The Diamond Upgrade: Diamond-II

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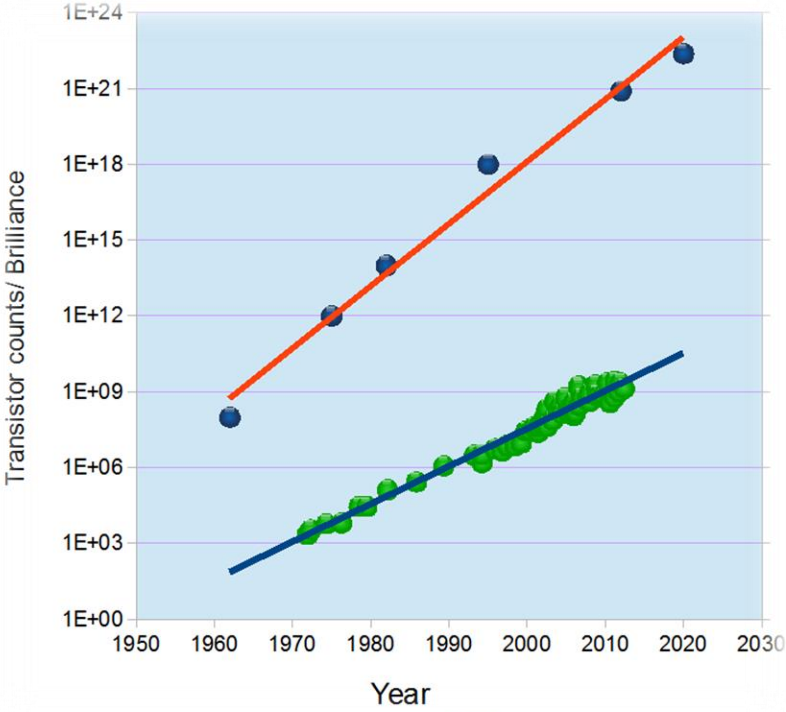
Scope

- Diamond Baseline Design
- Mini-Beta upgrade for I13 and I09
- DDBA upgrade with mid-section straights
- Proposed Diamond-II Upgrade
- Energy Factors
- Beamlines: critical, new
- Timescales

Diamond



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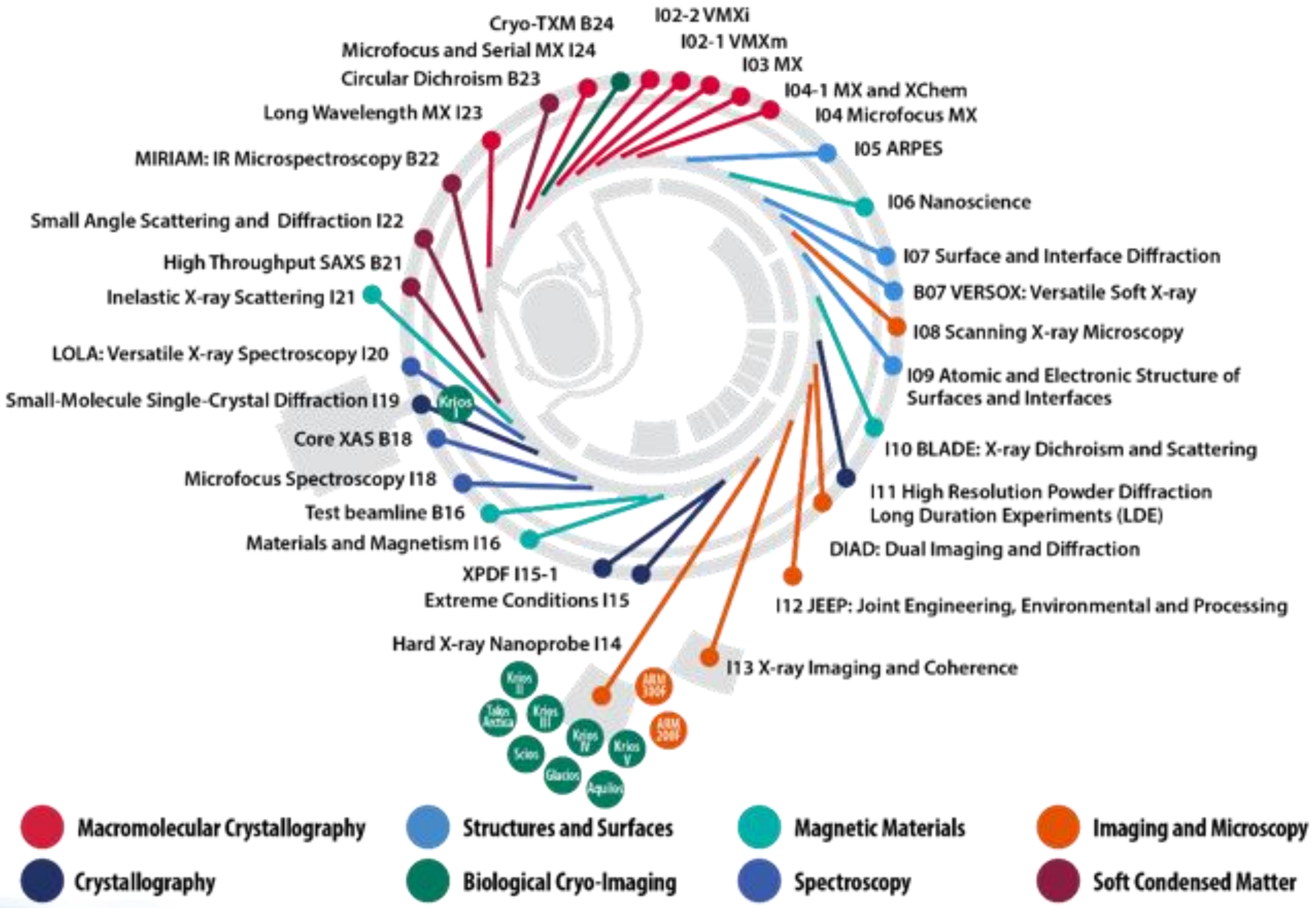
Beamlines by Science groups at Diamond



Complementary EM

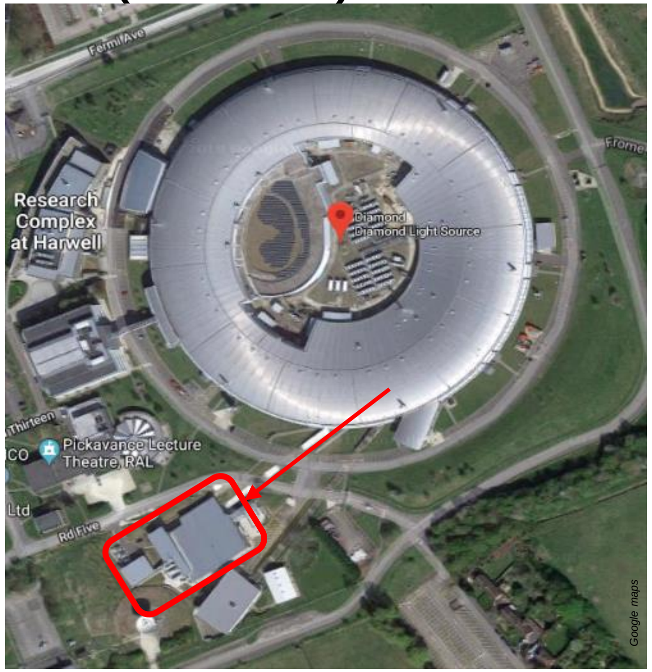
- National centres for Cryo-EM (eBIC) with 5 Titan Kryos and ultra-high resolution materials TEM (ePSIC)

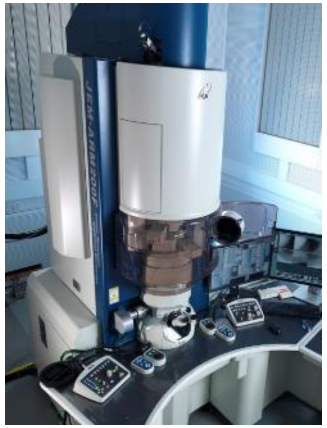
UKRI Biotechnology and Biological Sciences Research Council

UKRI Medical Research Council

wellcome

ThermoFisher SCIENTIFIC





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JM Johnson Matthey Inspiring science, enhancing life

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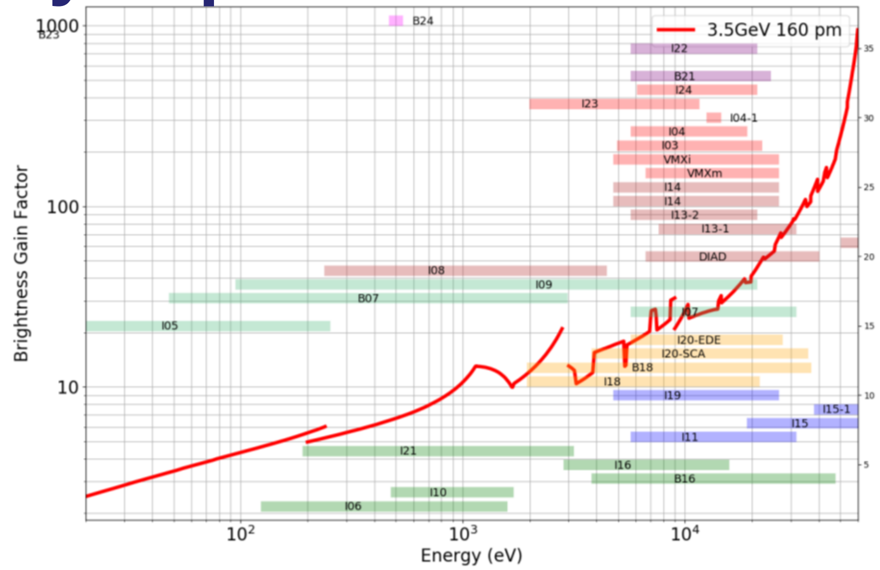
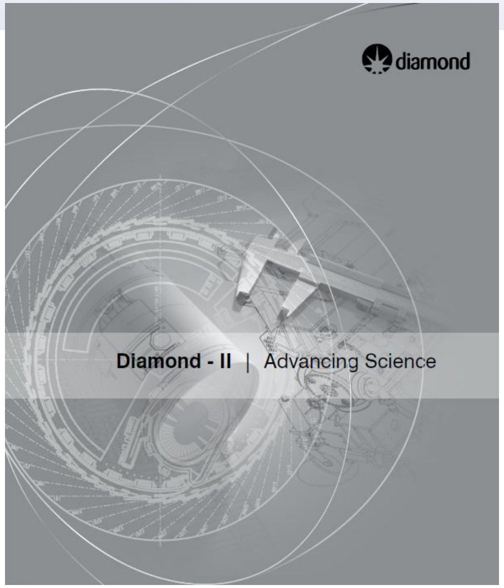
Diamond-II Multidisciplinary impact

