GM/CA CAT
Dual Canted Undulator Beamlines

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GM/CA-CAT
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What is GM/CA-CAT?

National Institute of General Medical Sciences
And National Cancer Institute
Collaborative Access Team
At the Advanced Photon Source
At Argonne National Laboratory

Mission: To develop and operate a sector at the APS consisting of two independent-insertion device beamlines and one bending magnet beamline for high-through-put macromolecular crystallography for targeted research projects of NIGMS and NCI and for General Users.
GM/CA CAT Staff & Advisors

Staff
- Janet L. Smith (Purdue) - CAT Director
- Robert F. Fischetti - Project Manager
- Sheila Rossi - CAT Administrator
- Ward Smith - Protein Crystallographer
- Ruslan (Nukri) Sanishvili - Protein Crystallographer
- Shenglan Xu - Beamline Engineer
- Rich Benn - Beamline Assistant Engineer
- Sergey Stepanov - Beamline Controls Scientist
- Oleg Makarov - Beamline Instrumentation Scientist
- Alex Urakhchin - Programmer

Technical Advisors
- Lonny Berman - NSLS
- Thomas Earnest - ALS
- Peter Kuhn - SSRL, Scripps
- Jim Viccaro - CARS
Why Do We Need More Beamlines?

- Human Genome Project
- Structure-Based Drug Design
- Improved High-Through-Put Cloning and Expression Techniques (Robotics)
- Recent Success with Improved Phasing Methods (Se-met)
- Over-subscription of Existing Beamlines

Number of Structures in the Protein Data Bank

Mb, J. Kendrew 1959
Why Dual Undulators?

- Limited number of sectors left
- Maximize use of floor space in a sector
- Increase capacity per sector and APS
Impact of Various Dual Undulator Designs on Scientific Capabilities

- Two fully functional beamlines vs one fully functional and a second with slightly reduced capabilities
- Impact on experimental layout
- Technical Design Issues
  - Energy range (3.5 – 35 keV)
  - Energy resolution (dE/E ~ 1 x 10^{-4})
  - Harmonic rejection
  - Intensity (>1 x 10^{13} photons/sec/0.1%BW)
  - Energy scan rate (350 –3500 eV/sec)
  - Flexibility of focal properties
  - Focal size (100 x 200 microns)
  - Beam stability (intensity and position) and feedback
  - Beam convergence/divergence angle
Other Design Issues

- Employ proven technology when ever possible
- Easy of use
- Independent operation (shuttering)
- Independent maintenance
- Adaptable to different source properties
Beamline Design Options

- First Optical Component has to handle high heat load from undulator (dual undulator) source
- Preserve vertical brilliance of source
- Cryo-Cooled Si-monochromator
- Water cooled Diamond monochromator
- Water cooled white beam mirror
Vertical Diffracting Monochromator

Energy Resolution vs Energy
Vertically Diffracting Monochromator

Emittance = 3.0 nm-rad; Coupling = 1.0%

Solid line - Resolution when Accepting Full Vertical Fan
Dashed Line - Best Achievable Resolution with a "Closed" Slit

Energy Resolution (FWHM, eV)

Energy (keV)

Si(111)
Si(220)
Si(400)

L3
K

Energy Resolution (FWHM, eV)

Energy (keV)
Horizontal Diffracting Monochromator

Energy Resolution vs Energy
Horizontally Diffracting Monochromator
Emittance = 3.0 nm-rad; Coupling = 1.0%
Solid line - Resolution when Accepting Full Horizontal Fan
Dashed Line - Best Achievable Resolution with a "Closed" Slit

File: E_Res__Hor_3nm-rad
Dual Undulator Beamlines Layout

- Option 1 – Vertical monochromator offset
- Option 2A – Outboard line deflected horizontally with monochromatic mirrors
- Option 2B – Inboard and Outboard lines each deflected horizontally with monochromatic mirrors
- Option 3 – Large horizontal offset monochromator (2 m)
- Option 4 – Horizontal deflecting white beam mirrors
Conceptual Design Issues

