Hard X-ray systems progress

HXR Self Seeding
(V-pol, and extra degree of freedom)

XPP cryo-chamber (20K)
for time-resolved diffraction
Hard X-ray operations 18-24 keV

- **XCS**: femtosecond liquid-phase wide angle scattering extended up to 24 keV.

- **CXI**: femtosecond gas-phase wide angle scattering at high photon energy with enhanced UV excitation capability.

*Courtesy: Natan, Gaffney, van Driel*
L2S-I Update: ChemRIXS preparation, and TMO progress

TMO – successfully fielded 3 endstations:
- LAMP
- cVMI
- Magnetic bottle

4th system tested next month (MRCOFFEE)
L2S-I Update: qRIXS Spectrometer progressing well
1. **L2S-I Soft X-ray Imager down-select review** later this week for near-term deployment for REXS and XPCS in qRIXS.

2. Early **SparkPix-ED** prototype ASIC results are encouraging, with results now up to 1 MHz for initial electronics tests. Key rare-event 'information extraction engine' for experiment-specific detector toolkit, funded by SLAC LDRD.

3. **ePix10k** ASICs have been bonded to CdZnTe sensors (Ge in work) in support of the **BES Hi-Z Collaboration**.

4. First mock-up of the shingled ePix detector for TXI instrument.

5. LCLS-sponsored **MCP/Timepix** study to explore XFEL response and saturation behavior has begun reporting preliminary results, with several more geometries to test (Anton Tremsin @UCB/SSL).

6. A joint **Detector Calibration Team** with direct participation of LCLS detector scientists and TID detector developers now working for continuous improvement of calibration accuracy (e.g. ePix10k).
Introduction

Optical Laser Systems

High power laser system R&D
Wavelength conversion from UV to THz
Timing synchronization: pulse fiber timing system
Timing diagnostics: high sensitivity at high rate

Sample Environment & Delivery

Microfluidic Injector R&D: thin jet, hydrodynamical focusing, in-line anti-clogging filter, in-chip mixer.
Drop-on-demand sample delivery system
LCLS-II readiness: high rep-rate tests, sample damage, low sample consumption thin jets.

Beam Delivery and Manipulation

Beam transport: transient thermal mechanical modeling, high heat load optics design for LCLS-II
X-ray pulse manipulation: split-delay system design, dispersion control of femtosecond x-ray pulses, single crystal diamond optics, Nano diffractive optics
Optics for source development: seeding, cavity-based XFEL project, cavity optical layout design, cavity optics and diagnostics

New Experiment Methods

High throughput soft x-ray XES/RIXS: PAX
High sensitivity absorption spectroscopy using capillary optics
ML based new measurement modalities
IXS spectrometer design for LCLS-II HE
Outline

Laser and Timing
- OPCPA Production System and R&D system status
- OPCPA R&D update and PULSE lab collaboration
- Timing synchronization system update and next cross-correlator project plan
- First time tool results from TMO with attosecond pulses

Advanced Optics and Diagnostics
- Split-delay optics, amplitude-splitting system, and XPCS.
- SRW modeling of the LCLS-II HE DXS monochromator and X-ray Cavity
- Thermal mechanical modeling of crystal optics

Sample Delivery
- Quick review of past projects
- Drop-on-demand Roadmap and Project Status

Experimental Methodology
- Latest SSRL results on PAX for soft x-ray spectroscopy
- Polycapillary optics for XAS in the hard x-ray regime
- Examples of machine learning applications
OPCPA R&D System

• R&D project started in 2015 for LCLS-II Experiment Laser Delivery.
• 24/7 operation with minimal human intervention at 800 nm, 100 kHz, 1 mJ, ~16 fs.
• Final stage kW pump amplifier needs reliability improvement.
First ‘User Delivery’ System for LCLS-II Soft X-ray Instruments will be a 40W system. System assembly is underway in the ASC laser laboratory. Expected completion within FY21.

- Design based on R&D.
- Optical parametric amplification at 800 nm
- Single oscillator for both pump and signal
- 31 kHz – 1 MHz operation possible
- Pumped with 350 W Amphos Yb:YAG amplifier
- Compressed pulse duration: <20(15) fs
- >30 W output power
- 24/7 operation
- Upgradable to >100W at a later point
OPCPA R&D Activities Summary

Current R&D focus: nonlinear conversion stages to address the spectral ranges from UV to THz.

- Multiple conversion stages have low conversion efficiency and partially fail to deliver parameters for LCLS-II FY22 operation at 100 kHz and higher.
- Objective is to develop simple and robust methods with fewer nonlinear conversion stages, to deliver high power pulses in the entire range from UV to THz. We use current R&D and production system equipment for upgrades.