1. Brightness
2. Increased capacity
3. Higher energy





Quantum materials

Energy materials

Chemistry & Catalysis

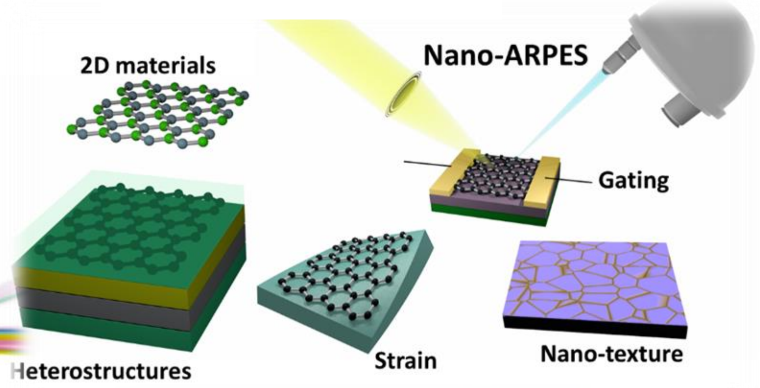
Environment

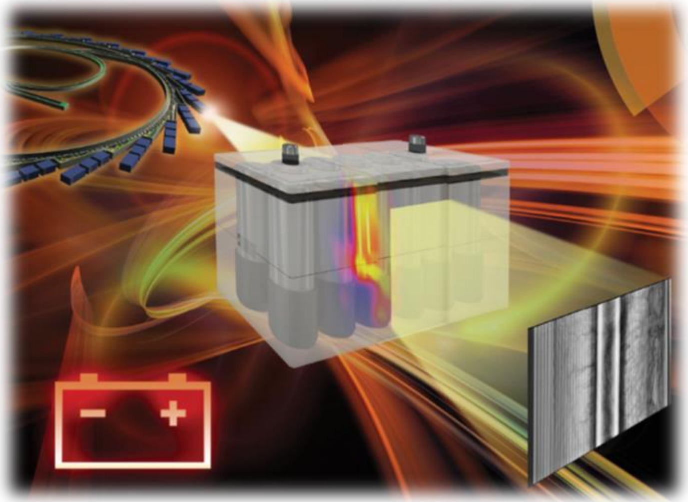
Materials Engineering & Processes

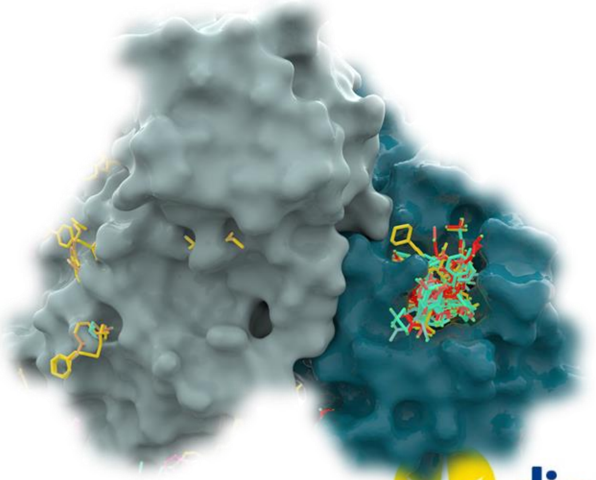
Integrated structural biology

Biotech & biological systems

Health & well-being







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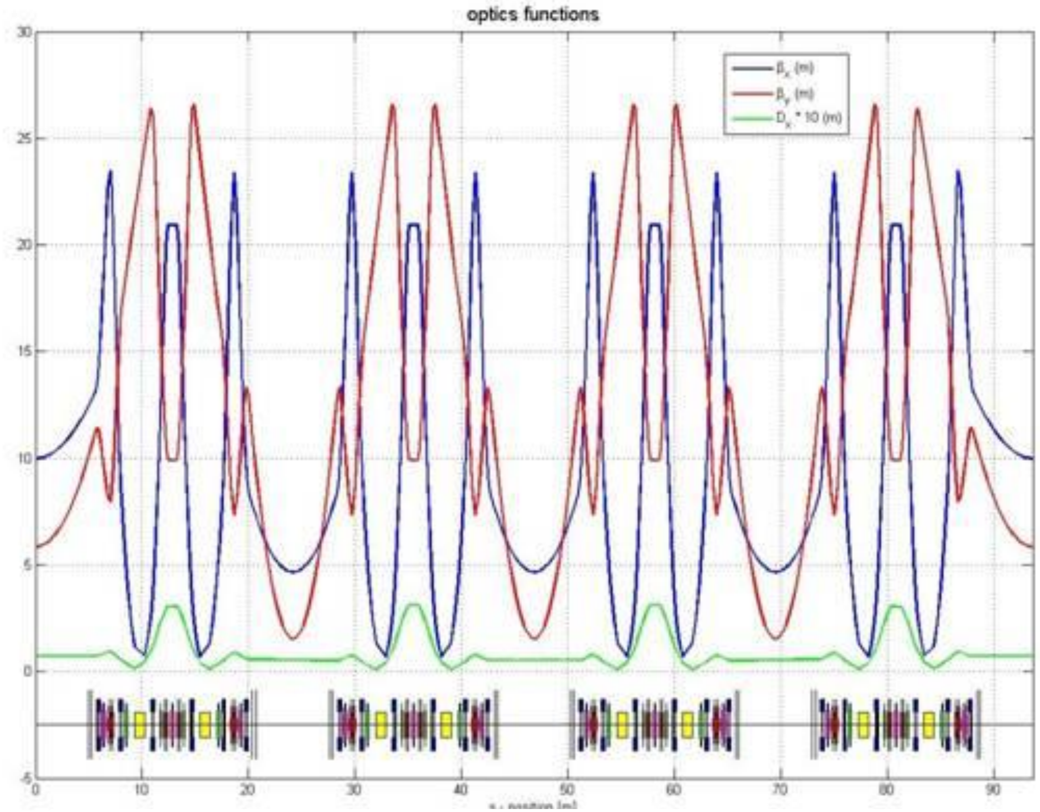
Diamond storage ring

Diamond was designed (2003) and commissioned (2006) as a

24 cells DBA lattice with 6 super-periods



Energy	**3 GeV**
Circumference	**561.6 m**
No. cells	**24**
Symmetry	**6**
Straight sections	**6 x 8m, 18 x 5m**
Insertion devices	**4 x 8m, 18 x 5m**
Beam current	**300 mA (500 mA)**
Emittance (h, v)	**2.7, 0.03 nm rad**
Lifetime	**> 10 h**
Min. ID gap	**7 mm (5 mm)**

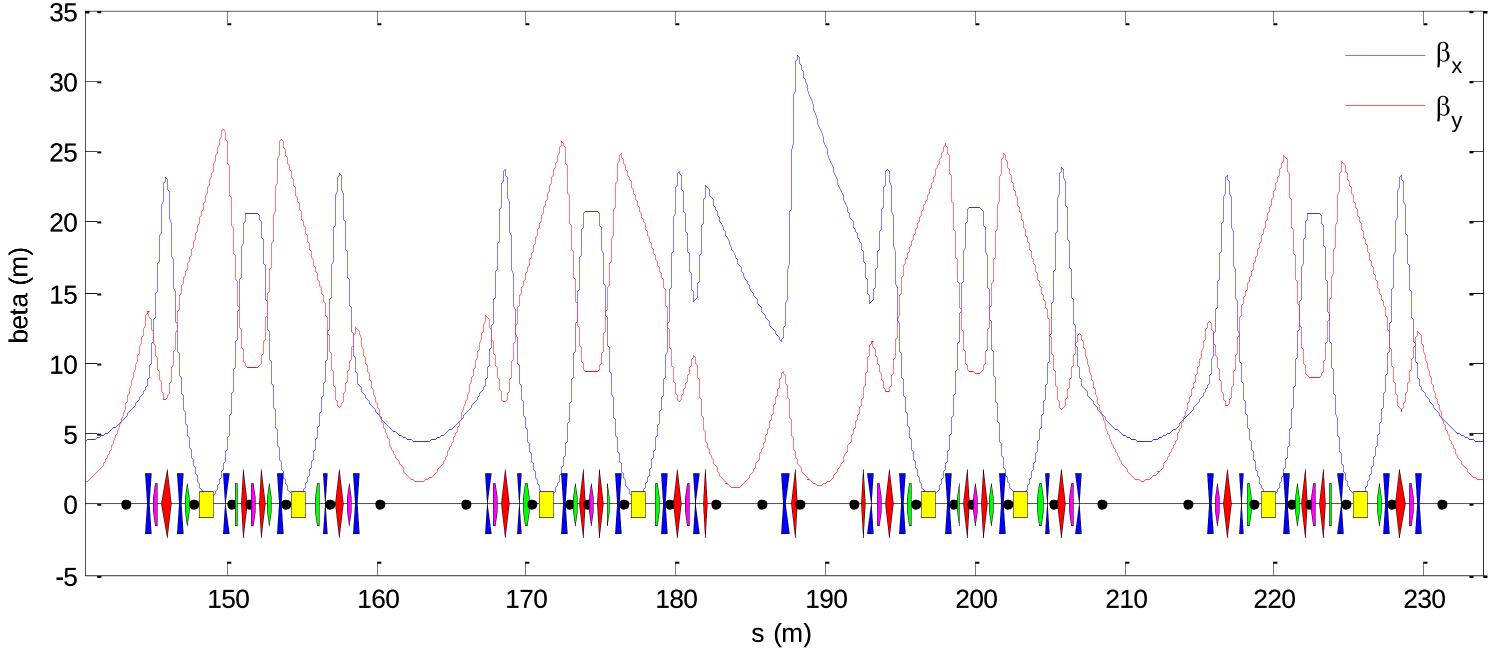
48 Dipoles; 240 Quadrupoles; 168 Sextupoles; 3 SC RF cavities; 168 BPMs

Sextupoles have H and V orbit correctors and skew quadrupoles (96)

Quads + Sexts have independent power supplies

I09 and I13 straight sections

In 2009 and 2010 two straight sections were modified to accommodate customised optics in straight 9 and straight 3



- In straight I09 and I13 we introduced two quadrupoles doublets to reduce the V beta functions and allow two independent beamlines with in-vacuum undulators.

