

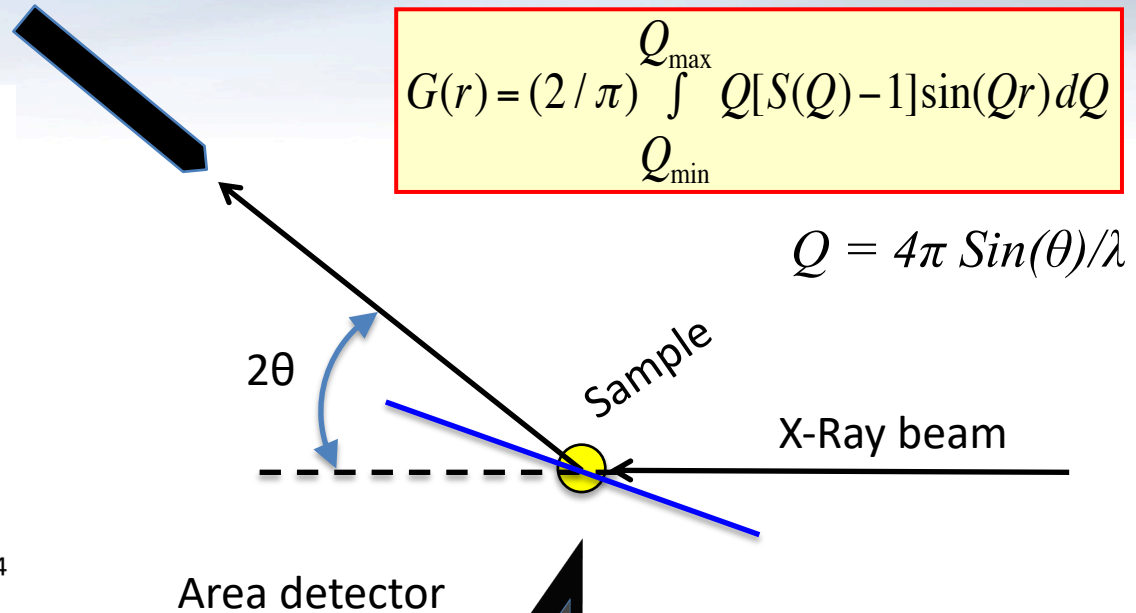
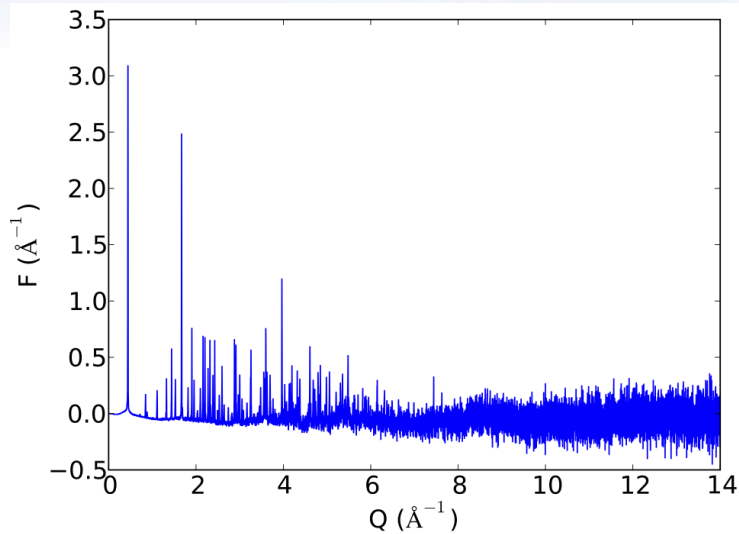
X-PDF Experimental Setup & Data Reduction Work-flow

M. Abeykoon
NSLS-II PDF School 2018

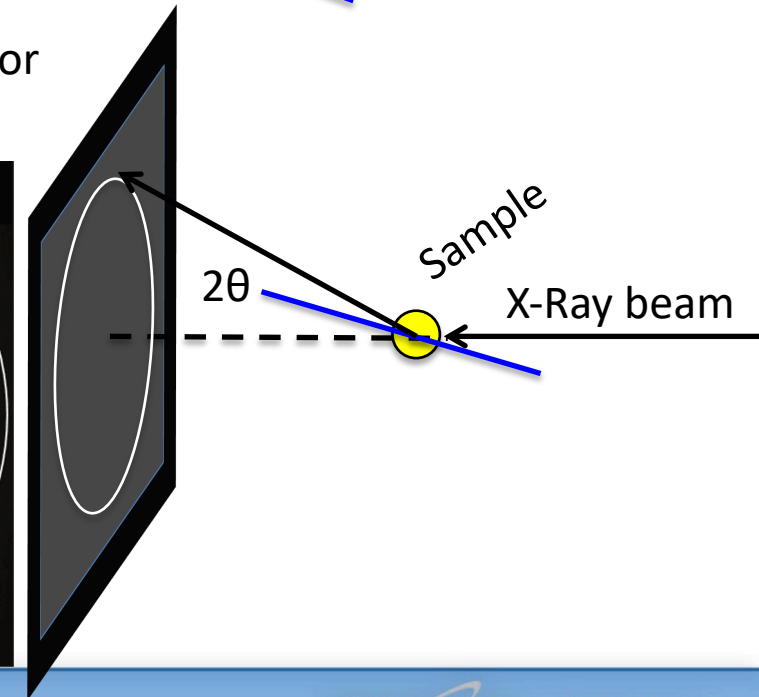
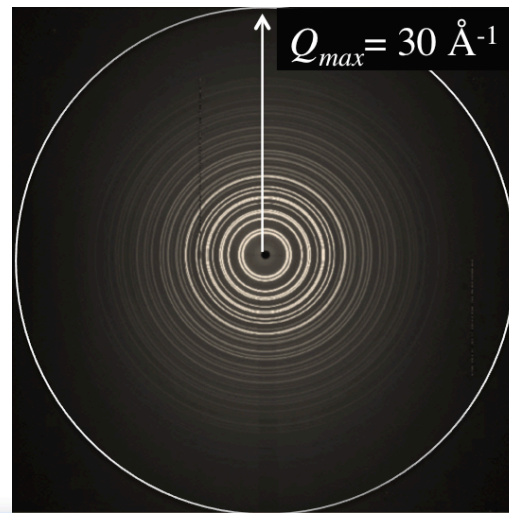
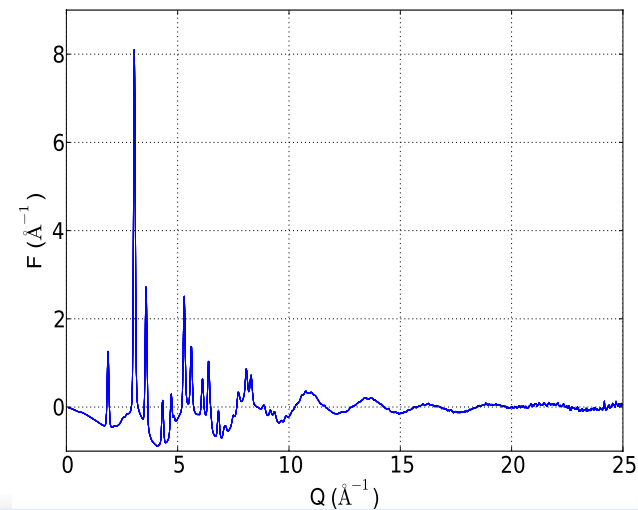


