10th Annual
CLS MX Data Collection School
VIRTUAL EDITION

CMCF Upgrades

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- *ActaCryst.(2020). D76, 630–635*
- *Also check CMCF website*

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Timeline…

Two beamlines: CMCF-ID and CMCF-BM

1999 — CLS construction started

CMCF-BM:
- Minor upgrade completed
- Open to users

2001 — CMCF-ID construction started

2004 — Grand opening of the CLS

CMCF-ID:
- Major upgrade in progress since March 2020
- Currently not available to users

2005 — 1st CLS users; CMCF-ID construction completed

~ 14 yrs — 2006 — CMCF-ID 1st users; CMCF-BM construction started

2009 — CMCF-BM construction completed

Upgrade goals:
- Boost beamline performance
- Improve data quality while reduce collection time
  - More intense and smaller x-ray beams, faster detectors etc.

~ 10 yrs — 2010 — CMCF-BM 1st users

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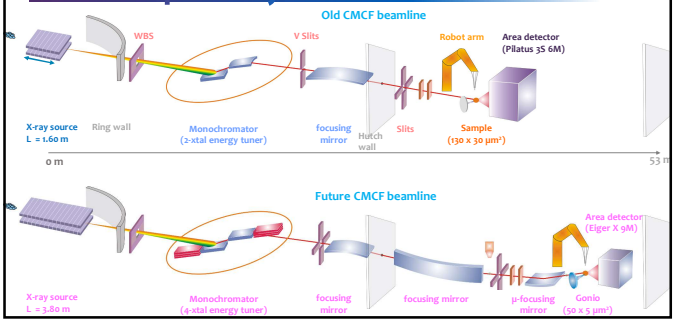
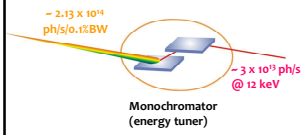
2

CMCF-ID optical layout

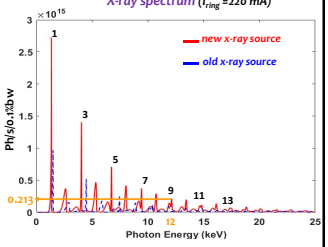


X-ray source characteristics

- Energy range: 5 – 20 keV (usable)
- More intense beam due to longer source (~ 2x)
- Beam intensity at 12 keV



X-ray spectrum (I_{ring} =220 mA)



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X-ray source – in-vacuum undulator

Vacuum chamber + Frame

- Chamber contains the magnet lattice
- Pressure < 1 x 10^{-10} mbar (10 trillion times smaller than 1 atm)

Complete assembly

- Weight ~ 11 Tons
- Length > 4.5 m

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X-ray source – in-vacuum undulator

Delivered September 2019

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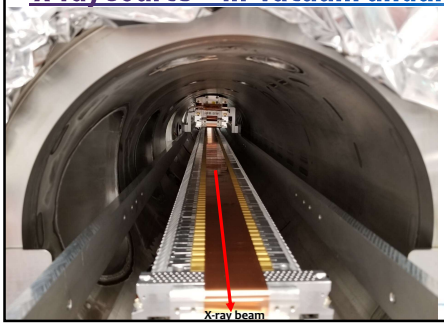
X-ray source – in-vacuum undulator

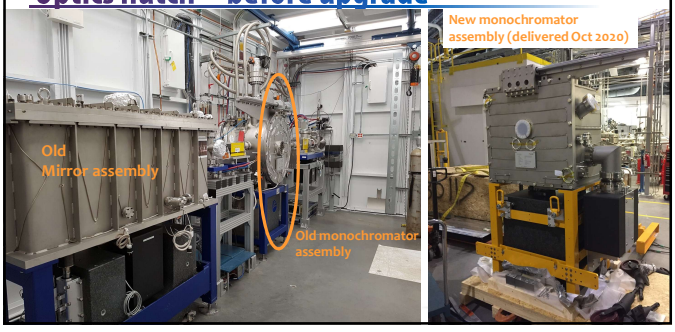
Installed in the synchrotron tunnel May 2020

X-ray source – in-vacuum undulator



- Array of magnets
- Number of periods = 191
- Periodic length = 20mm
- Peak magnetic field ~ 1T