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<tr>
<td>1</td>
<td>Direct nonlinear compression of 1.03 µm (Yb:YAG amplifier)</td>
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<td>2</td>
<td>Infrared OPA pumped at 1.03 µm.</td>
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<tr>
<td>3</td>
<td>4-wave mixing of 1.03 µm and 0.51 µm in gas-filled capillary to replace harmonic generation in crystals (high power alternative for UV generation. Note: this is also beneficial R&amp;D for the LCLS-II photo-injector)</td>
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<tr>
<td>4</td>
<td>Soliton self-compression in gas-filled capillary of infrared OPA. Potential for direct 100-900 nm tunable range with high energy and ultra-short pulses.</td>
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spectral broadening and direct compression
hollow core capillary (25W input power)
tunable colinear OPA, towards mid IR via DFG
Applications and Collaboration with PULSE

Beam Transport to PULSE Lab

High harmonic generation beamline (XMAS collaboration with PULSE)
- The non-collinear OPA delivers short pulses <30fs
- Spectral broadening multi-pass cell
- Output power is ~30W (>40W, work in progress)

Applications: few cycle pulse generation with self-compression in multi-pass cell; soliton self-compression in gas-filled capillary for UV-VIS pulse generation; HHG for x-ray multi-edge absorption spectroscopy (XMAS)

Joint laser lab layout in the new ASC building

Additional dedicated R&D space as well as ‘endstation’ laboratory.
Overall Timing System Layout

New architecture based on Cycle™ pulsed-fiber timing system aims at delivering <10fs RMS stability across the near experimental hall.
System Installation and Cross Correlator R&D

- Optical Master Oscillator (OMO) installed and performing well within spec.
- Out-of-loop motorized delay lines (OL-MDLs) installed and aligned.
- Timing jitter of 2 links against each other: \( \sim 0.7 \, \text{fs (rms)} \); Drift: \(< 1 \, \text{fs (rms)}\) over 8 hours
- Full characterization expected over upcoming months before moving system to NEH.

**Next Major R&D Activity**: direct cross correlation between pulse train from the fiber to the x-ray beam.

- Cycle proposed using their SOPRANO platform to boost PFTS output to 5 uJ pulse energy at 1 MHz rep rate.
- Amplifier section can be actively timing stabilized.
- Cycle currently investigating possibilities and limitations.
- Will investigate suitable target and required feedback bandwidth etc.
Arrival Time Monitor Sensitivity Improvement

- R&D aims at delivering increased sensitivity to low x-ray fluence, critical for sub-10 fs experiments.
- First ATM signal and timing correction for XLEAP pulses.
- In-house grown targets (MOCVD @SNF) alone provided a x10 boost of sensitivity.
- Interferometric probing implementation to be tested.

**400 - 500 eV X-ray**

**10s of μJ pulse energy**

**2 x 3 mm beam FWHM**

**Next Steps:**
- Better understanding of the cause of target damage, improve damage thresholds.
- Understand the performance at high repetition rate (response recovery).
- Develop diamond-based transmission type targets for hard X-ray applications.
Split-Delay Over the Years

**2011-2015**: Fixed energy design. Takes many days to complete alignment.

**1st DESY SD prototype**

**2016-2018**: LCLS IH design and commissioning of a variable energy system. <30min alignment, < 1 urad and < 1 um stability. Unable to scan, limited profile similarity.

**XCS SD rebuild**

**2018**: All-channelcut design enabling fly-scan with 100nrad and 100 nm focus stability, limited mutual coherence.

**Compact all-CC system**

**2020**: dispersion compensation + amplitude splitting: sub-100 nrad stability and high degree of mutual coherence at the same time.
Approaching the Pulse-Twin Requirements for XPCS

- Combination of transmission grating beam splitter and channel-cut crystal delayline resolved the stability and beam similarity challenge at the same time.

- Prototype provide bandwidth <0.4 eV, delay time range ~10ps at 10keV.
Almost identical looking small angle speckle patterns indicating high degree of mutual coherence between the two foci. (a) fixed-delay branch. (b) delay branch. (c) both branches.

Delay scan showed a little bit of pointing hysteresis. Positive direction showed nearly flat contrast response.

Overall ‘overlap factor’ dropped only about 10% over the 10ps delay scan range. This provide a solid baseline for observation of dynamics induced decorrelation within this time window.

Science application to follow in two experiments the coming summer.
The Monochromator System for DXS at LCLS-II HE

**Background:** high resolution monochromators at synchrotron sources have not considered pulse duration preservation in the past.

**Requirement:** rethink the monochromator design process including time domain considerations!

**Resolution vs. photon energy**

- FT-limited, tunable pulses. Design allows variable pulse duration and corresponding energy resolution.
- Large operation energy range enables RIXS at all transition-metal K-edges, and 5d L-edges.

At 18 keV, the preliminary design estimates ~3 meV with 50% efficiency. More careful exploration of the parameter space may lead to further improvements.

*This is the current baseline design for the DXS instrument of LCLS-II HE. We need to support more detailed system level performance modeling under HE and future source beam loading conditions.*
Beam propagation modeling of the DXS monochromator system has been now adopted to run on NERSC. Memory CAP currently at 750GB, allowing simulation up to 3eV total bandwidth for this system.

Currently finalizing modeling result by cross-validating with a few alternative local code.