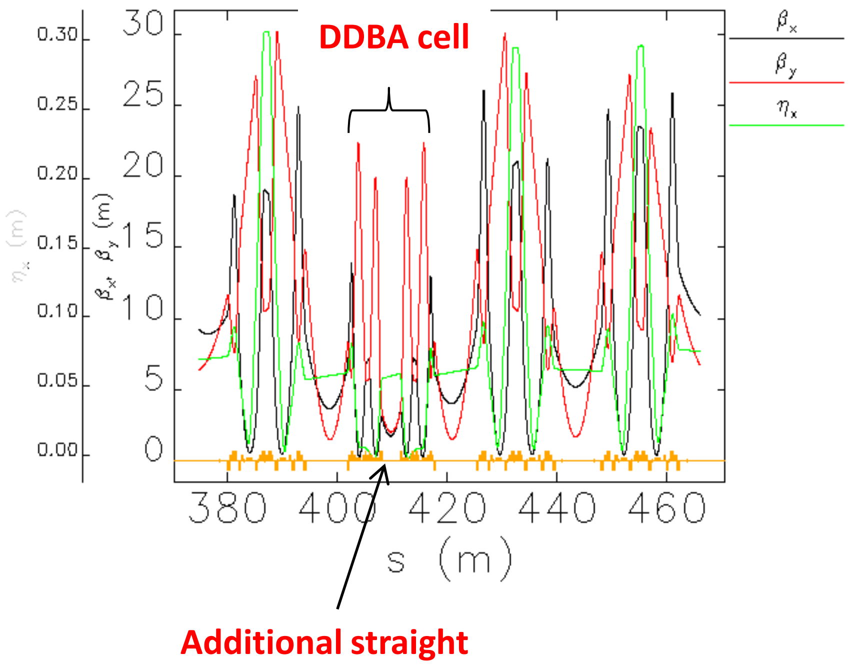
- The straight sections have a double waist in Y and a decreasing slope in H

- The 6-fold symmetry of the ring is broken

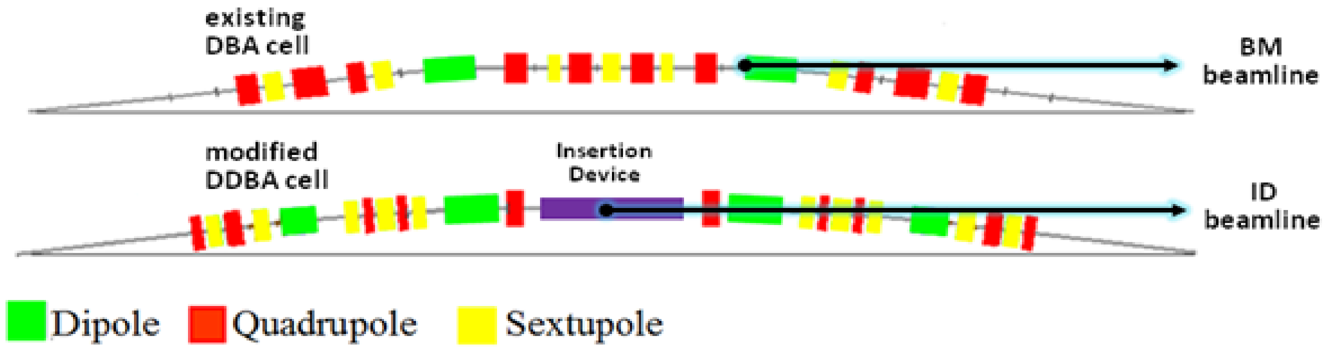
DDBA project 2013-2016

Replacing the existing cell2 with a DDBA cell

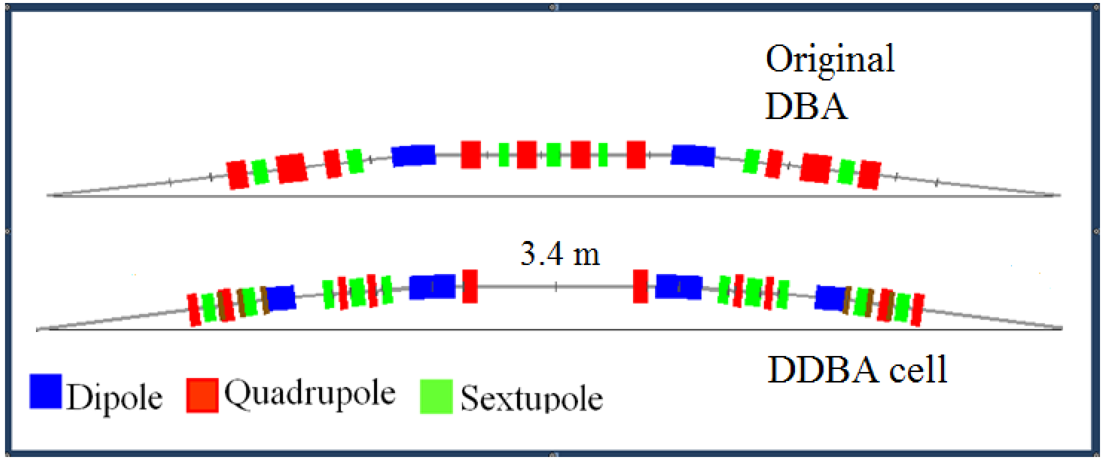
- **Introduces an additional straight section (beamline upgrade bending magnet to ID beamline) Complete (and aggressive) break of the symmetry**
- **Serves as a prototype for low emittance lattice upgrade**
- **Lots of R&D required (magnet design challenging, vacuum with small apertures, engineering integration, etc)**

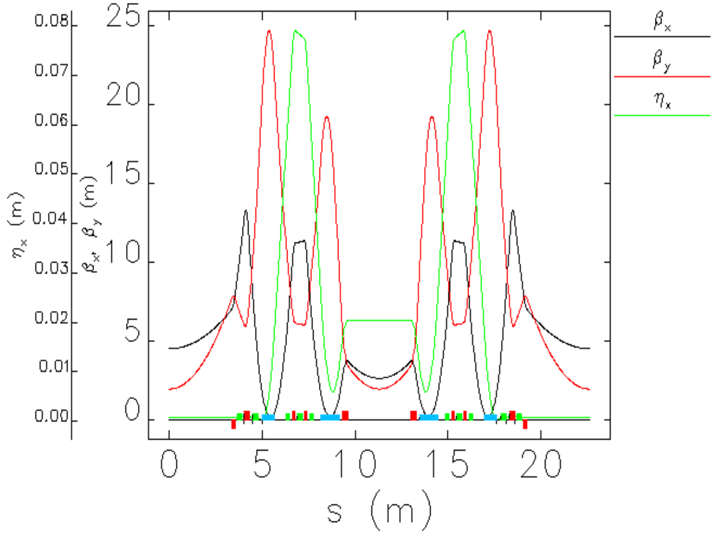


- VMXm MX beamline ~< 0.5μm X-ray spot at sample



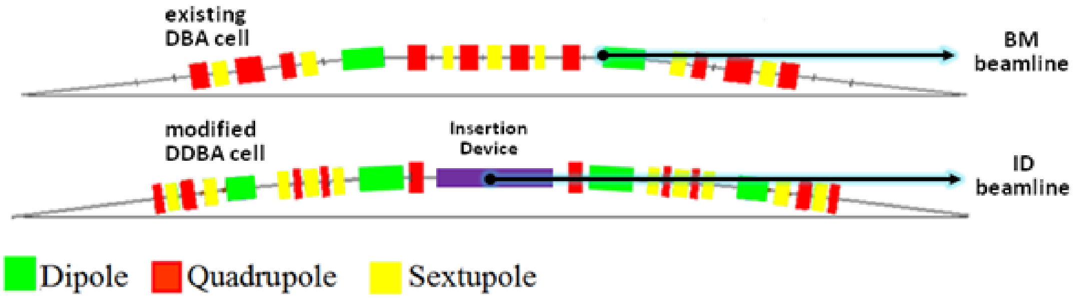
Diamond-II: modified 4BA – 270 pm





This lattice combines the idea of doubling the capacity of the ring with the low emittance

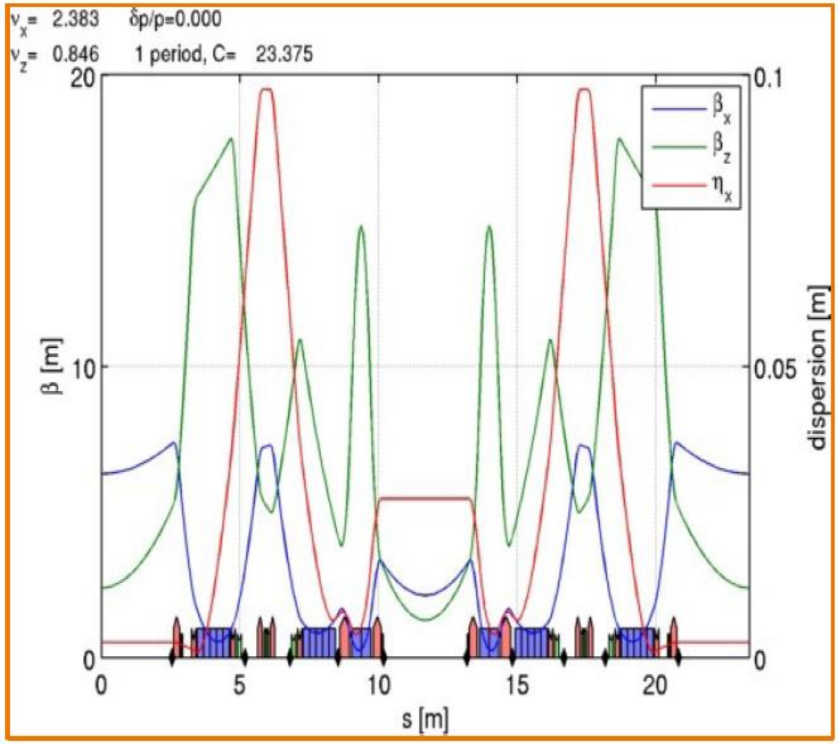
The Diamond Board approved the project to replace the existing cell2 with a DDBA cell – it was Diamond-II baseline design until end 2015