Optics hutch – before upgrade

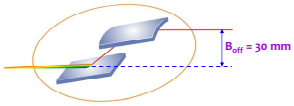


Optics hutch – now

- Monochromator ready to be installed

Optics – monochromator

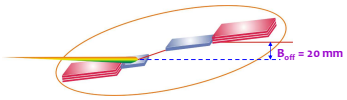
Old (2 crystals)



- Double crystal monochromator
- Old design with:
- 'Problematic' sagittal bending on 2nd crystals (horizontal focusing)

Mechanical stability issues
Beam not stable enough for sample < 5 µm
Horizontal focusing is limited at sample

New (2 crystals + 2 multilayers)

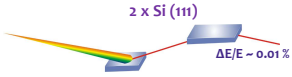


- Double crystal multilayer monochromator
- New more compact design with:
- 2nd flat crystal (no bending, another mirror does horizontal focusing)

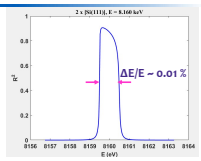
In-line multilayer and smaller beam-offset for more compactness & mechanical stability
Easy switch from Si to multilayer mode

Optics – multilayer crystals

2 x Si (111)

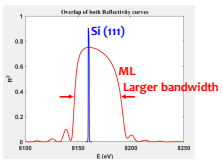


+ High (energy) resolution
+ Energy range: 5 – 20 keV

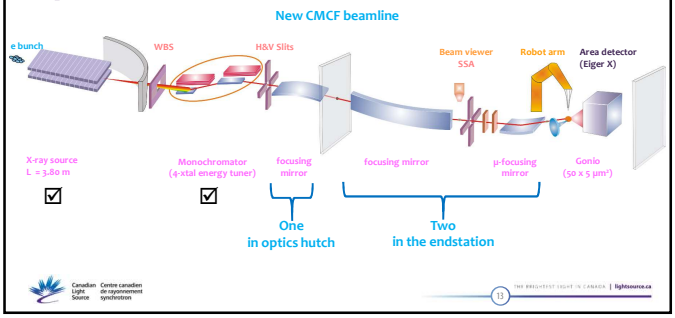


2 x Multilayers

+ High beam intensity ~ 100x stronger 50x (ML) and 2x (new undulator)
– Lower (energy) resolution
– Energy range: 7.2 – 10.4 keV



Optics – mirrors



Endstation – before upgrade (April 2020)

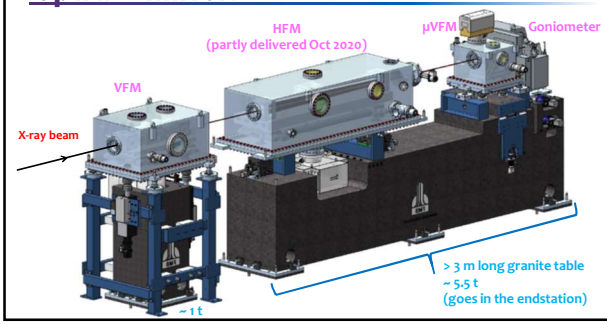
All components still in

- Robot arm
- Detector
- Goniometer
- Beam conditioners
- Controls system

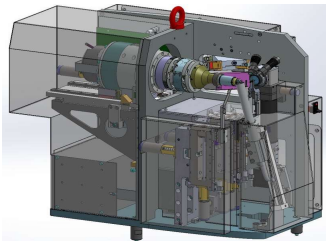
Endstation – before upgrade (now)

All components removed

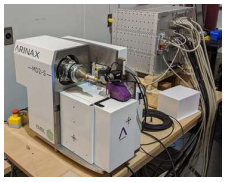
Optics – mirrors



Goniometer – MD2S



- Delivered November 2019
- Compact system
- On-axis sample visualization
- Multiple apertures and capillary included
- Movable beamstop and beamviewer
- Controls system included



CMCF storage area

- Sphere of confusion < 2 µm at 100 deg/s
- Rotation speed (500 deg/s) with air-bearing gonio
- Minimum oscillation angle 0.1 mdeg (typically 0.1 deg is 'enough')

