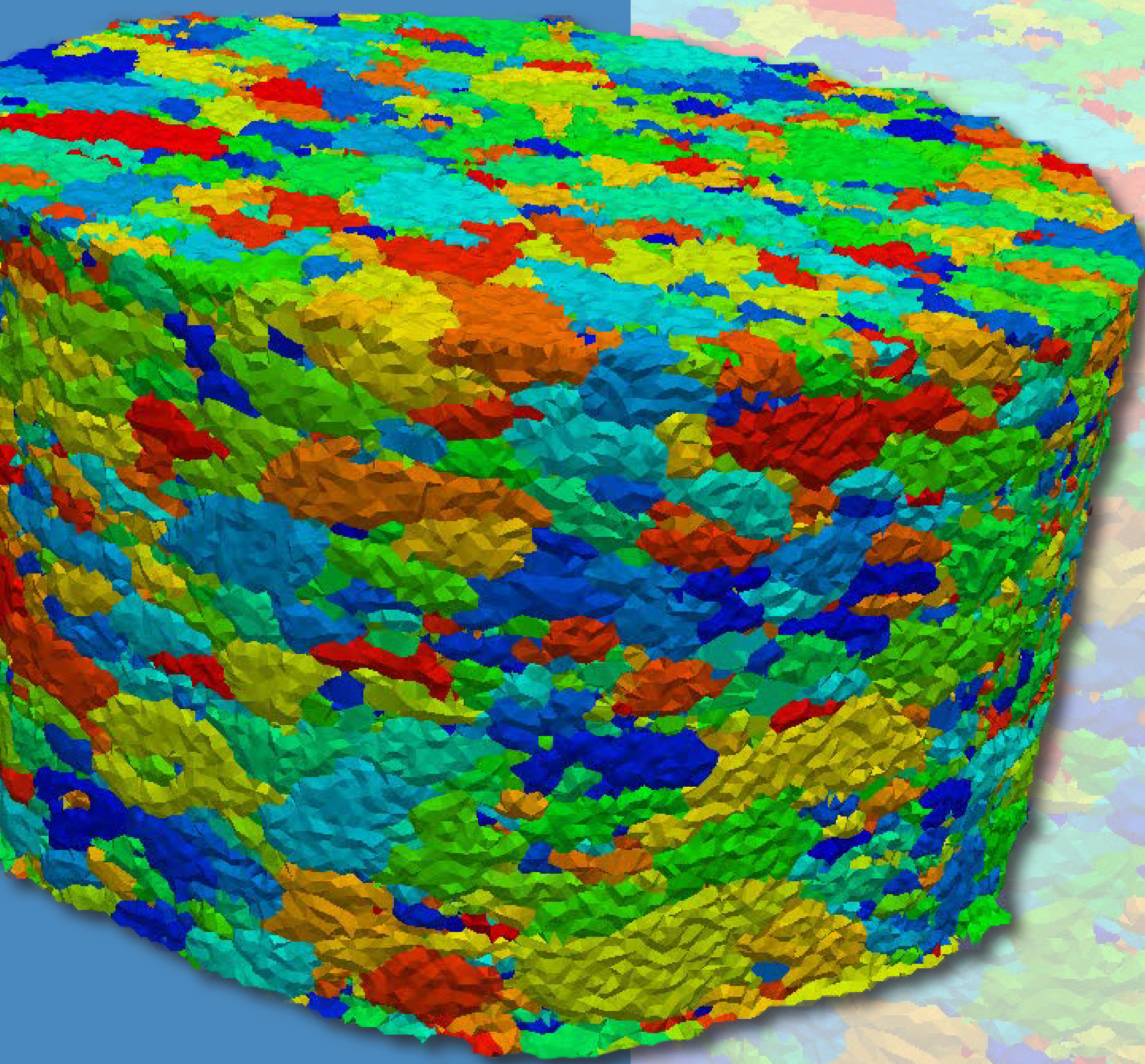
XMAT

eXtreme MATerials beamline

Advanced Photon Source *In situ* X-Ray Study of Materials in Extreme Environments



A PROPOSAL

Argonne NATIONAL LABORATORY

More advanced, capable nuclear materials are needed to increase accident tolerance, extend fuel burn-up, enhance waste storage security, and reduce facility costs.

XMAT enables rapid evaluation of advanced materials and fuels to high DPAs, under conditions that can be confidently extrapolated to nuclear environments.

The XMAT user facility combines the ultra-high-energy ion acceleration capability of Argonne's Tandem Linac Accelerator System (ATLAS) with the high-energy X-ray analysis capability of the Advanced Photon Source (APS) user facility to enable rapid, *in situ* mesoscale "bulk" analysis of ion radiation damage in materials.

