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Decoding Early Candidacy of High Entropy Alloys for Nuclear Application using the Advanced Test Reactor through Predictive Methods and Combinatorial Testing

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Decoding Early Candidacy of High Entropy Alloys for Nuclear Application using the Advanced Test Reactor through Predictive Methods and Combinatorial Testing

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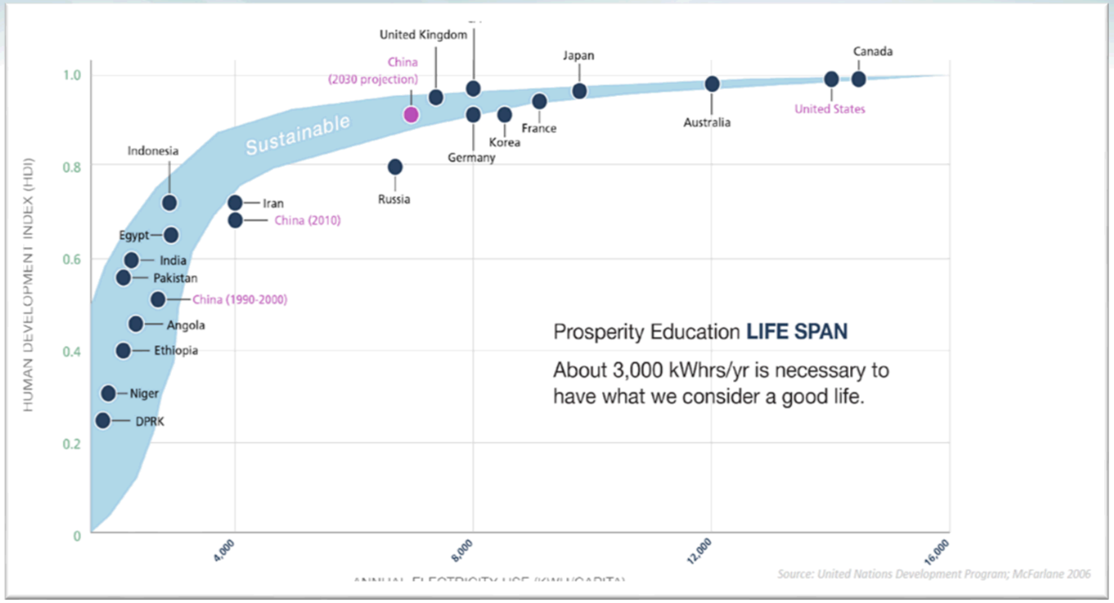
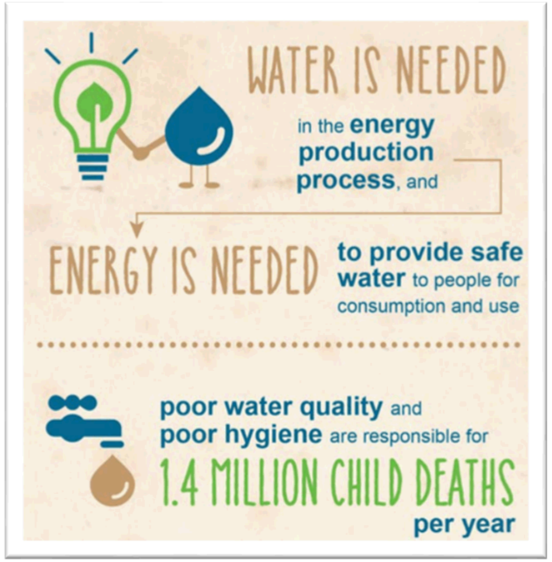
1. Idaho National Laboratory
2. University of Utah
3. CalNano Inc.

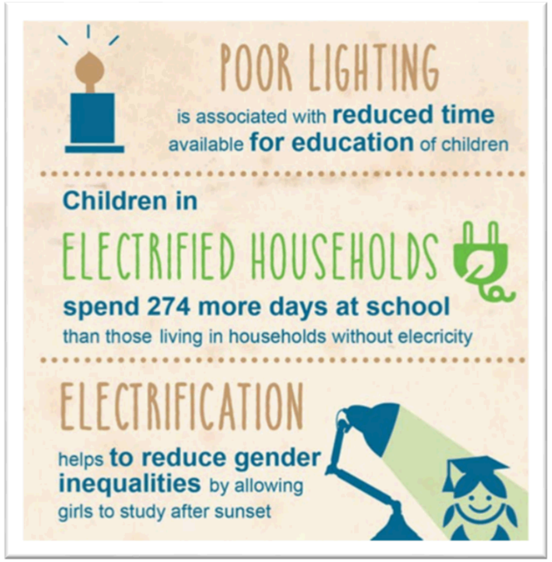
Idaho National Laboratory

First, why nuclear?

- **By 2040 the world population is expected to surpass 9 billion people and electricity demand is expected to increase by 93% - UN/UNICEF**
- **Quality of life is intrinsically linked to power generation**
- **Education opportunities are directly linked with access to reliable electricity**
- **Gender equality is highly dependent upon access to reliable electricity**
  - **E.g., 95% of the Bangladeshi communities rely on biomass for cooking & 46,000 die prematurely from respiratory infections caused by solid fuel use within the home. Women and children are disproportionately affected.**

