The Extreme Materials Beamline for the accelerated study of radiation damage: XMAT

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Argonne National Laboratory

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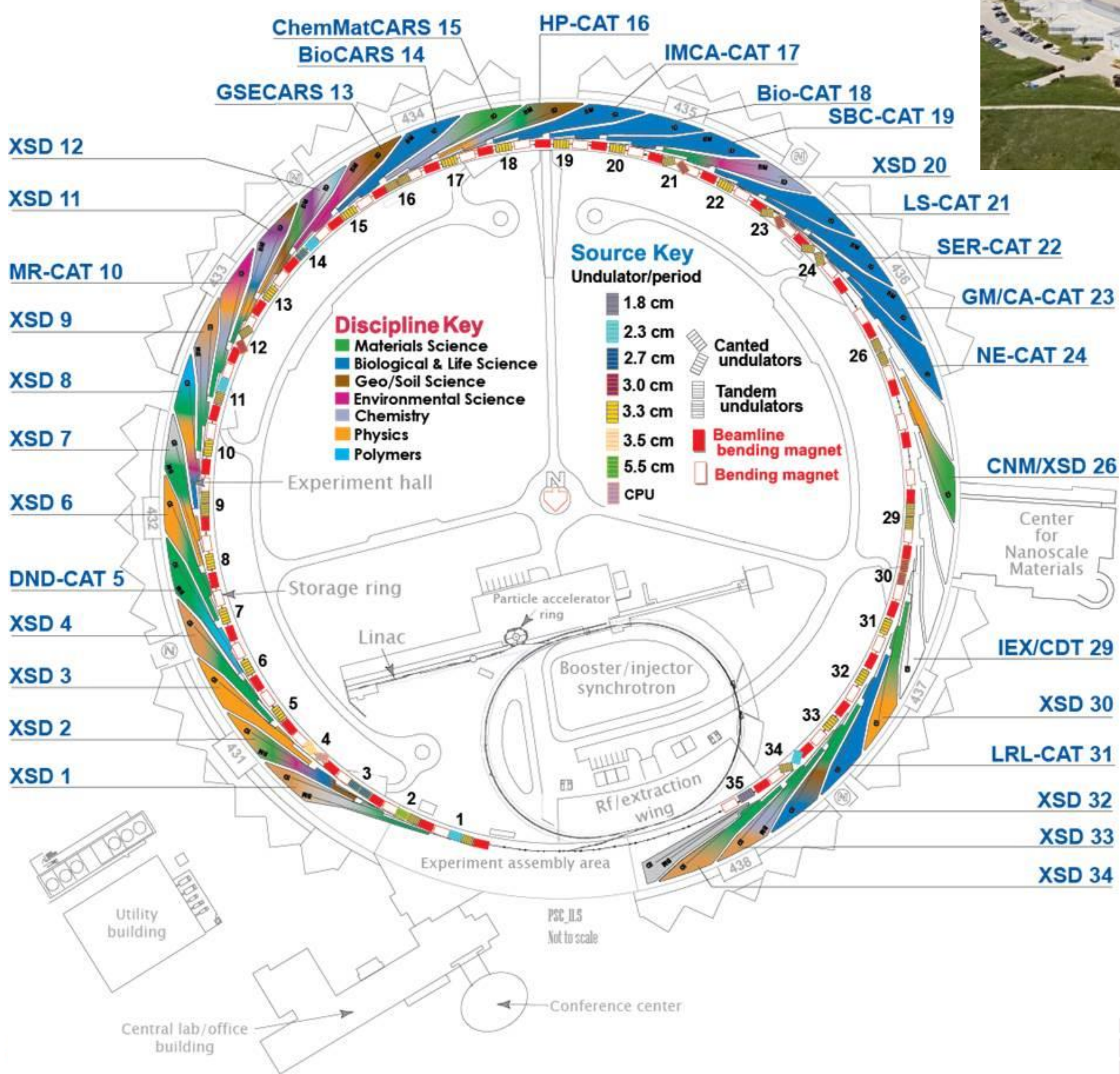
Advanced Photon Source, ANL