Point vs Area Detectors

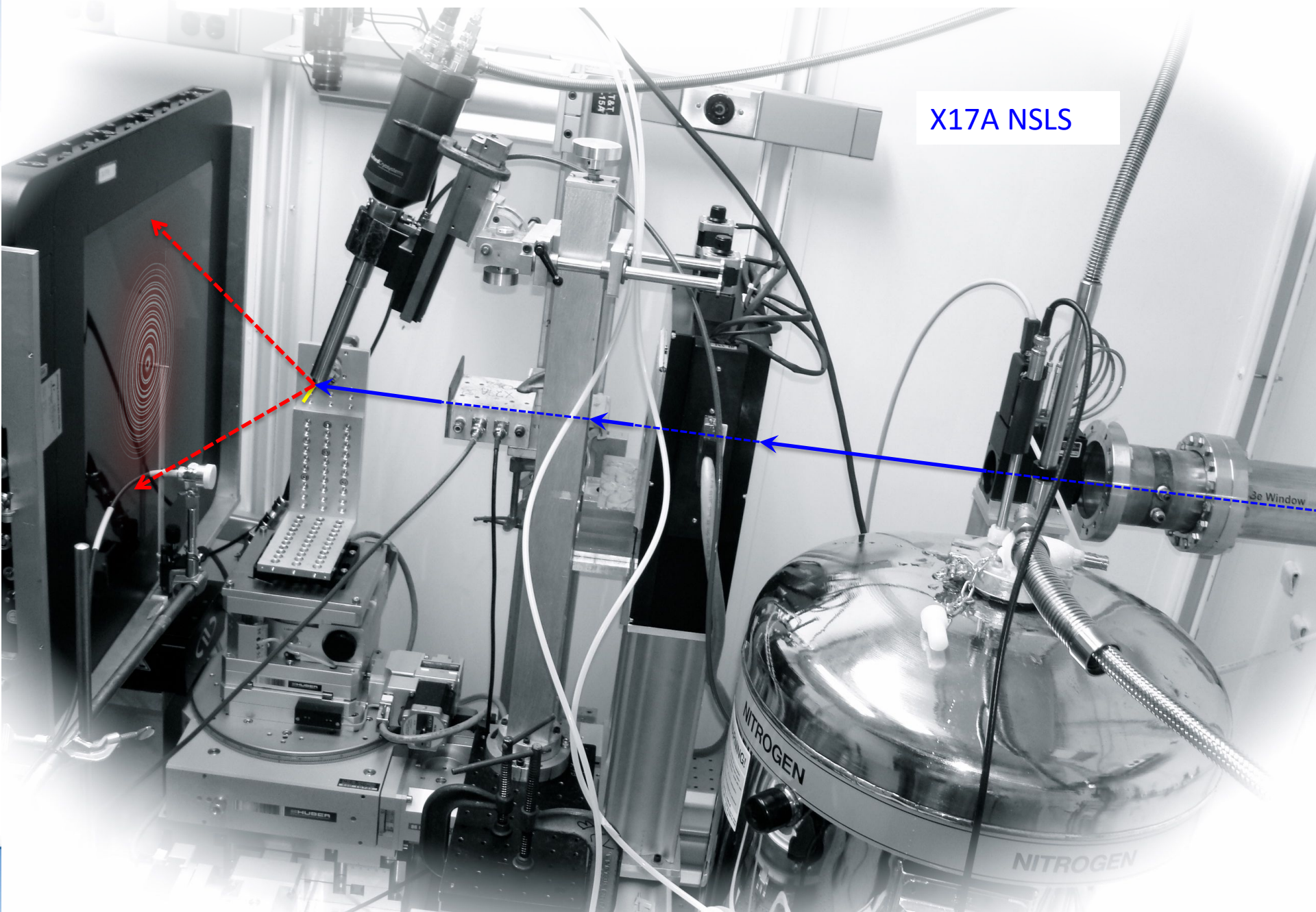
Point detector



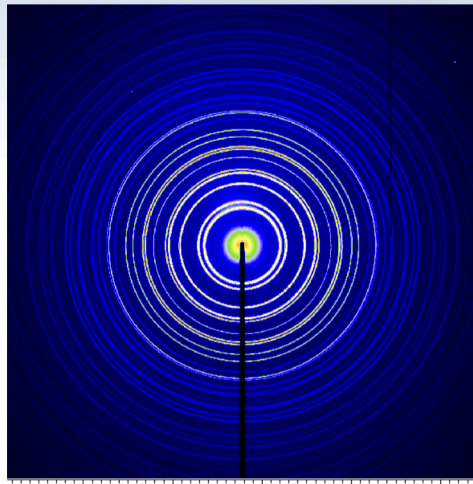
Area detector



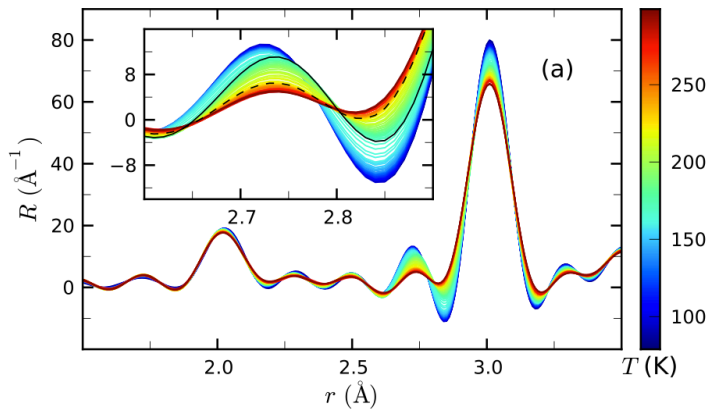
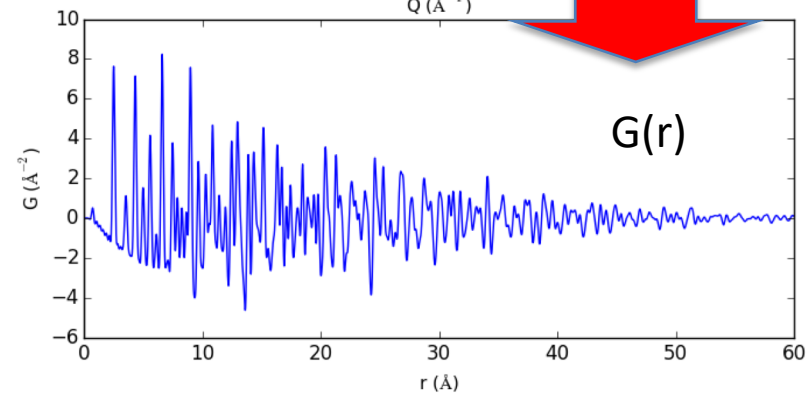
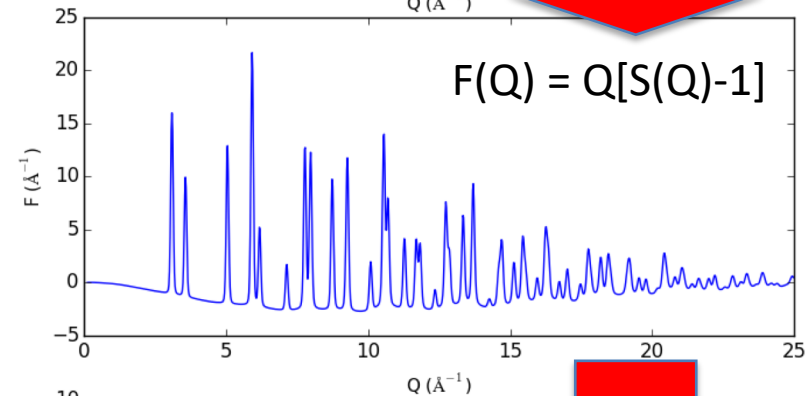