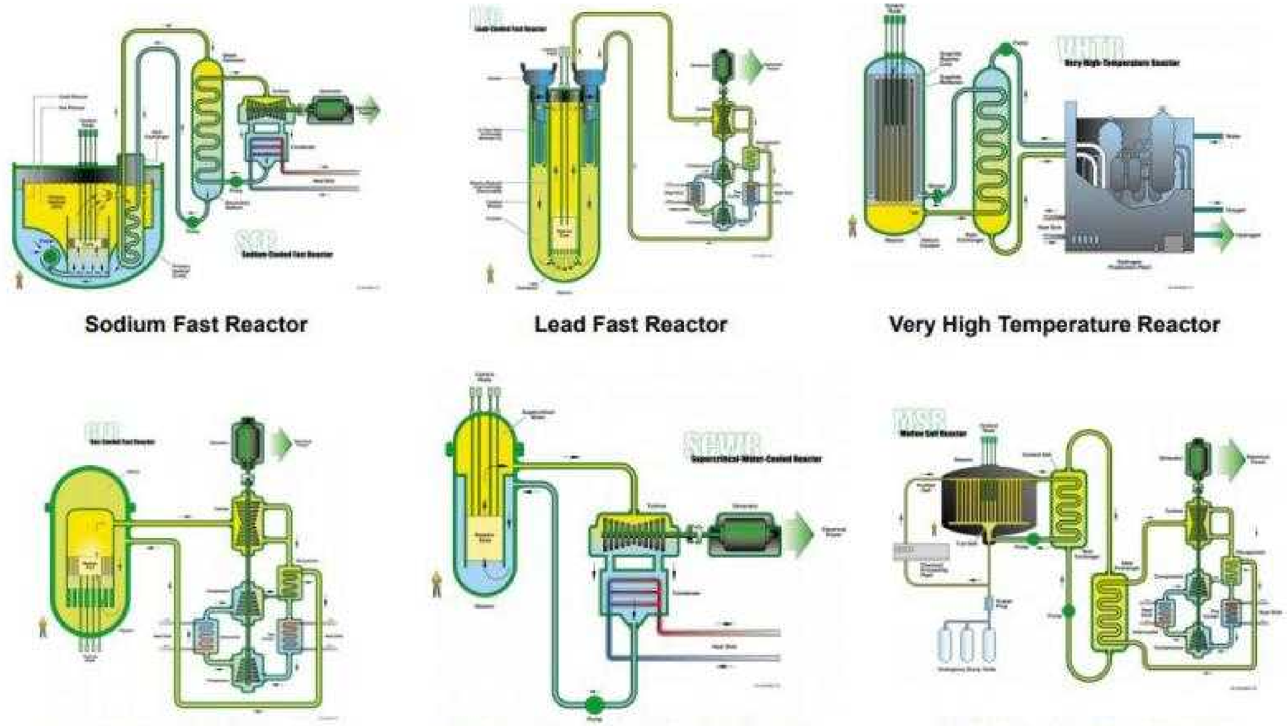






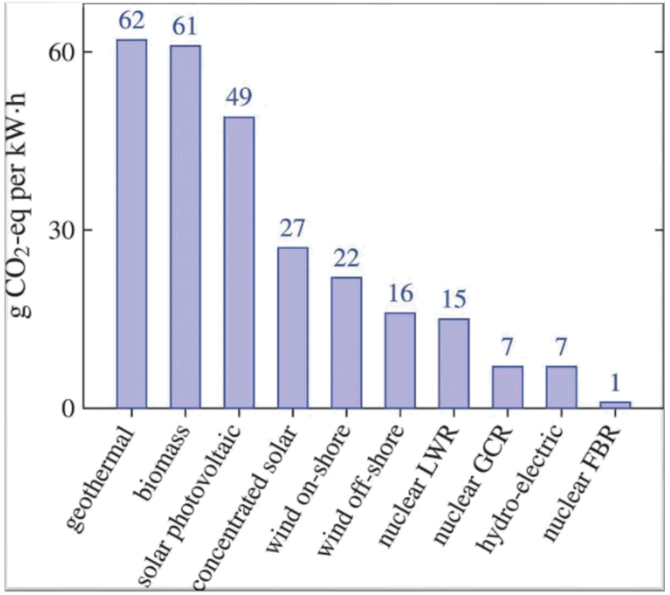
What do we want from a 'nuclear material'?

- What are 'nuclear materials'?
- What is a Gen IV reactor?
- Why is nuclear important compared to other energy sources?



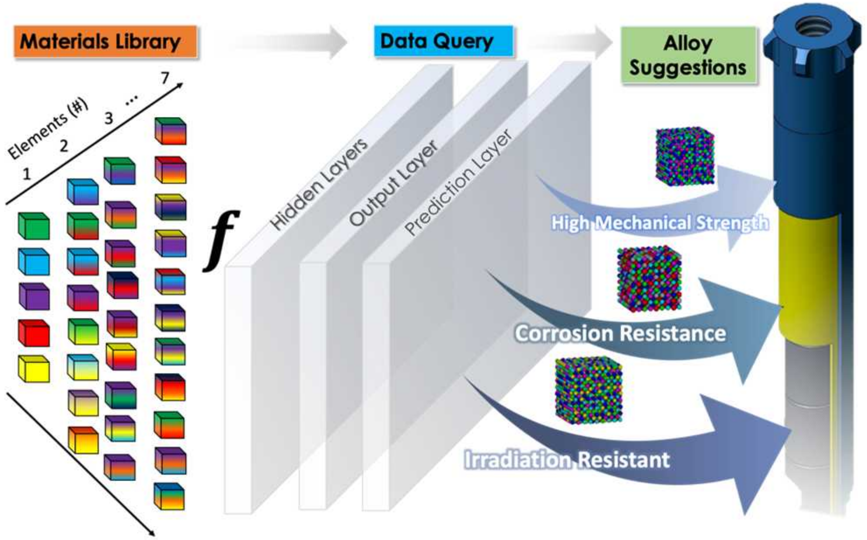
Sodium Fast Reactor | Lead Fast Reactor | Very High Temperature Reactor

Gas Cooled Fast Reactor | Supercritical Water Cooled Reactor | Molten Salt Cooled Reactor

