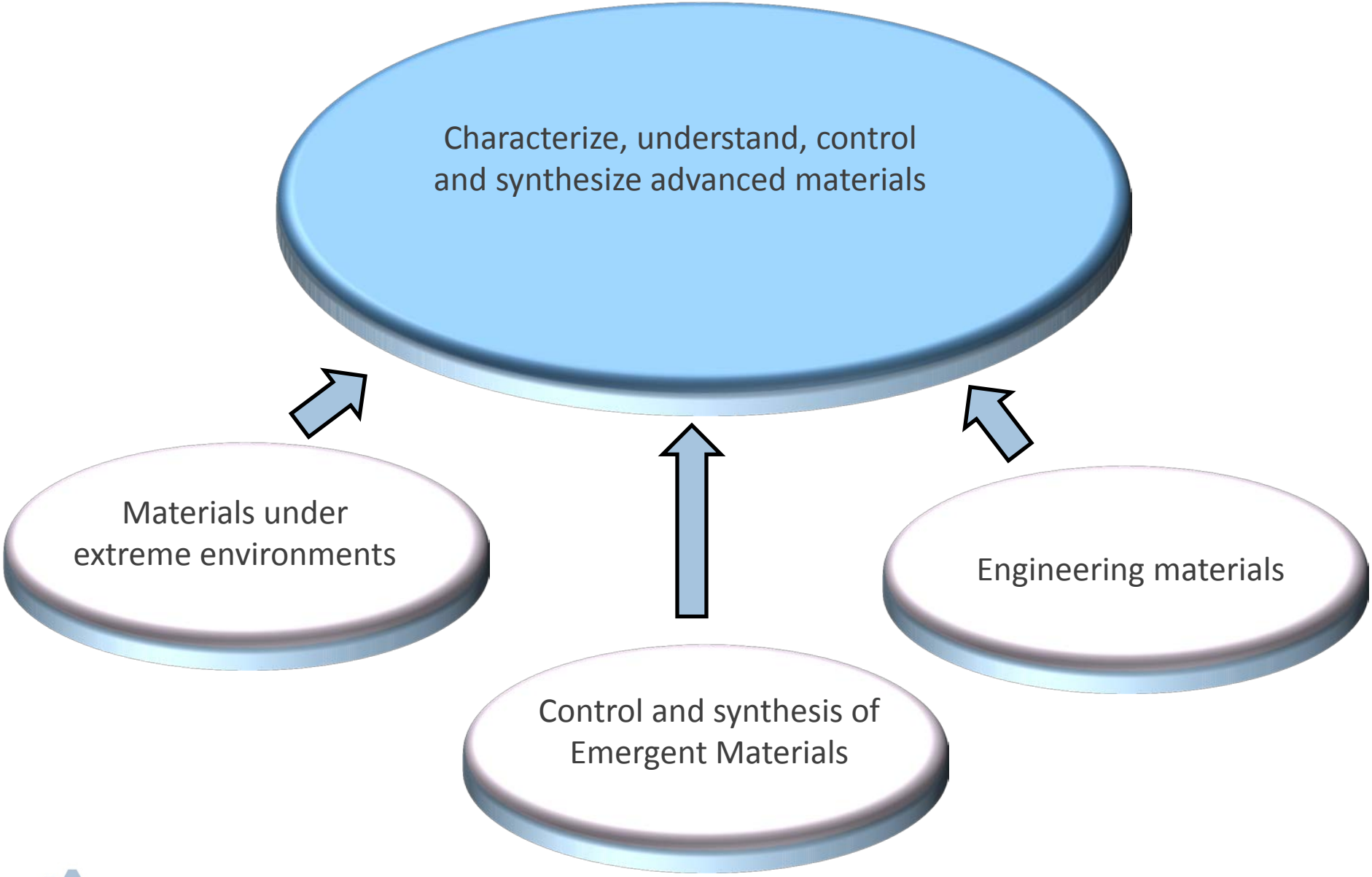
Materials Science and Condensed Matter Physics

What sets the APS apart from other synchrotrons, facilities, probes?

- **High energy storage ring -> High energy x-rays (>20 keV)**
  - ✓ True bulk measurements
  - ✓ *In-situ In-operando* studies (synthesis, reactions, ….)
  - ✓ Extreme environments (pressure, field, radioactive,…)
- **High brilliance (APS-Upgrade – MBA)**
  - ✓ High coherent x-ray flux (CDI, XPCS)
  - ✓ µm to nm focusing
- **Unique Timing structure**
  - ✓ Pump-probe techniques run majority of they time.
- **Co-location with a programmatic research lab**
  - ✓ Large built in user base with unique expertise
  - ✓ Opportunities to develop larger scale complex experiments (*in-situ, in-operando*).