Conceptual Layout Summary
• Inboard ID-line – best possible ID-beamline, vertical offset monochromator, K-B mirrors, performance specifications
• Outboard ID-line – vertical offset monochromator, horizontal deflecting mirrors, K-B mirrors, performance specifications
• Bending magnet line – collimating mirror, monochromator, focusing mirror, performance specifications

Design Issues
• Sufficient vertical separation to introduce horizontal mirrors
• Monochromator, precision, reproducibility, stability (tune and position)
• Monochromator Cryo-crystals, first and ideally second
• Compton scatter shield
• Focusing mirrors – highly demagnifying, mirror length
• Beam transport – joint or separate
• Independent operation/shuttering of ID-lines
Schematic View of the Canted ID-Beamlines

Sector-23 Canted Insertion Device Beamlines
GM/CA CAT Sector Layout
GM/CA ID_out Experimental Station
# Beam Separation vs High Energy Cut Off

Based on Option 2A

<table>
<thead>
<tr>
<th>Mirror Surface</th>
<th>Si</th>
<th>Cr</th>
<th>Ni</th>
<th>Rh</th>
<th>Pd</th>
<th>Pt</th>
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<tr>
<td>E*Theta at 8 keV</td>
<td>keV*mrad</td>
<td>3.276E-02</td>
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<table>
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<th>Mirror Angle (mrad)</th>
<th>Hor (mm)</th>
<th>Ver (mm)</th>
<th>Diag (mm)</th>
<th>E_critical (keV)</th>
<th>E_max (keV)</th>
<th>E_critical (keV)</th>
<th>E_max (keV)</th>
<th>E_critical (keV)</th>
<th>E_max (keV)</th>
<th>E_critical (keV)</th>
<th>E_max (keV)</th>
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<td>3.50</td>
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<td>16.0</td>
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<tr>
<th>Edges</th>
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<th>E(keV)</th>
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<td>M(II)</td>
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<td>M(I)</td>
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<td>L(III)</td>
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<td>K</td>
<td>23.220</td>
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<td>78.395</td>
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Reflectivity of Multiple Mirror Surfaces

Reflection from 1 and 4 Rh surfaces each at 4.0 mrad
Reflectivity of Multiple Mirror Surfaces

Reflection form 2-Pt at 4.0 mrad and 2-Rh at 3.0 mrad
vs
2-Rh at 4.0 mrad and 2-Rh at 3.0 mrad
Reflectivity of Multiple Mirror Surfaces

Reflection form 1 and 4 Pt surfaces each at 4.0 mrad
## Beamline Characteristics

<table>
<thead>
<tr>
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<th>ID</th>
<th>BM</th>
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<tr>
<td>Energy Range (keV)</td>
<td>3.5 - 16, 3.5 - 35</td>
<td>3.5 - 35</td>
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<td>Energy Resolution (%)</td>
<td>&lt;0.02</td>
<td>&lt;0.02</td>
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<tr>
<td>Flux @12 keV (photons/s/100 mA/0.02% BW)</td>
<td>&gt; 1.0 x 10^{13}</td>
<td>&gt; 1.0 x 10^{11}</td>
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<td>Harmonic contamination (%)</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
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<td>Rate of energy change (eV/sec)** at 6.5 keV</td>
<td>350</td>
<td>350</td>
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<tr>
<td></td>
<td>at 20 keV</td>
<td>3500</td>
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<tr>
<td></td>
<td>3500</td>
<td>3500</td>
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<td>Beam positional stability for 100 eV change (% of beam size)</td>
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<td>&lt;5</td>
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<td>Beam positional stability for 1000 eV change (% of beam size)</td>
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<th>Vert</th>
<th>Hor</th>
<th>Vert</th>
<th>Hor</th>
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<td>Beam size at crystal (microns) *</td>
<td>50</td>
<td>200</td>
<td>100</td>
<td>200</td>
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<td>Beam divergence at crystal (mrad) *</td>
<td>0.05</td>
<td>0.25</td>
<td>0.25</td>
<td>2.0</td>
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</table>
Hockey Puck Cryo-Crystal
Thermal Effect on 2nd Crystal

Detune due to Heating of the 2nd Crystal

Change in 2nd Crystal Angle (microradians) vs. T(k)
Closed Loop Positional Feedback

