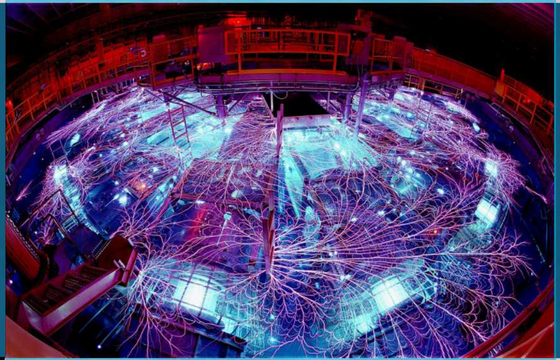
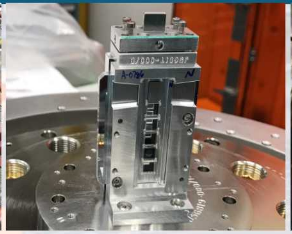
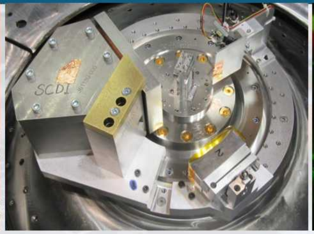
Sandia National Laboratories

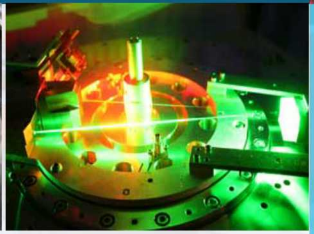
SAND2020-7806C

Status of x-ray diffraction of dynamically compressed matter on Z









PRESENTED BY

Tommy Ao, Marius Schollmeier, Patricia Kalita

Z Fundamental Science Workshop, Albuquerque, NM
August 3-4, 2020

U.S. DEPARTMENT OF ENERGY NNSA

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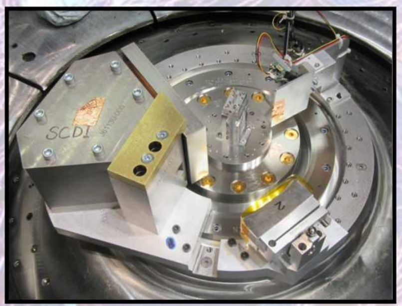
Outline

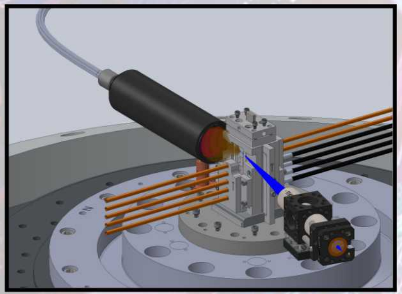
Background

- Z-Accelerator and Z-Backlighter capabilities
- Challenges of x-ray diffraction on Z



X-ray Diffraction on Z

- Spherical crystal diffraction imager
- Recent results



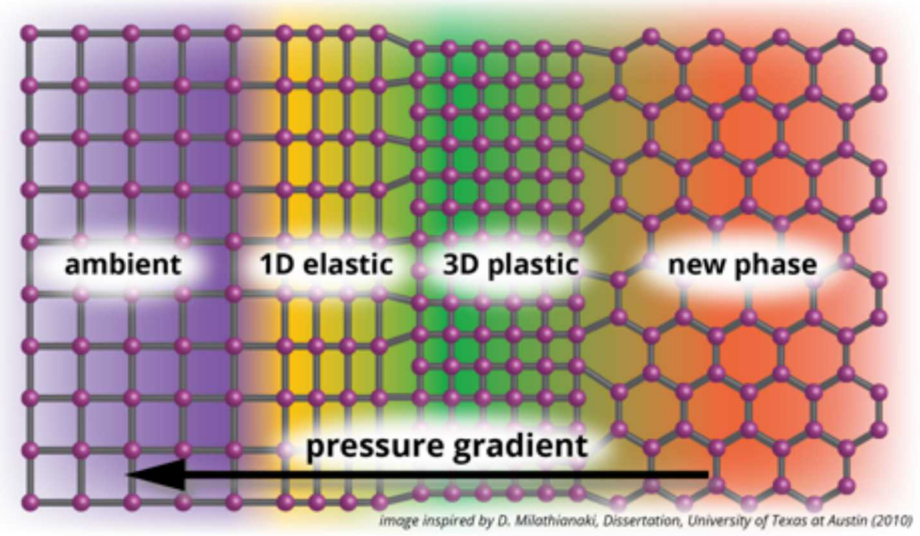
Future Developments

- Time-gated -ray diffraction detector
- X-ray sources

X-ray diffraction to infer dynamic material properties

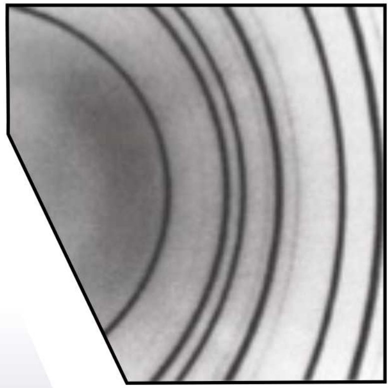
Goals

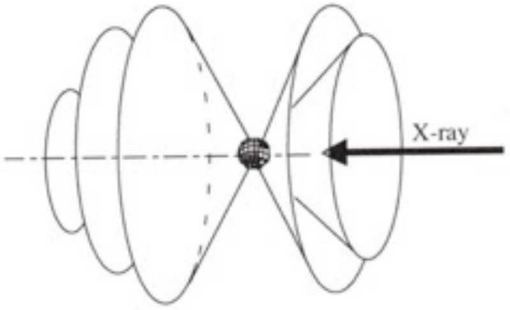
- Characterize both phase transitions and their kinetics that occur in dynamically compressed condensed matter on ns time scales and nm spatial scales
- Determine at atomic scale how materials behave under extreme pressure & temperature conditions; velocimetry gives only continuum scale information



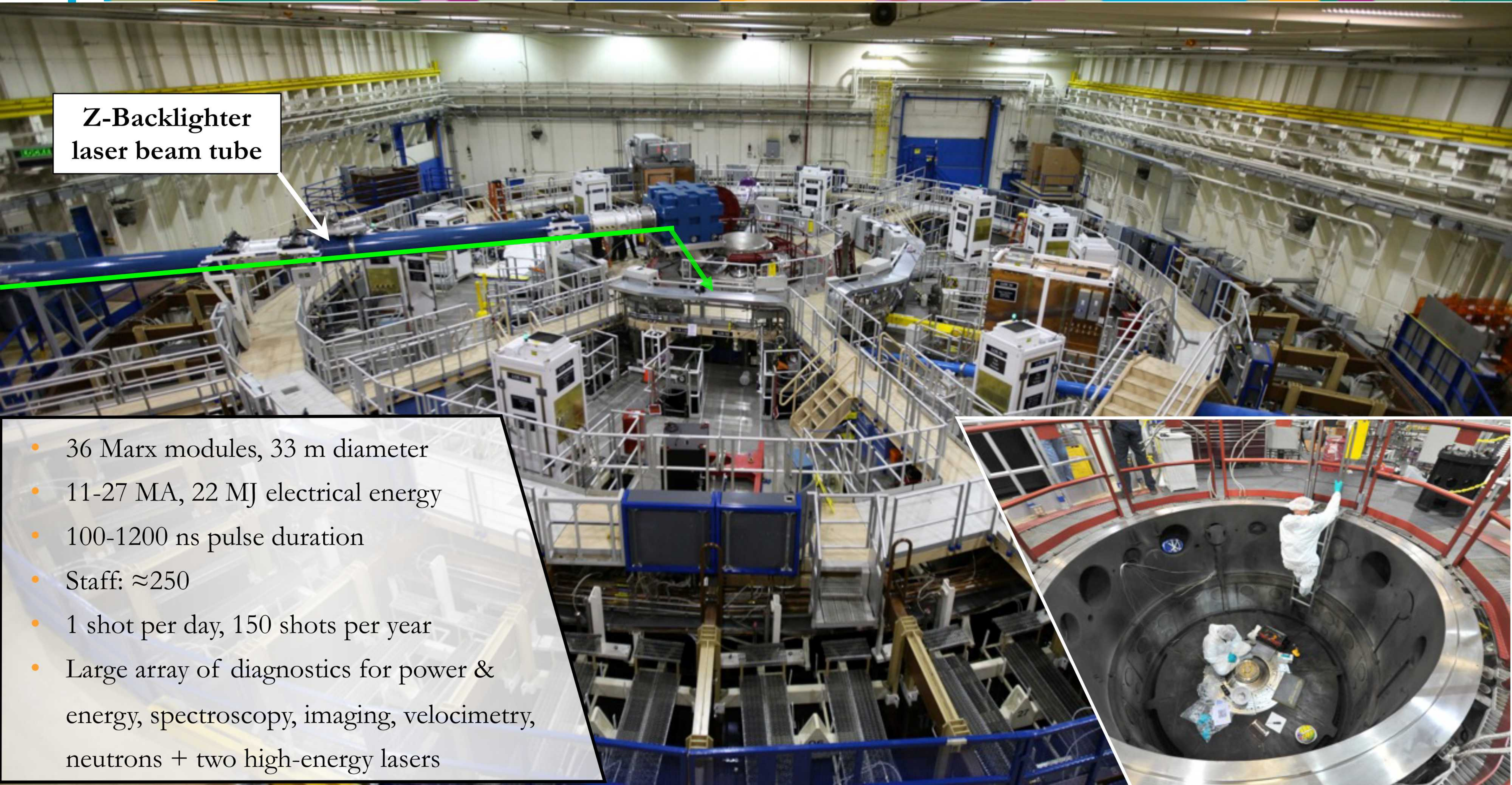
Approach

- Produce source x-rays with ZBL/ZPW laser
- Generate high-pressure state with Z-DMP load
- Detect diffracted x-ray pattern