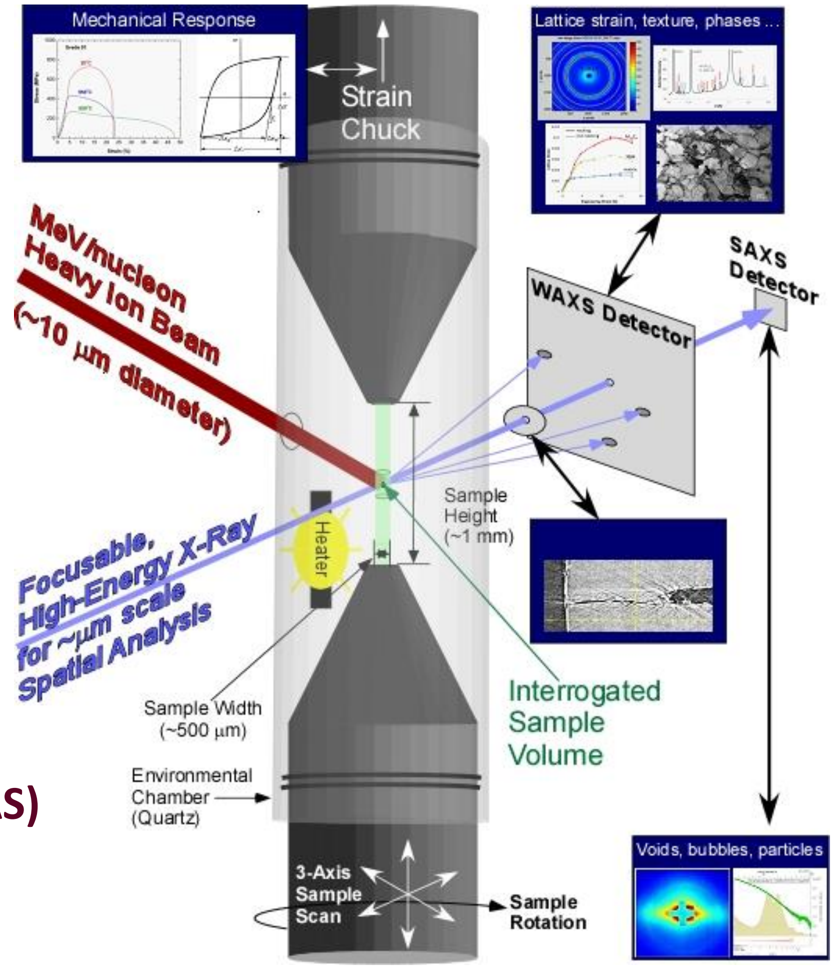
Advanced X-ray Characterization Techniques

- Scattering & diffraction
- Imaging & Microscopy
- Spectroscopy
- *In situ*, time-resolved studies of "real" materials in "real" environments

Proposal - eXtreme MATerials beamline (XMAT)

A new beamline at APS for *in situ* studies of nuclear energy materials under irradiation, temperature, stress, and environment.

XMAT will provide x-ray probes for *in-situ* study of materials in simulated nuclear reactor environments, enabling rapid evaluation of new materials performance under extreme service conditions including structural materials and for the first time nuclear fuels.



XMAT is made possible by combining two of Argonne's unique capabilities:

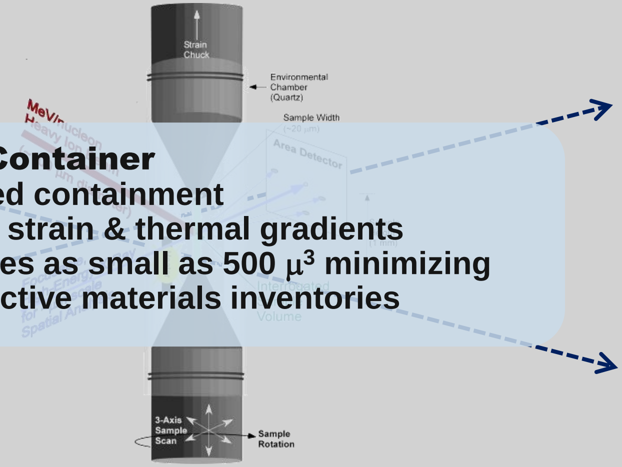
1. **Energetic, Heavy Ion Beams (ATLAS)**
2. **Focusable, High Energy X-Rays (APS)**