Future investments need to leverage these unique capabilities.

Materials Science and Condensed Matter Physics



Engineering Materials

Can we understand failure mechanisms and create engineering materials with better properties?

Unique capabilities at APS

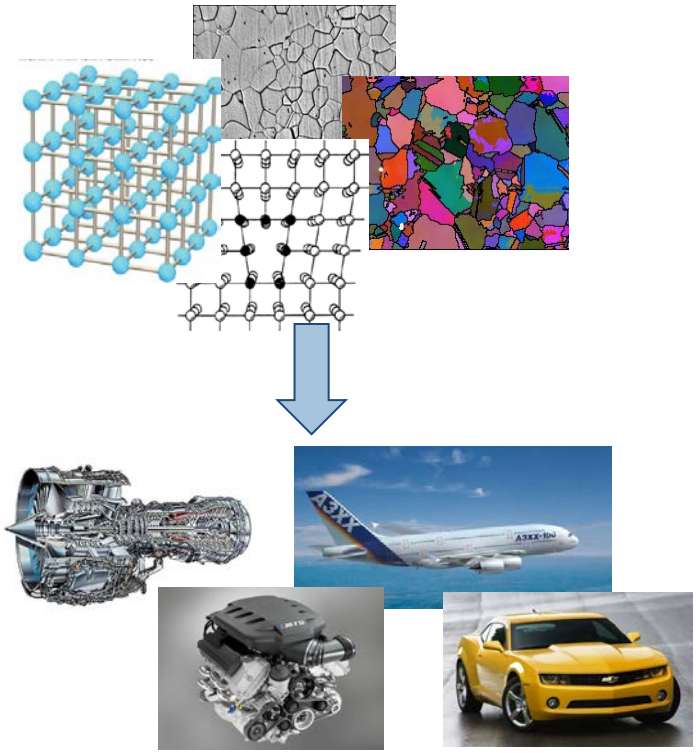
3D grain mapping of polycrystalline materials under thermomechanical loading (T:1200 C).

High Energy Diffraction Microscopy (1-ID)
5µm resolution, mm thickness
White beam Laue Diffraction Microscopy (34-ID)
100 nm resolution, 100 µm thickness

Additional capabilities at the APS

Tomography (2-BM, 26-ID, 32-ID)
Imaging (2-ID, 26-ID)
Powder diffraction (11-BM, 17-BM, 6-BM)
PDF (11-ID)
USAXS, SAXS (12-ID, 15-ID)

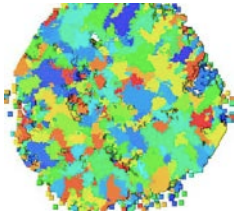
Hierarchical information on atomic, mesoscopic, and macroscopic length scales

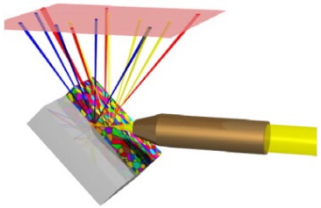


Improved performance and properties at continuum length scales

Engineering Materials: Future directions

- Push resolution limits (optics)
  - ✓ HEDM (5→1 µm); nano-Laue (500 → 100 nm)
  - ✓ Nano-fluorescence mapping



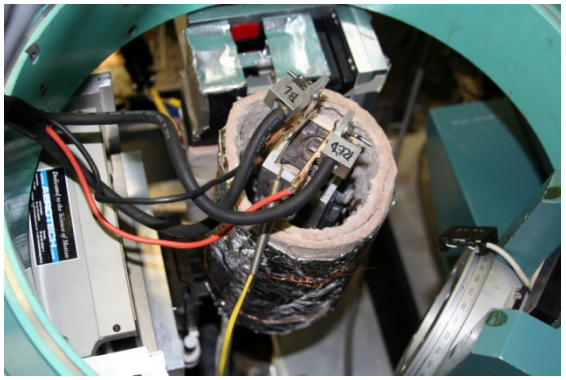


- Improve *in-situ/in-operando* environments
  - ✓ Develop in-house engineering expertise
- Big Data – HEDM (1-10 TB/day); Imaging
  - ✓ Engage ANL-MCS/ALCF in processing and data storage
    - Virtual Data Facility (host large data sets)
    - Materials Genome Initiative (NIST)