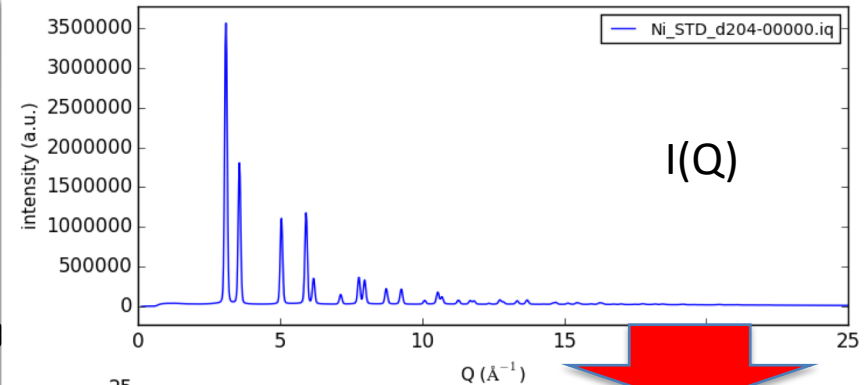
PDF experimental setup



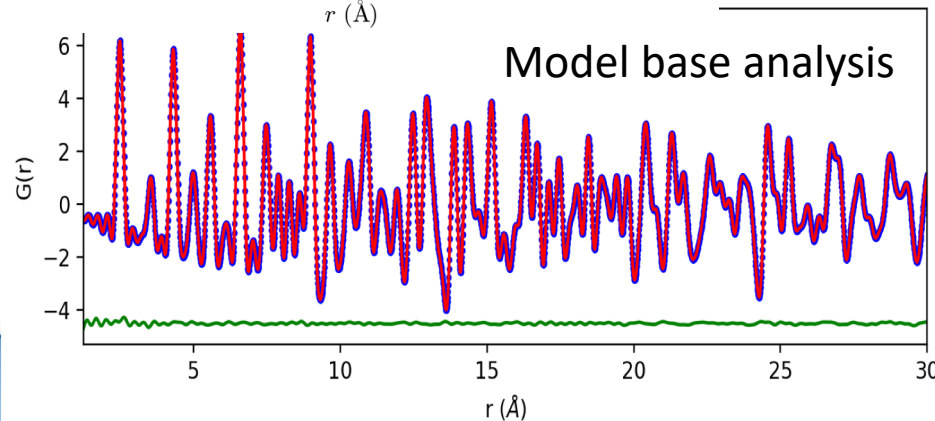
Data reduction workflow



2D → 1D

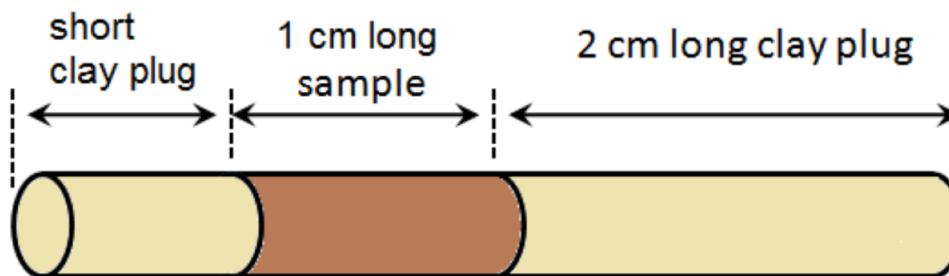
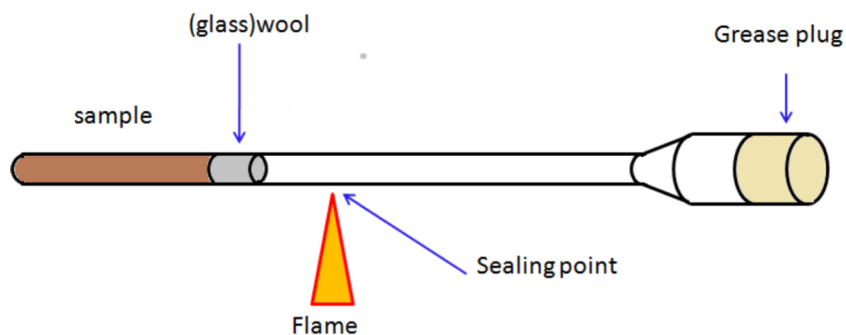