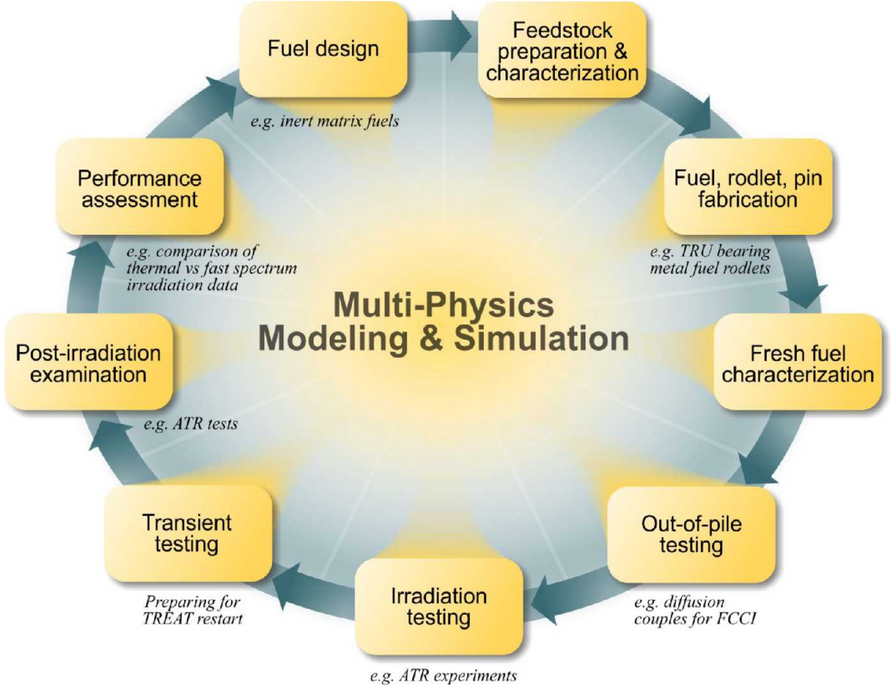


Nuclear Materials Challenges and High Throughput HEAs

- The deployment of advanced reactor cores, like Gen IV reactors, relies upon the development of advanced materials
- The traditional trial and error approach to nuclear material development (cook and look) is slow and expensive
  - Roughly 25 year R&D cycle
  - Qualification notionally requires 10 years and $500m

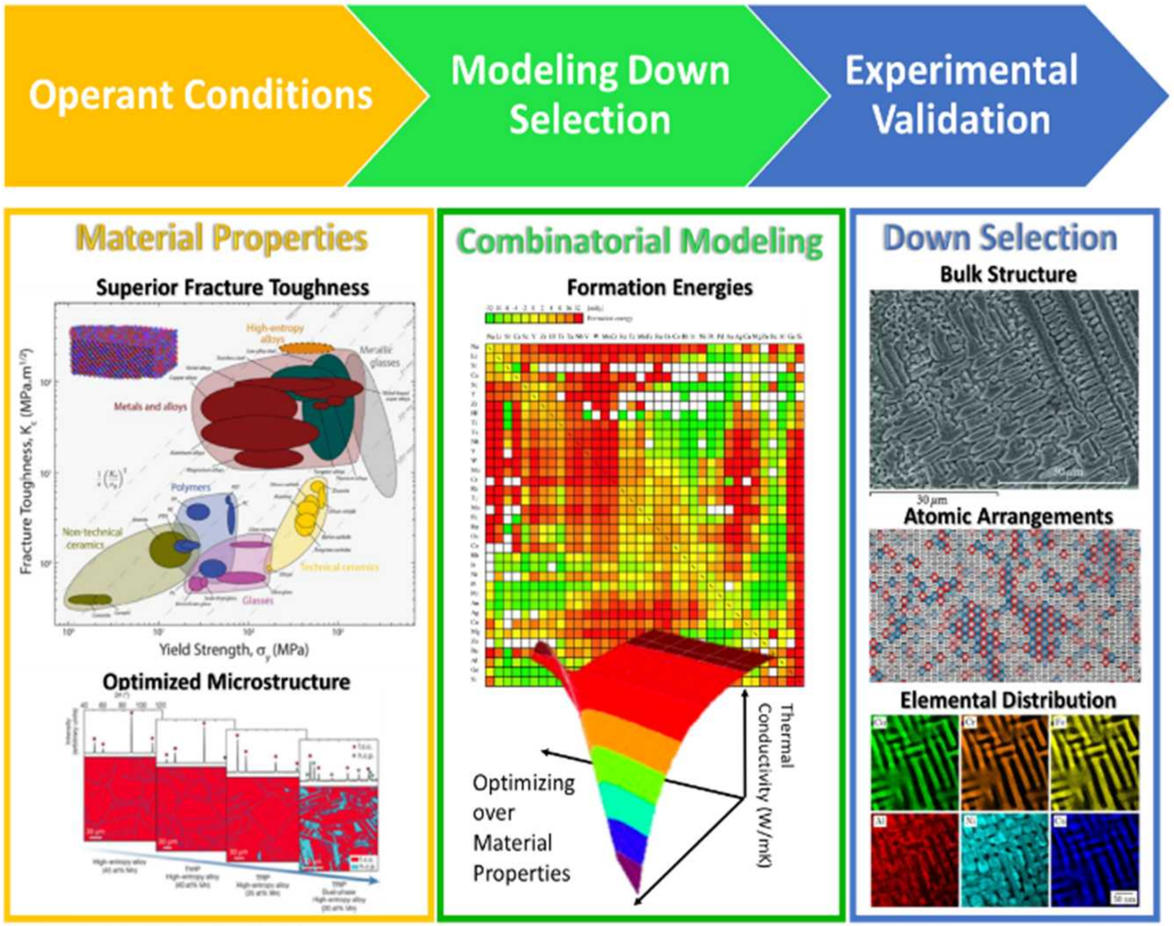


Nuclear Fuel Development Lifecycle



- Modernization of nuclear R&D is required
- Advanced materials, such as HEAs or MPEAs, can provide material performance previously unavailable to reactor designers

Designing the Alloys



1. Huang, Jen-Ching. *Scanning*, 2012, **34**, 325-31.
2. Z. Li, K. Pradeep, Y. Deng, D. Raabe, and C.C., *Nature*, 2016, **534**, 227–230.