- Expand multi-modal characterization capabilities
  - ✓ HEDM + Tomography (1-ID)
  - ✓ USAXS + SAXS + WAXS (15-ID)
- Foster partnerships with industry
  - ✓ Metals Affordability Initiative (75 companies)

Carnegie Mellon University

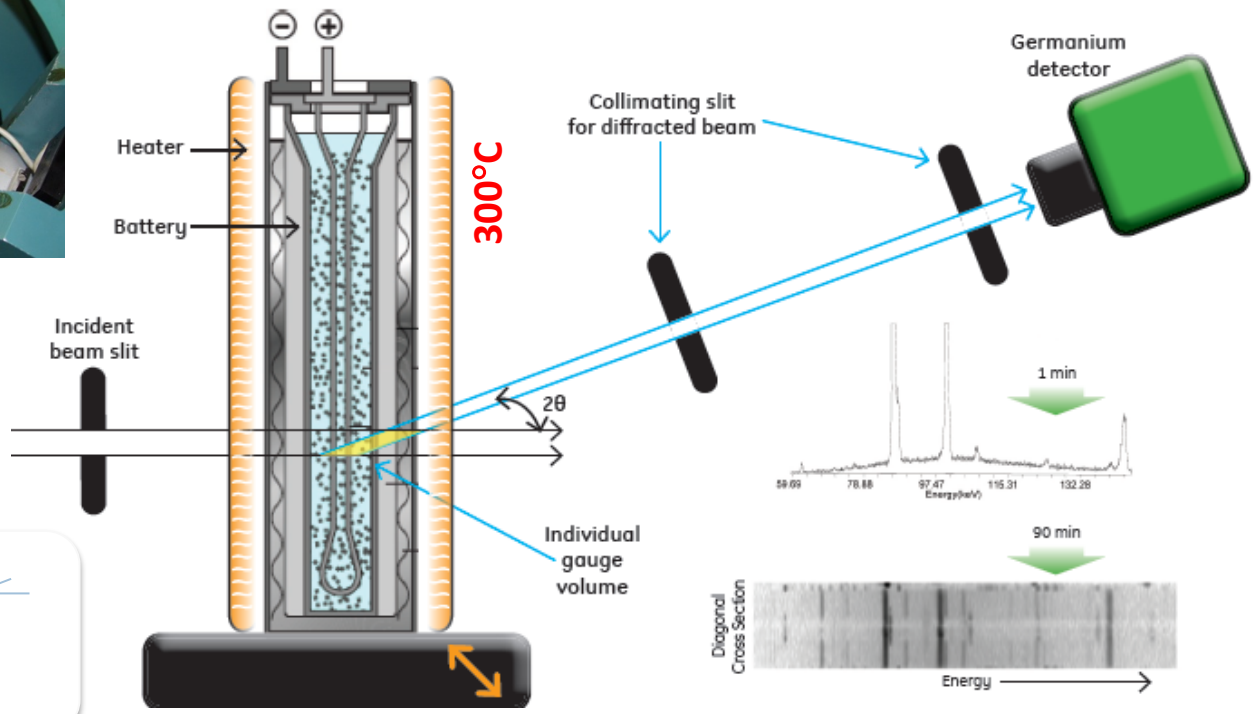
Engineering Materials: In-situ EDD of "real" battery



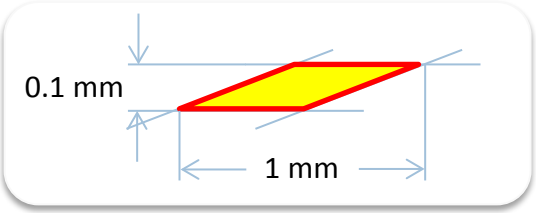
Setup at X17B1

To cycler

Charge/discharge time: a few hours



High-energy white beam (50-150 keV)