Model independent analysis

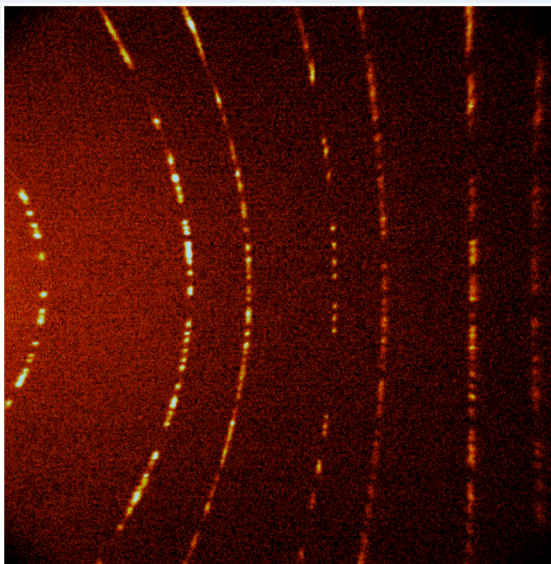


Sample Types and environments

Capillaries filled with powder



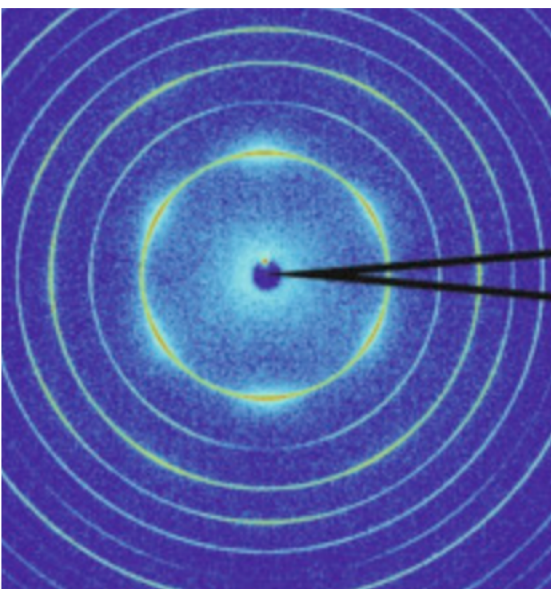
Sample Types and environments



What to avoid when using capillary samples

1. Bad powder average: When there are not enough crystals oriented in all directions diffraction patterns become grainy.

- Pack the sample well
- Grind the sample well
- Spin the sample
- Use area detectors and integrate the entire ring

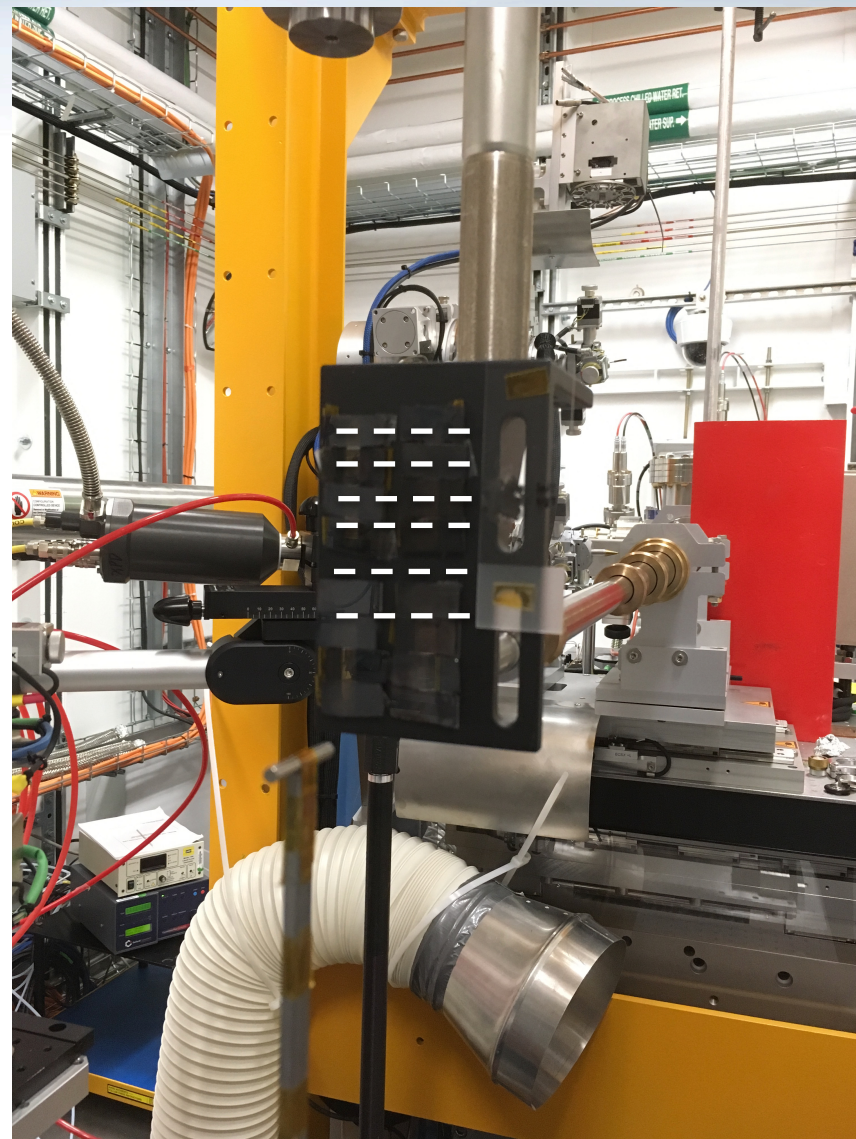
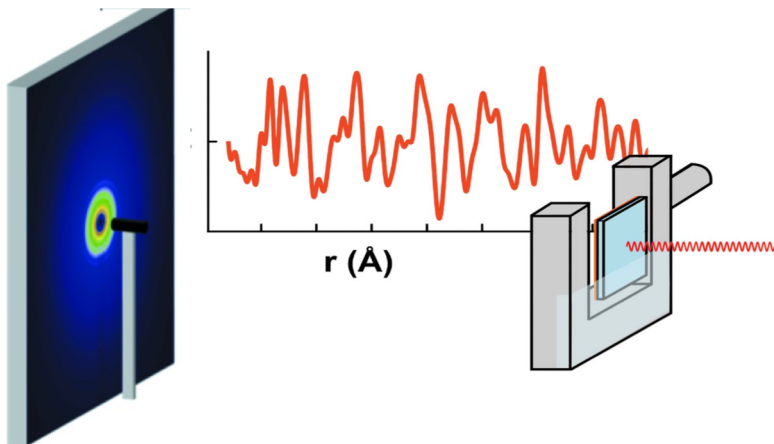


2. Preferred orientation: When powder particles in the capillary prefer to pack in certain direction (Ex: needle shape particles along the walls of capillary) certain rings become more intense than other rings.