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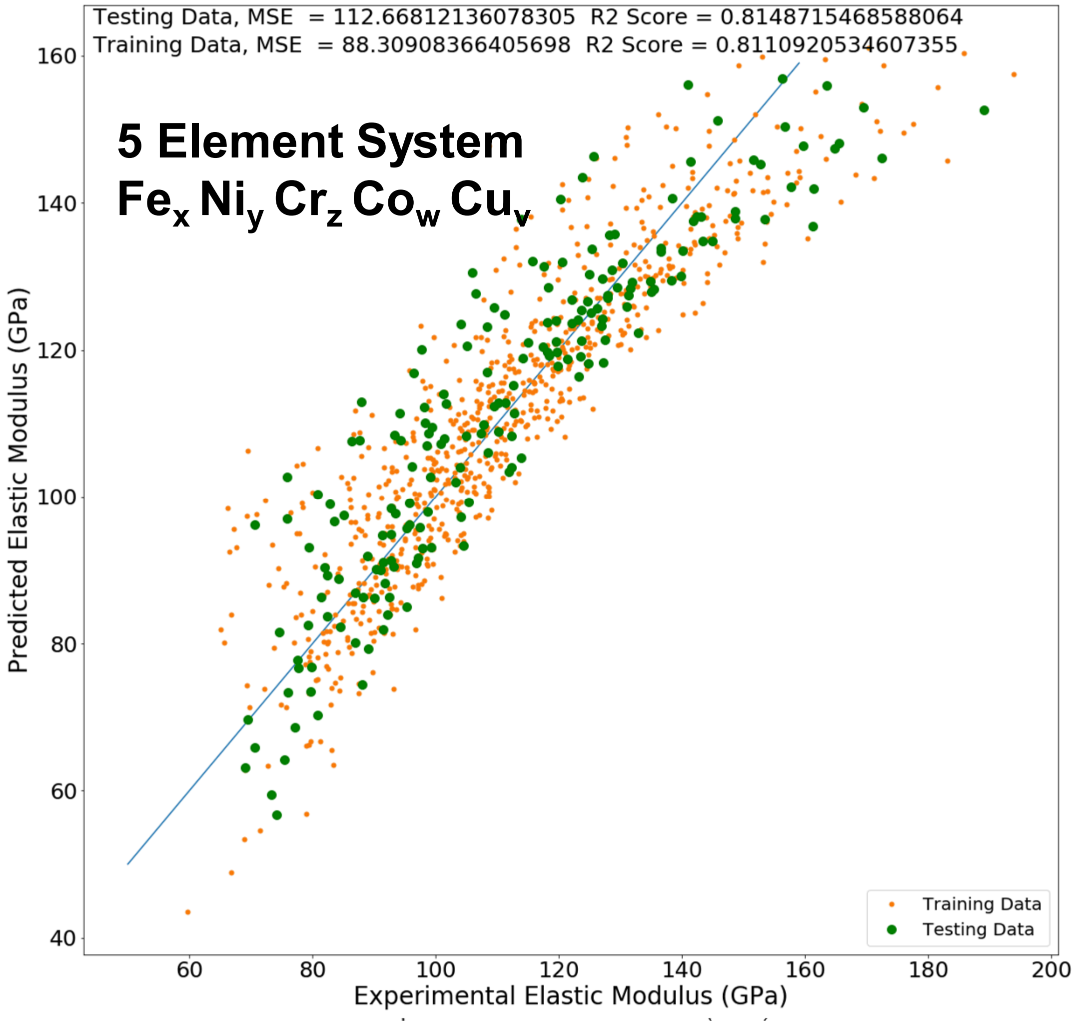
https://www.rrutc.msm.cam.ac.uk/research-themes/high-entropy-alloys

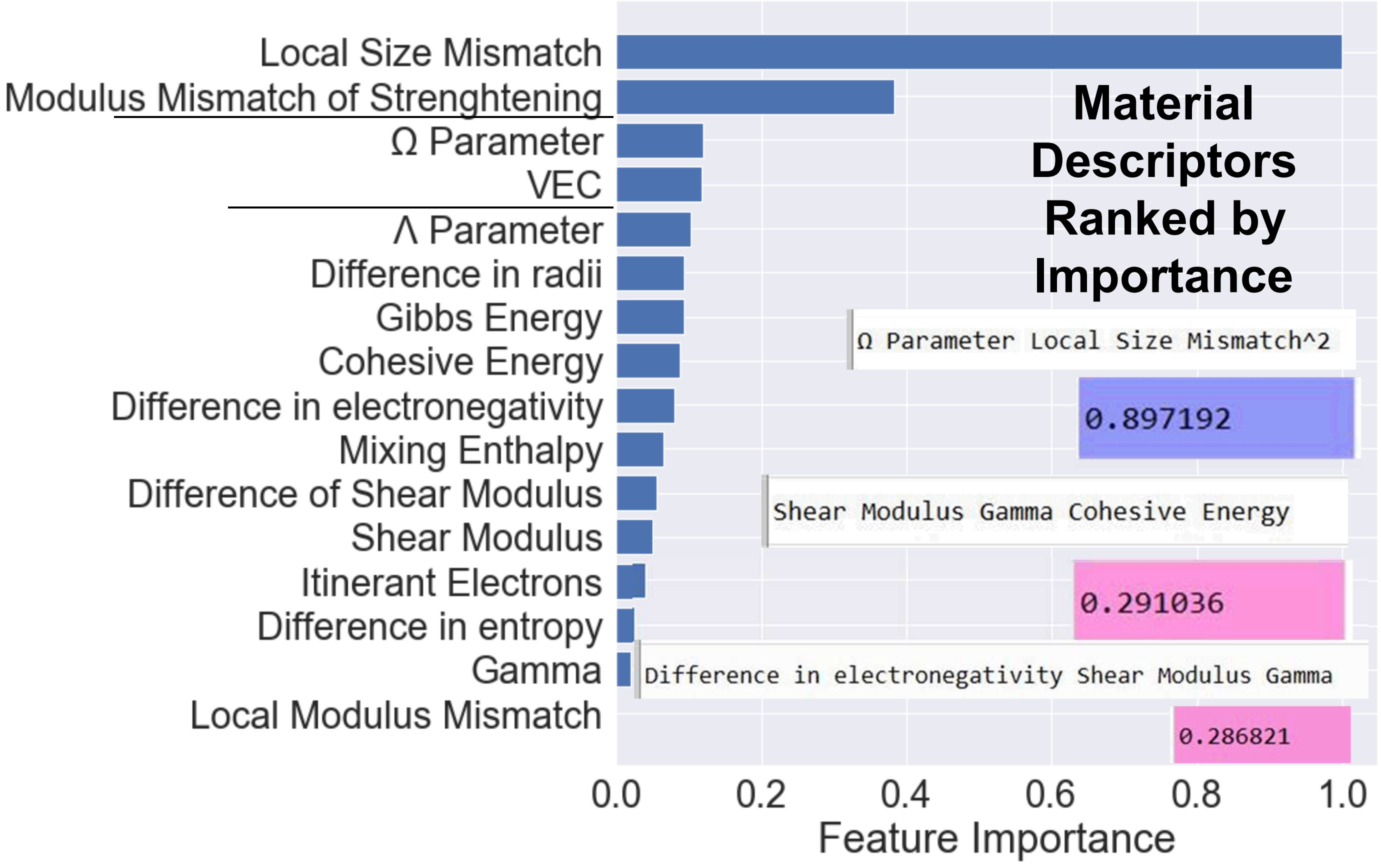
- Accelerated approach to materials research through intelligent materials design.
- Combinatorial materials modeling and electron microscopy accelerates the pace at which researchers converge on potential high-entropy alloy candidates from an early stage
- Down selection of material possibilities (over 2.3 million 3-6 element systems) to a dozen distinct options for insertion to the Advanced Test Reactor (ATR)