Probe volume

Sample stage

Data collection: 30-60 sec/pattern

Phase and strain mapping with spatial selectivity

imagination at work

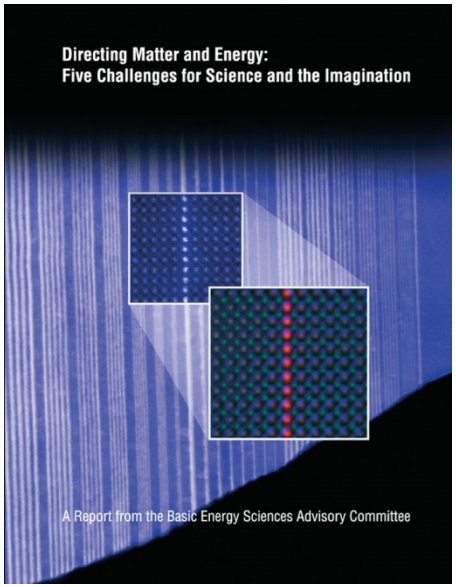
EDD@APS: 1-BM starting March 2013; 6-BM in near-future

GE Global Research, Rutgers University, BNL

Emergent Materials

How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?

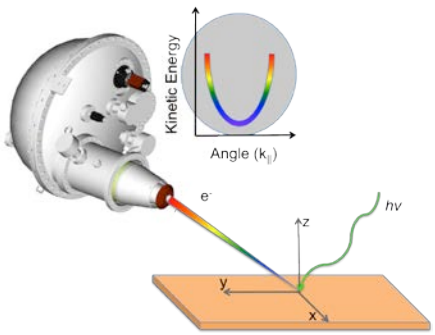
Nearly all XSD beamlines provide *ex-situ* characterization tools for emergent materials



- Correlated electron systems & quantum matter
  - Scattering ⟶ Atomic and micro scale structure of a material
  - Spectroscopy ⟶ Magnetism, dynamics
  - Imaging ⟶ Phase segregation on nm length scales
- Soft matter systems
  - Scattering ⟶ Particle sizes, ordering, dynamics (SAXS, GISAXS, XPCS).
- In-situ synthesis
  - Scattering ⟶ *In-situ* growth characterization direct feedback loop

Emergent Materials: Near term developments

New beamlines and capabilities for looking at correlated electron systems & soft matter:



IEX (29-ID) - Partnership with Univ. of Illinois (NSF funded)

- **ARPES** – Electronic excitations in Energy/Momentum
- **RSXS** – Spatial ordering of excitations

RIXS (27-ID) – APS upgrade

- Electronic excitations (5d systems)

