

Synchrotron and Free electron laser Radiation: generation and application (SFR-2016)

Possibilities for Future SR and FEL Development in the UK.

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SR-86 ... a lot's changed since then !



Diamond Light Source

Fil



Beamline Delivery Schedule BLS-GEN-REP-0011 October 2015

Beamline	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020
Phase 1		-				-									1				
102 Macromolecular Crystallography																			
103 Macromolecular Crystallography																			ĺ
104 Macromolecular Crystallography																			
106 Nanoscience																			
115 Extreme Conditions																			
116 Materials and Magnetism						1													
I18 Microfocus Spectroscopy																			ĺ
Phase II		-				-									¥.				
122 Non-Crystalline Diffraction		1																	
B16 Test Beamline																			
111 High Resolution Power Diffraction			1											Soo	n cc	omir	ng ta) the	
124 Microfocus MX														000			.9 .0		
119 Small Molecule Diffraction			E											end	of I	Phas	se-II	l:	
B23 Circular Dichroism																	_		
I12 JEEP (Engineering, Environment & Processing)														Dia	mor	d w	ill h	21/0	
104-1 Monochromatic MX				5				3										ave	le la
120 - EDE Branchline														36 i	nde	nen	den	t	
120 - XAS Branchline				1										501	iiuc	PCII	acii	L	
107 Surface and Interface Diffraction (XENA)														bea	mlir	าe b	rand	ches	
B22 Infrared Microscopy																			
110 BLADE: X-ray Dichroism & Scattering					1														
B18 Core EXAFS																			
113 X-ray - Coherence Branchline											1								
113 X-ray - Imaging Branchline																			
109 SISA: Surface and Interfaces																			ĺ
Phase III								<i>i</i> te											
B21 High Throughput SAXS																			ĺ
123 Long Wavelength MX																			ĺ
105 ARPES												13							ĺ
B24 - Cryo Transmission Microscope																			
108 Soft X-ray Microscope (STXM)																			
114 Hard X-ray Nanoscale Probe for Complex Systems (HXNP)																			
121 Inelastic X-ray Scattering (IXS)	Beam	line Sta	tus							1									ĺ
B07 Versatile Soft X-ray (VERSOX)	Op	erationa	ı			1									3				
115-1 X-ray Pair Scattering Distribution Function	Lin	der Con	struction																
VMXi Versatile MX in situ		uer con	auction								Č.								l
VMXm Versatile MX microfocus	Pla	nned																	ĺ
DIAD Dual Imaging and Diffraction	Off	line				J													



Insertion Devices

	Type of Device
01	(injection)
02	in-vacuum undulator
03	in-vacuum undulator
04	in-vacuum + short ex. vac. undulators
05	5m APPLE undulator
06	2 APPLE undulators
07	cryogenic in-vacuum undulator
08	4.5m APPLE undulator
09	in-vacuum + APPLE undulators
10	2 APPLE undulators
11	in-vacuum undulator
12	superconducting wiggler

Type of Device

13	2 in-vacuum undulators
14	in-vacuum undulator
15	superconducting wiggler
16	in-vacuum undulator
17	(RF)
18	in-vacuum undulator
19	in-vacuum undulator
20	2 permanent magnet wigglers
21	5m APPLE undulator
22	in-vacuum undulator
23	in-vacuum undulator
24	in-vacuum undulator

27 discrete IDs ... all straight sections are occupied !



Increasing demand - over 9000 "user-visits" last year:



Increasing science output:





Industrial Impact

Increasing impact – now 100 companies engaged in industrial use of Diamond





Examples of industrial use of Diamond

Engineering

diamond



Rolls-Royce Strain scanning in aerospace components

Drug design



Heptares **Designing drugs** for Parkinson's disease treatment

Consumer products



Unilever Microstructure in a new hair care product



Catalysis

Johnson Matthey Platinum speciation in three way catalysts

Medical

devices

Fuel additives

Infineum **Crystallisation** processes in biofuels

> Diagnosing disease



Drug

manufacture

GlaxoSmithKline Controlling a manufacturing



NHS Understanding failure in MOM hip replacements Synchrotron and Free Electron Laser Radiation: Generation and Application (SFR 2016), BINP, 4-7 July 2016



NHS Speeding up cancer diagnosis using IR



Planning for the Future

The 10-year Vision:



available from: http://bit.ly/Diamond10yearvision



... which led to the Diamond Upgrade proposal:

presented to the Diamond Science Advisory Committee (27th-28th April 2016) and Board of Directors (1st June 2016). The Diamond Upgrade

A next generation light source for UK science and innovation

Executive Summary

Diamond has established itself in its tenth year of operation as a world-class synchrotron, enabling research by leading academic and industrial groups in physical and life sciences. However, the technology for light sources, including detectors, optics and scientific computing, is developing at a tremendous pace and Diamond must take advantage of this if it is to continue to provide first-class opportunities to meet the scientific and societal challenges of the future.