Next steps are modeling the misalignment parameter space in order to define system engineering requirements and to include SASE input for performance estimation.

Thermal mechanical deformation will be included in the next step simulation as well.
A rectangular x-ray cavity was built and tested at the X-ray Pump Probe instrument at LCLS. This is an early demonstration of the optics feasibility, as well as an opportunity to test/refine the alignment procedure.

Cavity was aligned down to <500 nrad precision, limited by available mechanics, with 3 meV energy accuracy. Cavity loss modeling indicate good crystal quality. Impact of input beam jitter is currently being investigated in detail.
• **Challenges of the LCLS-II HE beam:** high peak power, the single shot XFEL introduces non-uniform temperature change, leading to non-uniform thermal stress. The non-uniform thermal stress generates elastic waves

• **How to model it:** both heat transfer and the elastic waves can be modeled by Finite Element Analysis (FEA). Commercial tools (ANSYS, COMSOL) are being scaled up to run on SLAC clusters to include full crystal in the model and increase spatial/temporal resolution.

• **How to measure it:**
  - Locally persuing 2-bunch-type x-ray pump x-ray probe characterization with wavefront sensor to obtain the required calibration data.
  - Collaboration with EuXFEL where long bunch train studies with crystal optics.
Sample Delivery R&D Overview

Gas accelerated thin sheet jet, for soft x-ray spectroscopy and scattering experiments at UED.

Feasibility study of droplet injection on demand for sample consumption reduction.

Standard multi-functional chip format for streamlined and robust operation.

In-chip mixer, from handmade prototype to 3D printed production on chip format.
Drop-on-Demand: R&D Goals

**Near-Term Goals:** enable broadband at-atmosphere sample delivery for biology and chemistry scattering experiments by

- significantly reduce sample consumption compared to current methods
- automate liquid phase sample handling and delivery
- improve photon usage by increasing sample hit rate and reducing down time

**Mid-Term Goals**

- expand the range of liquid phase spectroscopy and correlation spectroscopy experiments
- develop fast mixing capability, hard X-ray spectroscopy on timescale of 100’s µs and longer

*Preliminary study:* drop stability in space/time sufficient across a large range of sample parameters.

*Next Step:* procure customized system that is compatible with the MFX instrument, optimize workflow for SFX and trWAX experiments.

*Commercial system From Scienion.*

*Customization for beamline deployment*
2021: LCLS Run 19, MFX first trial

2022: Test deployment in Run 20/21 for rapid sample screening program

2022: standalone trial operation.

2023: LCLS Run 22 SFX/trWAX routine user deployment

2023-24: Beyond run 22, broader deployment at additional LCLS Instruments. Spectroscopy at TXI

2024+: development of higher repetition rate, in-vacuum delivery, broader sample compatibility, crystal-on-demand, fast mixing, tighter integration for continuous unmanned operation ...

* Current scope focuses on near term deployment and optimization of ambient pressure systems. In-vacuum droplet delivery will be addressed most likely in parallel by a separate project at a later point.
The PAX spectrum is a convolution of RIXS spectrum and converter response.

Incoming x-rays, well defined in energy

Au converter coated Aluminum filter: convert photon to electrons & block Auger/secondary electrons from the sample

Scattered x-rays, over a range of energies

Hemispherical electron analyzer

Sample to be measured

Electrons

SSRL BL13-1 Installed in Feb. 2020

- Procure the most efficient electron spectrometer on the market for this project (Scienta-Omicron EW4000)
- Extensive testing at SSRL BL13-1 to maximize the count rate

Resolution
- At the moment it is feasible to carry out RIXS measurements with ~0.6-0.7 eV resolution throughout the soft x-ray range, using the 4f lines of Au.
- The resolution is dominated by the natural width of the doublet lines, ~0.5 eV, with typical beamline and spectrometer resolutions of ~0.2 eV.

Path forward & Applications
- Currently the limiting factor is the throughput of the hemispherical analyzer (1/1000 transmission). This limits the possibility to use the Fermi edge as the PAX ‘converter’.
- A massive improvement can be achieved with momentum microscope analyzers, combining the HSA and TOF.
- Surface science spectroscopy: straightforward to incorporate.
- Liquids: need to overcome challenges with relatively high pressure.
- Solids: high throughput XAS in PFY mode, similar to TES.
Jitter correction for pump/probe and mixing-jet experiments

Zhen Su, Chuck Yoon, et al.: diffusion map method able to filter the diffraction patterns and correct effective delay time for mixing type protein crystallography experiments.

Adopting ML software/hardware ecosystem for temporal reconstruction

Ryan Coffee et al.: Edge AI driven ‘cookie box’ data extraction and reduction is being developed to reduce Tbps data stream to Mbps ‘information stream’.
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High sensitivity absorption spectroscopy using capillary optics
ML based new measurement modalities
IXS spectrometer design for LCLS-II HE

Welcome comment from the SAC on overall program balance, approaches of specific areas and projects, suggestions on potential new impactful areas.