Opportunity Window -> APS/ATLAS Upgrades

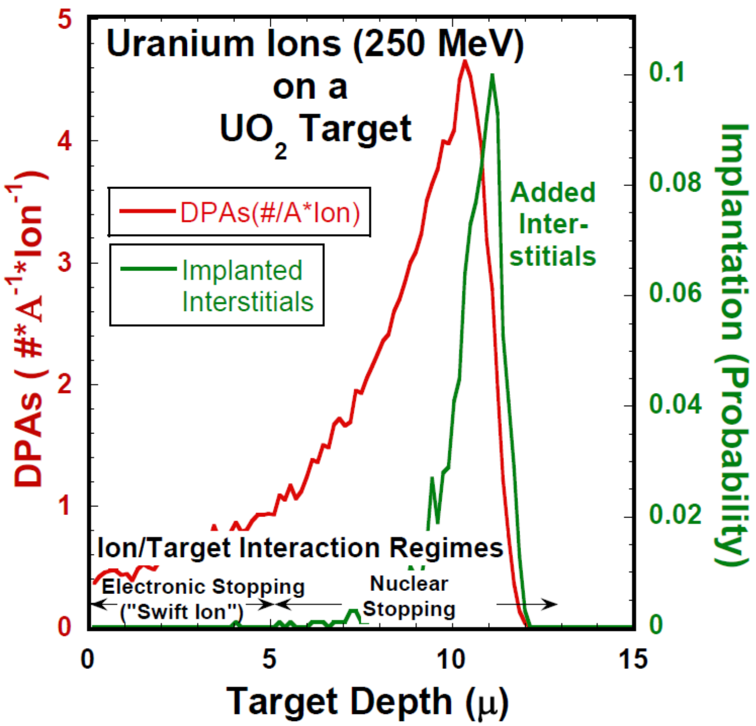
What's Unique? - High-Energy, Heavy-Ion Irradiation

***In Situ*, High Energy Ion Irradiation (HEI)**
- Damage Rates to 25 DPA/hour (controllable)
- Damage Doses to >2000 DPAs
- ~ 1 MeV/nucleon heavy ion irradiation (e.g. 150MeV Xe)

X-Ray Line (30<E<60 keV)
- Diffraction: Shape, size, orientation of single grains
- Scattering: defect distributions, aggregate response
- SAXS: nanoscale voids, bubbles, particles
- Tomography: three dimensional imaging, scattering



Sample Container
- Isolated containment
- *In situ* strain & thermal gradients
- Volumes as small as 500 μ^3 minimizing radioactive materials inventories



Ion damage provides rapid controllable, non-activating radiation damage, but material interactions are more complicated than neutrons.

HEI/X-Ray study allows interpretation by:
- Spatial separation of irradiation effects
- Deeper penetration removing "surface sinks"
- 6-8 μm depth damage close to neutron

While providing
- Damage Doses to > 2000 DP
- Controllable damage rates up to 25 DPA/hour

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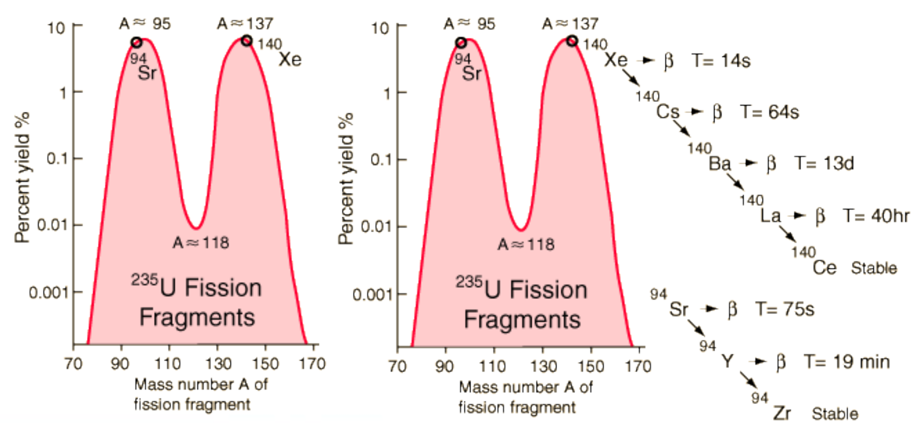
In nuclear fuels the complexity of fission fragment damage, the high total dose, and the chemical complexity has made

XMAT irradiates with fission fragments!