This document outlines some of these challenges, shaped by the strategic priorities of our shareholders, STFC and the Wellcome Trust, and informed through input from our user community. It also presents an Upgrade programme for the period 2016-2024, whose timescale is set by the length of time it will take to design, build and commission a new, low-emittance storage ring, and this part of the Diamond Upgrade is called Diamond-II.

The new storage ring will be built within the existing footprint and offer more than 10-fold increase in brightness, with much enhanced coherence. In addition the unique machine design gives the potential to introduce more high performance insertion device beamlines, as well as providing flexibility for implementing other source improvements in the future.

Equally important for effective science delivery will be upgrades at every other stage of the measurement process - from brighter insertion devices, through nanofocus optics to faster detectors offering far greater resolution/range in time and space, and near real-time comprehensive data analysis. These developments will provide transformative opportunities across science, engineering and medicine. Specifically Diamond will build on its position as a leading global centre for materials discovery, processing and integrated structural biology to maximise the impact of the ongoing revolutionary developments.

April 2016

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Enabling technology to maintain competitiveness:

- Improved sources CPMUs and potentially SCUs
- Improved optics
- Improved detectors
- Improved/greater range of sample environments and sample transfer systems
- Continuing upgrades to data handling infrastructure
- Significant upgrades to beamlines
- A new low emittance lattice: Diamond-II



The "Data Deluge"

6

5

4

3

2

1

0

янв.07

янв.08

янв.09

янв.10

Increasing data rates from detectors (MB/s):

Increasing data storage requirements:

Cumulative data taken

by Diamond (PB)

янв.12

янв.11

янв.13

янв.14

янв.15

янв.16



Increasing use of automation:



Detector Controller 1 sample/minute EPICS Area Detector 1 dewar of 592 Processing samples in 10 hours Detector Memory: Detector enough to fit a full **GDA** Control scan 5 PB online rapid access storage high performance cluster for near real-time data analysis **Data Visualisation** Storage Cluster



When Diamond was built .. it was the largest, and lowest emittance "medium energy" SR source:





but now ...





and soon ...





so we are beginning to think seriously about Diamond-II ...





Initial studies of low emittance lattices started with Multi-Bend Achromats (MBA) with M=4,5,7



Increasing M reduces emittance, but results in diminishing dynamic aperture:

No. of Bends (M)	Emittance	Dynamic Aperture
4	270 pm	± 5 mm
5	140 pm	± 3.5 mm
7	45 pm	± 1 mm

courtesy of R. Bartolini, DLS



DDBA

This led to the concept of a modified 4BA, or "double-DBA" (DDBA)



Allows a bending magnet beamline to become a new insertion device beamline

- Will be carried out in one cell of the ring in Oct./Nov. 2016 to create a new ID beamline
- Converting the whole ring to DDBA became the initial design for Diamond-II
 - Natural emittance 275 pm.rad (factor 10 reduction on present lattice)
 - 24 additional straight sections for further ID beamlines or other machine components



DDBA

take out a complete arc, 3 girders:



and replace it with 2 completely new girders: (new magnets, vacuum vessels, BPMs, girders, cabling, controls etc.)





DDBA



Installation of one DDBA in Oct./Nov. 2016

- New magnets & vacuum vessels delivered
- Girder assembly well underway





Diamond-II

In the summer of 2015 a new concept emerged – the modified 6BA, or "double triple bend achromat" (DTBA) lattice.

This has been developed in collaboration with ESRF, adapting their hybrid 7BA lattice, with longitudinal gradient bends, to our 6BA.



Promising design:

emittance ~120 pm dynamic aperture ~ 8-9 mm lifetime ~ 2-3 h

Gives the benefits of both lower emittance and additional straight sections !

Study of a Double Triple Bend Achromat (DTBA) Lattice for a 3 GeV Light Source, A. Alekou et al., Proc. IPAC 2016



Diamond-II



	Diamond	Diamond-II
Emittance	2700 pm	108 pm
Tunes H, V	27.20, 13.36	58.38, 22.30
Chromaticity H,V	-54, -90	-79, -123
Momentum compaction	1.7 10-4	1.1 10 ⁻⁴
Bunch length	3 mm	2.4 mm



Diamond-II

Full ring dynamic aperture and momentum aperture



- Dynamic Aperture of -8.5 +7.5mm, can accommodate the injected beam
- Momentum aperture of ~3% gives a Touschek lifetime of ~2.5h (300 mA 1 % coupling) without bunch lengthening

DTBA is a promising candidate for Diamond-II !

