

XRD Breakout Summary

Experiment types

- Liquid Phase Scattering
 - Molecules
 - Nanocrystals
 - Anomalous option
- Single crystal diffraction
 - Bulk
 - Thin films
 - Bragg, diffuse
 - Resonant diffraction
 - GID
 - Laue
 - Proteins
- Reflectivity
- Powder
- Gas phase
- Amorphous solids
- Single particle imaging?

Experiment types: XFEL specific challenges

- Reversible vs. irreversible processes
 - Sample replacement
 - Burst mode
- Possibilities for multi-color XFEL experiments
 - X-ray pump/probe
 - Stimulated Raman

Beam parameters

- Energy tuning:
 - Non-resonant scattering: high energies
 - Liquid phase wants about 20 keV (as much as possible)
 - Global fundamental tuning range 4-14 keV for resonant or anomalous scattering seems OK.
 - No plans for “fast” (< a few minutes) tuning
 - ~10 eV range of tuning for resonant diffraction
 - ~100 eV for anomalous scattering
- Bandwidth
 - 0.08% BW acceptable for amorphous scattering
 - 0.015% BW for resonant diffraction
 - Increasing BW very useful for Laue (> 1%)
 - 10^{-6} harmonic rejection OK

Beam diagnostics

- LCLS “baseline” is 10^{-3}
- Diffuse scattering (liquids, amorphous, etc.):
 - 10^{-4} (or 10^{-5}) desirable for scaling shots
- Should be “just before” sample
- Slits: lower intensity & more intensity fluctuation, but better position stability
- May be able to use “total integrated” scattering for some experiments
- Need for accurate spectral characterization for liquid scattering
- Heat load effects in burst mode on monochromator?
- Angular stability better than 0.1 mdeg
- Time stamping: < 100 fs (or < 10 fs)

Sample environment

- Pre-alignment station for “next” experiments
- Cryo-jet
- Goniometer with cryostat (solid state samples)
- Heavy-duty alignment stages
- Sample refresh mechanism for solids
- What is facility provided? What is user provided?

Consortiums?

The “pump”

- Far-IR to UV range
- Intense THz
- Space to “roll your own” (OPA, NOPA, etc.)
- Electrical & magnetic pulses
- Optical pump-probe at same time (sample accessibility)

Detectors

- Linearity: $\ll 1e-3$
- Liquid scattering: LPD acceptable
- LPD may be OK for some Bragg-type experiments if detector moved back
- I-D with higher resolution (~ 100 micron) useful for “single shot” GID experiments
- Data analysis tools on-site & on-line

Miscellaneous

- Burst mode:
 - May be useful at lower rep rates for “long time” dynamics (esp. proteins)
 - ~40 kHz OK for some experiments (~10 pulses)