- XMAT achieves >2000 DPA total doses because of the unique properties of MeV/nucleon ions
- Controllable damage rates
- Effects of gaseous, immiscible and miscible fragments can be studied individually or in combination.
- Multiple mass irradiations (for ions with same charge to mass ratio)
  - e.g. $^{+15}Sr_{86}$ and $^{+23}Xe_{132}$
  - e.g. Ce / Zr



What's Unique? – High-Energy, Focusable X-Rays

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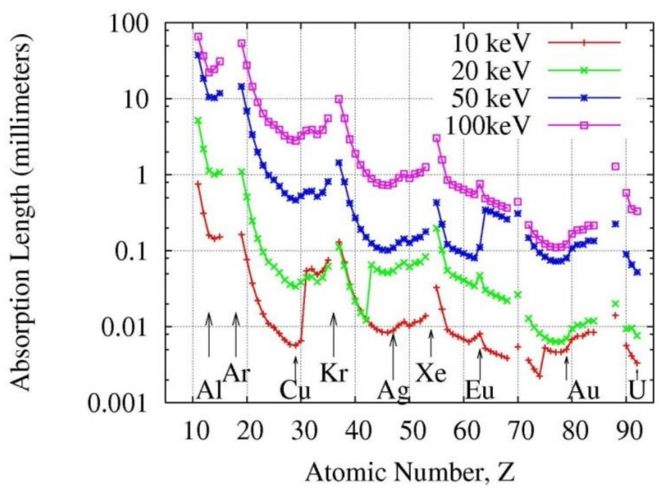
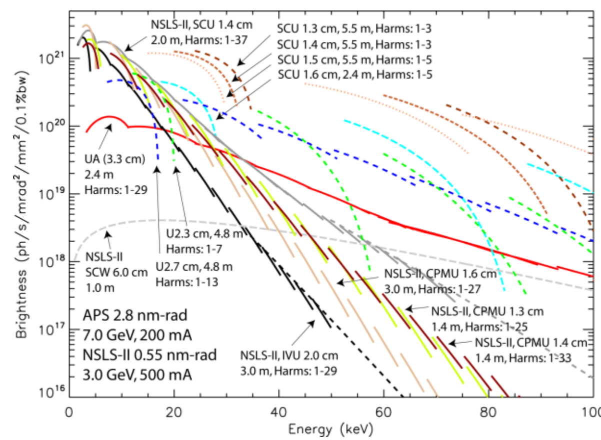
Sample Container
- **Isolated containment**
- ***In situ* strain & thermal gradients**
- **Volumes as small as 500 μ^3 minimizing radioactive materials inventories**

The key to understanding radiation damage is *in situ* study of the 3-dimensional evolution of microstructure at the mesoscale.



Higher x-ray energy->penetrate deeply into a sample – "**bulk" effects (including actinides)**.



High brilliance, high flux ->high resolution (mesoscale analysis)

Hard X-rays Critical to Radiation Research
- Real materials, real environments, real time