BPM at 59350 mm drives angle of second crystal
BPM at 60450 mm records position further downstream
Comparison of Undulator A and Short-Undulator A

Low Emittance Mode (3.0 nm-rad, 1% coupling, 7 GeV, 100 mA)
Comparison of Undulator A and Short-Undulator A Low Emittance Mode (3.0 nm-rad, 1% coupling, 7 GeV, 100 mA)
Comparison of 3.0-cm and 3.3-cm Short Undulators
Low Emittance Mode (3.0 nm-rad, 1% coupling, 7 GeV, 100 mA)
Comparison of 3.0-cm and 3.3-cm Short Undulators
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Comparison of 3.0-cm and 3.3-cm Short Undulators
Low Emittance Mode (3.0 nm-rad, 1% coupling, 7 GeV, 100 mA)

Energy (keV)

Brilliance/Total Power

Comparison of 3.0-cm and 3.3-cm Shortened Undulators
Low Emittance Mode (3.0 nm-rad, 1% coupling, 7 GeV, 100 mA)
# Properties of Synchrotron Sources

<table>
<thead>
<tr>
<th>Particle Beam Properties</th>
<th>APS ID, July 1999</th>
<th>APS ID, Low Emittance</th>
<th>APS BM, July 1999</th>
<th>ESRF High Beta</th>
<th>ESRF Low Beta</th>
<th>ESRF Bending Magnet</th>
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</thead>
<tbody>
<tr>
<td>Natural Beam Emittance, $\varepsilon$</td>
<td>8.18E-09</td>
<td>3.00E-09</td>
<td>8.18E-09</td>
<td>4.00E-09</td>
<td>4.00E-09</td>
<td>4.00E-09 m-rad</td>
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<tr>
<td>Coupling Constant, $k_{xy}$</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
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<tr>
<td>Horizontal Beam Emittance, $\varepsilon_x$</td>
<td>8.10E-09</td>
<td>2.97E-09</td>
<td>8.10E-09</td>
<td>3.96E-09</td>
<td>3.96E-09</td>
<td>3.96E-09 m-rad</td>
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<tr>
<td>Vertical Beam Emittance, $\varepsilon_y$</td>
<td>8.10E-11</td>
<td>2.97E-11</td>
<td>8.10E-11</td>
<td>3.96E-11</td>
<td>3.96E-11</td>
<td>3.96E-11 m-rad</td>
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<td>Horizontal Beta function, $\beta_x$</td>
<td>15.90</td>
<td>15.90</td>
<td>1.64</td>
<td>35.60</td>
<td>0.50</td>
<td>2.20 m</td>
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<td>Vertical Beta function, $\beta_y$</td>
<td>5.30</td>
<td>5.30</td>
<td>15.90</td>
<td>2.50</td>
<td>2.73</td>
<td>34.90 m</td>
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<td>Horizontal Beam Size, $\sigma_x$</td>
<td>358.85</td>
<td>217.32</td>
<td>115.25</td>
<td>375.49</td>
<td>44.50</td>
<td>93.34 microns</td>
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<td>Vertical Beam Size, $\sigma_y$</td>
<td>20.72</td>
<td>12.55</td>
<td>35.89</td>
<td>9.95</td>
<td>10.40</td>
<td>37.18 microns</td>
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<td>Horizontal Beam Divergence, $\sigma_{x'}$</td>
<td>22.57</td>
<td>13.67</td>
<td>6000.00</td>
<td>10.55</td>
<td>89.00</td>
<td>m</td>
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<td>Vertical Beam Divergence, $\sigma_{y'}$</td>
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<td>2.37</td>
<td>47.00</td>
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<td>3.81</td>
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<td>the Straight Section</td>
<td>-1.25</td>
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<td>0</td>
<td></td>
<td>m</td>
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<table>
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<tr>
<th>ID X-ray Source Properties from WEB Document</th>
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<tr>
<td>Horizontal Beam Size, $\Sigma_x$</td>
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<td>Vertical Beam Size, $\Sigma_y$</td>
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<td>Horizontal Beam Divergence, $\Sigma_{x'}$</td>
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<tr>
<td>Vertical Beam Divergence, $\Sigma_{y'}$</td>
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