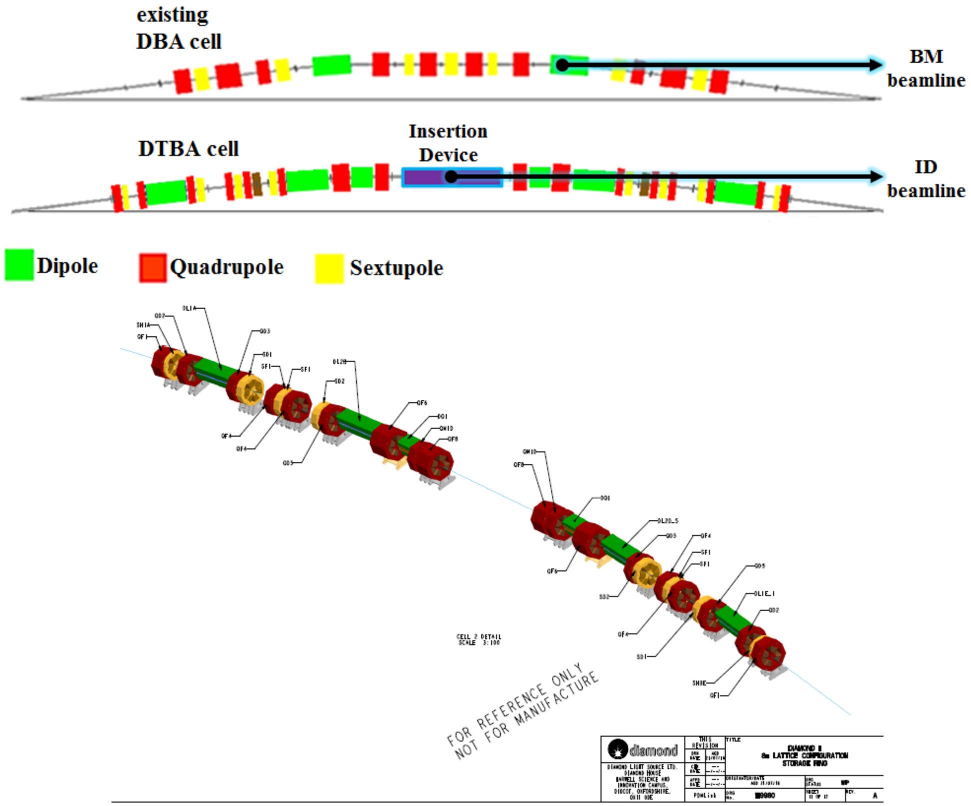


Diamond II: DTBA cell – 120 pm

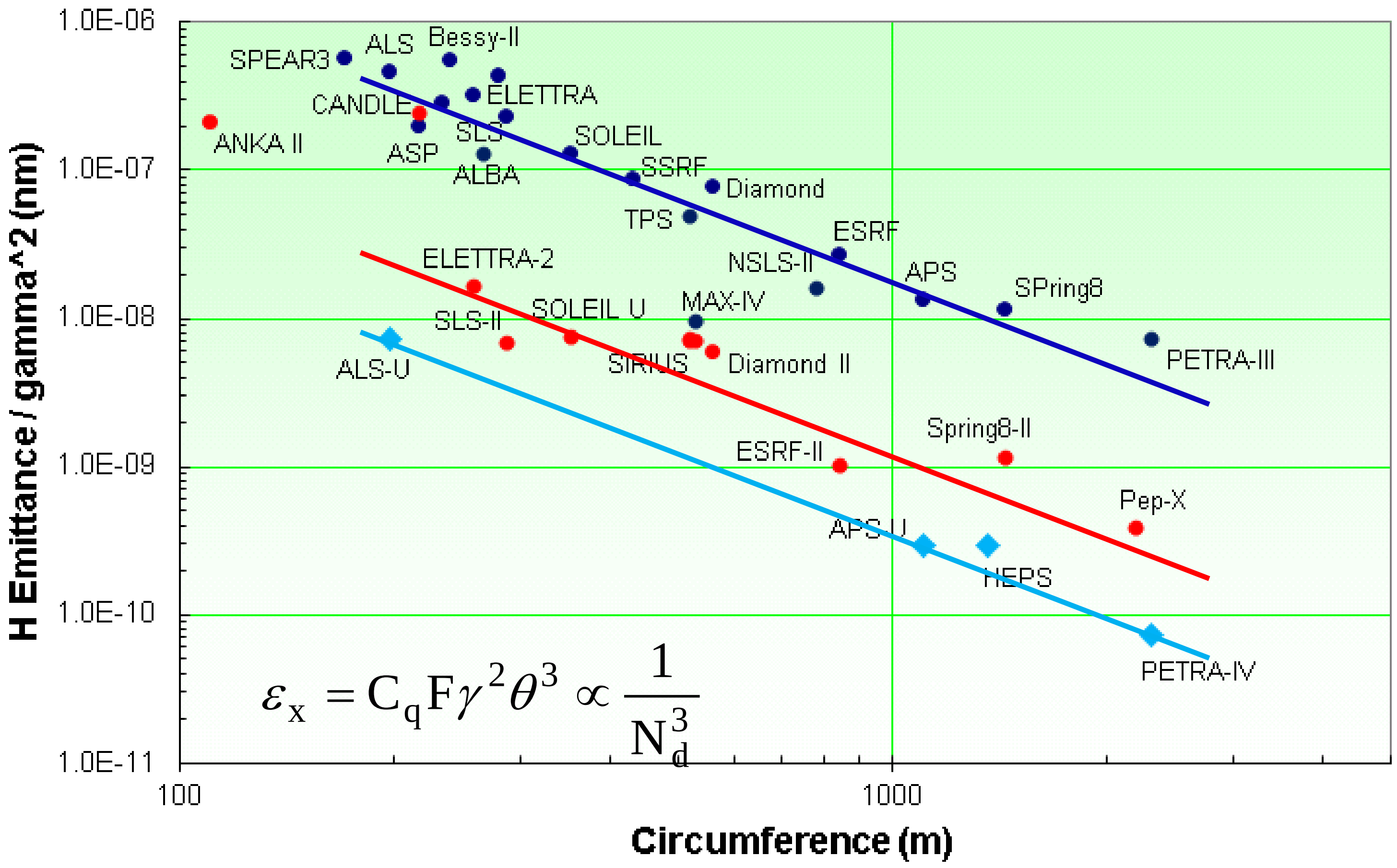
A more aggressive design was then proposed that merges the ESRF HMBA concept with the Diamond DDBA mid straight section taking the best of both

Use the ESRF cell (7BA with longitudinal gradient dipoles) – removing the mid dipole to make it a 6BA with a straight at the centre





Survey of low emittance lattices for light sources



$$\varepsilon_x = C_q F \gamma^2 \theta^3 \propto \frac{1}{N_d^3}$$

MBA

On axis injection
Antibend
…
Full symmetry

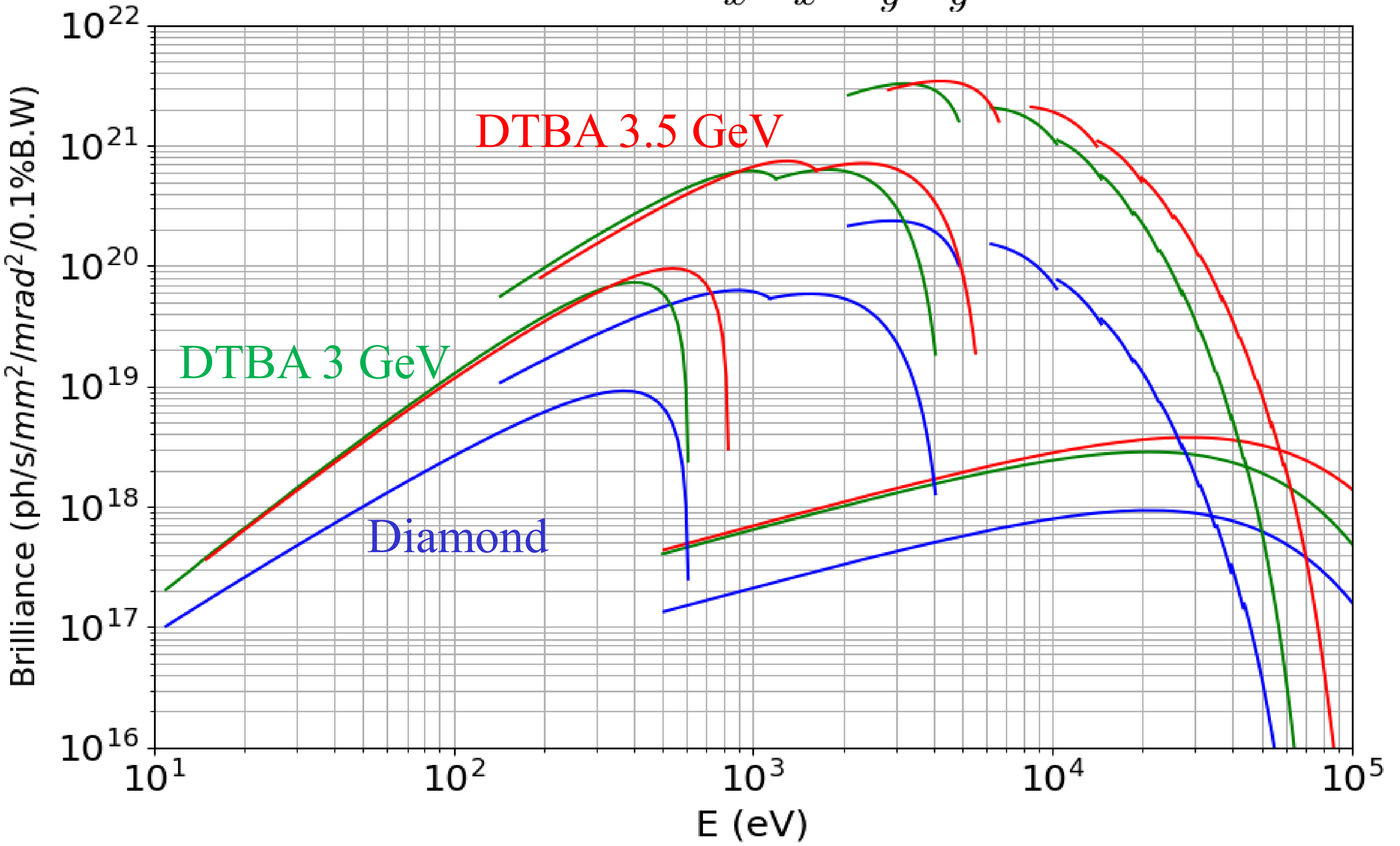
The DTBA lattice places Diamond in line with the new upgrades with the advantage of increasing the capacity of the ring, albeit without pushing the emittance down as much as done in other projects e.g. ALS-U, …

Diamond-II – 3.5 GeV

$$\mathcal{B} = \frac{\Phi}{4\pi^2 \Sigma_x \Sigma_{x'} \Sigma_y \Sigma_{y'}}$$

“By the end of the 1990s, it had become clear that a medium-energy (3–4 GeV) machine would be in many ways a perfect SR source. User requests in the UK (number of proposals versus photon energy) clearly pointed to a source optimized for the photon energy range of 4–20 keV”