Evaluating Properties Alloy Design through Machine Learning

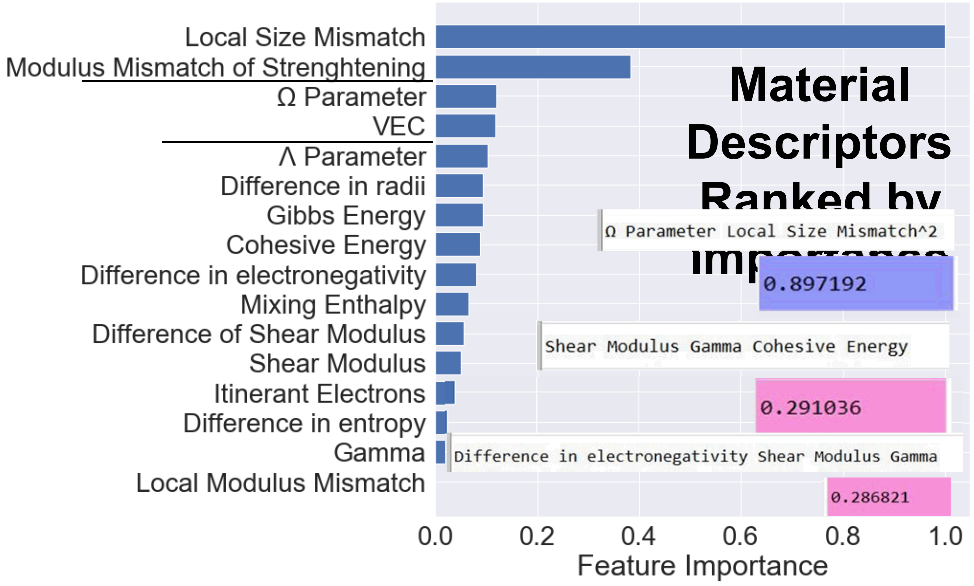
Prediction and Training on Elastic Modulus

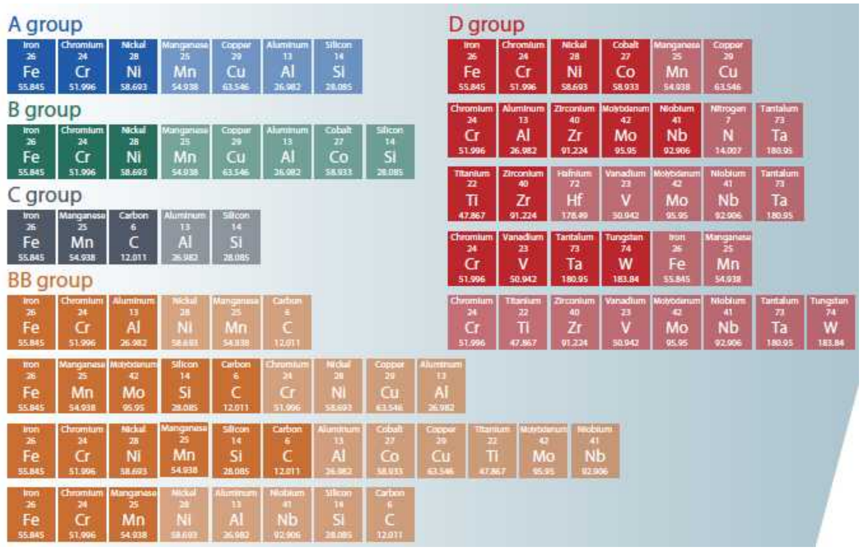


- **Training & evaluation dataset: 30,000+ alloys** containing varying concentrations from **0 °K to 1673 °K**.



Alloys selected





B Group:

- FeCrNiCoCu
- FeCrNiCo
- FeCrNiMnCo

BB Group:

- FeCrNiMnSiC
- FeCrNiMnSiCMo
- FeCrNiMnAlCoSiCCuTi
- FeCrMn
- FeCrMnCo
- FeCrMn*

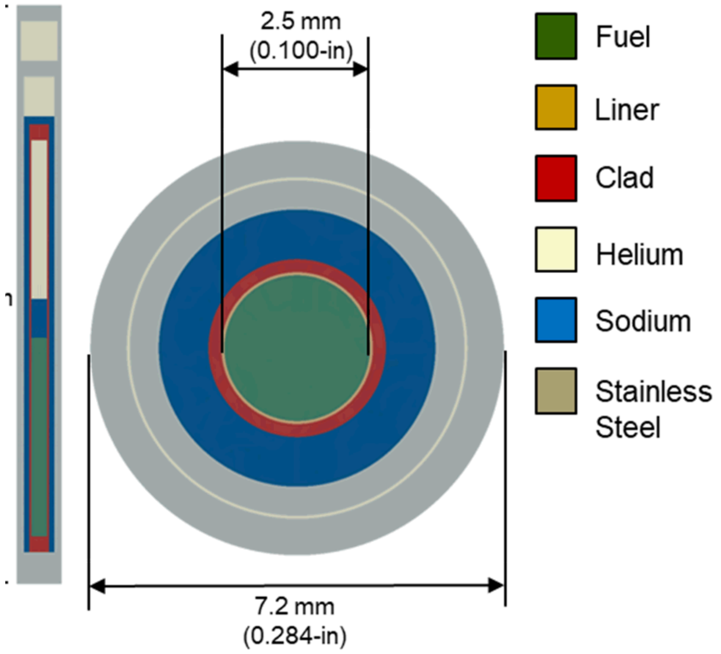
D Group:

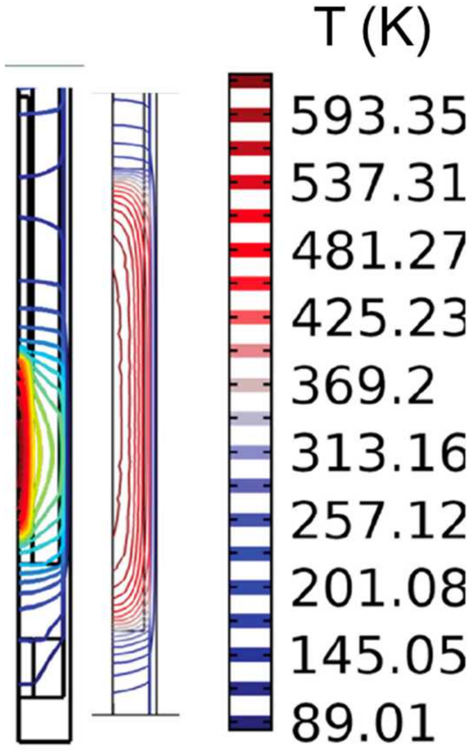
- CrAlZrMoNbTa
- CrAlZrMoNb
- CrAlZrMoNbN
- $CrAlZrMoNbNTa_2$
- TiZrVMoNb
- $Ti_2ZrHfV_{0.5}Mo_{0.2}$
- TiZrHfNb
- TiZrHfNbTa
- FeCrVTaW
- CrVTaW
- CrMnVTaW

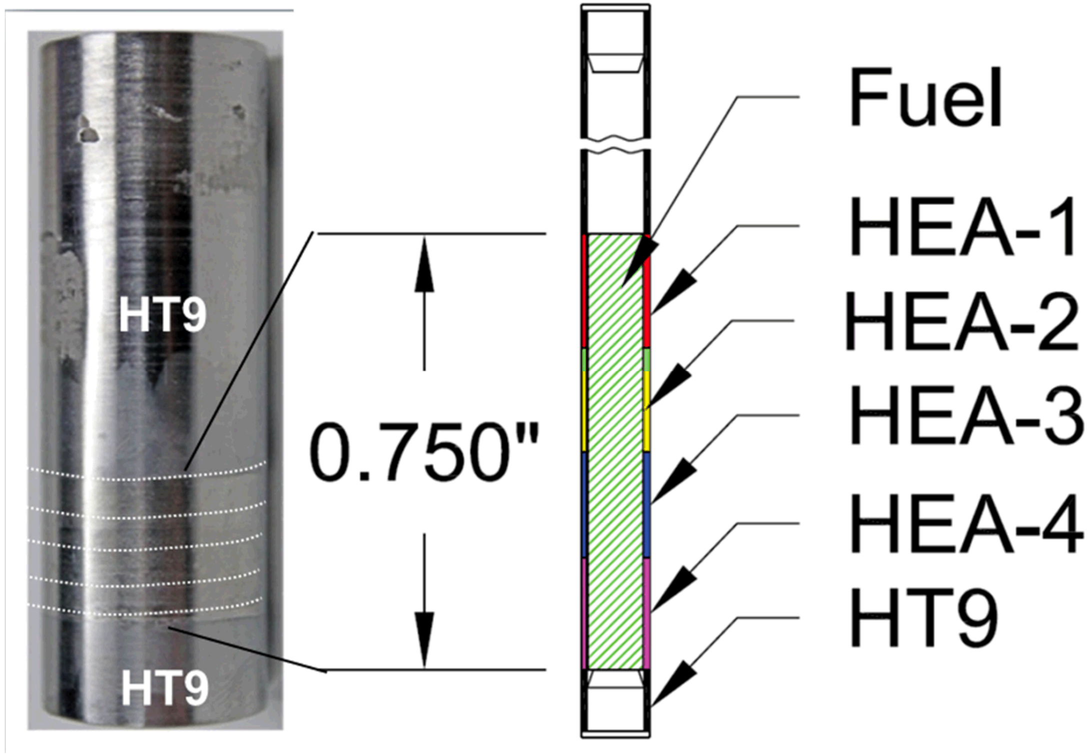
Irradiation Test Strategy – FAST

Fission-Accelerated Steady-State Testing in the ATR

- Accelerated fuel irradiation test: Up to 10x burnup rate
- Double Encapsulated design facilitates versatile experiment design opportunities
- Improved sensitivities to fabrication eccentricities and variations