THz Pump (7-ID) - Strategic LDRD

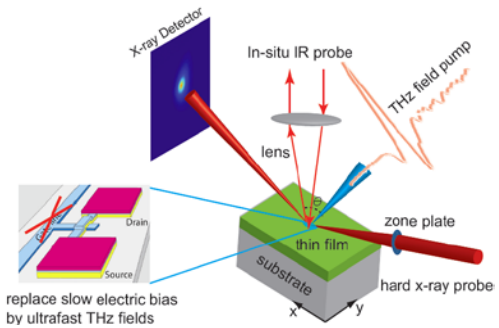
- Selective pumping of quasiparticles

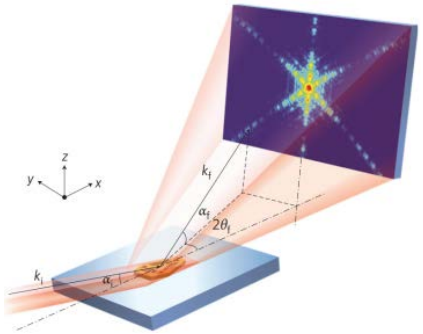
X-STM (26-ID) – DOE young investigator

- Atomic Chemical & Magnetic Imaging

In-Situ Nanolighography (8-ID) – IME partnership

- GISAXS of self-assembled microelectronics templates



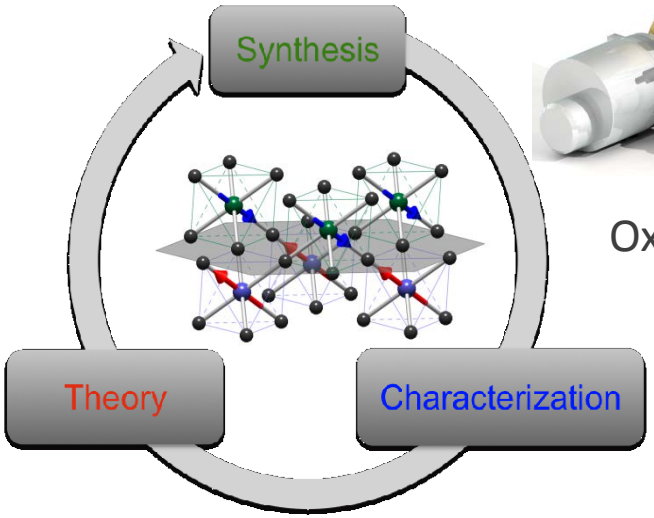


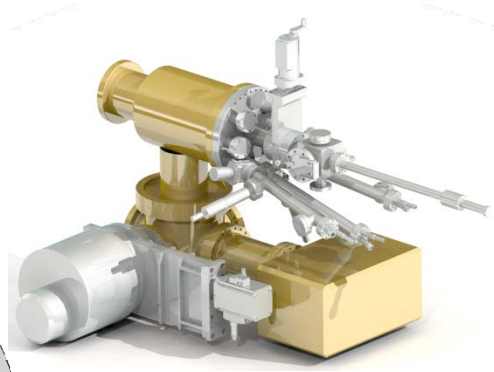
Opportunities for leveraged funding for new instrument development

Emergent Materials: In-situ Synthesis

Can we harness the power of computation to synthesize novel functional materials?

Materials by Design





Oxide MBE (33-ID)

X-rays can provide key feedback on materials growth in real-time, greatly reducing the time to materials discovery.

In-situ synthesis

- Oxide MBE (33-ID) MSD/CSE partnership Materials for Energy LDRD funded
- PLD + HE-XPS (33-ID) MSD Partner
- MOCVD, ALD (12-ID) MSD programmatic research
- Microwave nano-particle synthesis (1-ID) CNM Materials for Energy LDRD funded
- In-situ nanoparticle self assembly (8-ID) IME partnership
- A number of beamlines are involved in EFRC rational materials discovery (11-ID, …)

DOE thrust this year in Computational Materials Science

Materials under Extreme Environments

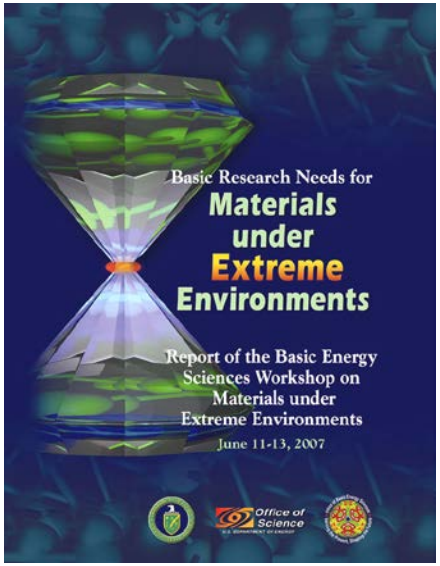
What new materials and phenomena will we discover under extreme conditions?

Most extreme environments (P,T, H, …)

- small sample volumes

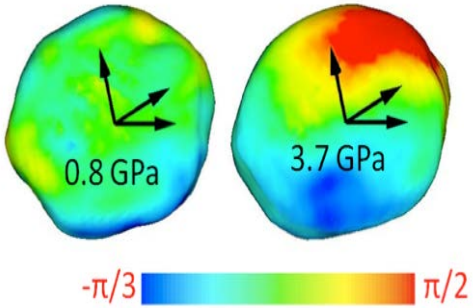
High-brilliance hard x-rays

- structure, electronic properties, and dynamics of materials in extreme environments.



Extreme environments

- Pressure (core strength of APS; HP & GSE)
  - ✓ XSD : XMCD, NRS, PDF, IXS, RIXS, CDI, µDiff, …..
- Magnetic and Electric fields (pulsed and static)
  - ✓ Static (7 Tesla); Pulsed (30 Tesla; 1 ms)
- Temperature
  - ✓ Low-T cryostats & high-T furnaces & Laser heating
- Shock compression (32-ID, 35-ID)
- "Extreme samples" Radioactive and Irradiated



Extreme Environments: Future directions

- Future opportunities lie at the extremes

  Field, Pressure, Temperature, Stress

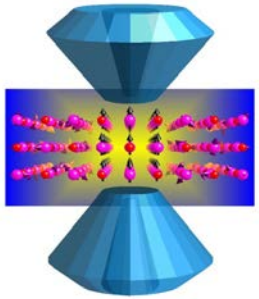
- Expand accessible multi-parameter phase space
  - ✓ Pressure >100 GPa, H > 7 Tesla, T< 2K
  - ✓ Pulsed Fields 40T & 10 ms