G. Materlik et al., [Philos Trans A Math Phys Eng Sci](). 2015 Mar 6; 373(2036): 20130161.



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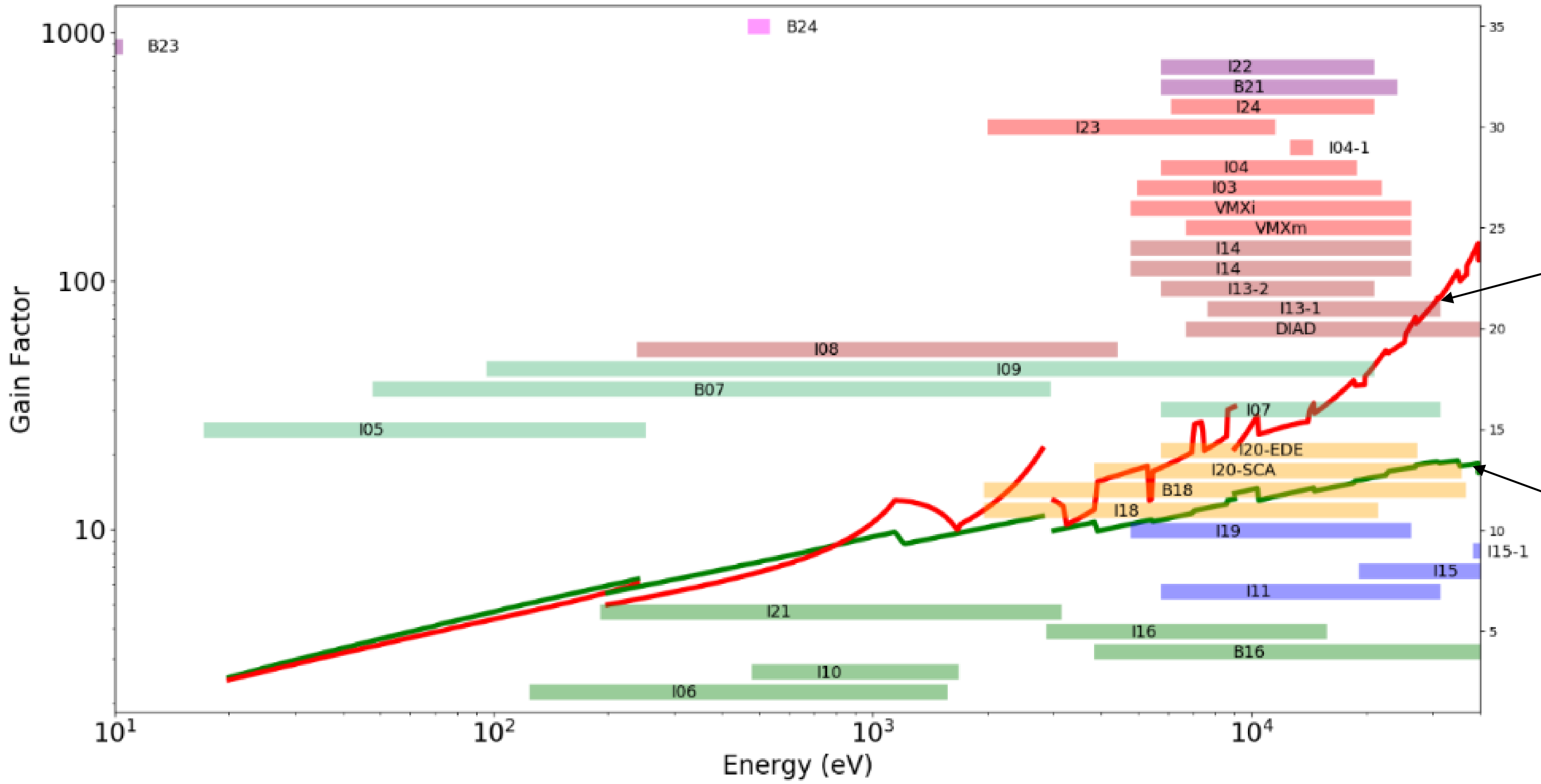
Brightness gain 3 GeV v 3.5 GeV



160 pm.rad
@3.5 GeV

118 pm.rad
@3.0 GeV

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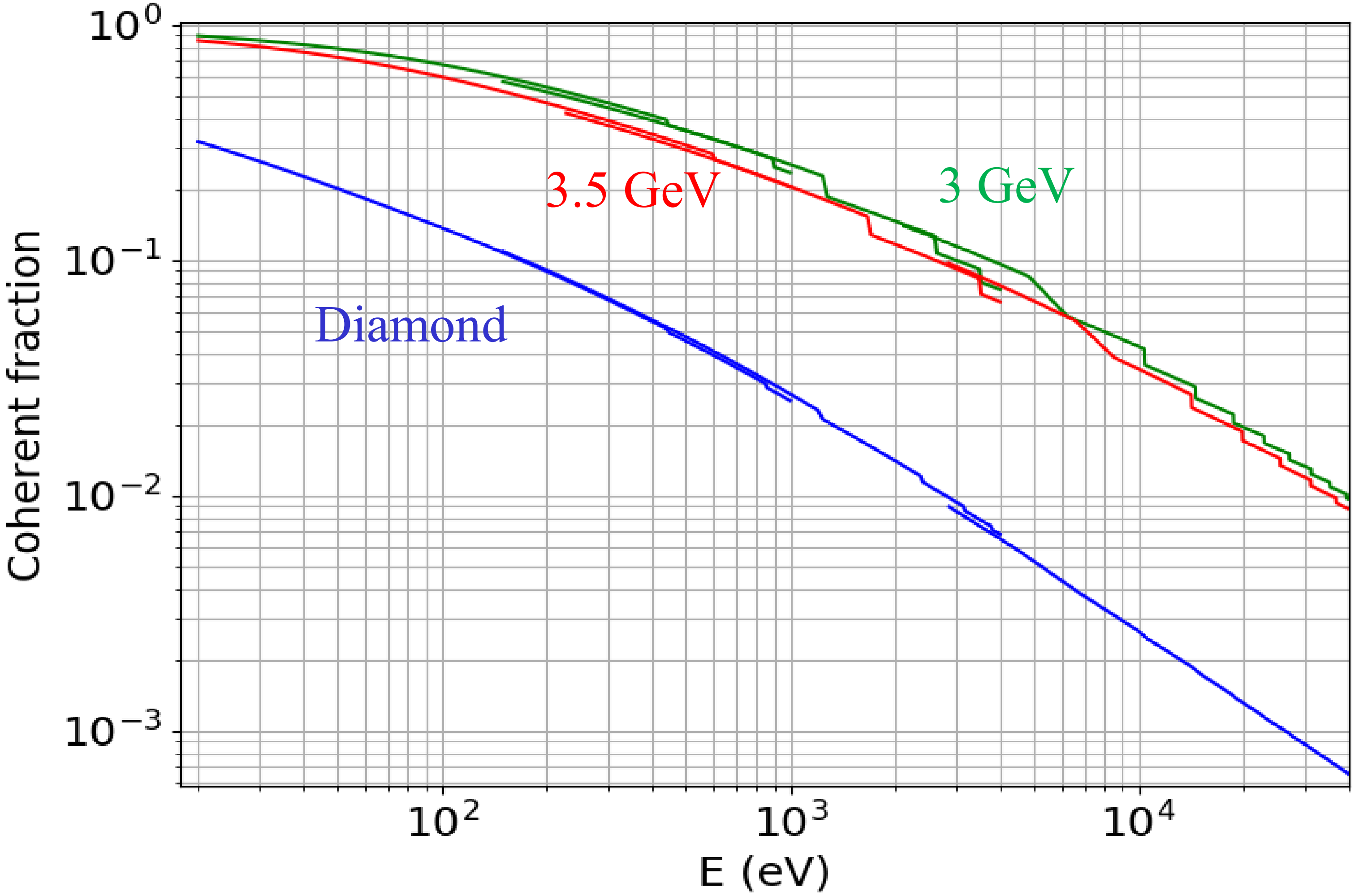
Coherence



The improvement in coherence is approximately a factor of x3 at 100 eV and x10 at 1 keV, the main benefit coming from the reduction in the horizontal source size

Energy spread effect, medium energy rings

Harmonic

Periods

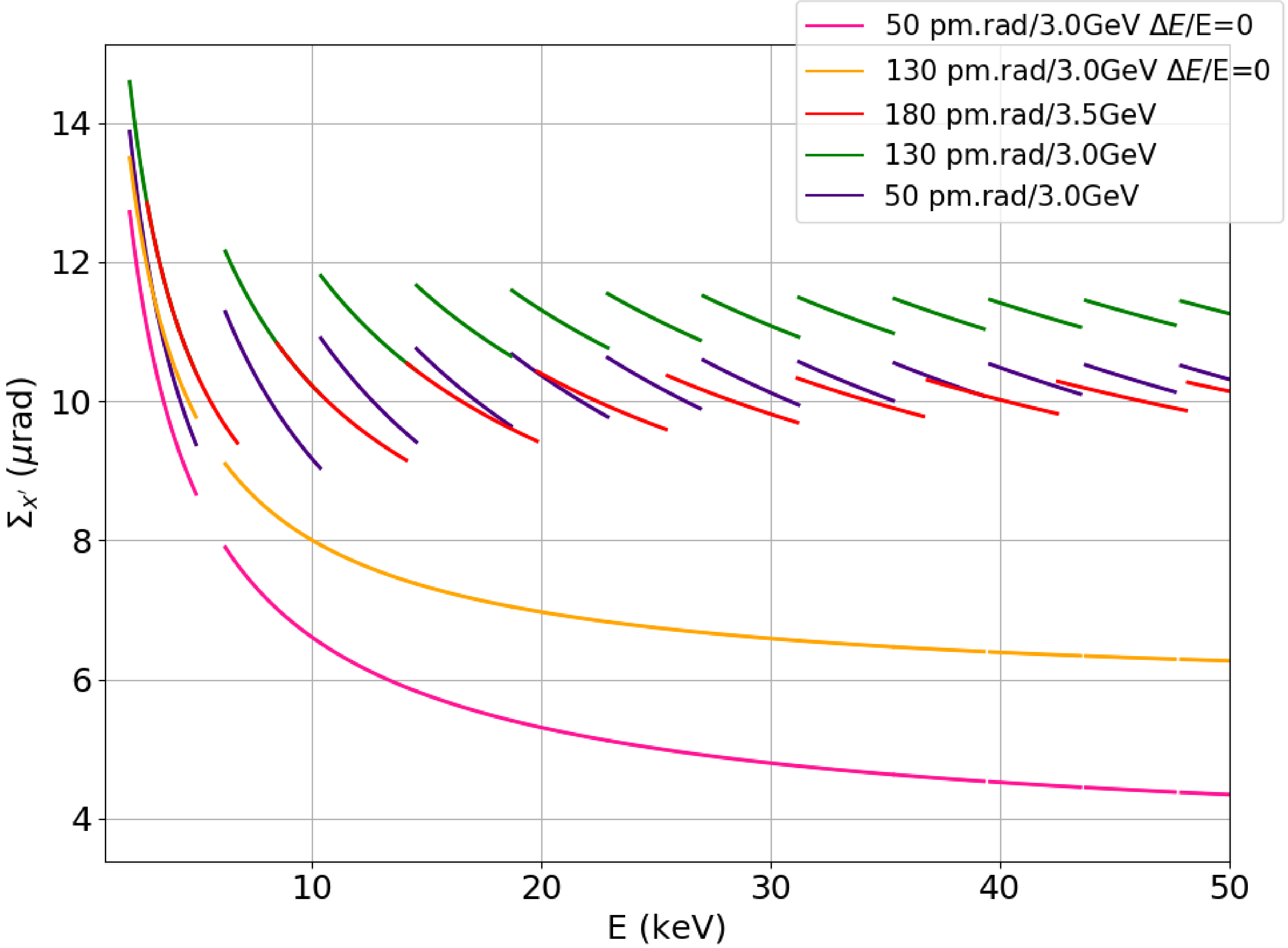
Energy spread

$$\sigma_e = 2\pi n N \frac{\Delta E}{E}$$

$$\sigma_{r'_B} = Q_a(\sigma_e)\sigma_{r'}$$

$$Q_a(x) = \sqrt{\frac{2x^2}{e^{-2x^2} + \sqrt{2\pi}x \cdot erf(\sqrt{2}x)) - 1}}$$

*[1] T. Tanaka and H. Kitamura,
"Universal function for the brilliance of undulator radiation considering the energy spread effect,"
J. Synchrotron Radiat., vol. 16, no. 3, pp. 380–386, 2009.*