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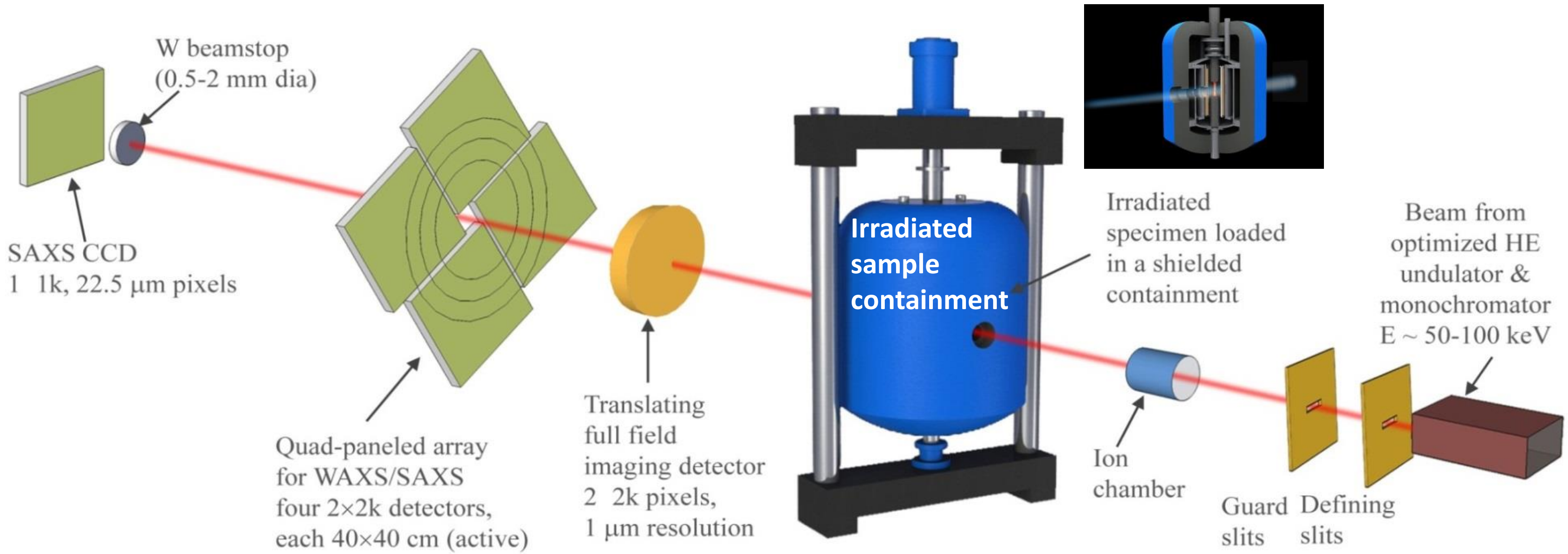
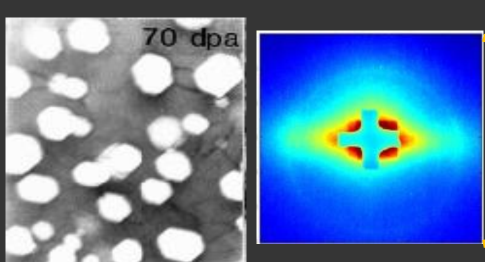
- ***Focusable*** allows mesoscale 3-D imaging
- Deep penetration
  - Bulk behavior
  - Environmental chambers
- Spatially resolved (inhomogeneity)
  - Resolve complex structures
  - Direct comparison with simulations on same length scales
- In situ, real-time studies
  - Dynamics
  - structural evolution
- Unit mechanisms and collective effects in complex engineering materials
  - Multiple probes for concurrent, multi-scale characterization

Concurrent, Multi-scale, Real-time Characterization of Irradiated Materials

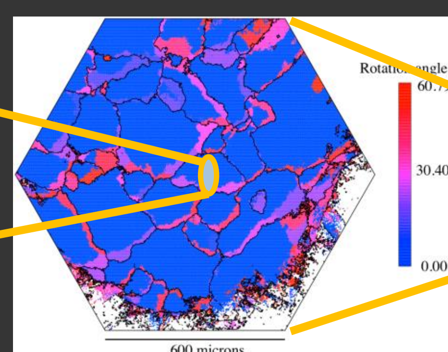
M. Li (NE), J. Almer (XSD), E. Benda (AES), Y. Chen (NE), A. Mashayekhi (XSD), K. Natesan (NE), D. Singh (NE), L. Wang (NE), F. Westferro (AES)



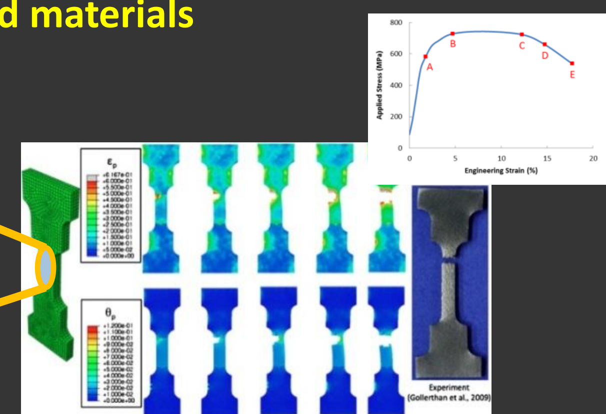
Combined techniques and intense, penetrating hard x-rays will visualize material evolution across relevant length scales under thermal-mechanical loading in irradiated materials