Z Pulsed Power Facility for HEDP research

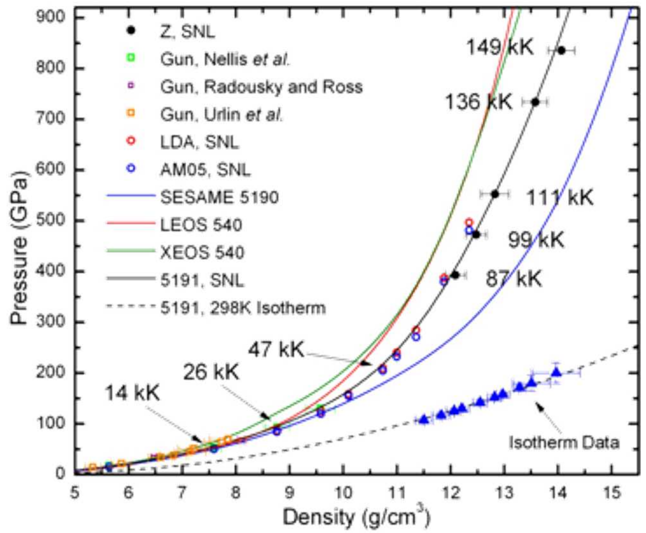


- 36 Marx modules, 33 m diameter
- 11-27 MA, 22 MJ electrical energy
- 100-1200 ns pulse duration
- Staff: ≈250
- 1 shot per day, 150 shots per year
- Large array of diagnostics for power & energy, spectroscopy, imaging, velocimetry, neutrons + two high-energy lasers

Z can perform both shockless and shock wave experiments

Z creates high pressures without directly heating materials:

- Long time scales (100-1200 ns) with control over the time history
- Large samples (cm): HED conditions for volumes ≫ sample grain boundaries dimensions
- One Z-DMP (Dynamic Materials Properties) experiment can field 6-20 samples

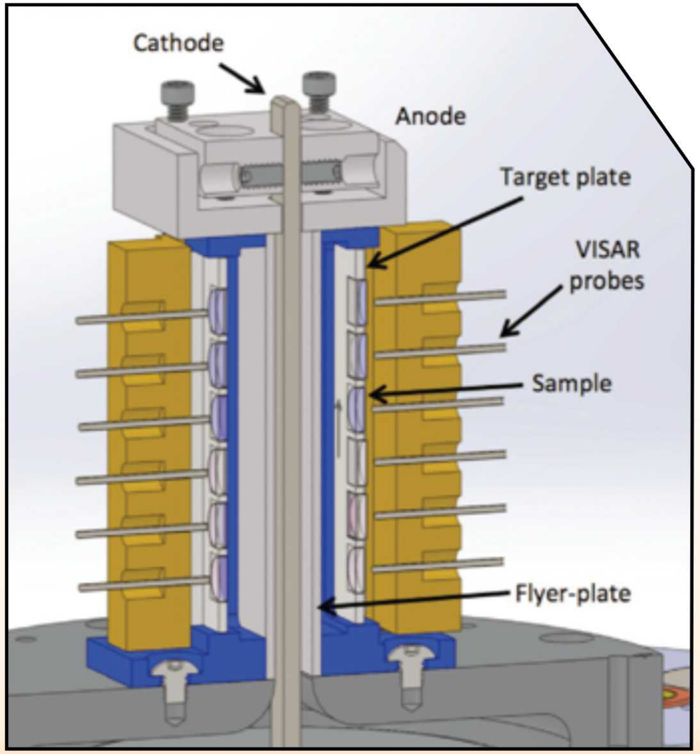


P-ϱ Hugoniot plot of Xenon*

Key physics questions:

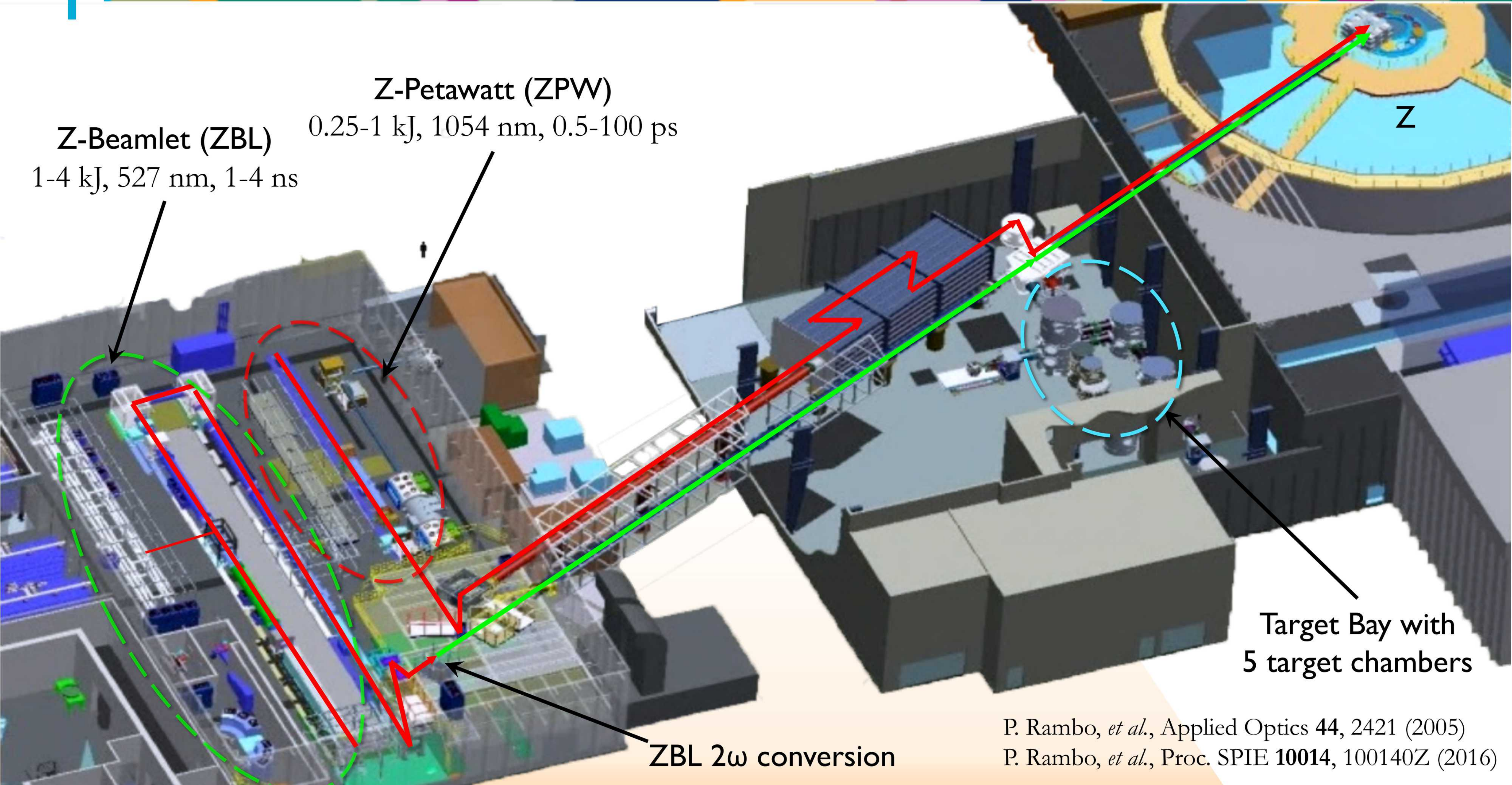
- Role of microstructure
- Kinetics and phase transitions
- Strength
- Transport properties
- Radiation shock

⟶ Theory & data almost always diverge in previously unreachable regimes



*S. Root, *et al.*, Phys. Rev. Lett. **105**, 085501 (2010)

Z-Backlighter Facility



P. Rambo, *et al.*, Applied Optics **44**, 2421 (2005)
P. Rambo, *et al.*, Proc. SPIE **10014**, 100140Z (2016)

Challenges for implementing XRD on Z

Load parameters

- Large and thick samples; high-Z samples and hardware
- Reflection geometry limits accessible angles

Destructive environment of Z-DMP load

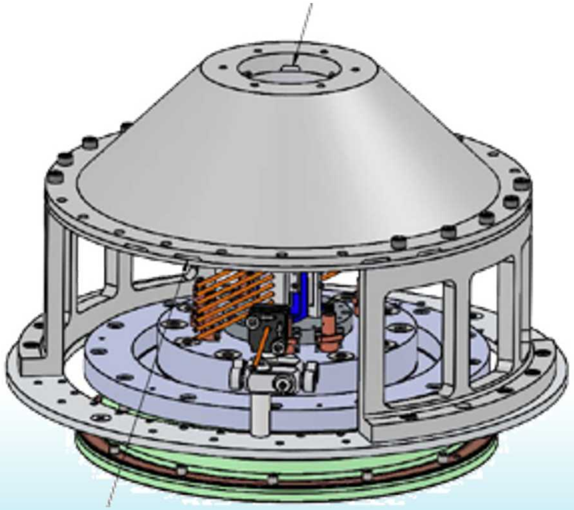
- **Minimum distance ~5 cm**
- Data retrieval?
- Protect Z-Backlighter laser optics

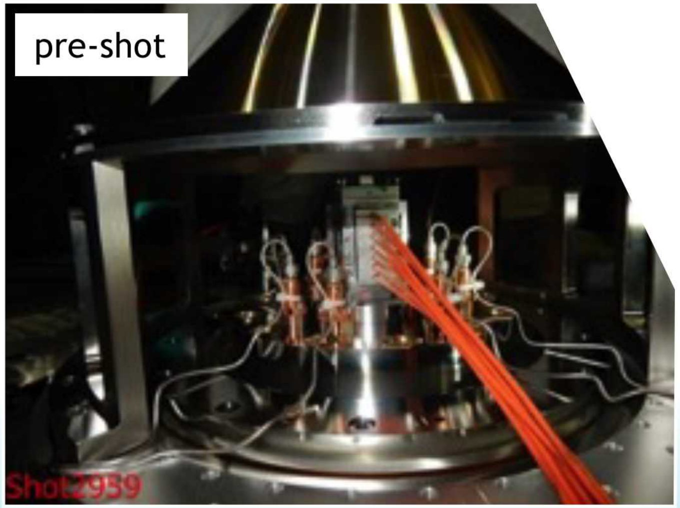
X-ray background

- High energy photons (MeV) produced near load
- Sufficient signal-to-noise?