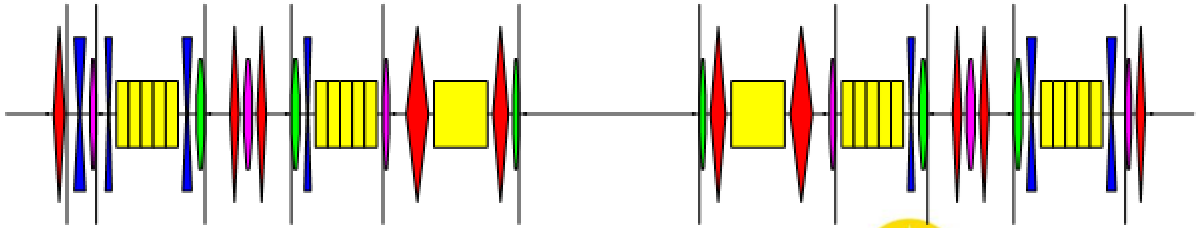


Diamond-II is a 'Modified Hybrid 6 Bend Achromat'

Combines two concepts:

- The ESRF-EBS upgrade lattice*
- The Double-Double Bend Achromat cell**

	CDR Lattice	M-H6BA-28-1-1	M-H6BA-28-2-1
Injection scheme	off-axis	off-axis	on-axis
Offset of mid-straights (mm)	-190.79	-190.792	-190.792
bx, by, hx (Long Straight)	8.37, 4.4, 0	8.90, 4.07, 0	5.8, 3.18, 0
bx, by, hx (Standard Straight)	5.68, 2.1, 0	6.24, 1.99, 0	2.4, 2.35, 0
bx, by, hx (Mid Straight)	2.2, 1.85, 0.0249	2.34, 1.92, 0.0253	2.24, 1.38, 0.0227
Operational parameters (with IDs, IBS and 3HC) (pm)			
Emittance (pm)	147.45	148.96	110.4
Energy spread ($x10^{-3}$)	1.030	1.090	1.082
Effective emittance of mid straights (pm)	257.78	263.55	204.69



*ESRF Technical Design Study, "The Orange Book" (2014)
R. Bartolini et al., PRAB **21, 050701 (2018)

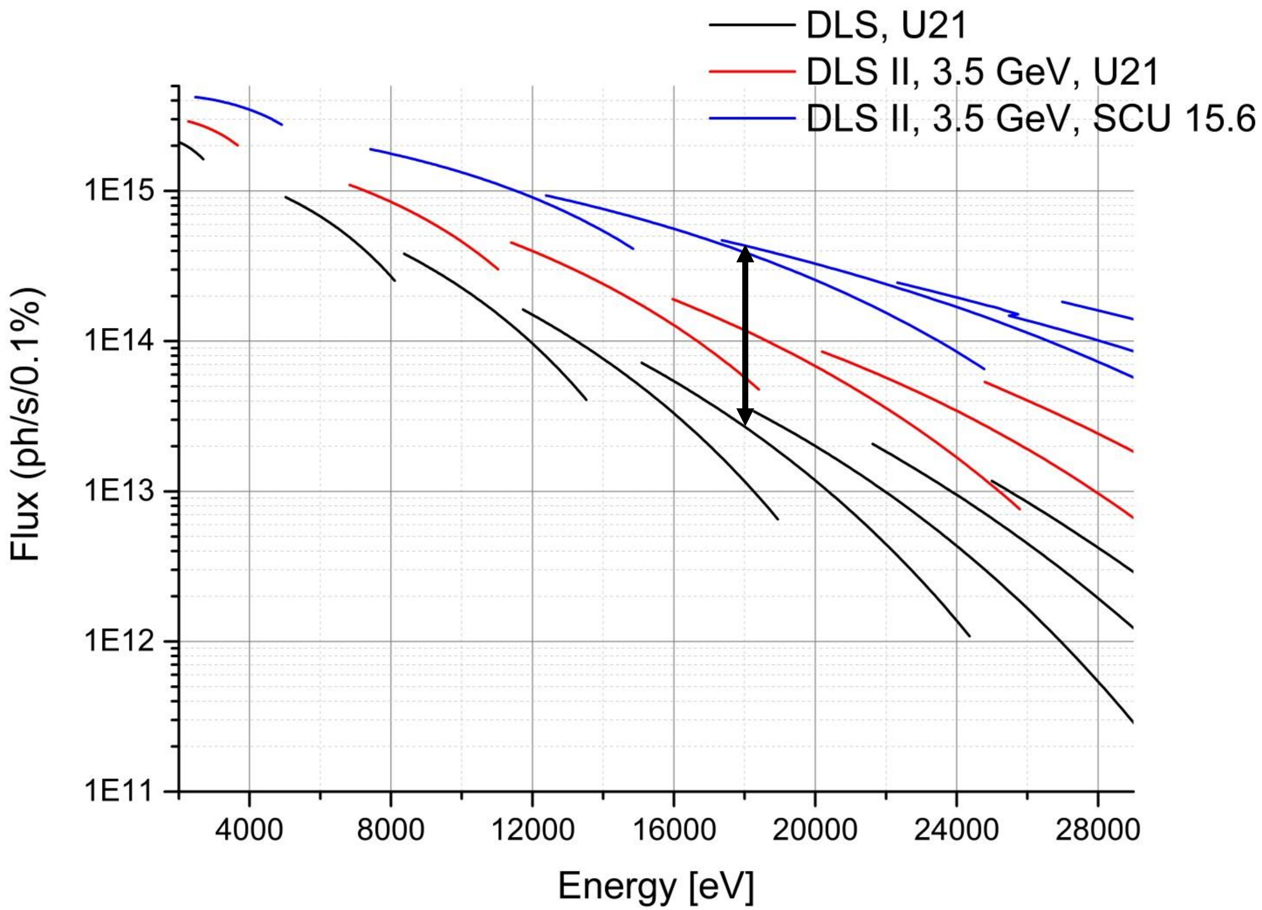
Beamlines

Calculations being made to understand:

- Standard in-vac ID and CPMU beamlines: calculations for flux, coherence gains and smaller spot sizes, and benefits of higher energy.
- Wiggler beamlines benefit from higher energy but factor x2 heat load on optics
- I05 ARPES (18 – 240 eV) (APPLE-Knot undulator)
- Consider sources for current BM beamlines, which may now move to an ID

✓ Flux for higher energy ring, power load etc (SPECTRA code)
✓ Ray-tracing for beam size and flux at sample (Oasys – ShadowOUI)

Impact of Upgrade: Peak flux



Flux at peak position for **E = 18 keV:**

- ✓ U21 DLS: 2.7E13 ph/s/0.1%BW
- ✓ **U21 DLS II: 4.4 times more flux**
- ✓ **SCU 15.6 DLS II: 16 times more flux**

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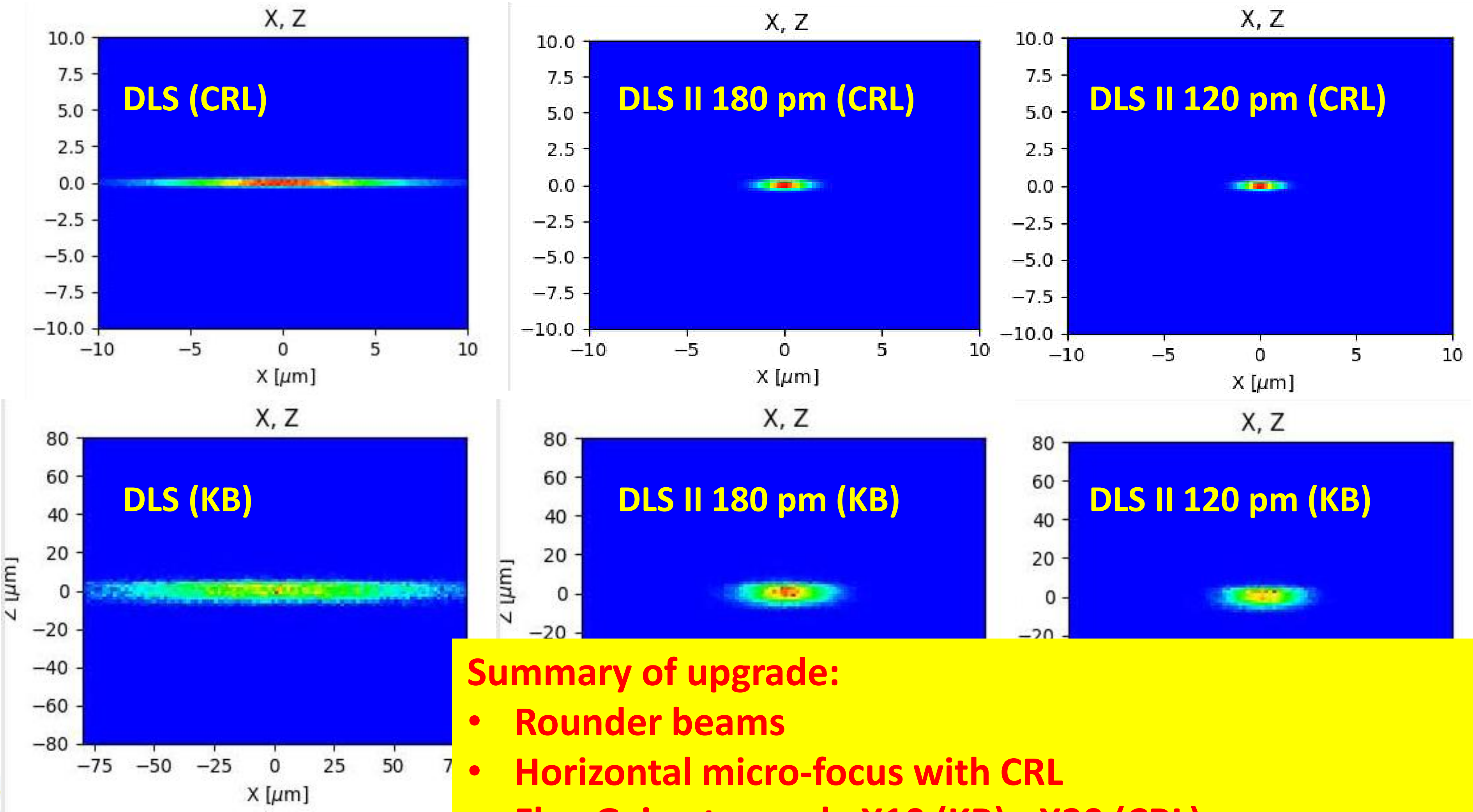
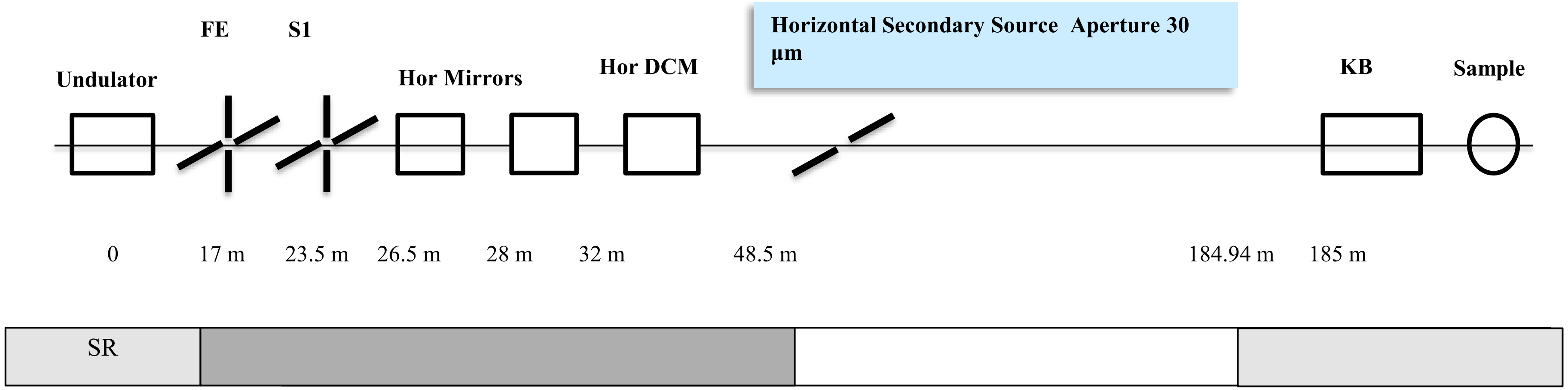
Ray-tracing simulations