New Beamline Concept

The Advanced Photon Source (APS) provides open access to specialized instrumentation and expertise that enables scientific users from universities, national laboratories, and industry across the nation to carry out experiments and develop theories that could not be done at their home institutions.

The APS upgrade opens a window of opportunity to build a new beamline that will provide users across the U.S. with the capability to conduct *in situ* real-time monitoring of radiation damage to new nuclear materials.

The proposed beamline will bring together two technologies, high-energy, heavy ion irradiation and high-energy X-ray scattering, to enable the interrogation of samples subjected to radiation, strain, and thermal gradients. The high-energy ions and X-rays are well matched — allowing radiation damage deposition and interrogation to depths exceeding 10 microns even in actinide materials. Energetic heavy ion irradiation produces a range of spatially separated radiation damage phenomena. Argonne's APS produces focusable, intense 50-100 keV X-rays capable of probing each of these damage regions.

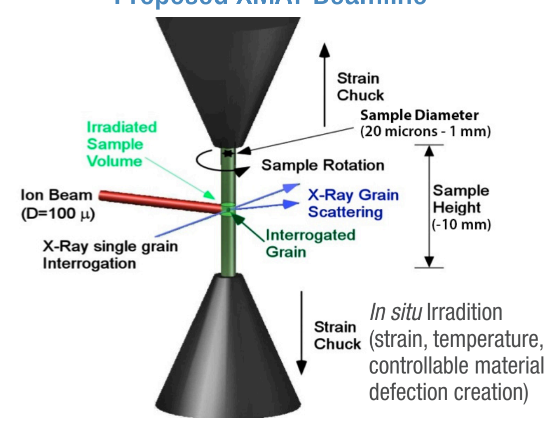
The *in situ* experimental information will be coupled with high-performance computing simulations to analyze the dynamics of irradiation-induced changes and predict the response of materials in extreme nuclear environments.

What's Unique?

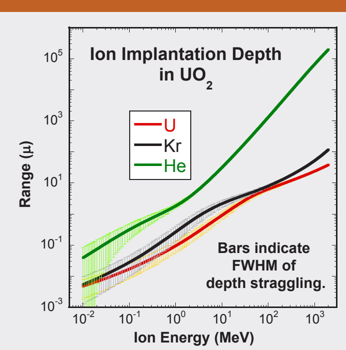
We're Not Just Scratching the Surface!

- High-energy, heavy ion irradiation (e.g., 250 MeV U)
- High-energy, focusable X-rays
- Three-dimensional mesoscale *in situ* study of radiation damage beyond the range of surface effects
- High damage doses and rates allow rapid material screening
- Combination allows users to follow all aspects of fission fragment damage at temperatures appropriate for used fuel storage or in the reactor
- Computer simulations informed by materials parameters measured, for the first time, can confidently extrapolate material response in a nuclear environment

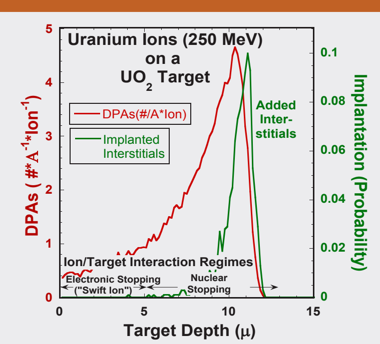
Proposed XMAT Beamline



MeV/nucleon ion acceleration can create bulk damage; allows >10 µm penetration.



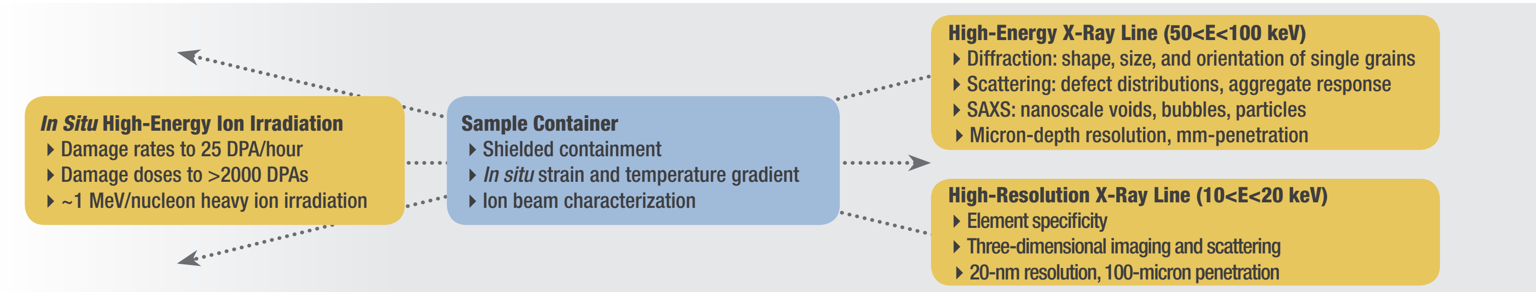
The energetic X-ray, ion combination reveals the phenomena that make ion and neutron damage different.