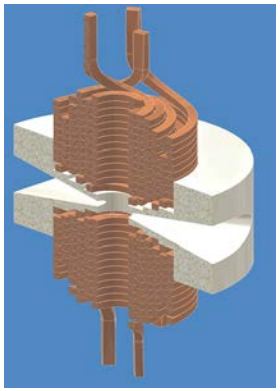
- Develop extreme environment capabilities across more techniques.
  - ✓ e.g. Magnetic fields -> IXN, RIXS, CDI, …

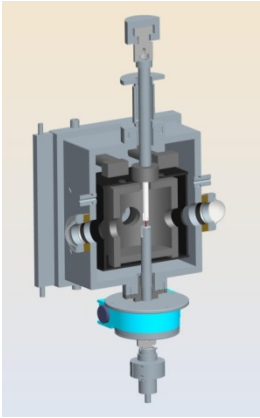
- Engineer new sample containments for probing radioactive materials
  - ✓ Are facilities needed at the APS for rad sample handling?

- Standardize sample environments across beamlines (cross-modal studies)
  - ✓ Do we need a sample environments group?

- Mitigation strategy for controlling operational costs of liquid Helium

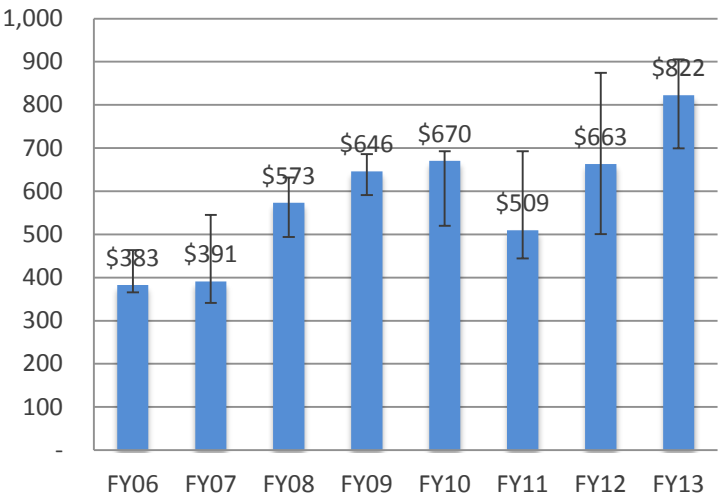






Extreme Environments: Helium Costs

Helium cost per 100 liter

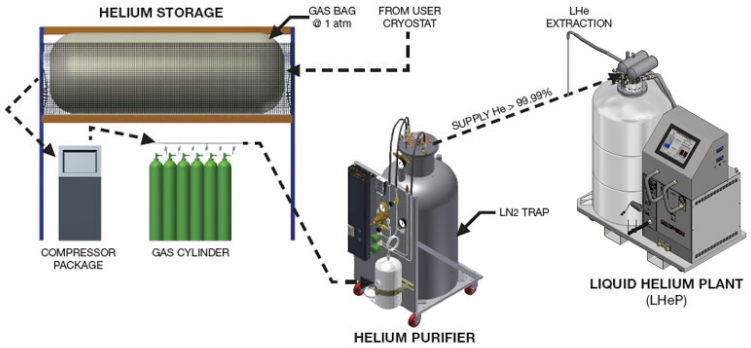


4-ID-C 7T Magnet
(largest consumer)

Cryogen-Free Magnet

Cost of liquid helium rising and unpredictable

Helium Recovery System



- ~<u>700% increase</u> in operating cost over 7 years
  - ✓ Cost/liter x2.5 ($3.50 ➜$9.00)
  - ✓ Usage x2.5 (increased demand, instruments)

At current Helium price recovery system would pay for itself in 4-5 years

Materials Science and Condensed Matter Physics

- **3 years outlook**
  - Engineering Materials
    - Improved instruments & methods for high-resolution grain mapping, big data sets, in-operando,..
  - Emergent Materials
    - New beamlines/instruments IEX, RIXS, THz, X-STM, ….
    - Look for opportunities in Computational Materials Design initiative
  - Extreme Conditions
    - Expand accessible phase space using common cross-beamline platforms
  - Dedicated end-station/sample environment engineering (sub-)group

- **APS Upgrade-MBA**
  - Nurture new coherence and nano-focusing capabilities for imaging and dynamics studies of materials.