Nanoscale: diffraction and SAXS



Mesoscale: diffraction microscopy



Macroscale: mechanical loading

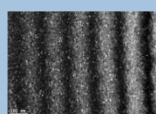
Predict Neutron Damage using Ion Damage Data

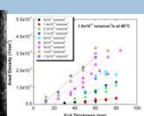
Meimei Li (NE/ANL), Mark Kirk (MSD/ANL), Donghua Xu, Brian Wirth (U. Tennessee)

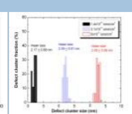
Collaborative and iterative process between experiments and computer modeling has led to an accurate model that can be used to predict radiation damage in nuclear reactors.

In situ Ion Irradiation Experiments

Well-controlled TEM with *in situ* ion irradiation experiments of thin films were designed to improve and validate computer models. Experimental data provide a complete set of high-quality, quantitative information, and described the defect behavior at a level of detail unavailable before.

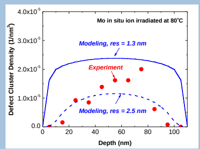


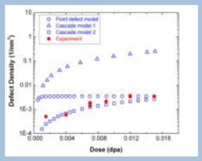




Experiment-Simulation Comparison

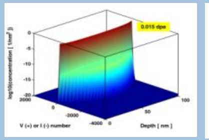
Quantitative, absolute comparisons between experiments and modeling at the same spatial and time scales have led to the establishment of accurate, reliable computer models.

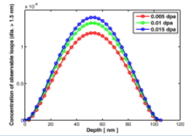


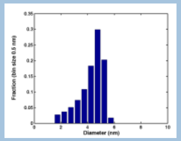


Computer Simulations

Multiscale modeling to simulate defect evolution from atomic-scale, pico-second events to nanometer-scale, hour evolution of defect structures.

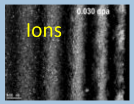


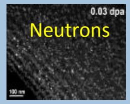


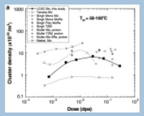


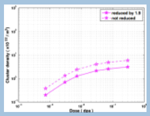
Prediction of Radiation Damage in Reactors

The experimentally-validated model for ion irradiated thin foils is used to predict neutron damage in Mo irradiated in a reactor, and validated by neutron irradiation data