← At far left, XMAT's 250 MeV U ions (~1 MeV/nucleon) penetrate 10.5 microns into solid UO_2 (the most difficult case). Other ions (e.g., 84 MeV Kr, 4 MeV He) that can be accelerated with U, show similar penetration depths.

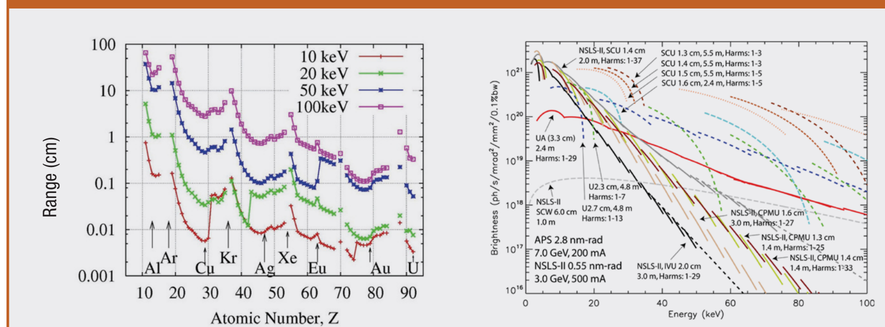
← At near left in red, the large, depth-dependent UO_2 DPAs per incident ion is shown. Fission fragments have similar energies. The APS X-rays' probing micron scale regions allow assessment of individual damage mechanisms (e.g., added interstitials [green] can be deconvoluted from DPA effects).

New Beamline Goals



- Couple new materials synthesis, predictive modeling, and accelerated ion beam testing to enable transformative breakthroughs in advanced nuclear fuels and materials, waste forms, and separation technologies.
- Remove uncertainties, as much as possible, in understanding the differences in ion and neutron irradiation. This will be accomplished by
  - Energetic heavy ions, which produce damage deep in the sample, enabling the role of surfaces as damage sinks to be understood.
  - Damage rates to 25 displacements per atom per hour (DPAs/hr) with minimal sample heating allows rapid materials testing and an assessment of the damage rate dependence of a materials response.
- Provide insights into the extended response of materials radiation damage for the first time by employing the large damage rate/surface erosion rate of high-energy, heavy ions, which allows total damage doses to exceed several thousand DPAs.
- Provide, for the first time, both *in situ* X-ray scattering and three-dimensional characterization of defect dynamics. This will validate information for computer simulations which, in turn, will predict defect evolution under extreme irradiation.
- Enable study of a wide range of nuclear materials, including actinides and claddings by: 1) the penetrating nature of both X-rays and ions; 2) the small sample size required (allowing radioactive samples to be handled safely); and 3) the low sputtering yield of these ions (allowing 100-nm films to provide sample containment).
- Improve understanding of damage and aid in material design through simulations of irradiation effects such as point defects and clusters, voids and gas bubbles, and dislocations.
- Provide physical parameters to accurately model nuclear fuels.
- Enhance the Advanced Test Reactor (ATR) materials and facility by enabling further (and higher dose) study of ATR's current materials library while screening materials that would otherwise require extended testing.