Electromagnetic pulse (EMP)

- Fry electronics
- Early triggers



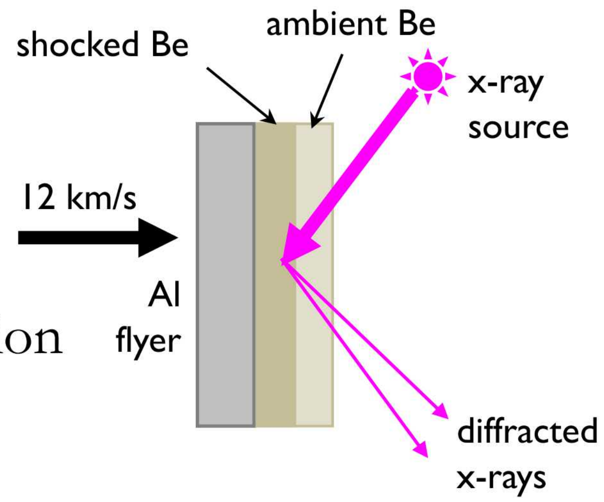


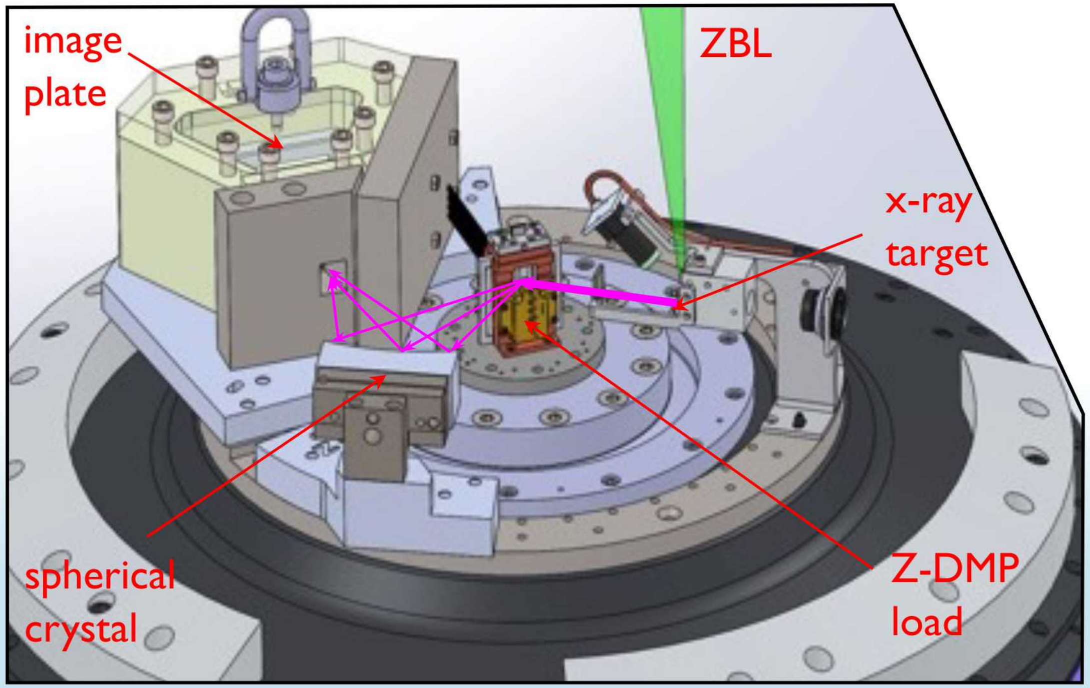
Direct x-ray detection (image plates, CCDs) is infeasible

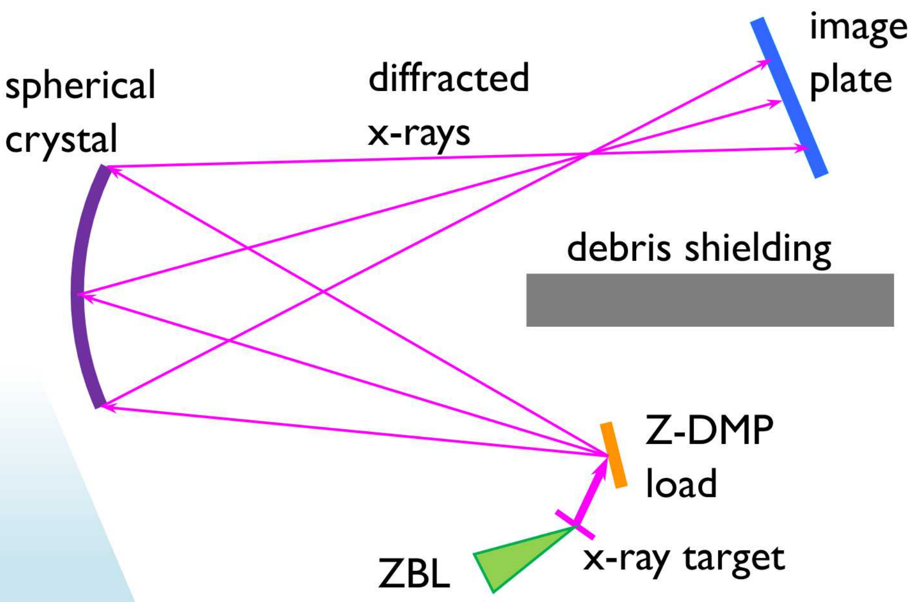
Spherical Crystal Diffraction Imager (SCDI)

Experimental parameters

- Z-Beamlet laser ⟶ 6-8 keV x-rays
- HOPG spherical crystal ⟶ collect and reflect diffracted x-rays
- Image plate ⟶ record data
- Be sample ⟶ low mass attenuation coefficient, high XRD cross section
  - Serves as its own x-ray window
  - Possible hcp-bcc phase transition at ~2 Mbar, 3000 K*





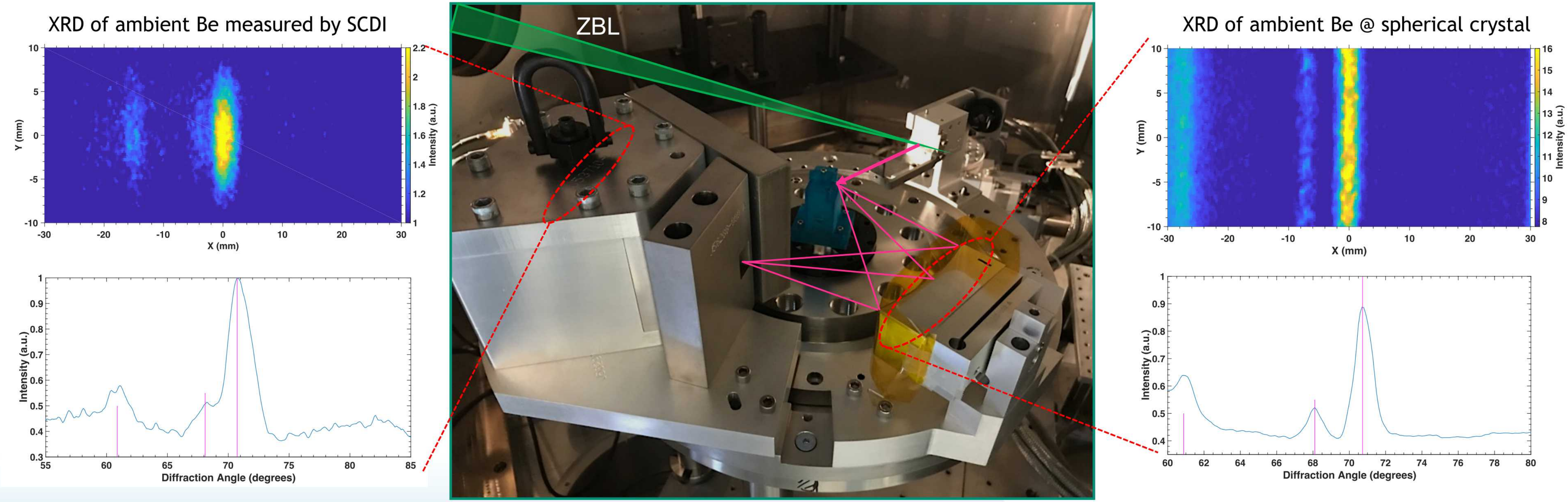


*A. Lazicki, *et al.*, PRB **86**, 174118 (2012)

SCDI diagnostic validated in Chama target chamber

Duplicate SCDI hardware with surrogate Z-DMP load

- HOPG crystal collects diffracted x-rays and focuses into detector housing

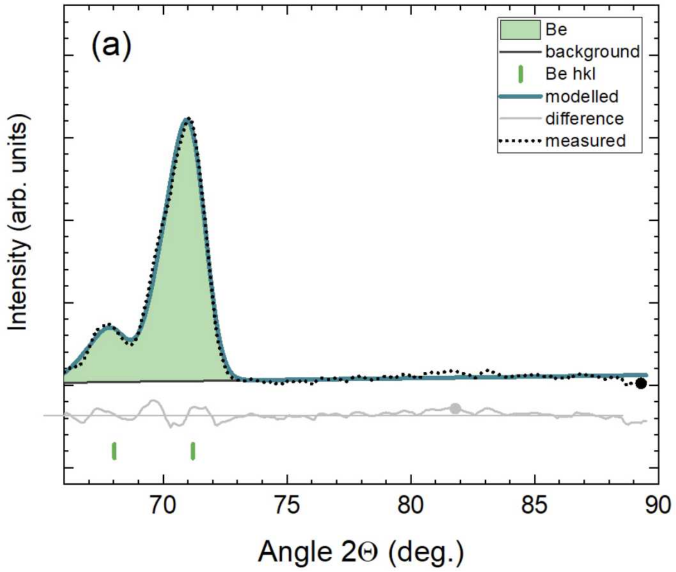


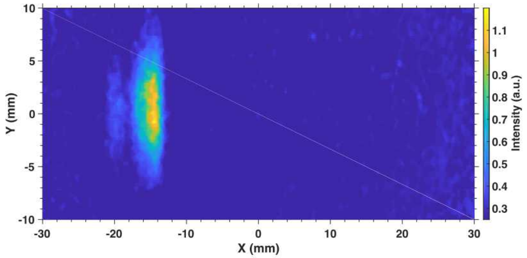
SCDI design and Chama measurements:
T. Ao, M. Schollmeier, P. Kalita et al., Rev. Sci. Instrum. **91**, 043106 (2020)

SCDI measured XRD of shocked beryllium ~165 GPa

SCDI diagnostic has been fielded on Z-DMP experiments (7)

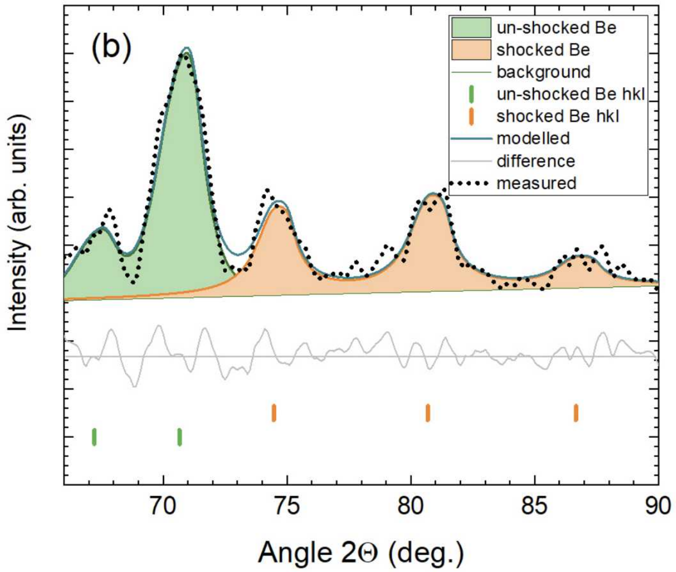
- 25-mm thick tungsten box with 12 x 3 mm slit
- IP survives shot, no debris penetration
- Strong, MeV-level x-ray background
- Inferred shocked x-ray density matches pressure measurement

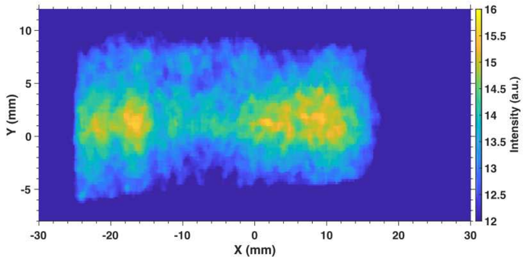




X-ray density of ambient Be ~ 1.85 g/cm³

SCDI housing survives!