Electron beam sizes and photon phase space

Parameter (rms values)	Diamond	Diamond-II
Horizontal size, σ_x [mm]	123.5	23.6
Vertical size, σ_{y} [mm]	3.5	3.5
Horizontal divergence, $\sigma_{x'}$ [mrad]	24.1	5.1
Vertical divergence, $\sigma_{v'}$ [mrad]	2.3	2.3
Product	2.38 10 ⁴	9.60 10 ²
Electron beam brightness ratio	1	24.8

NB] with the same vertical emittance of 8 pm.

electron & photon horizontal phase space at 1Å

diamond





Brightness improvement with Diamond-II (120 pm)

Hard X-ray undulator

Soft X-ray undulators (APPLE-II for I05, I06, I08, J09, I10 and I21)



NB] this assumes the same vertical emittance of 8pm in Diamond-II brightness ratio = x 17 at 20 keV for emittance of 2 pm



Coherent fraction improvement with Diamond-II (120pm):

$$F = \frac{\lambda^2 / (4\pi)^2}{\sum_{x} \sum_{x'} \sum_{y} \sum_{y'}}$$

Hard X-ray undulator

Soft X-ray undulators (APPLE-II for I05, I06, I08, J09, I10 and I21)



The improvement in brightness/coherence is approximately a factor of x3 at 100 eV x10 at 1 keV, x12 at 10 keV, the main benefit coming from the reduction in horizontal source size



Note – effect of energy spread on the radiation brightness is increased for low emittance, with high harmonic numbers !



$$\mathbf{B} = \frac{F}{\sum_{x} \sum_{x'} \sum_{y} \sum_{y'}}$$
$$\Sigma_{x',y'} = \left(\boldsymbol{\sigma}_{x',y'}^2 + \boldsymbol{Q}_a^2 \boldsymbol{\sigma}_{R'}^2\right)^{1/2}$$
$$\boldsymbol{Q}_a(x) = \left(1 + \frac{2x^2}{\pi}\right)^{1/4}$$

 $x = 2\pi n N \boldsymbol{\sigma}_{E}$



Pinhole Flux

Smaller pinhole needed to collect the same fraction of flux:

- \rightarrow smaller mirror sizes, higher quality
- \rightarrow reduced power loading, better thermal stability



Flux through a 40 μ rad * 40 μ rad aperture for the CPMU in the existing ring (red) and in Diamond-II (black).

Impact of Diamond-II on Beamlines

- Several existing Bending Magnet beamlines can convert to Insertion Device beamlines.
- Some lower intensity beamline branches based on short ex-vacuum, Insertion Devices can move to longer in-vacuum IDs.
- New beamlines can be built without impact on existing beamlines.
- Higher brightness/coherence will provide more flux and/or better resolution for nanoprobe beamlines:
 - tender/hard Xray experiments at 10 nm resolution will become routine
 - challenging experiments with < 10 nm resolution will become possible
- Greater exploitation of coherence e.g. ptychography, CDI, CXRD, XPCS etc.
- For crystallography, higher brightness will lead to better signal to noise in diffraction data, higher throughput and increased use of microbeams.

diamond

😍 diamond

Impact of Diamond-II on Beamlines

Beamline Name and Number	Diamond II	Insertion device	0ptics	Detectors	Sample environments	Beamline Name and Number	Diamond II	Insertion device	Optics	Detectors	Sample environments	
Macromolecular Crystallography						Engineering and Environment						
102-1 - Versatile MX micro (VMXm)						111 - High Resolution Powder Diffraction						
102-2 - Versatile MX in situ (VMXi)						I12 - JEEP: Joint Engineering,						
103 - MX						Environmental and Processing						
104 - Microfocus MX						115 - Extreme Conditions						
104-1 - Monochromatic MX						115-1 - XPDF: X-ray Pair Distribution Function						
123 - Long Wavelength MX						Spectroscopy						
124 - Microfocus MX						108 - Scanning X-ray Microscopy						
B24 – Cryo Transmission						114 - Hard X-ray Nanoprobe						
Soft Condensed Matter				118 - Microfocus Spectroscopy								
B21 - High Throughput SAXS												
122 - Small Angle Scattering and Diffraction						120 - 101 A: Versatile X-ray Spectroscopy						
B22 - MIRIAM: Multimode InfraRed Imaging And Mircrospectroscopy						I21 - Inelastic X-ray Scattering						
B23 - Circular Dichroism						Materials						
Surfaces & Interfaces						113 - X-ray Imaging and Coherence						
105 - ARPES						116 - Materials and Magnetism						
106 - Nanoscience						B16 - Test beamline						
107 - Surface and Interface Diffraction						119 - Small-Molecule Single-Crystal Diffraction						
B07 - VERSOX: Versatile Soft X-ray												
109 - SISA: Surface and Interface Structural Analysis												
110 - BLADE: Beamline for Advanced Dichroism Experiments						KEY: NEW OPPORTUNITIES CLEA	R SCIENCE BENE	FIT MODI	ST BENEFIT	NO BEN	EFIT	