- Loosely pack the sample
- Use a foil to vibrate the capillary to break preferred orientation

Sample Types

Polycrystalline thin films



Sample Environments



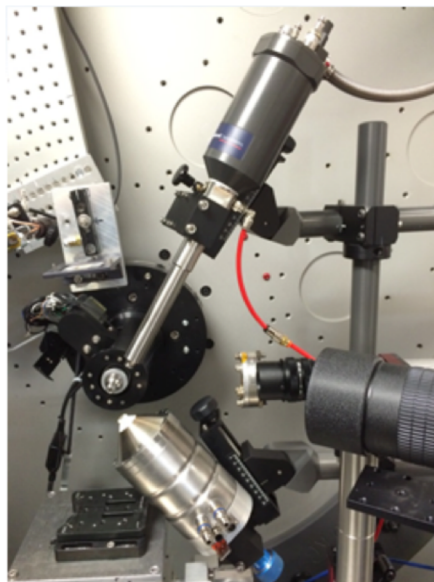
(80-500) K LN2
cryostream



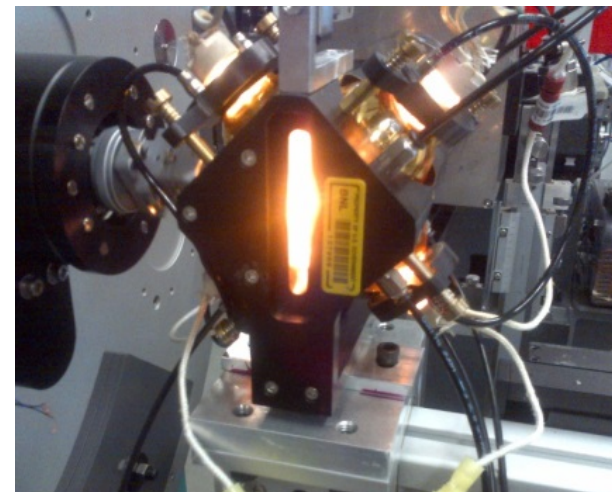
(0-5) T
Superconducting
magnet



(5-500) K Liquid
He cryostream



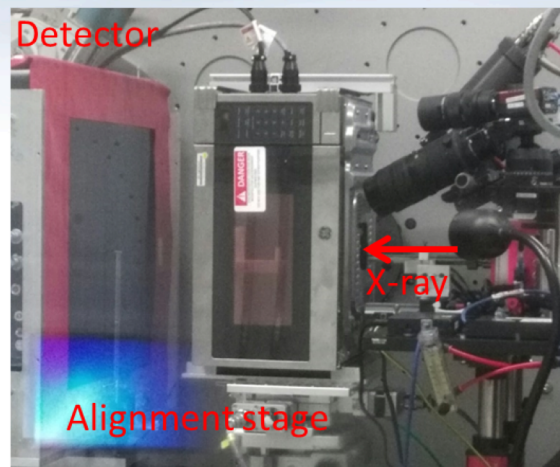
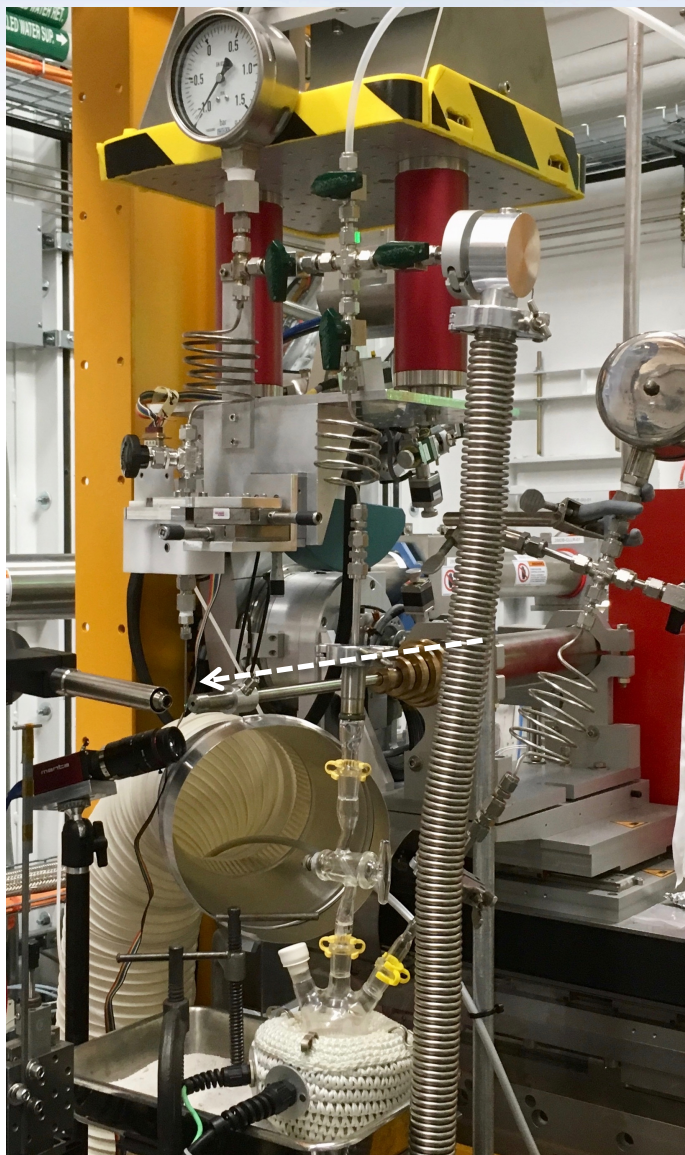
Hot air blower



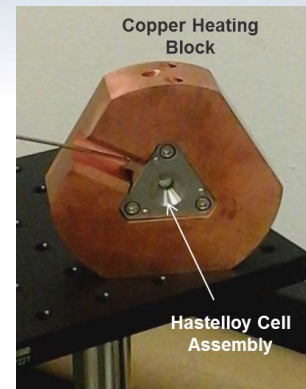
Quadruple Lamp Furnace
(2000°C)

Sample Environments

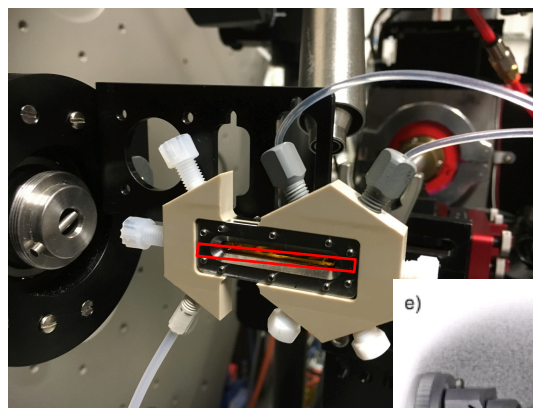
Custom reaction cell



Microwave reactor

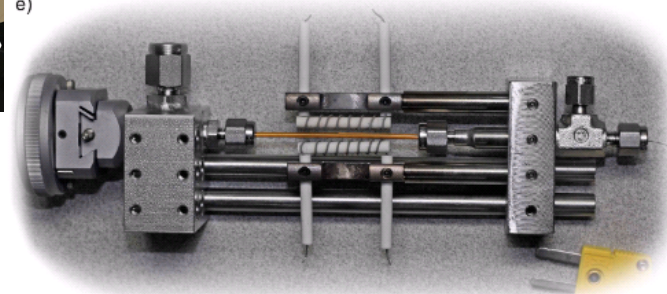


Oxidation/corrosion chamber
(steam at 400°C and 1,500 psi)