Sample changer

Former ID sample changer (SAM)

New sample changer (ISARA – operational since Nov 2017)

Single gripper
Full cycle time ~ 120 s
Dewar capacity:
12 pucks x 16 pins
= 192 crystals

Single gripper
Full cycle time ~ 25 s
Dewar capacity:
29 pucks x 16 pins
= 464 crystals

Detectors

Pilatus 3S 6M
(currently operational on CMCF-BM)

Number of pixels	2463 x 2527 (> 6M)
Pixel size	172 x 172 µm²
Max frame rate	25 Hz (40 ms)
Readout time	2000 µs
Max count rate	3.3 x 10⁸ ph/s/mm²
Readout noise	None

Eiger X 9M
(delivered Dec 2019)

Number of pixels	3110 x 3269 (> 10M)
Pixel size	75 x 75 µm²
Max frame rate	238 Hz (4 ms)
Readout time	3 µs
Max count rate	5 x 10⁸ ph/s/mm²
Readout noise	None

Upgrade milestones and costs…

	Cost	Estimated installation date
☑ X-ray source (undulator)	2,600,000	May 2020
☑ Front-end modification	350,000	Mar – Oct 2020
☑ Monochromator	560,000	Nov – Dec 2020
Mirrors	1,200,000	Jan - Mar 2021
☑ Endstation (Gonio)	600,000	
☑ Detector Eiger X 9M	1,700,000	
Other components + labor	840,000	
Beamline integration	250,000	
Commissioning		April 2021
☑ Sample changer (Robot)	400,000	Nov 2017
☑ Detector Pilatus 3S 6M	1,500,000	May 2017
Total (CAD)	10,000,000	

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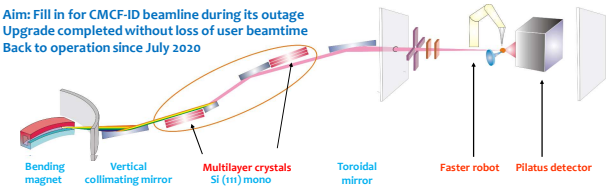
CMCF-BM Upgrade

Aim: Fill in for CMCF-ID beamline during its outage
Upgrade completed without loss of user beamtime
Back to operation since July 2020



- Added multilayer crystals
- Reduce sample exchange cycle time (25 sec)
- Transfer Pilatus 3S 6M from ID to BM

→ More intense x-ray beam (36x)
→ Faster data collection

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CMCF-BM Upgrade

Dataset collected at upgraded CMCF-BM beamline

Angle/frame = 0.2 deg
Exposure/frame = 0.2 s
Attenuation = 0 %
Aperture = 200 µm

Typical values used at old CMCF-ID beamline

1800 Frames (1-1800) | Meta-Data

Delta_Angle:	0.2
Start_Angle:	0.0
Resolution:	2.2999999999999994
Detector_Type:	PILATUS 6M
Detector_Size:	2463
Pixel_Size:	0.172
Beam_X:	1231
Beam_Y:	1263

Res: 1.51 Å

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Beamlines deliverables

Ring current (220 mA)	Former beamline	Upgraded beamline
Spectral range (keV)	6.5 – 18.0	5.0 – 20.0
Flux on the sample (ph/s)	BM: ~ 0.1 x 10^{12} (Si @ 8 keV)	~ 36x better with ML crystals (8 keV) ☑ ~ 2x better with Si crystals (8 keV) ☑
	ID: 1.0 x 10^{12} with Si (12 keV, 50 µm aperture)	~ 10x better with Si (12 keV, 50 µm aperture) ~ 500x better with ML (12 keV, 50 µm aperture)
Focal Size @ 12 keV	(H) 130 µm (V) 30 µm	(H) 50 µm (V) 5 – 50 µm variable
Sample exchange time	120 s (old SAM robot)	25 s (on both beamlines) ☑
Sphere of confusion	10 µm (sample)	< 2 µm with MD2S µ-diffractometer ☑
Detector (frame rate)	ID: 172 um x 172 um (25 Hz) BM: 73 um x 73 um (1 Hz)	75 um x 75 um (238 Hz) ☑ 172 um x 172 um (25 Hz) ☑