shutter</th>
<th>Layer</th>
<th>Neutron Dose in mR/hr</th>
<th>Gamma Dose in mR/hr</th>
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September 24, 2002

Collin L. Broholm
Timothy D. Pike
MACS Shutter
Perspective
Cryo (77K) Filter Exchanger

• Engineering Challenges
  77K, Multiple filter positions, gamma rays

• Design Approach
  Key Plate & Selector tabs, SS tube lift

• Optimization
  Minimize Dewar surface area, Integral shielding,
  Super insulation, Sliding rails; Step plates top & bottom
  for conductivity cold head

• What’s Next?
  Detail Drawings, Bidding, Dewar Vendor Selection;
  Cold head sizing
Cryo Filter Exchanger (CFX)
Plan View Reference
Filter Exchanger Selector
1st Position
Filter Exchanger Selector
9 Positions

1  A

2  A+B+C

3  B+C

4  B

5  A+C

6  A+B

7  C

8  A+B

9  A+C
Cryo Filter Exchanger (CFX)
Perspective
Cryo Filter Exchanger
Perspective 2
In-Line Collimator Exchanger

- **Engineering Challenges**
  Multiple levels of collimation, size, motion & registration

- **Design Approach**
  Inline Collimators of length 2/5 & 3/5 Produce denominators 2, 3 & 5; Side Rails with Kinematic Registration for In-Beam Position

- **Optimization**
  MCNP, Collimator lift mechanism above with Counter balances to increase motor life

- **What’s Next?**
  Prototype & testing: Lift, Registration, Counterbalance, Neutron Testing
In-Line Collimator Exchanger (ICX)
Plan View Reference
In-Line Collimator Exchanger (ICX)
Perspective 1
Variable Beam Aperture

• Engineering Challenges
  Near Aperture Face too close to Shields

• Design Approach
  Split Shutter on Analyzer Side

• Optimization
  Sliding Rail System, Counter balance linkage matches RHS /LHS, Top & Bottom

• What’s Next?
  Drive Mechanism and Position Sensor Design
Variable Beam Aperture (VBA)

Plan View Reference
Variable Beam Aperture
Perspective
Super-mirror Guide

• Engineering Challenges
  Minimize background

• Design Approach
  Multiple radial “cuts” prevent LOS radiation, Spherical Dome top & Bottom (w/ center flats)

• Optimization
  Arrangement to maximize shielding volume

• What’s Next?
  Re-optimize with new values for maximum opening (Removable Shielding to allow extra wide angles);
  Physical (scale) model
Super-mirror Guide (SMG)
Plan View Reference 1
Super-mirror Guide (SMG)
Plan View Reference 2
Super-mirror Guide (SMG)
Perspective 1
Part IV

Detector
Strategy and Components for Detection System

- Goals for Detection System
- Active Components in detector system
- Modes of Operation
Goals for Detection System

- Maximize solid angle at fixed $E_F$
- Minimize background count rate
- Variable $E$ and $Q$ resolution
- Alignment once a year at most
- Maximize rejection ratio for $E_l$ neutrons
- Energy integrating “two-axis” detectors operating simultaneously
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Twenty-one Channel Analyzer System

Design by C. Brocker
BeO filter
BeO filter
Be filter
Be filter
PG filter
PG filter
Collimator 1
Collimator 1
8° vertically focusing Analyzer crystals
Energy integrating Detector
“TAS” detector
Design by C. Brocker
Neutrons detected left and right

Length of principal axes of projection of resolution function on scattering plane

\[ E_F = 3.7 \text{ meV} \]

60'-60'-20'-20'

Left at analyzer

Right at analyzer
Elastic Scattering left and right

EF = 3.7 meV
60'-60'-20'-20'

\[ FWHM (\text{Å}^{-1}) \]

\[ Q (\text{Å}^{-1}) \]

-3 -2 -1 0 1 2 3

Left at analyzer
Right at analyzer
Fixed vertical focusing of analyzers

Double analyzer is “compound lens” efficient vertical focusing
Constant energy transfer slice \[ E_f = 3.7 \text{ meV} \quad \hbar \omega = 1 \text{ meV} \]
Assembling slices to probe Q-E volume

-2  -1  0   1   2

$Q_x$ (ÅÅ$^{-1}$)

0.0  0.5  1.0  1.5  2.0

$Q_y$ (ÅÅ$^{-1}$)

0 meV  1 meV  2 meV
• Powder sample Q-E map
  – 8 x 30 pts x 0.2 min. = 1:00

• Single crystal constant-E slice
  – 8 x 100 pts x 0.5 min. = 6:40

• Single crystal complete Q-E Volume
  – 8 x 100 x 10 pts x 0.5 min. = 3 days
Part IV
Detector