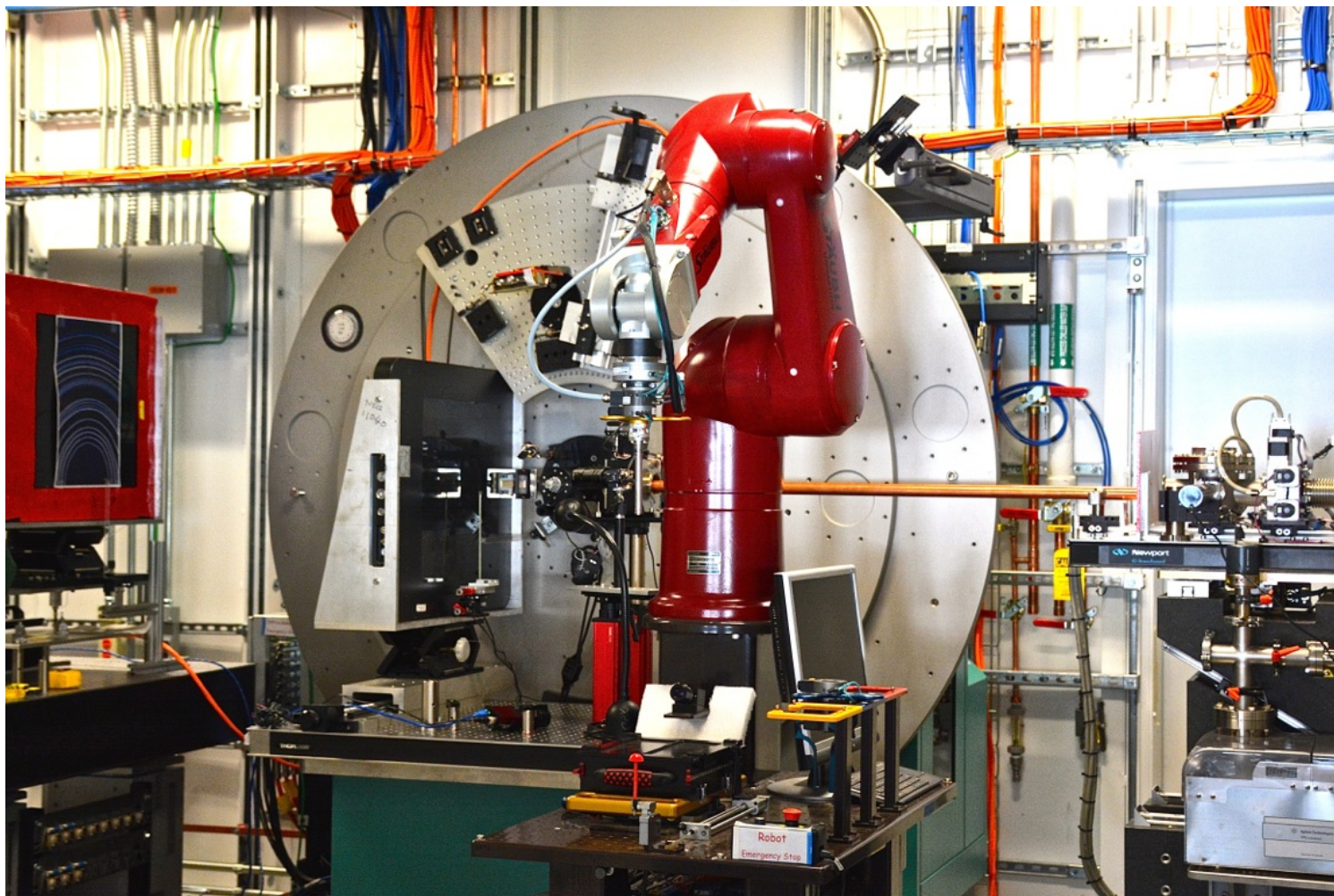


Multi-Solvent
Liquid reaction
cell

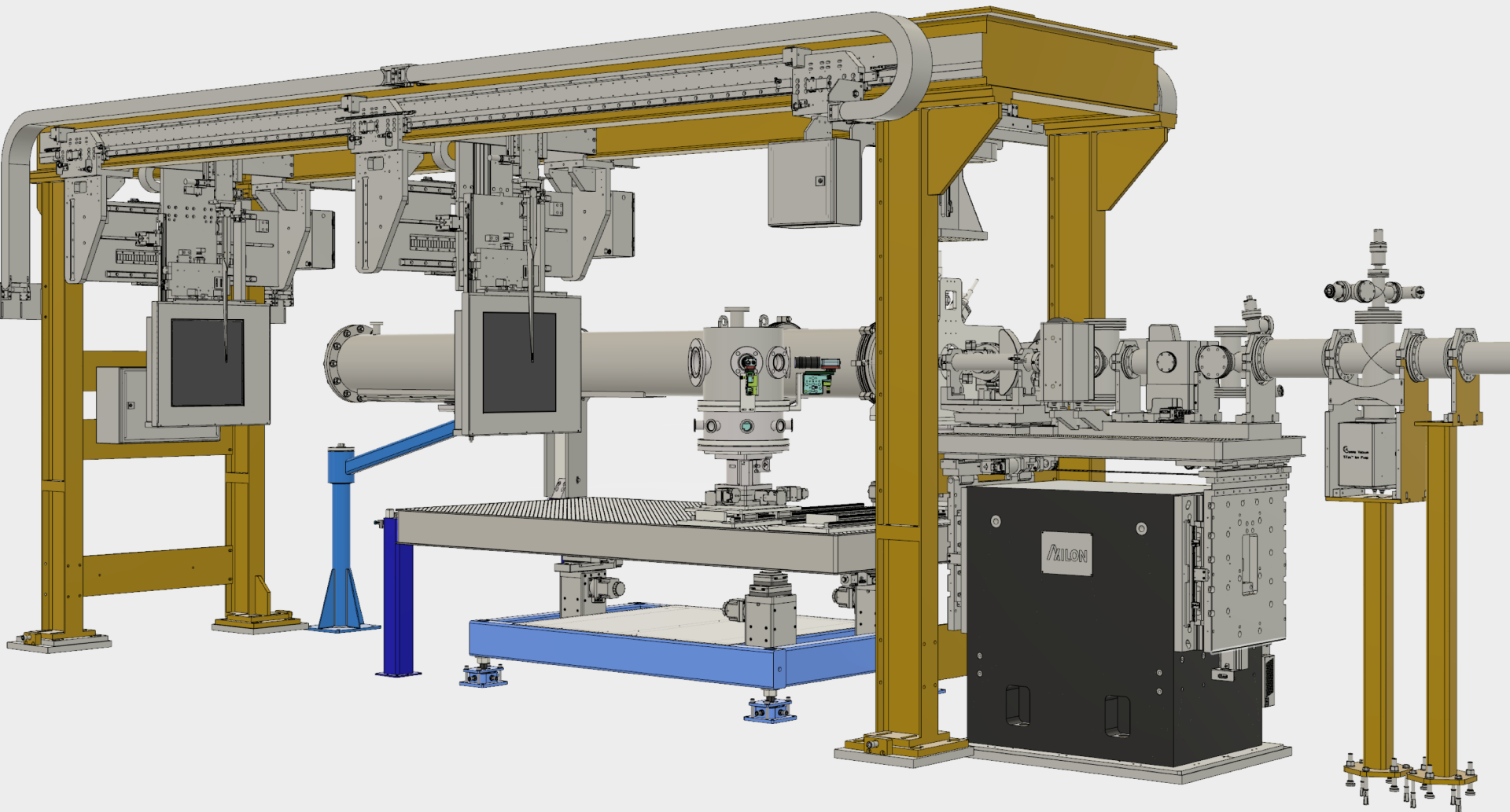
Gas flow cell with
resistive heater (800°C)