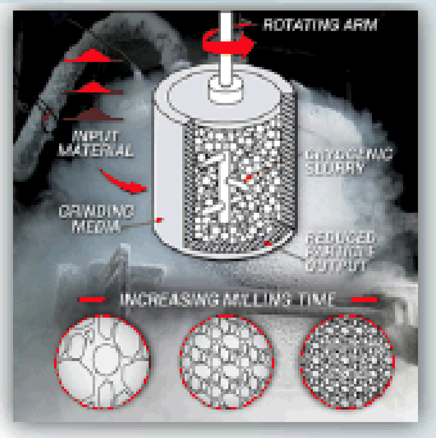






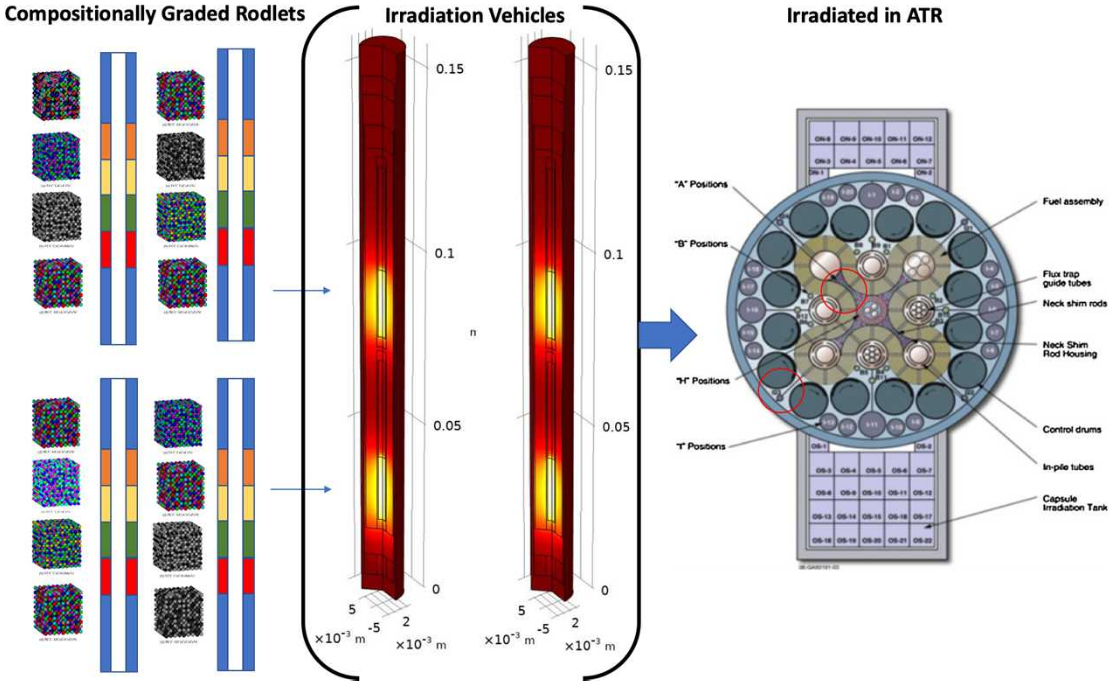
Material Fabrication

- Supporting efforts in alloy design and selection by fabricating 100+ alloys.
- Single and compositionally graded specimens.
- Alloys extensively characterized (in progress) to assess microstructure, structural uniformity, mechanical response, and thermal stability.



Cryogenic Milling

SPS



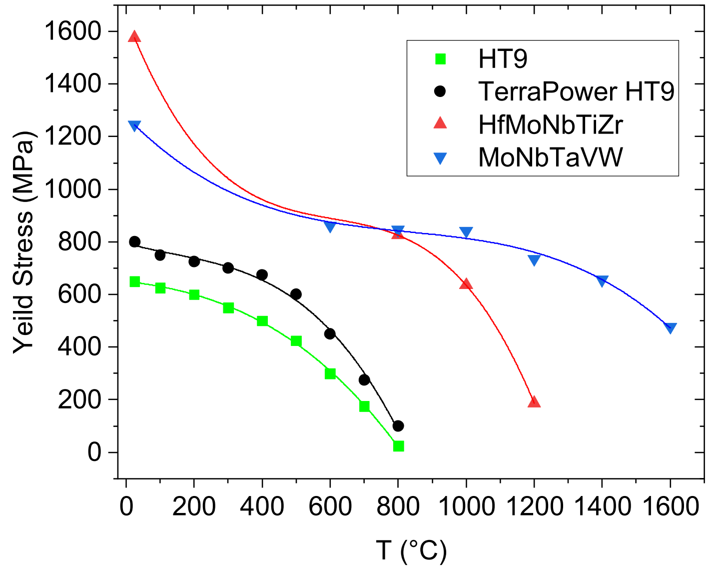
Irradiation Test Strategy – FAST Rodlets

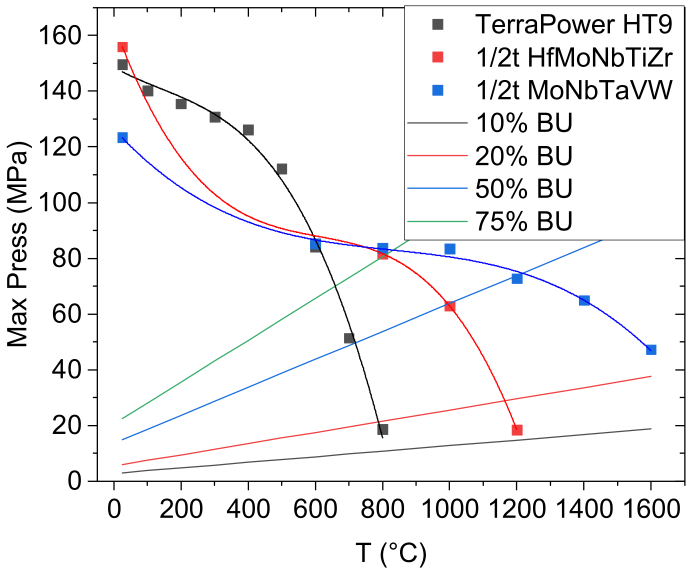
- ASME circumferential pressure limit is dependent upon the yield stress and wall thickness of the tubing