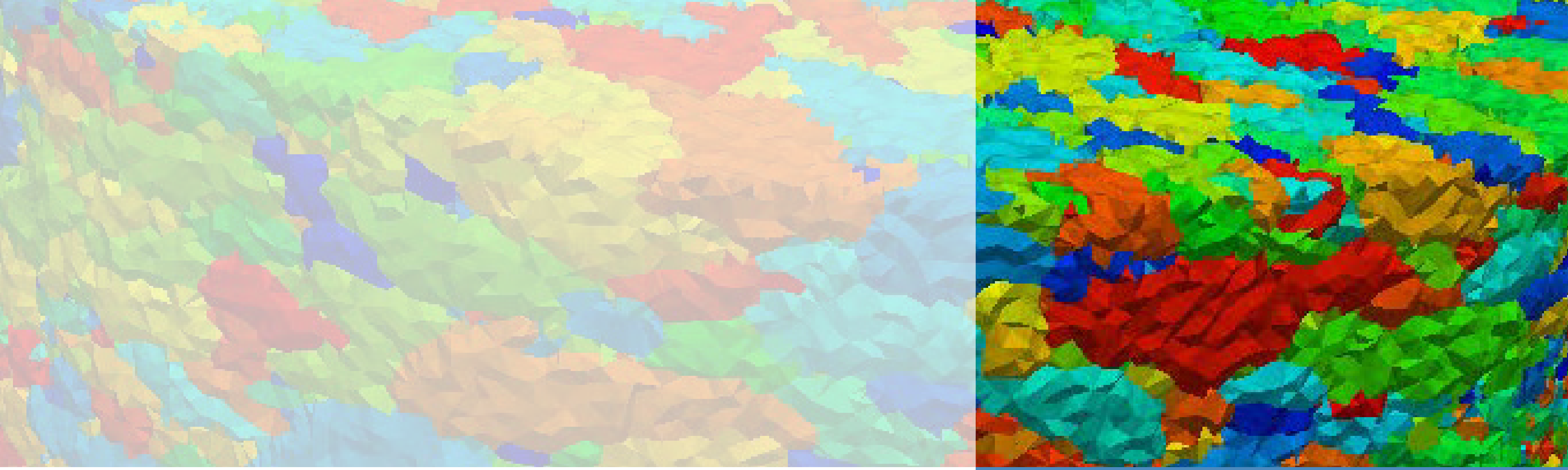
APS 50-100 keV X-rays probe samples with three-dimensional resolutions to 1 micron.

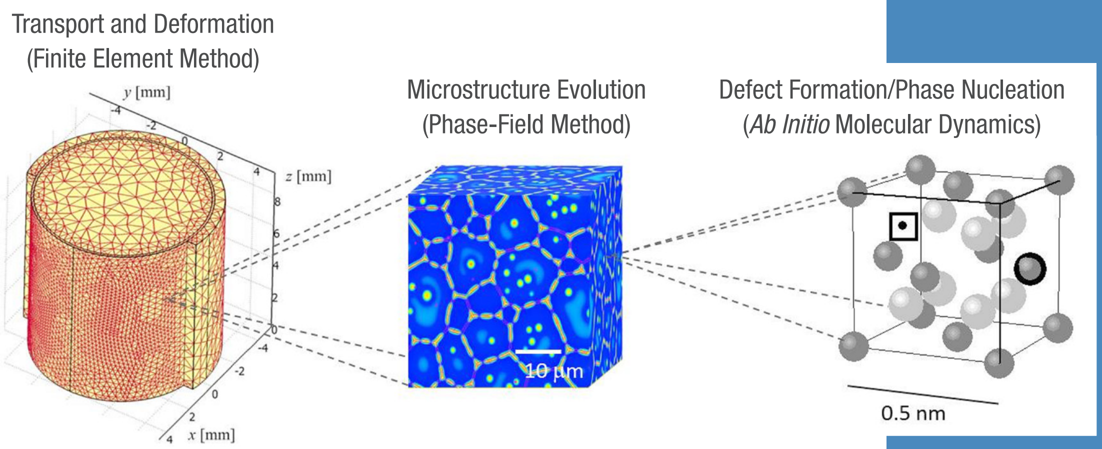


The APS's high-energy undulator X-rays penetrate (even actinide) samples with a beam brightness capable of isolating micron-scale sample voxels.

← At far left, the penetration depth of different X-ray energies is displayed as a function of sample composition. This penetration depth allows study of actinide samples and accommodates environmental studies, safety constraints, etc.

← At near left, the brightness of the APS X-rays are compared to other possible sources. Brightness is the ability to focus the X-rays' small volumes while maintaining sufficient beam intensity for rapid-sample analysis.





Multiscale simulations predict radiation damage effects on heat transport and deformation in UO2 nuclear fuel elements with metallic cladding. The information is exchanged between scales via file transfer using a “sampling” technique that selects representative computational domains at each scale.

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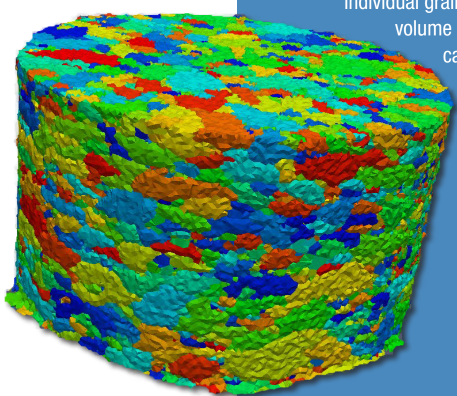
On the cover



Individual grains can be seen in a $0.79 mm^3$ volume of copper. These measurements can be undertaken as a function of temperature, permitting new three-dimensional insight into the thermal evolution of grain boundaries. Image courtesy of Bob Suter, Carnegie Mellon University, taken at the Advanced Photon Source.

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