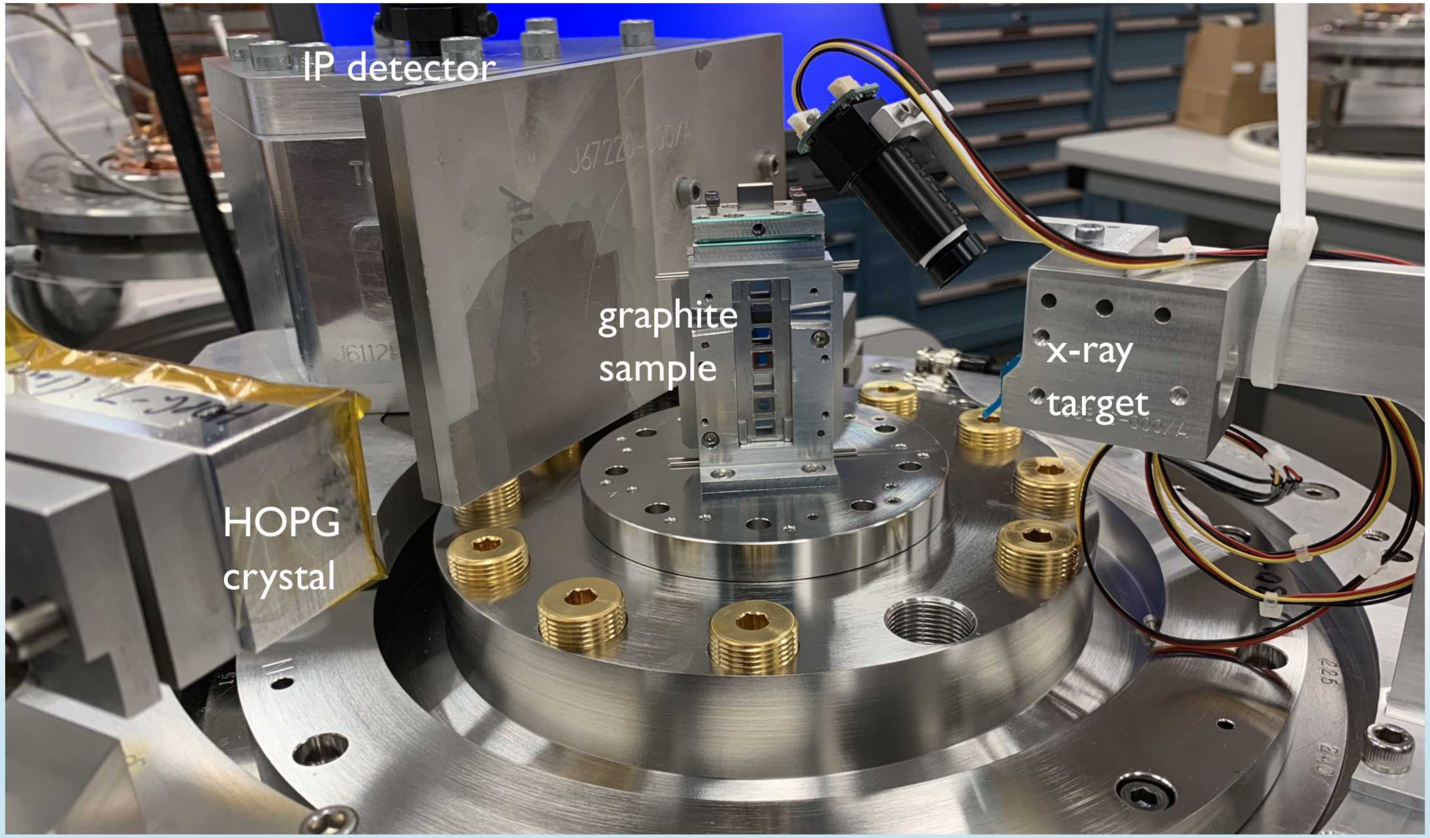
X-ray density of shocked Be ~ 3.1 g/cm³

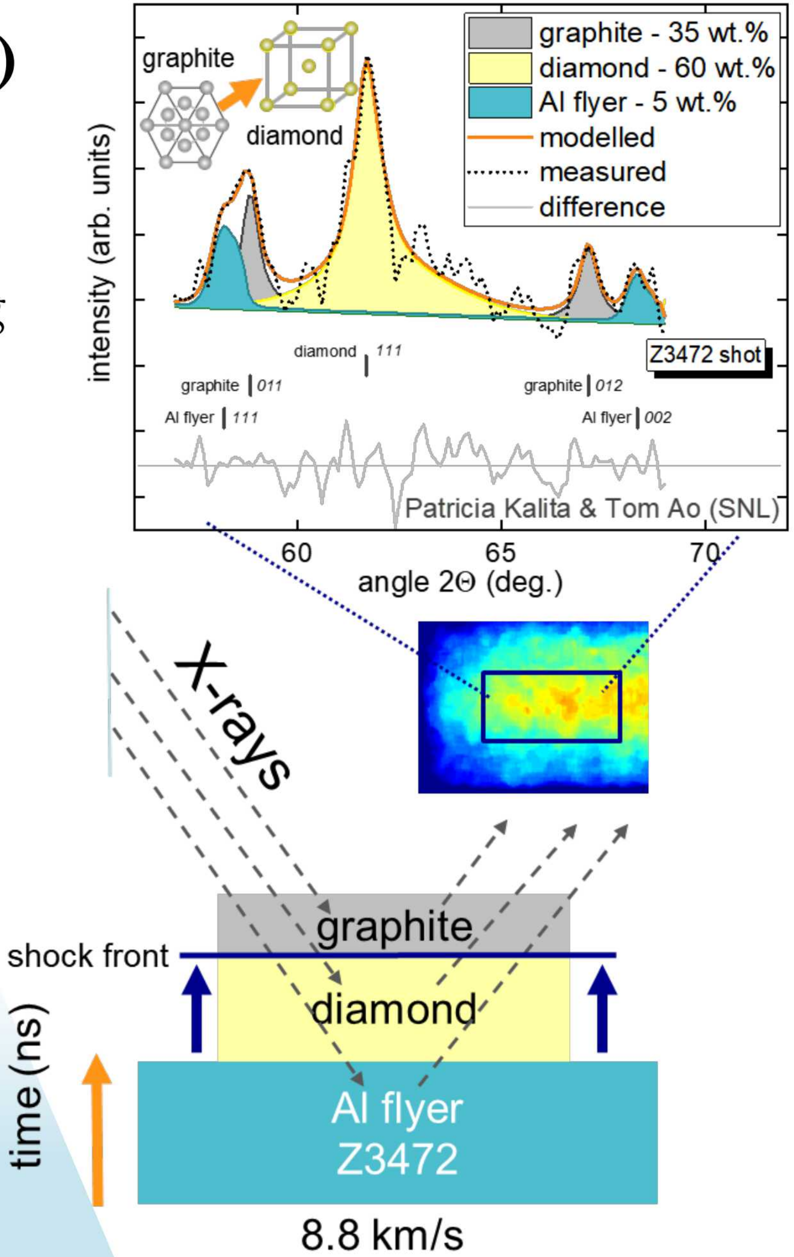
FY19 Milestone Sandia Report:
T. Ao, M. Schollmeier, P. Kalita et al., SAND2019-11868

Making diamonds on Z

SCDI diagnostic measured phase change on Z (3/2020)

- XRD measured transformation of graphite to diamond at the atomic scale
- Nanosecond-scale formation of diamond during shock loading to 130 GPa





XRD quantitative analysis

XRD image

XRD geometry

DIffraction SCintillator Objective (DISCO)

Limitation of existing SCDI diagnostic?

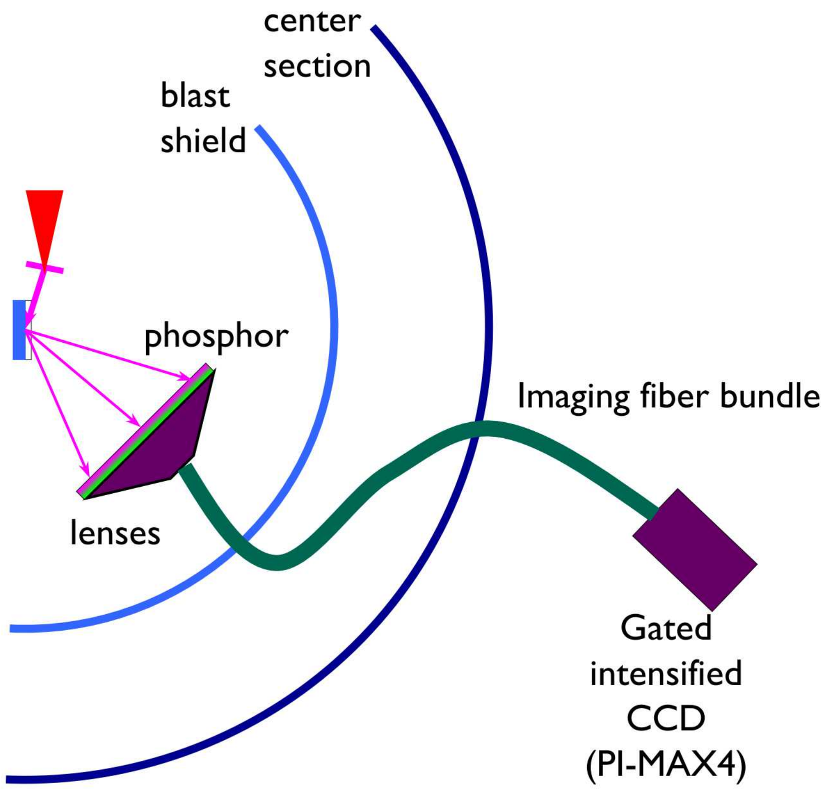
- Low signal-to-noise ratio due to crystal reflection and distance from Z load
- Time-integrated detector (image plate)
- Incompatible with Z-Containment