Comments from the Diamond Science Advisory Committee (April 2016)

"... there are major opportunities both for scientists to exploit the beam coherence and to improve the flux density and hence move to higher spatial, temporal or spectral resolution on beamlines (especially those already using micro-focussing) which exploit the brilliance of the storage ring."

"SAC agree with the conclusion of the upgrade document: that a major upgrade of DIAMOND Light Source, to achieve a source of radiation of much higher brilliance, is required in order to maintain the excellence of the facility ... and recommends that a decision on the trajectory towards an upgrade of DIAMOND is urgent."

Prospects for an Advanced FEL-based Light Source for the UK



Two Previous Proposals:

2006: 4GLS





Since then:

- Dec. 2014 announcement that UK will join European XFEL
- Mar. 2015 STFC started a Review of provision of FEL radiation for the UK:

FEL Strategic Review

STFC is carrying out a review to determine a strategy for the UK's Provision of Free Electron Laser (FEL) facilities.

The purpose of the FEL strategic review is to develop:

- a 15 20 year vision for UK FEL science;
- a 7 year strategy for FEL access, UK FEL facility provision, community development, and underpinning technology/skills.

The major focus of the review will be X-rays, but it will also examine the UK community's needs for lower energy machines and incorporate this into the strategy. The UK has committed to becoming a full member of the European XFEL facility (now under construction near Hamburg, Germany), and so this review will provide the framework for making decisions on any further FEL commitments the UK may make.

http://www.stfc.ac.uk/about-us/our-purpose-and-priorities/planning-andstrategy/fel-strategic-review/



FEL Review Summary

(as presented to STFC Science Board Feb. 2016)

<u>Needs</u>

"The UK needs to increase its investment in the XFEL.EU ...recognising that there will be the need for a UK facility in the future"

"In the long term, the UK's capacity requirements will be best served by constructing a UK FEL facility"

"Doing nothing is not an option. FEL science is advancing rapidly..."

Timescales

"STFC should be in a position to take the final decision on whether to build an X-ray FEL in the UK, and what kind of machine to build, in five years"

"The time taken form fully committing to the construction of a UK FEL facility to it being operational is likely to be at least six years. The final decision on whether to build an X-ray FEL in the UK and to what specification to build could be taken in five years, around 2020.



FEL Review Summary (ii)

(as presented to STFC Science Board Feb. 2016)

Type of machine

"In order to address the majority of the key science challenges, a UK facility would need to deliver hard X-rays.

To further broaden the range of science which could be tackled, the ideal machine would also have a high repetition rate. However, this is likely to be unaffordable as a national facility, so a best compromise specification will need to be defined to fit UK science.

This is expected to be an enhanced SwissFEL like facility: a high-energy non superconducting Xray FEL"



FEL Review Summary (iii)

(as presented to STFC Science Board Feb. 2016)

Location

"The UK has a unique opportunity to co-locate an X-ray FEL with the stateof-the-art ultrafast, high-energy and high-powered auxiliary laser sources currently located at the Harwell Campus.

This would equip the UK with world-leading facilities for creating and probing matter at extreme conditions, unmatched by any equivalent facility in the foreseeable future."











preliminary calculations by R. Bartolini, I. Martin, DLS



Desired enhancements / R&D topics:

- increased peak power (~TW) and photons/pulse (~10¹³)
- improve temporal coherence and pulse shape uniformity
- sub-fs / attosecond pulses
- two-pulse and two-colour operation
- reduce timing and wavelength jitter; improve laser & FEL synchronisation



FEL Review Summary (iv)

(as presented to STFC Science Board Feb. 2016)

<u>Actions</u>

"To prepare for this decision in five years' time the following actions are recommended in parallel with the development of the community:

- initiate a programme to define the specification that is required ...
- develop a fully coordinated FEL R&D programme...
- strategically plan the development of the skills base required to deliver the necessary technologies."

The UK FEL Community looks forward to a positive response from STFC !



Conclusion

Despite some dark clouds ... we remain optimistic for a bright future !





Thanks for Your Attention !

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