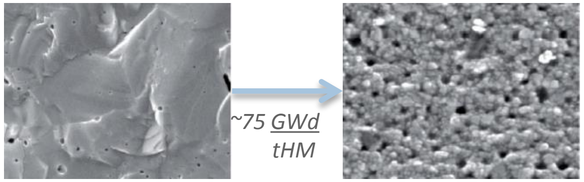


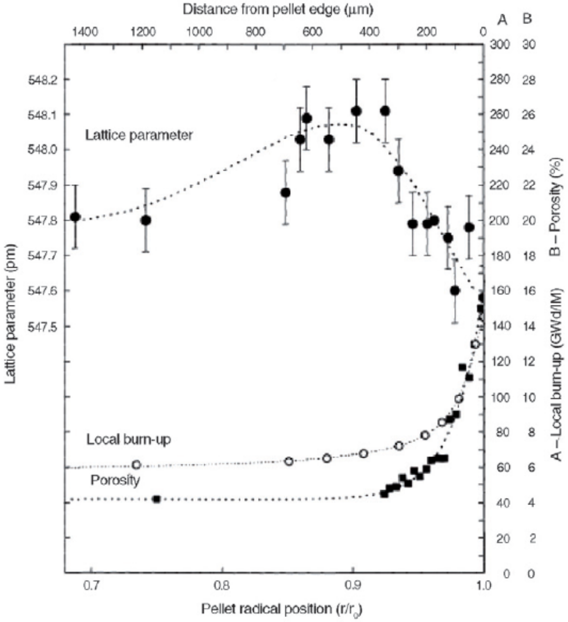
Neutron experiment

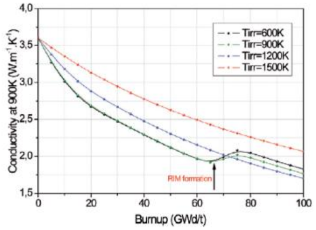
Model

Radiation Damage Challenge for Nuclear Fuels

- Fuel is subjected to ~1 displacement per atom (dpa) per day in Light Water Reactors (LWR)
  - High burn-up -> >2000 DPAs (cladding ~150 DPAs)
- >80% of the collisional damage is the result of fission fragments
  - Each fragment has ~ 1 MeV/nucleon
  - Electronic Energy Transfer to Fuel Matrix (excitation & ionization)
  - Nuclear Collisional Energy Transfer (responsible for DPA's)
- Fission products
  - Added Interstitials (extra atoms)
  - Chemical Distinct both in form and reactivity
    - **Volatiles -** Br, Kr, Rb, I, Xe, Cs, Te
    - **Metallics** - Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Se, Te;
    - **Oxides**
      - Precipitates: Rb, Sr, Zr, Nb, Mo, Se, Te, Cs, Ba
      - Dissolution: Rb, Sr, Y, Zr, Nb, La, Ce, Pr, Nd, Pm, Sm, Eu
- **Neutrons** – 3% of the energy, >20% of the collisional damage
- **Non-linearities** -> High Strain, Temperature & Temp. Gradients



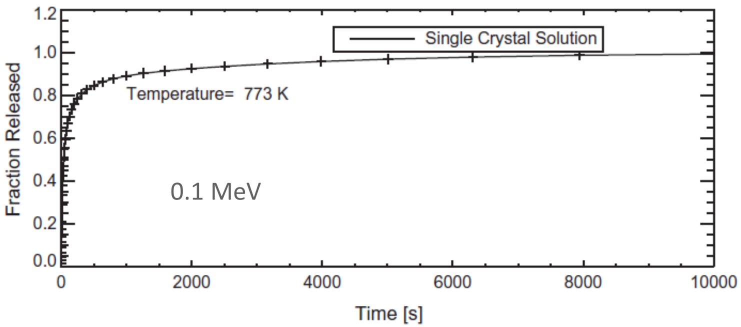




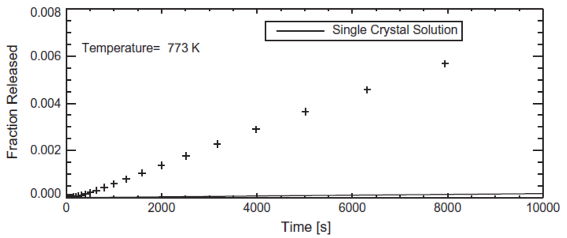
Predictive Modeling Requires an Understanding of Each Process!

Study at > 1000 DPAs

- Neutron Irradiaton
  - 3 Years in a reactor
  - 1 year to "cool down"
- Ion Irradiation (Fast -> DPA/minute)
  - Conventional Accelerators (>= 1 MeV/***ion***)
    - Limited to damage < ~200-400 DPAs
    - Surface Effects for T > 773 K (King, et al J. Nucl. Mat., 415, 38-54, 2011)
  - XMAT Facility (>= 1 MeV/***nucleon;*** *eg* U @ 235 MeV)
    - Damage to >2500 DPA (as fast as 20 hrs)
    - Surface does not play a role at relevant temperatures (~10 μ away)
- Rate Effects
  - Rates can be controlled (& rate effects studied)
  - Damage can be "seeded" by initial neutron exposure.
  - Competition between Diffusion, Strain and Radiation Damage can be monitored