DISCO:

- Sacrificial, time-gated detector close to load to cover large solid angle
- X-ray conversion to optical light via phosphor or scintillator
- Signal transport to a gated digitizer outside of Z center section
- Compatible with Z-Containment

Key specs:

- 23 mm active diameter, ~15 μm spatial resolution
- Phosphor decay: 70 ns now, <10 ns in development at subcontractor
- At 1 inch distance:
  - 50° angular coverage (SCDI: 30°)
  - 0.2° resolution (SCDI: ~1°)



Fast and bright scintillators

Detector	Chemical Formula	Decay Time (ns)	Emission Wavelength (nm)	Light Yield (photons/keV)
P-43	**$Gd_2O_2S:Tb$**	**10^6**	**550**	**95**
P-47	**$Y_2SiO_3:Ce$**	**70**	**400**	**38**
LSO	$Lu_2SiO_5:Ce^{3+}$	47	400	30
PreLude420	$Lu_{1.8}Y_2SiO_5:Ce$	41	420	32
BriLanCe380	$LaBr_3:Ce$	16	380	63
ZnO:Ga	ZnO:Ga	0.8	385	9
$LuI_3:Ce$	**$LuI_3:Ce$**	**3**	**575**	**70***
R42	?	68	510	11

*** Under consideration**

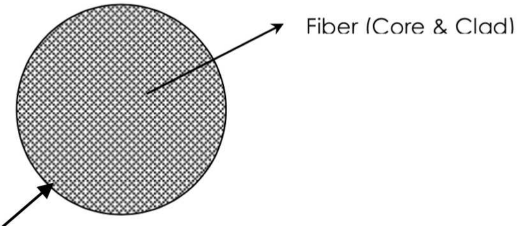
Working with vendor for $LuI_3:Ce$ to develop protective coating

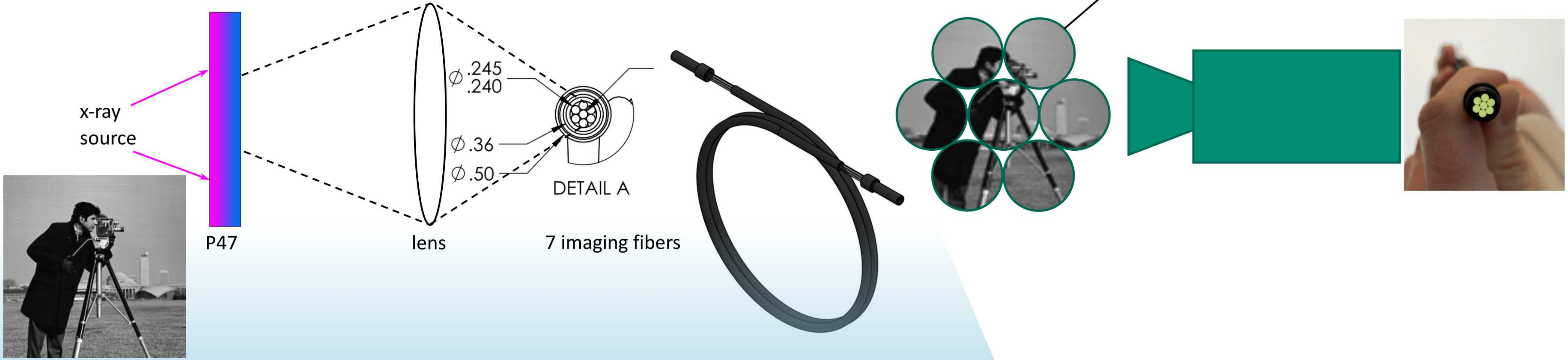
Bundle of 7 imaging fibers

Fiber-based optical relay

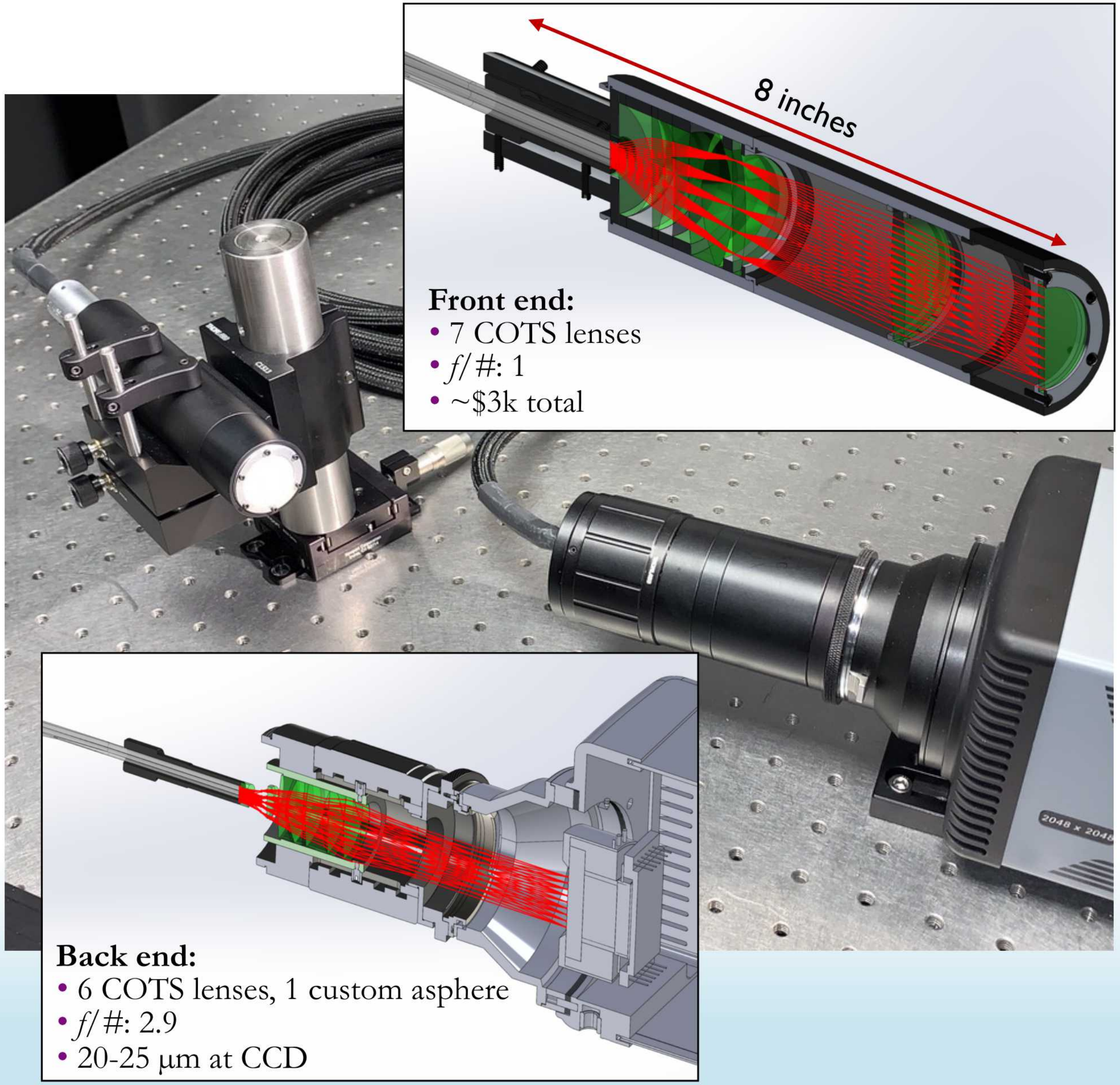
- Asahi Multi-core POF MBL-2000-24 PMMA imaging fiber bundle
  - 13,000 fibers, 15 μm, 2 mm total
  - NA = 0.485
  - \$33/fiber/m → \$230/m for bundle
- Super-bundle of 7 registered imaging fibers
  - Hexagonal pattern
  - Effective diameter: 6 mm/ 0.24 in

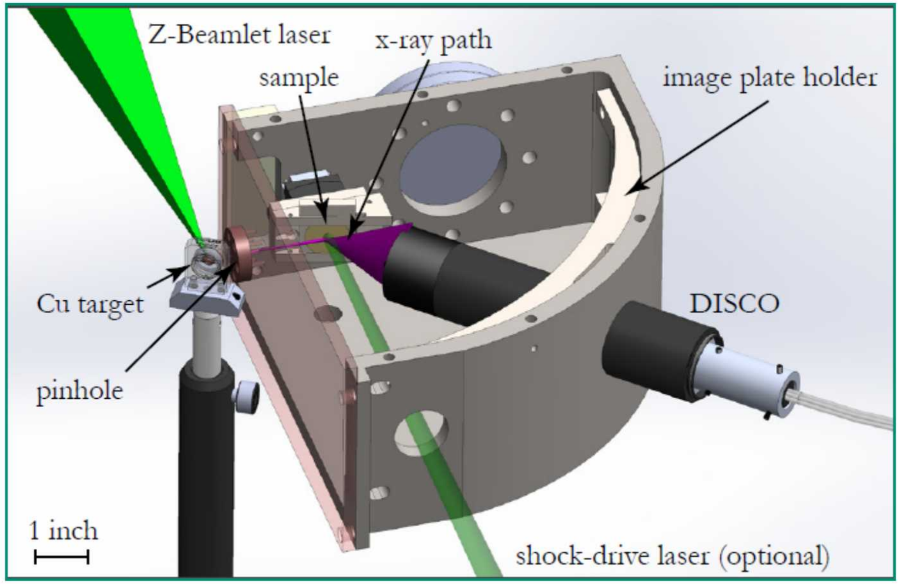
ITEM	UNIT	Specifications
Core Material		PMMA
Clad Material		Fluorinated Polymer
Fiber Diameter	μm	2000 ± 120
Core Number		13000
NA		0.5