Summary of upgrade:

- **Rounder beams**
- **Horizontal micro-focus with CRL**
- **Flux Gain at sample X10 (KB) - X20 (CRL)**
- **Flux Spatial Density gain at sample: X40 (KB) – X115 (CRL)**

I14 Nanoprobe



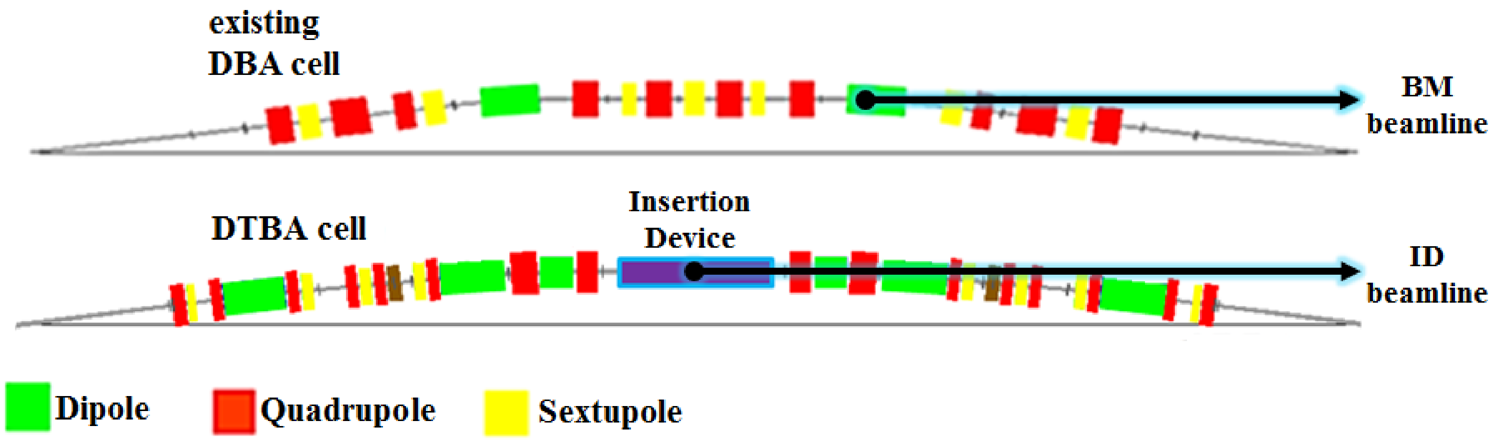
E = 12 keV

Scenario	ID	Flux after FE [ph/s/0.1%bw] X 1.73E14	Flux after SS [ph/s/0.1%bw] X 3.5E11	Flux at sample [ph/s] X8.3E9
DLS	U23	1	1	1
DLS	CPMU 17.6	1.6	1.6	1.6
DLS II 50 pm	**CPMU 17.6**	**1.6**	**6.2**	**28**
DLS II 120 pm	CPMU 17.6	1.6	5	17
DLS II 180 pm (3.5 GeV)	CPMU 17.6	2.5	7.3	20

Critical Beamlines: Mid-Section Straights (I)

Existing ID beamlines:

- I04-1 can be relocated to an improved ID source at B03, which would be significantly better than the current short ex-vac device.
- I20 EDE can be relocated to an improved ID source at B14 and be disentangled from I20 XAS.
- Without mid-straights J02 (VMXm) would be lost, since VMXm uses the mid-straight ID created by the recent DDBA insertion.
- DIAD (K11) can have a much better ID than the short mini-wiggler which has recently been installed.



Critical Beamlines: Mid-Section Straights (II)

An argument for the mid-section straights is for flexibility with the bending magnets

- B07 Two branches: could be split (undulator) and DQ?
- B16 test beamline: HPMU
- B18 Core XAS: 3PW
- B21 Bio-SAXS: HPMU
- B22 IR: long magnet (1 m), low field magnet (0.2 T)?
- B23 CD: long magnet, but higher field (0.34 T)?
- B24 Cryo-TXM: DQ magnet

Will need to be realigned to new source point

New Beamlines:
Up to 6 additional new ID beamlines could be built at B04, B08, B10, B12, B13 and B14?

Critical Beamlines: ID's

Source points for ID beamlines remains the same

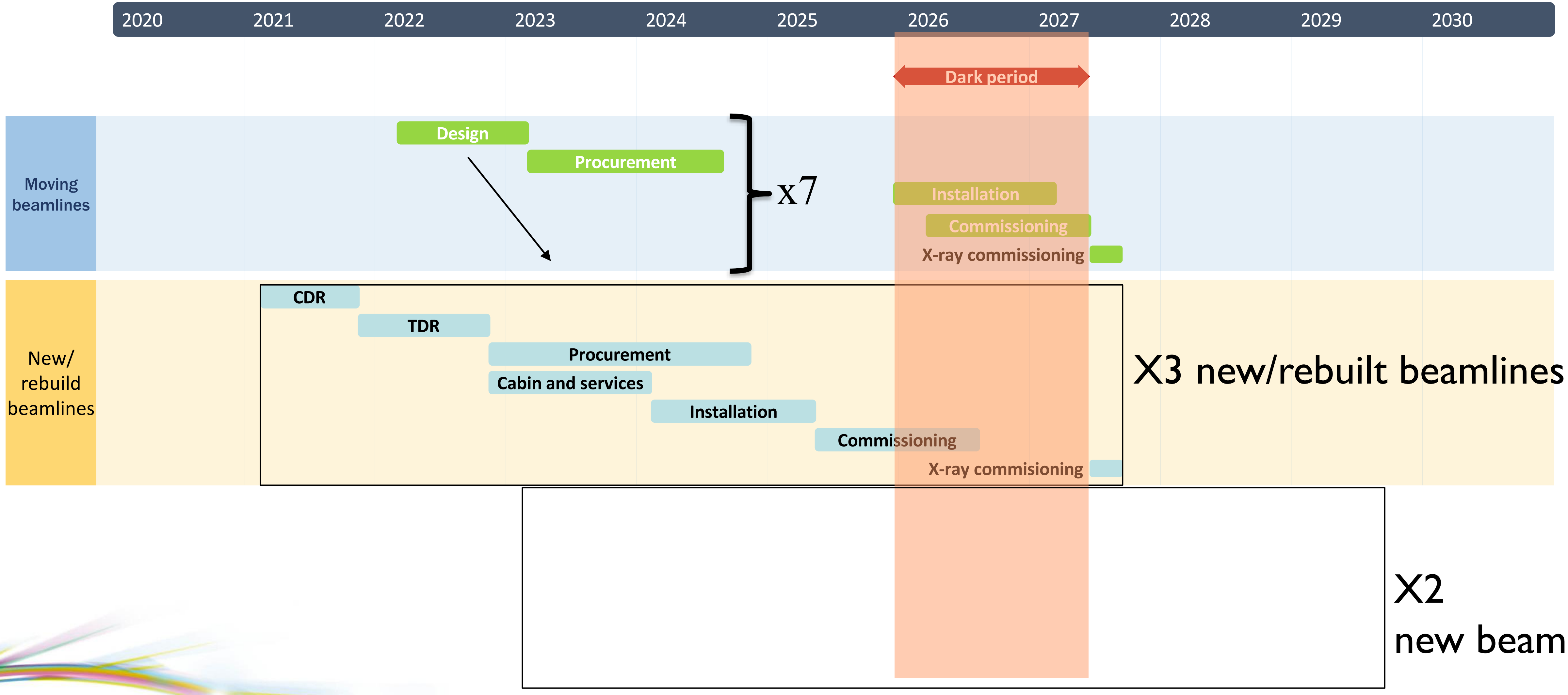
Diamond-I: 3 GeV, shielding and components designed for 500 mA, but only run at 300 mA
Upgrade to 3.5 GeV at 300 mA ~compensates, so no major shielding issues

Extra shielding for Wigglers being investigated.

Some upgrades to diagnostics, monochromators required.