• Detection System Shielding

Detector System Motion Control

• Post Sample Filter Exchanger

• Post Sample Collimator Exchanger

• Double Crystal Analyzer Linkage
Detection System Shielding

• Engineering Challenges
  Aggressively Reduce Background Radiation

• Design Approach
  Segments Match Radial Array of Analyzers & detectors; Fabricated to Reduce Streaming, High Precision Alignment & Location; Molded Plastic/ B4C blend and Water-jet cut borated Poly

• Optimization
  Plastic selection to maximize B4C for casting process, casting design; “permanent” interlock vs. modular design; Cd Sheet design, Poly blocks, Lid

• What’s Next?
  Model (full size) 3 channels using best design features
Detector Shielding
Plan View 1
Detector Shielding
Plan View 2
Detector Shielding
Perspective
Detector Shielding Segments

Perspective
Detector Shielding Multiple Segments

Perspective 1
Detector Shielding Multiple Segments
Perspective 2
Detector Shielding Segment Construction
Perspective 1
Detector System Motion Control

• Engineering Challenges
  5 tons of Shielding. 1/2 arc second Location Accuracy

• Design Approach
  2 Bearing Arcs & Intermediate Plate

• Optimization
  Radial (vertical face reading) Encoder Tape & Sensor

• What’s Next?
  Scale model, Transmission/ Feedback Development/ Life Estimates
MACS – a New High Intensity Cold Neutron Spectrometer at NIST

Detector System Motion Control

Perspective
Detector System Motion Control

Plan View
Post Sample Filter Exchanger

• Engineering Challenges
  Kidney Shaped Dewar on an Elevator

• Design Approach
  Follow approach of phase A study by IDG

• Optimization
  Elevator, Insulation, Cryo source

• What’s Next?
  Detail drawings, bidding, vendor selection; Fabricate
Post Sample Filter Exchanger
Plan View
Post Sample Cryo Filter Exchanger
Perspective Views
Illustrations Courtesy of JHU IDG
Post Sample Collimator Exchanger

• Engineering Challenges
  Multiple levels of collimation, size, motion & registration
  Inline Collimators of length: TBD

• Design Approach
  Side Rails with Kinematic Registration for In-Beam Position

• Optimization
  Collimator lift mechanism

• What’s Next?
  Prototype & testing: Lift, Registration, Neutrons
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Double Crystal Analyzer Linkage

• Engineering Challenges
  Precision Mechanism with 2 Theta Output

• Design Approach
  Adaptation of Golovchenko Mechanism

• Optimization
  Shielding, Tolerances

• What’s Next?
  Life testing, Accuracy Testing, Neutron Beam Testing
χ-ray monochromator system for use with synchrotron radiation sources

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A double crystal x-ray monochromator system has been developed for use on synchrotron radiation sources. The system consists of two separate Bragg reflecting crystals constrained by a mechanical linkage system enabling it to tune continuously in x-ray energy, always maintaining an exit beam of constant offset and direction relative to the incident beam. Accurate parallelism between the two crystals is maintained by a piezoelectrically-controlled analog feedback circuit.

PACS numbers: 07.85. + n

Monochromator Concept Basis

Figures 1 & 2
Monochromator Concept Basis
Figures 3 & 4
Monochromator Concept Basis
Figures 1 & 2 Repeated
Double Crystal Analyzer Linkage (DXAL)
Concept Plan View 1
Double Crystal Analyzer Linkage (DXAL)
Concept Plan View 2
Double Crystal Analyzer Linkage
Concept Range of Motion

1

2

3

4
Double Crystal Analyzer Linkage
Concept Perspective 1
Double Crystal Analyzer Linkage
Prototype Perspective 1
Double Crystal Analyzer Linkage
Prototype Perspective 2
Double Crystal Analyzer Linkage
Prototype Perspective 3
Double Crystal Analyzer Linkage
Prototype Perspective 4
Part V

Mechanical Summary
MACS General Layout
C-100 Perspective 1
MACS General Layout
C-100 Perspective 2
MACS General Layout
C-100 Perspective 3
Part VI

Remaining Design Work
Other Mechanical Design Tasks

- Sample Table
- Electronics Enclosures
- Cable Routing
- Incident Beam Stop
- Post Sample Beam Detection & Attenuation Module
- Monochromated (Sample) Beam Stop
- DFM Transit System
- DFM Exchanger
- Alignment System Hardware
Other Engineering Tasks

- Motion Control Software
- Signal Conditioning & Digitizing
Next Meeting:

Design Review of Individual Sub-Systems
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