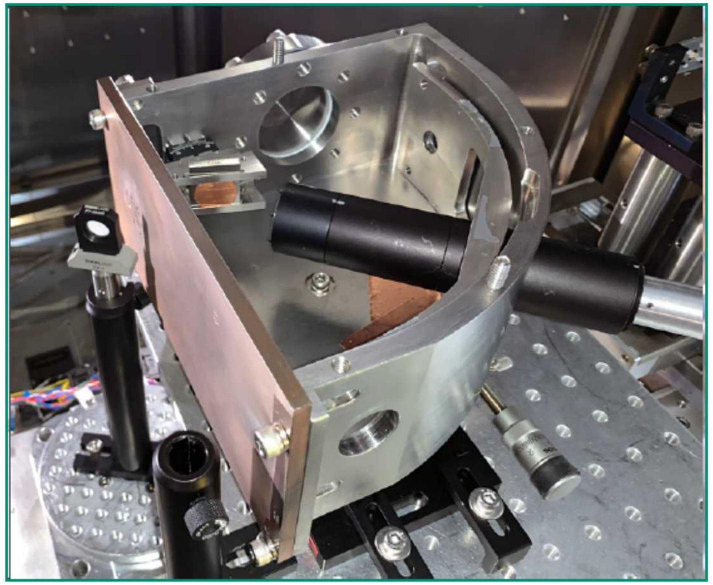




DISCO validated in Chama target chamber

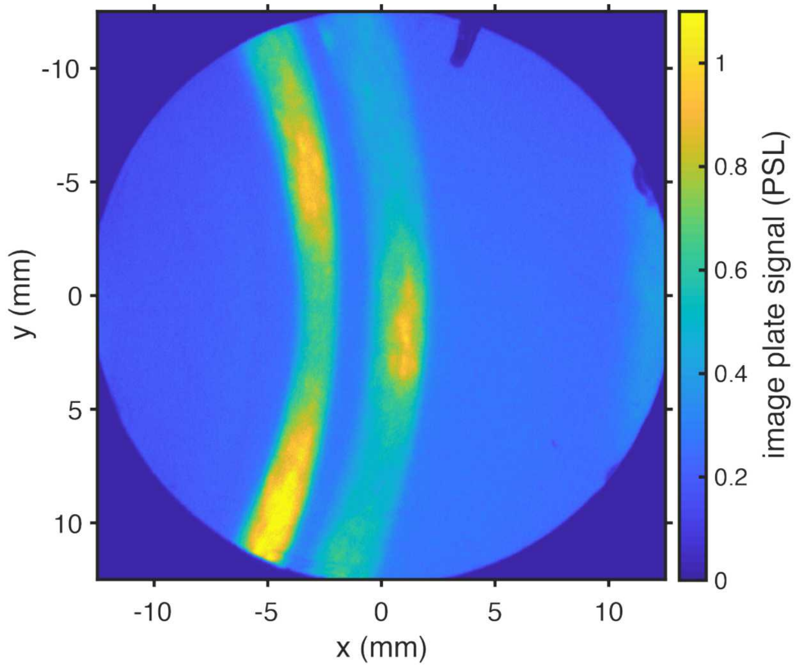




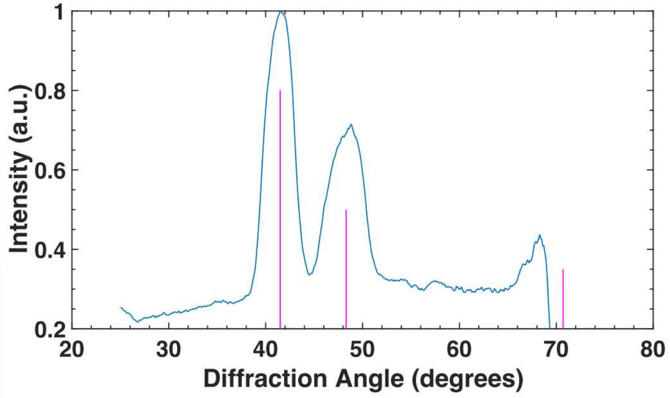


DISCO image comparison: Cu Heα (8.4 keV) on Cu sample

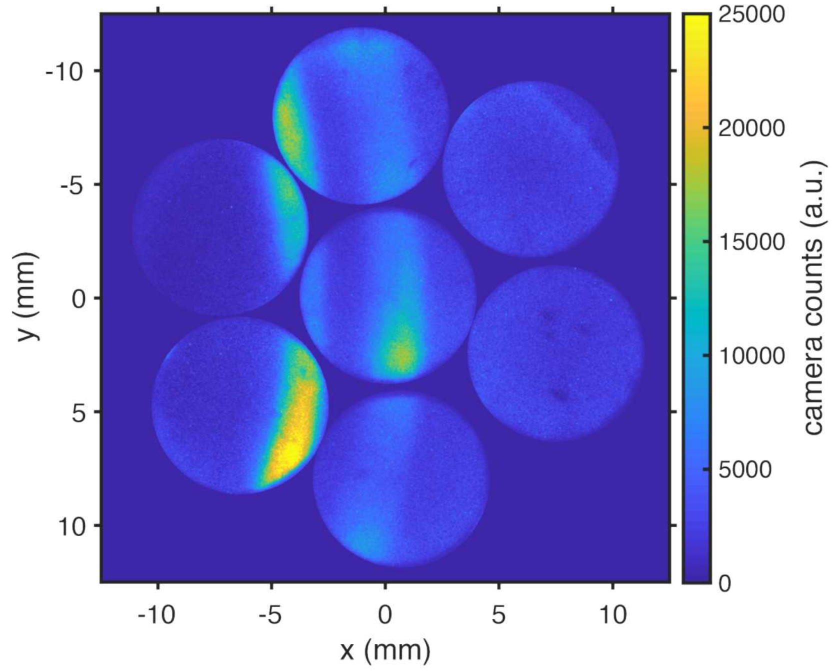
TR Image plate
Acquisition time: infinite



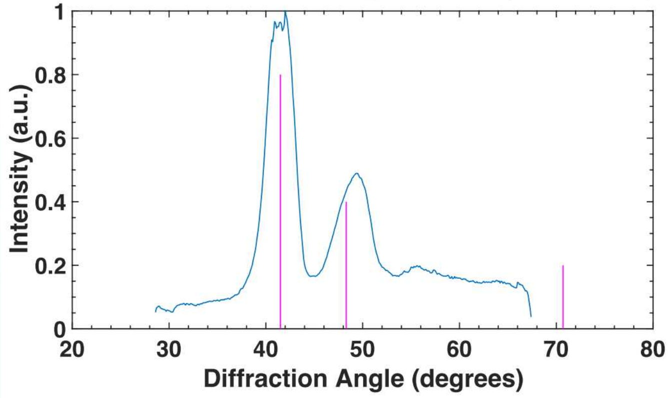
B20071501 - ZBL-XRD, Cu target, Cu sample, IP at DISCO



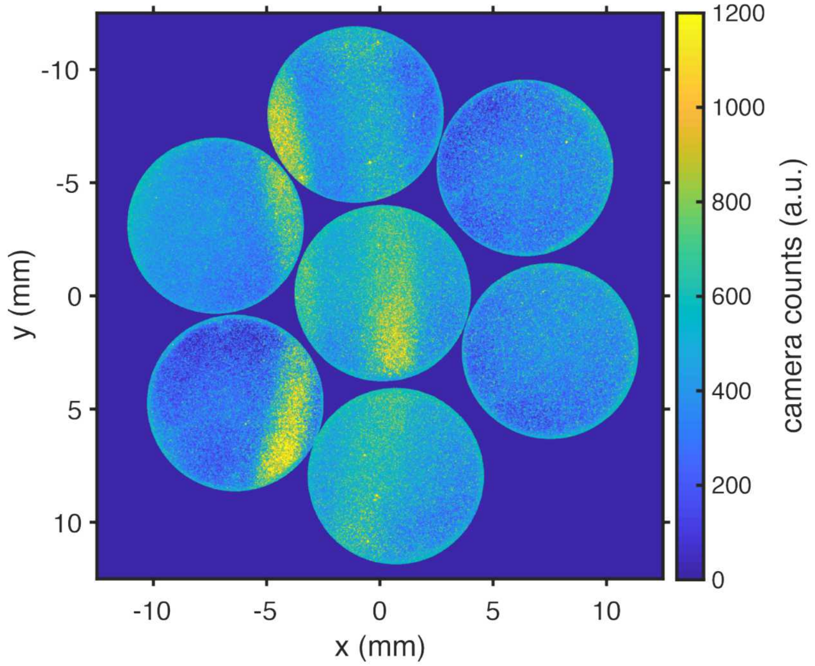
P43 phosphor, 10 µm thick
Acquisition time: 1.5 ms



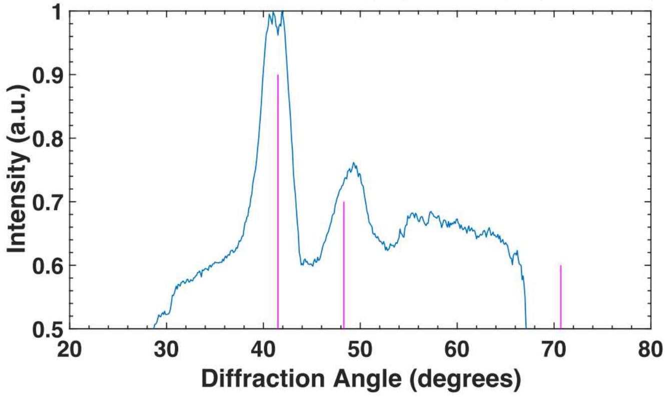
B20071602 - ZBL-XRD, Cu target, Cu sample, DISCO (P43)