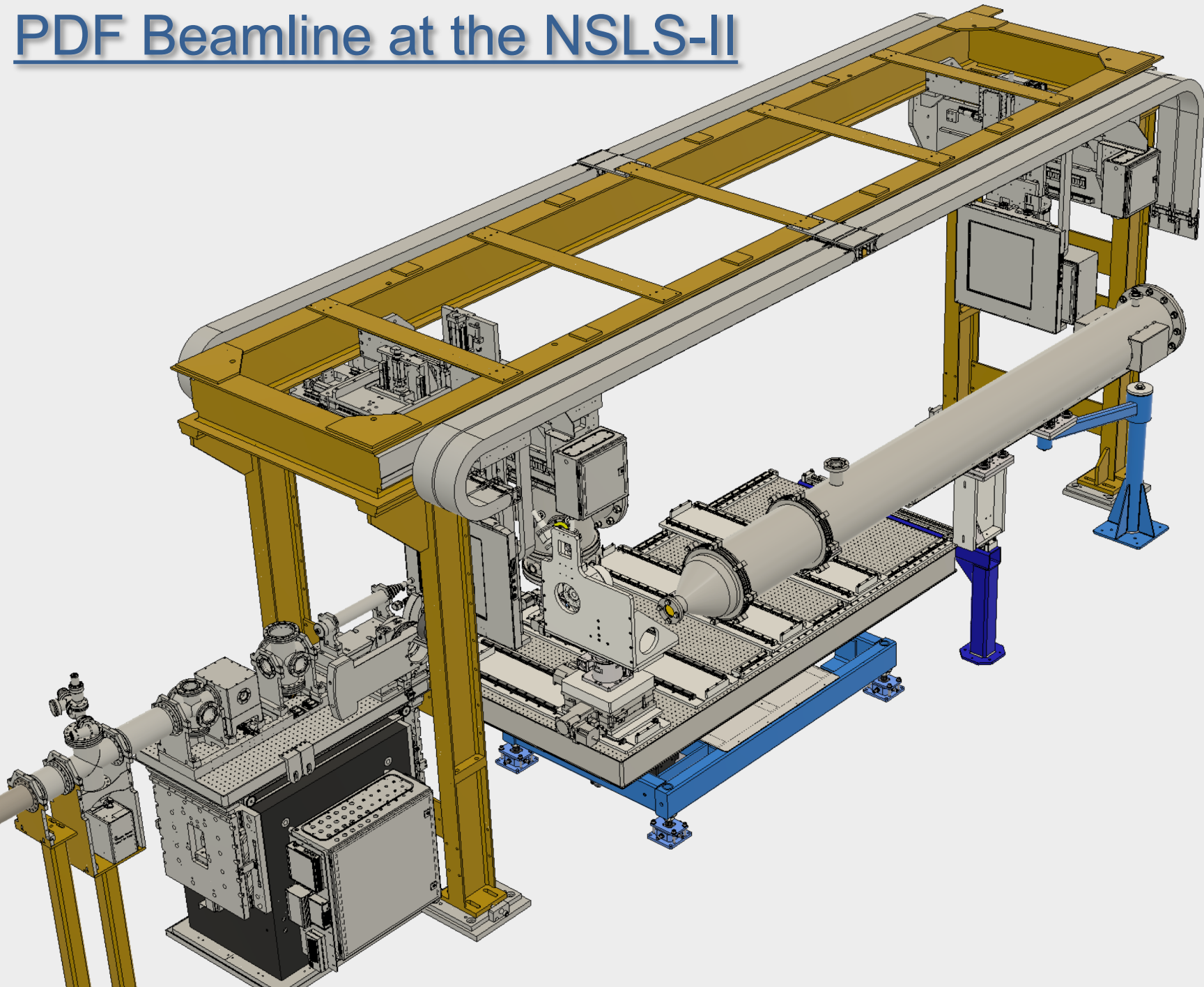
XPD Beamline at the NSLS-II



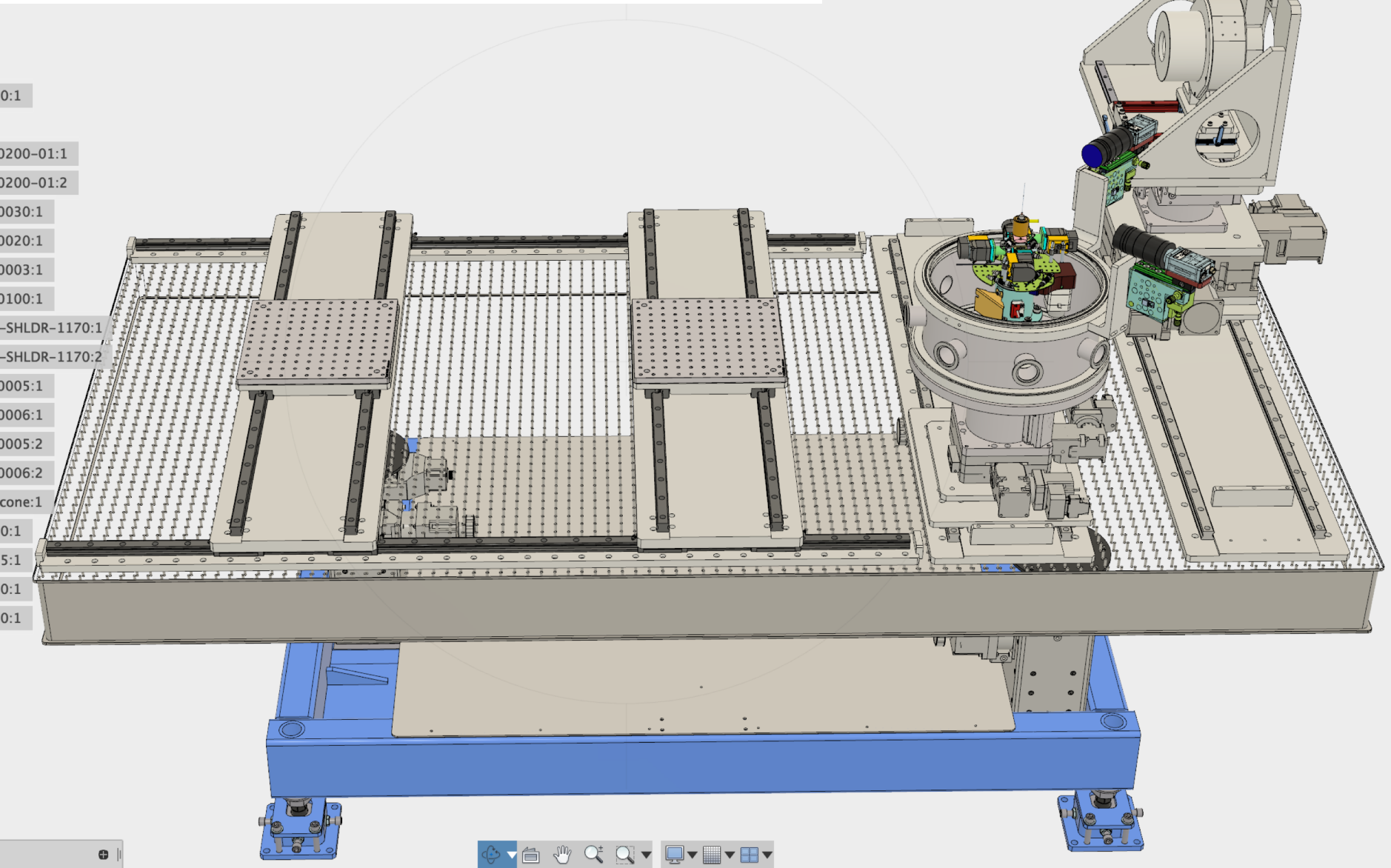
PDF Beamline at the NSLS-II



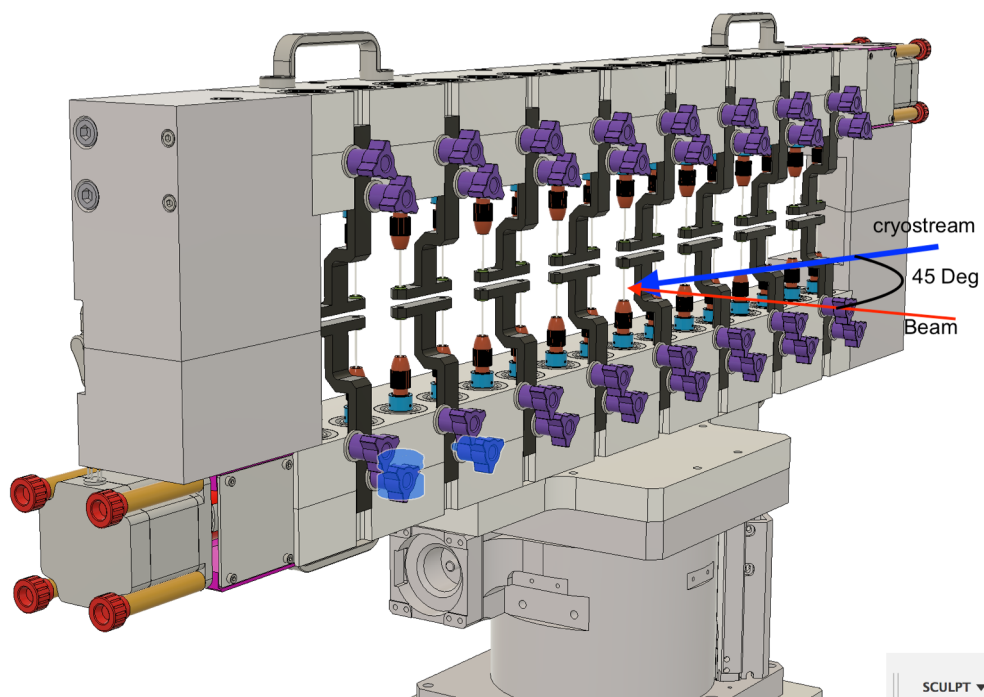