Implanted Xe in U



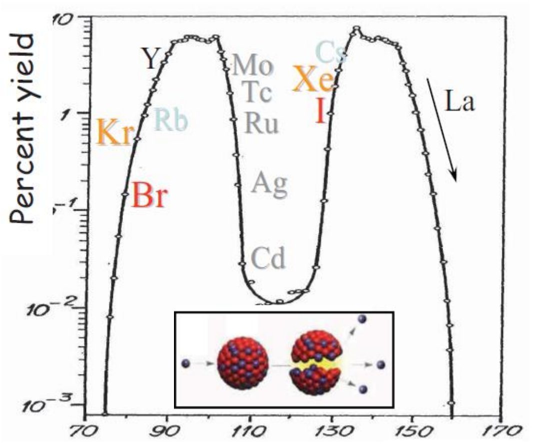
80 MeV

Grand Challenges

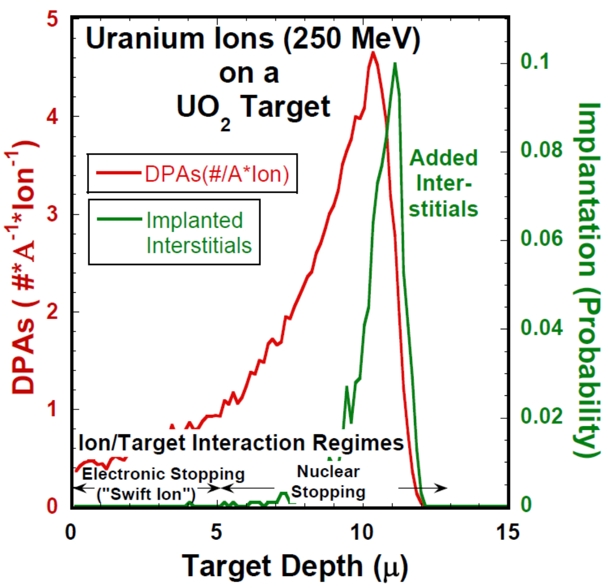
- **High Burn-up Structure**
- **Damage Delays**
- **Rate Competition (Rad Damage, Diffusion, Strain)**

Studies of Separate Effects with Controlled Parameters

- **XMAT Delivers Fragment Ions onto target @ Fission Fragment Energies**
  - Any Fragment Element is possible
  - Acceleration to > 1 MeV/*nucleon*
  - In essence XMAT's geometry allows study of each of the unique damage processes that occur in fuels.
  - Multiple Ions may be accelerated at once.
- **Added Interstitials (extra atoms)**
  - Separated in depth
  - Analysis as a function of depth allows assessment of the role of added interstitials
  - Chemical Effects can be studied since individual elements are delivered by the XMAT beam
- **Electronic Energy Deposition**
  - Swift Ion effects can be studied of varying nuclear damage
  - Light ion projectiles can be used to add varying mixes of damage
- **X-Rays provide a unique spatial probe**
  - Crystal Structure
  - Lattice Spacing
  - Thermal Transport



Mass (amu)



XMAT Status

Preliminary design has been developed

- Recent upgrade of both APS sector 1 and ATLAS have many similar pieces that would be combined here
- The success of these designs gives confidence in the XMAT design
- A more detailed accelerator design is underway to place it on the floor of APS.

The Advance Photon Source Scientific Advisory Committee agrees that XMAT is a good opportunity for the APS

- A key step in securing a "place" on the ring
- Working with APS management an "open" position on the ring has been found that would deliver appropriate X-Ray light for XMAT

The User Community is being engaged.

- An internal team has been assembled with the appropriate skills to move the concept forward.
- A distinguished external board has been engaged to help move the proposal forward.

A series of "first" experiments are underway to demonstrate the opportunity provided.

XMAT Members: First step in building community consensus for concept.

External Board

- **Todd Allen**, Idaho National Laboratory/ University of Wisconsin
- **Mark Kirk**, Argonne National Laboratory
- **Arthur Motta**, Pennsylvania State University
- **Bob Odette**, University of California at Santa Barbara
- **Simon R. Phillpot**, University of Florida
- **Andrew Sowder**, EPRI
- **Jim Stubbins**, University of Illinois (chair)
- **Jeff Terry,** IIT; Advanced Test Reactor National Scientific User Organization Executive Director
- **Gary Was**, University of Michigan
- **Brian Wirth**, University of Tennessee, Oak Ridge National Laboratory
- **Steve Zinkle**, Oak Ridge National Laboratory

Argonne Team

- **Michael Pellin**, PSE
- **Jon Almer**, APS
- **Tom Ewing, NE**
- **Hawoong Hong**, APS (XIS)
- **Meimei Li**, NE
- **Jerry Nolen**, PHYS
- **Marius Stan**, NE
- **Latif Yacout**, NE
- **Di Yun**, NE