P47 phosphor, 20 µm thick
Acquisition time: 70 ns



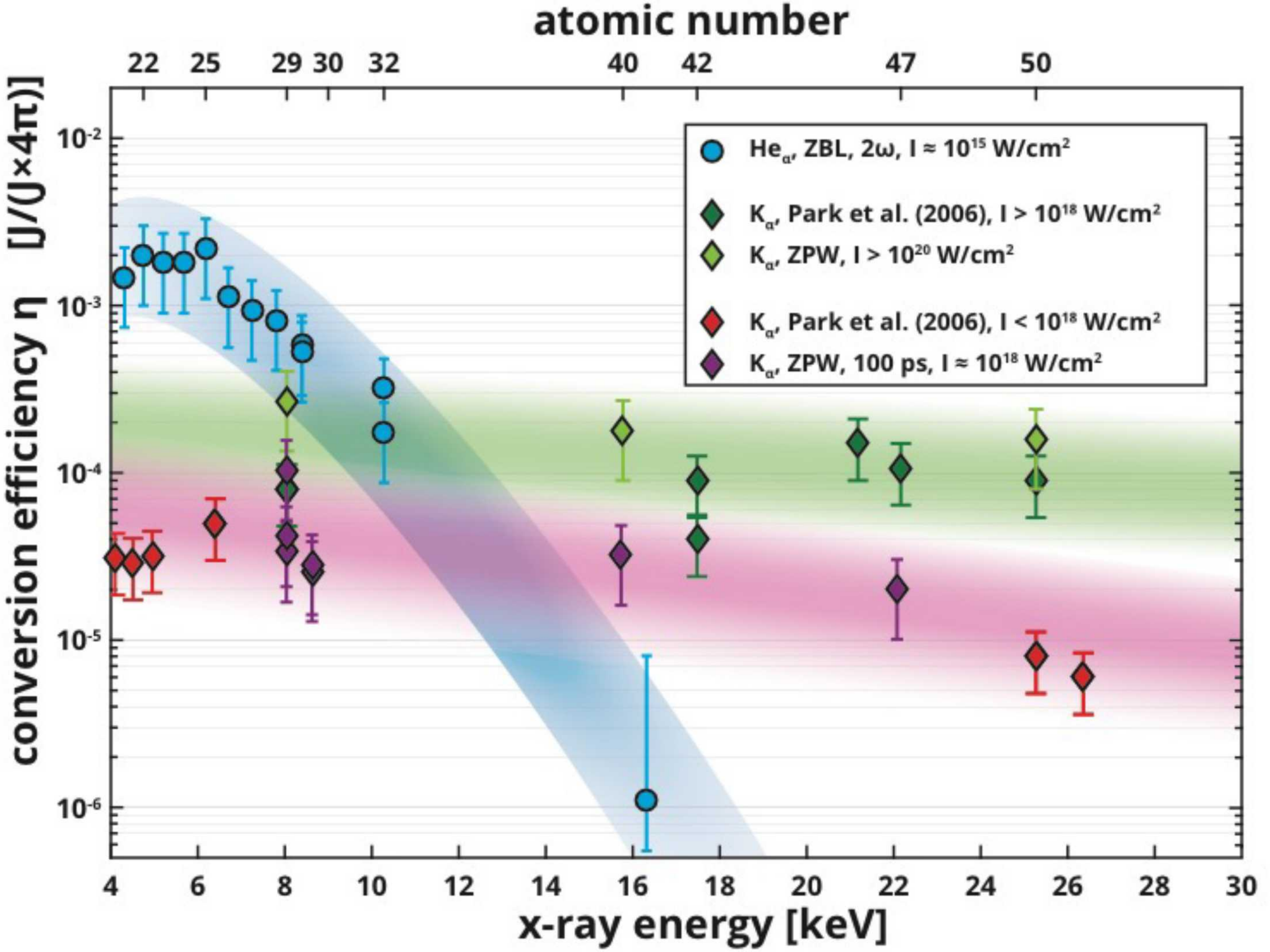
B20071604 - ZBL-XRD, Cu target, Cu sample, DISCO (P47)



Comparison of laser-to-x-ray conversion efficiencies

Single-shot diffraction requires both sufficient photon energy and fluence

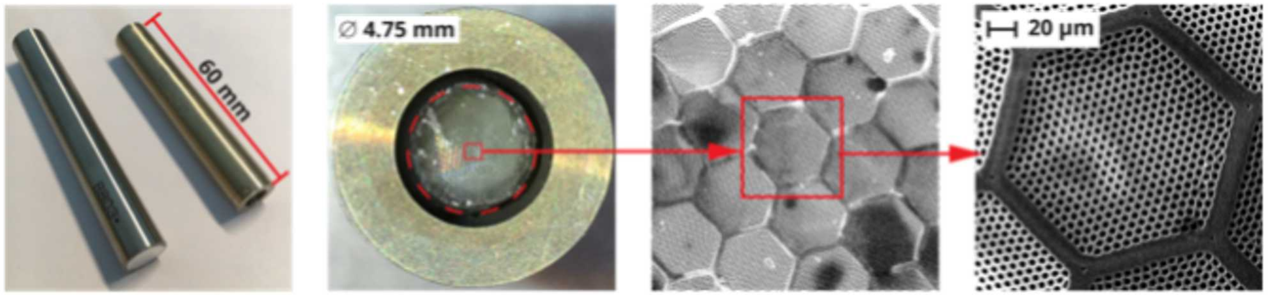
- Number of photons
  - $N_{photon} = \eta \times E_{laser} / E_{photon}$
- Z-Beamlet laser (ZBL): 1 – 4 kJ, 527 nm, 1 – 4 ns
  - 2 kJ → 6.2 keV → 10^{15} photons/4π
  - 2 kJ → 16 keV → 10^{12}
  - Minimal, low-energy background
  - Routinely used on Z
- Z-Petawatt laser (ZPW): 0.25 – 1 kJ, 1054 nm, 0.1 ns
  - 1 kJ → 16 keV → 10^{14}
  - Strong, MeV-level background
  - Not yet used on Z

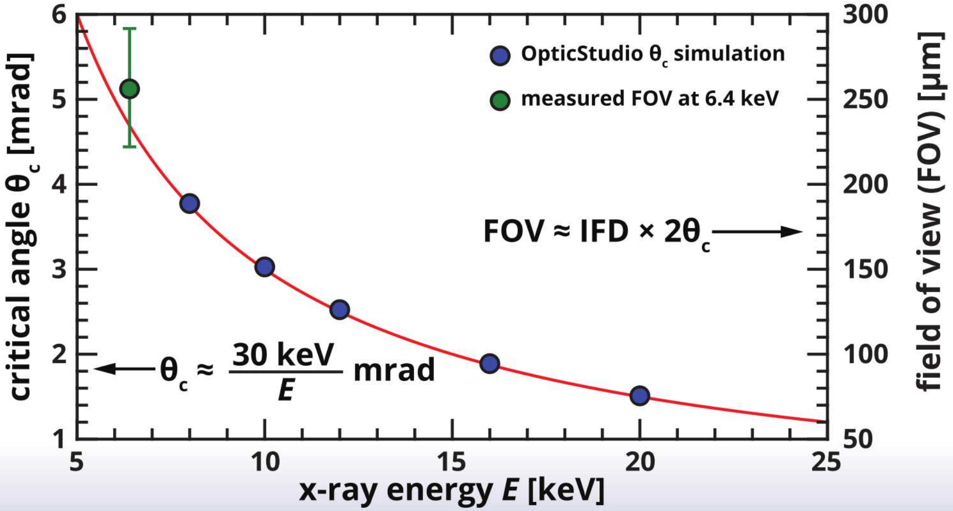


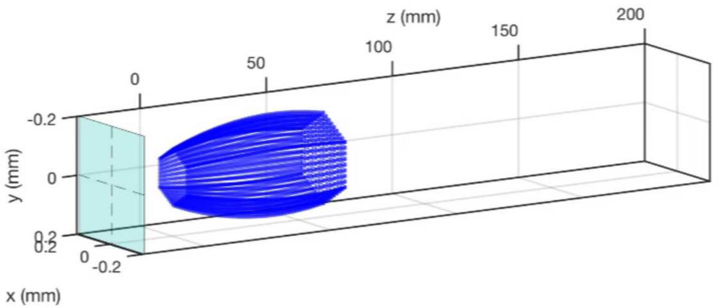
Polycapillary x-ray lenses

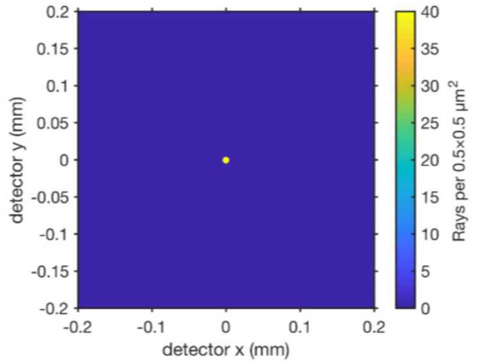
Enabling technology for ZPW XRD

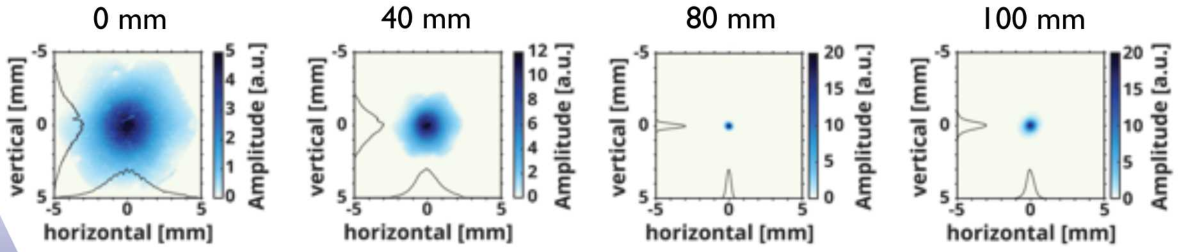
- Total external reflection focusing fiber bundle
- Throughput: $\Omega \times T \approx 5 \times 10^{-3}$
- X-ray flux gain vs. pinhole: 100 - 1000
- Number photons on sample: $10^{9} – 10^{12}$