PDF Beamline at the NSLS-II



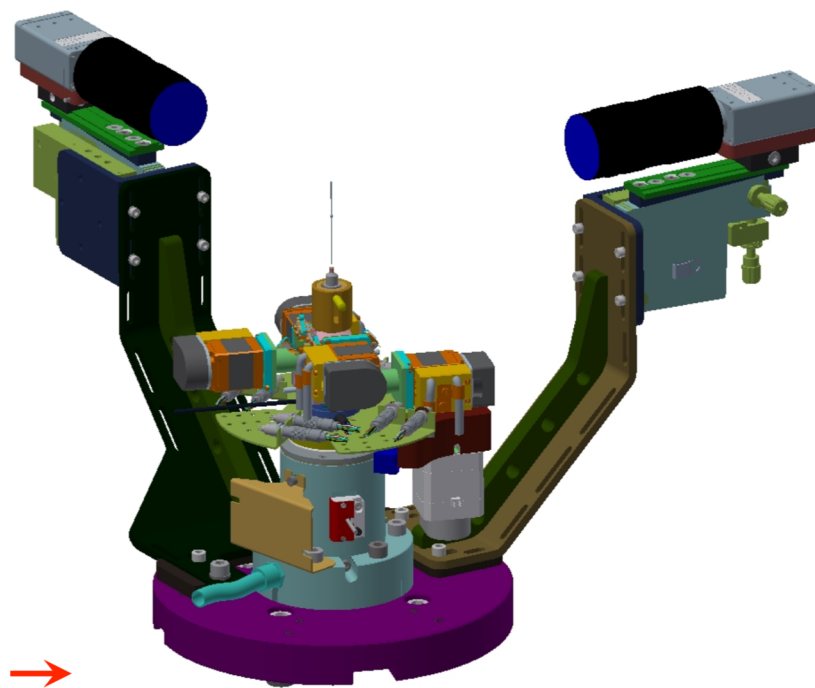
PDF Beamline at the NSLS-II



PDF Beamline at the NSLS-II



Multiple sample spinner



Automatic sample alignment system