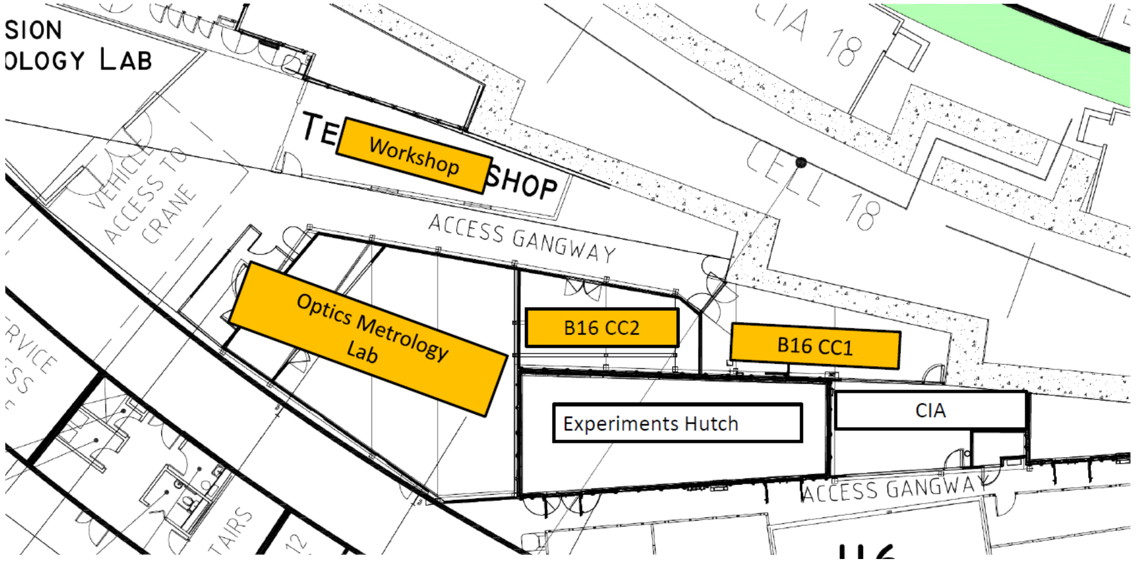
New Beamlines – Agreed scope: 3+2 model

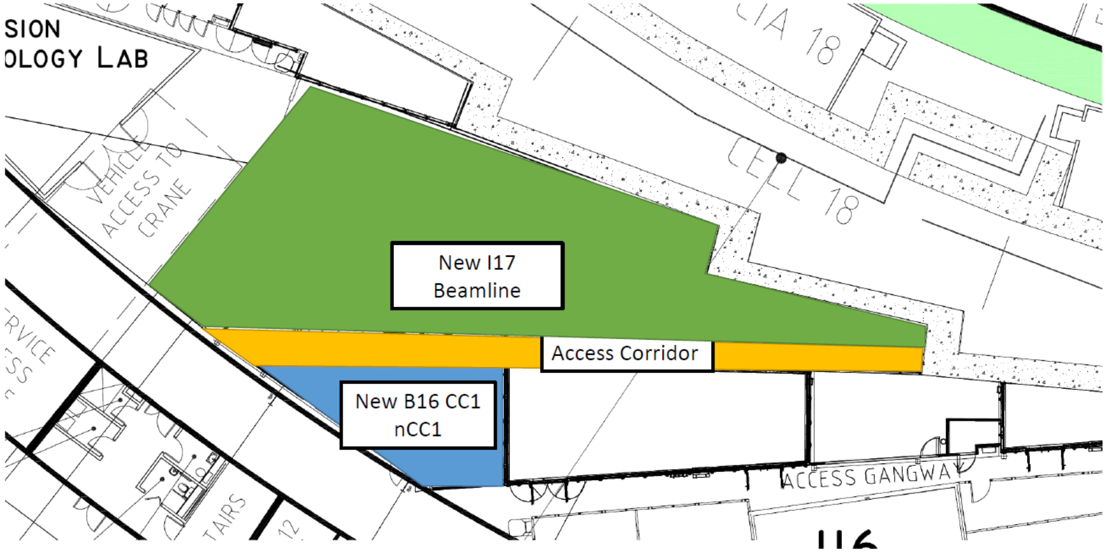
Dark period : 18 months   Current start of the dark period : Dec 2025,



New long straight I17

- Removal of 3 SC RF cavities in straight 17 frees up a long straight for a new ID beamline
- Reorganization of space is necessary of I17 instrument.
- This includes rebuilding the Optics Metrology Lab in a new area.





SAC/DISCo process

- Outline proposals for flagship projects new/rebuilt beamlines or upgrades
- Prioritisation in two steps:

May 2020

- Suite of beamlines proposed offer opportunities that were identified in the Diamond-II science case
- Identify key upgrades
- Validate group strategy
- Advise on developing full business cases

→

- Full business case prepared
- Projects developed with the community (UWG)
- Projects championed by academic/industrial user
- Broader stakeholder engagement (Webinars)

→

Dec. 2020

- External champions present full business case to SAC/DISCo
- Prioritization of new beamlines, first 3, and further 2 beamlines.
- Prioritisation of upgrade projects

→

Beamline delivery

- UWG develop CDR/TDR
- Oversight of construction
- Benefit realisation

Summary of new beamlines

Science Areas/technique	Instrument	Opportunity/benefit
MX	Protein crystallography, ultra-high throughput fragment screening	Ultra-high throughput (x10 faster than current capability) and transformation of fragment screening.
Soft-condensed Matter	Ultra-fast SAXS	New capability in the areas of soft materials, e.g. measuring response to out of equilibrium stresses and dynamic studies of protein transition states and conformational space. Micro-second resolution dynamic studies on proteins and research into hierarchical structures over 6-decades of length scale.
Bio-imaging	Coherent diffraction imaging	Develop the new area of large volume 3D imaging of biological cells and tissue in many areas of microbiology, cell and developmental biology.
Core Spectroscopy	Fast operando core-level spectroscopy	Support the increasing demand for fast in situ and operando characterisation of chemical systems and materials, electrochemical research. Augment capacity in this field of research currently extremely oversubscribed (3) and growing (electrochemistry, catalysis).
	Hard X-ray RIXS and valence to core spectroscopy	Offers new capability at Diamond (as provided on ID20 at ESRF or LERIX at sector 20 at the APS). Complement existing emission spectroscopy techniques by offering higher energy resolution exploiting a smaller spot provided by Diamond-II. Applications in chemistry, physics and materials science.
Crystallography	Nano-focussed crystallography	Step change in capability for high pressure/nanofocussed crystallography work for small molecules and materials science, using bright beams at high energy.
Surface Science	Nano-ARPES	Dedicated nano-ARPES beamline to study complex quantum materials and 2D system under external perturbation (gating, strain…). Augment capacity in this field of research (currently I05), currently extremely oversubscribed (4-5)
Magnetic Materials	Multiplexed soft X-ray RIXS	Provide a step change in the measurement of fundamental excitations in a variety of complex electronic systems and quantum materials by replacing energy scanning by single shot experiments, exploiting the hν2 concept.
	Coherent imaging	New capability to image magnetic domains using coherent diffraction techniques such as holography and ptychography using XMCD and XMLD. Will provide unprecedented spatial resolutions down to a few nanometres.

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Flagship projects

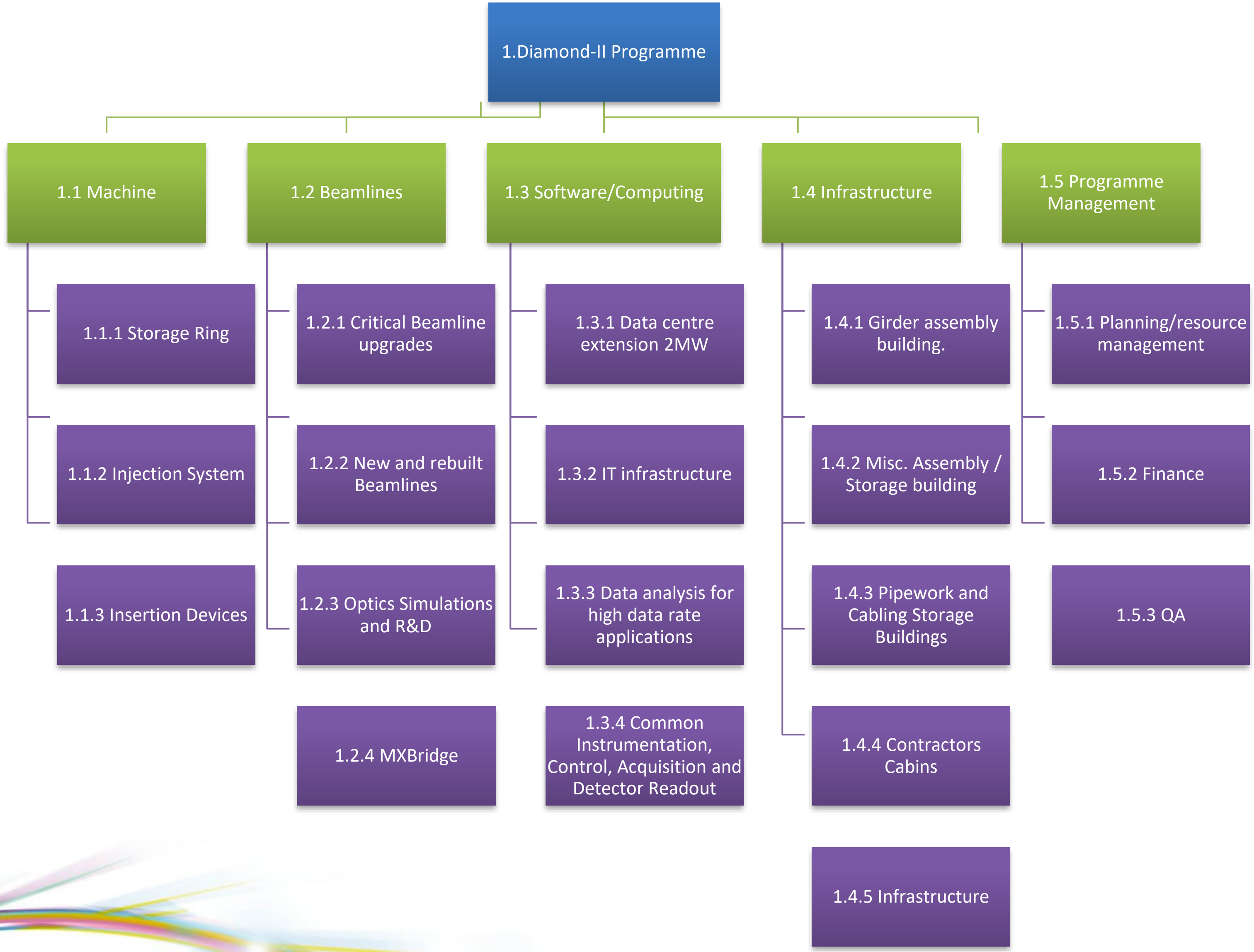
Beamline	Group	Type
I13L	Imaging	Upgrade
Versox-II	Surfaces	Upgrade
I16	Magnetic Materials	Upgrade
I21	Magnetic Materials	Upgrade
μ15	Crystallography	Upgrade
I24	MX	Upgrade
I04-1	MX	New *
Bio nanoimaging	Bio imaging	New
X4SCM	SCM	New
BERRIES	Spectroscopy	New **
SWIFT	Spectroscopy	New **
CSXID	Magnetic Materials	New
NexCube	Crystallography	New
Nano-ARPES	Surfaces	New

Long straight (17)

* I04-1 cannot continue to operate at its current position, so it is a new beamline but still different category to the others.

** Fast spectroscopy I20-EDE cannot continue to operate at its current position and will be close and replaced by more modern instruments such as SWIFT or/and BERRIES for fast and advanced spectroscopy.

Project Structure



1.1 Machine
1.2 Beamlines
1.2.1 Beamline critical surveys being finalised
1.2.2 Progressing with priorities from SAC
1.2.3 Optics simulations ongoing

1.3.1 Discussion with campus (STFC) for a large 10s MW data centre
1.3.2-1.3.4 Being fully scoped

1.4 Infrastructure

Milestones

Wellcome Application	OBC	TDR/CD2	FBC	2027	2030
Grant application reviewed by Wellcome. 4th Nov. 2020	Submission of Outline Business Case, 2021	Technical design review MAC/SAC Dec 2021 CD2 : approval of project baseline 2022	Full Business case 2022	**New facility with 3 new beamlines**	**New facility with 5 new beamlines**

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Acknowledgements

- Directors:
  Andrew Harrison, Laurent Chapon, Richard Walker
- Machine:
  Riccardo Bartolini, Ian Martin
- Beamlines: Science Group Leaders
  Martin Walsh (Bio-imaging), Sarnjeet Dhesi (Magnetism), Dave Hall (MX), Chris Nicklin (Surface Science), Paul Quinn (Imaging and Microscopy), Joe Hriljac (Crystallography), Sofia Diaz-Moreno (Spectroscopy) and Rob Rambo (Soft Condensed Matter)
- Optics: *Kawal Sawhney*

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