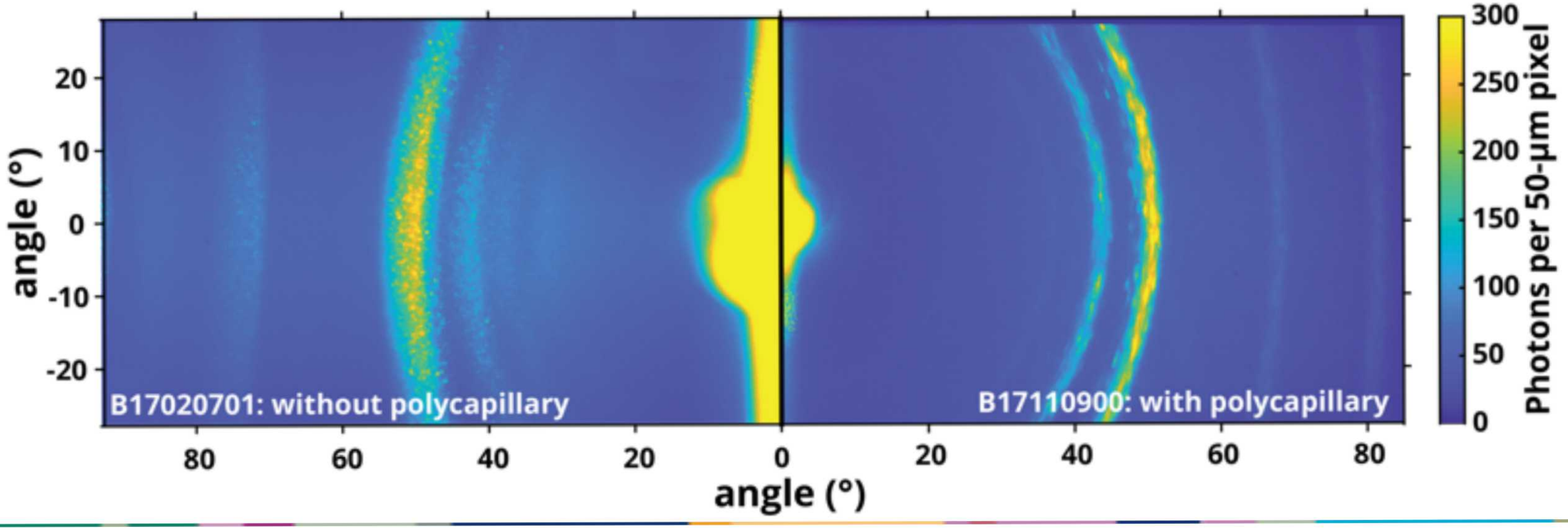




M. Schollmeier, T. Ao, *et al.*, RSI **89**, 10F102 (2018)

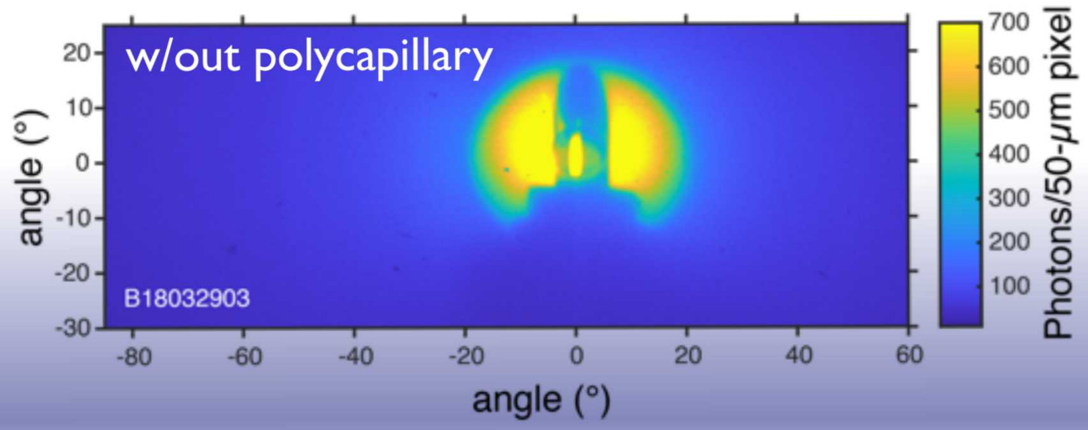
XRD data with ZBL (1 kJ, 1 ns, 10^{15} w/cm^2)

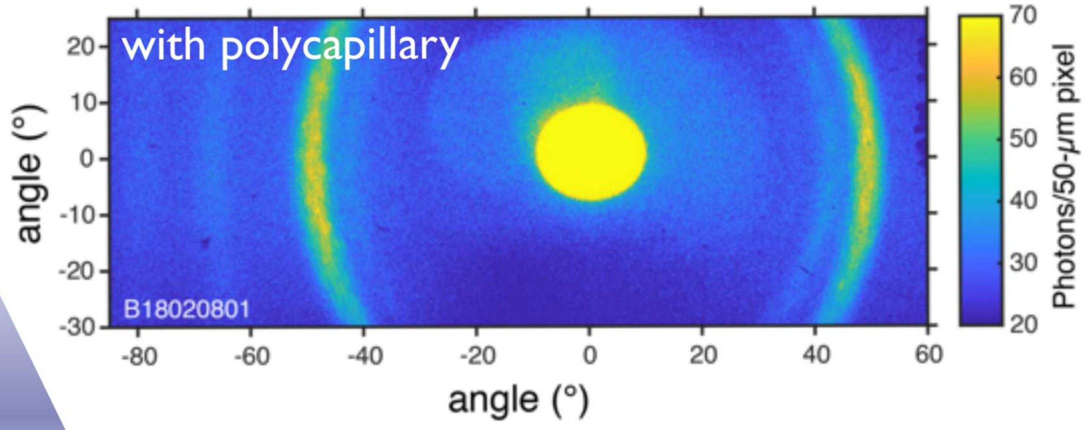
X-ray source: Cu He$_\alpha$, 8.4 keV. Diffraction sample: Be, 1.3 mm



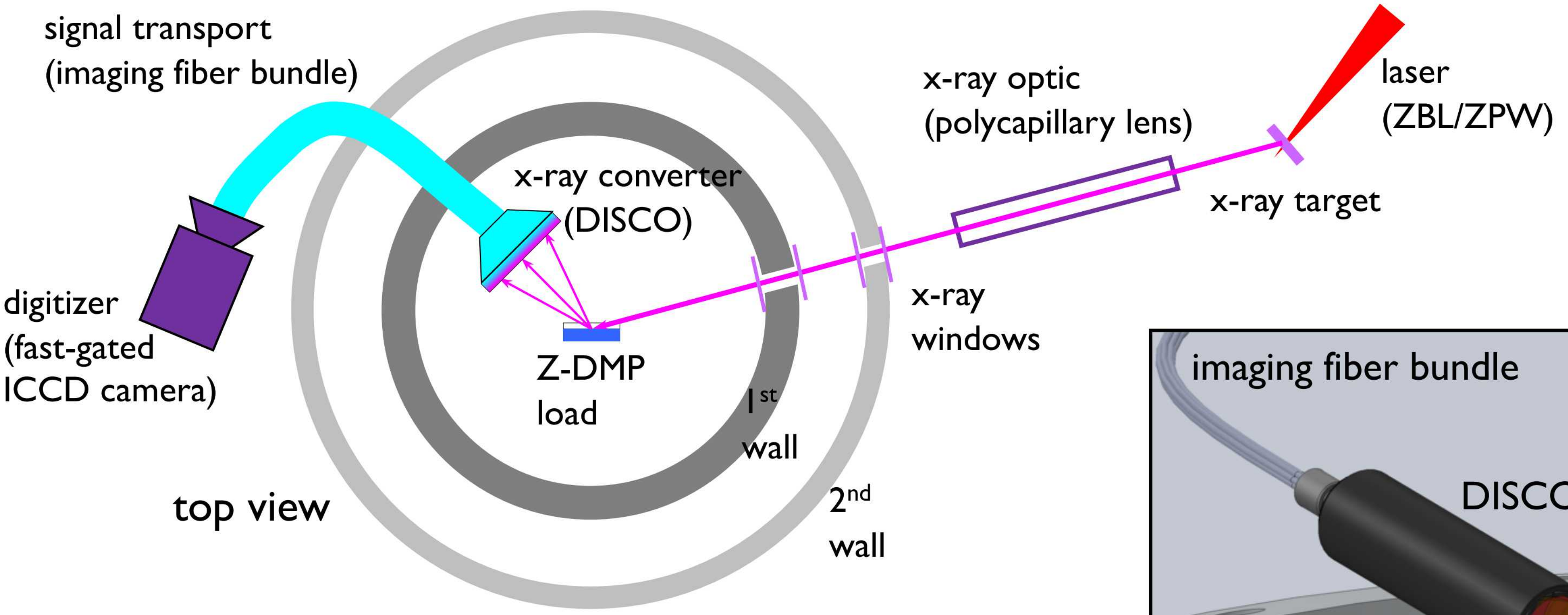
XRD data with ZPW (250 J, 100 ps, 10^{18} W/cm^2)

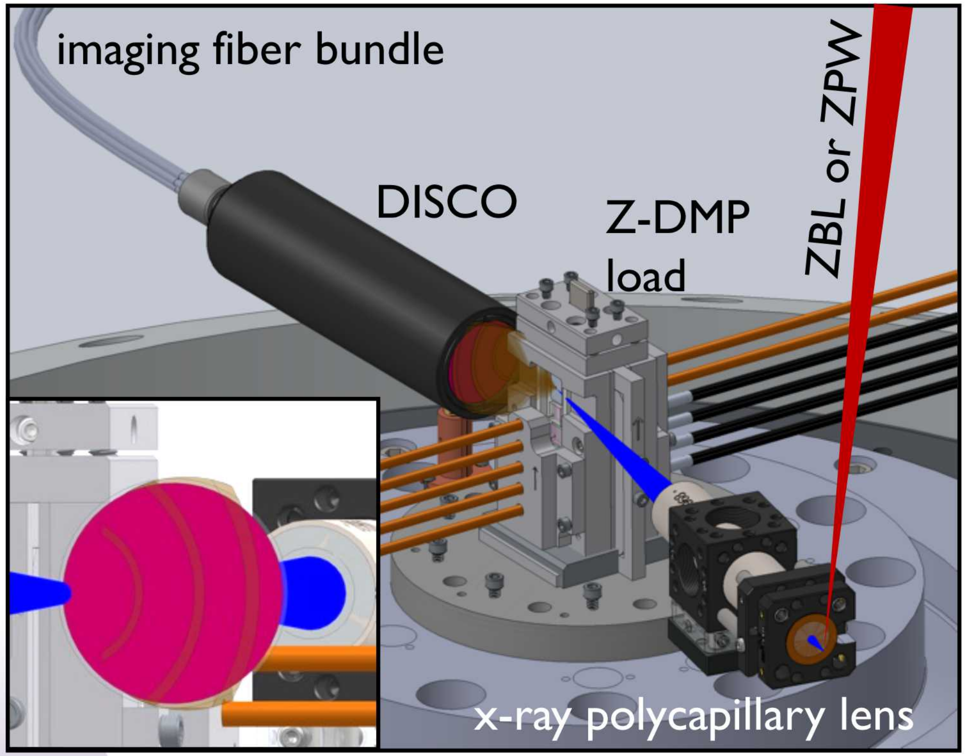
Cu K$_\alpha$, 8.05 keV. Diffraction sample: Be, 1.3 mm





X-ray diffraction diagnostic compatible with Z-Containment experiment





scintillator distance (mm)	Δ2θ (°)	Δθ (°)	signal for 8 keV (cts)	signal for 17.4 keV (cts)
45.8	30.5	0.1	46,000	1,100
25.4	**52**	**0.18**	**150,000**	**4,000**
18.3	69	0.25	280,000	7,250

Summary

X-ray Diffraction on Z

- Mitigation of load debris and x-ray background challenges
- Spherical crystal diffraction imager (SCDI) enabled time-integrated XRD measurements on Z

Future Developments

- New DIffraction Scintillator Objective (DISCO) detector scheme for time-gated/resolved XRD
- Higher photon energies (15-20 keV) x-ray sources using ZPW
- Polycapillary x-ray optics enhanced x-ray flux

Acknowledgements

- Anthony Smith, Paul Gard, Jim Williams, Caroline Blada, Heath Hanshaw, Ian Smith, Jon Shores, Shane Speas, Patrick Rambo, Ben Galloway, Chris Seagle, John Porter