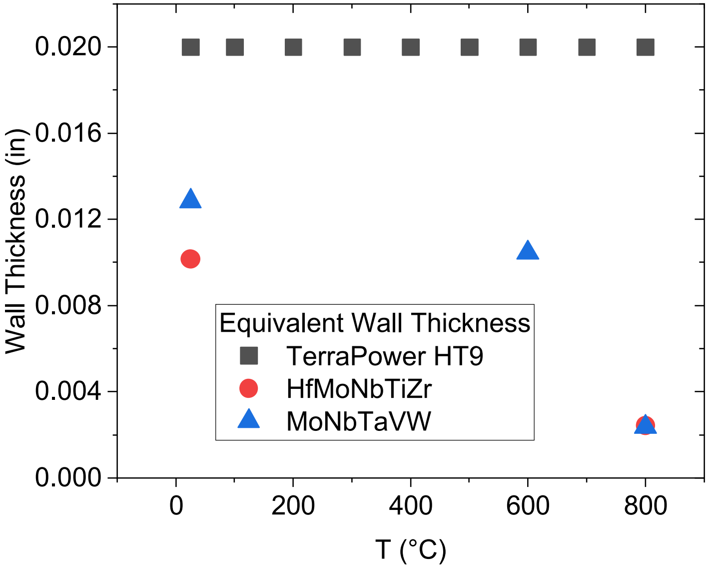
$$P_i = \frac{\sigma_Y t}{\frac{D}{2} + 0.6t}$$

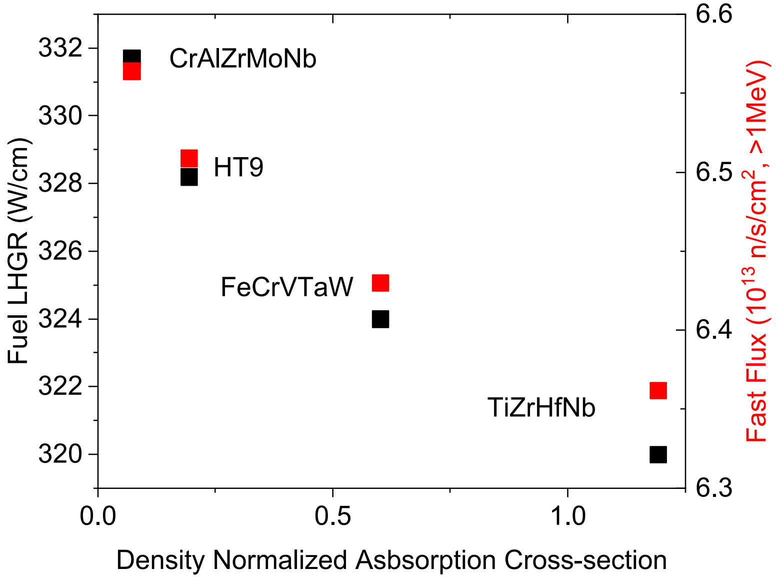
- Equivalent pressure retention can be obtained by thinner materials with higher yield stress

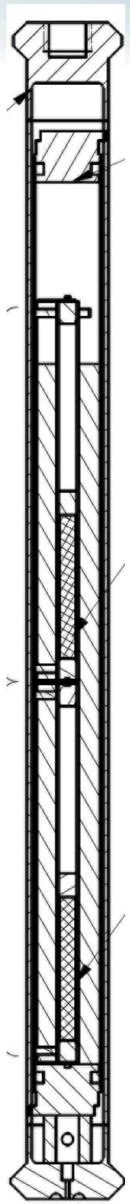
$$\frac{t_1}{t_2} = \frac{P-1.6667E_2}{P-1.6667E_1} \sim \frac{E_2}{E_1}$$





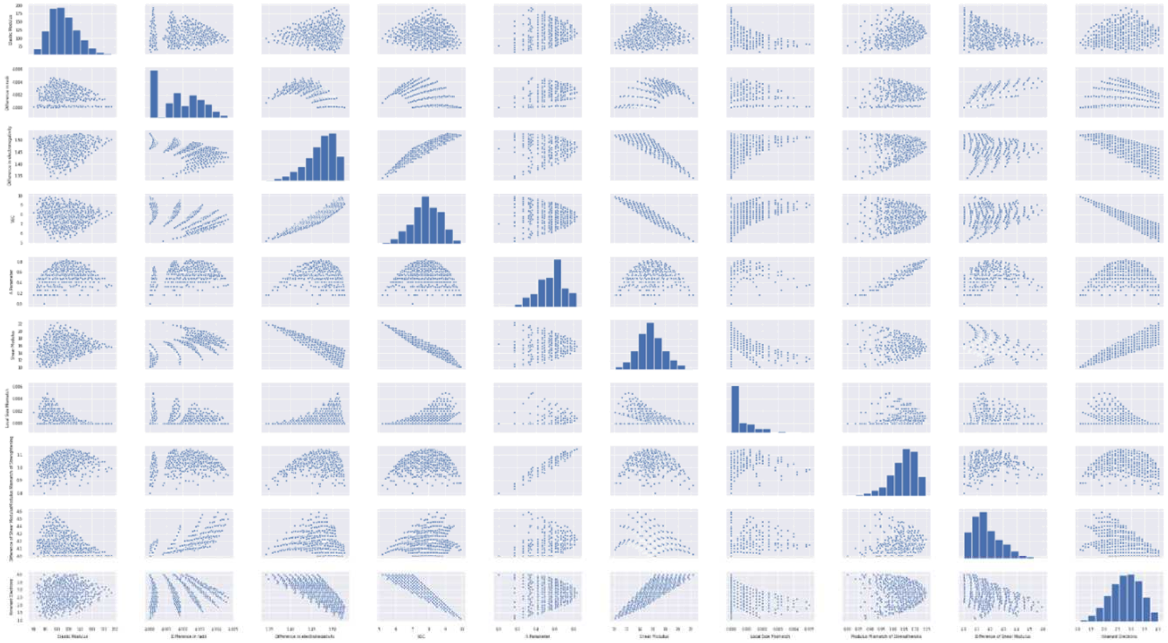






Combinatorial Nuclear Alloy Experiment and Design

The application of HEAs and MPEAs in advanced nuclear reactor concepts has the potential of unlocking unprecedented energy opportunities that are safe, reliable, and environmentally responsible.



This combination of materials by design with machine learning and advanced testing at ATR is the foundation of the Nuclear Materials Discovery and Qualification Initiative at INL.

Idaho National Laboratory

NSUF Nuclear Science User Facilities

NMDQi Nuclear Materials Discovery and Qualification Initiative

CAES Center for Advanced Energy Studies

Acknowledgement

THE UNIVERSITY OF UTAH

Idaho National Laboratory

RIT

Rochester Institute of Technology







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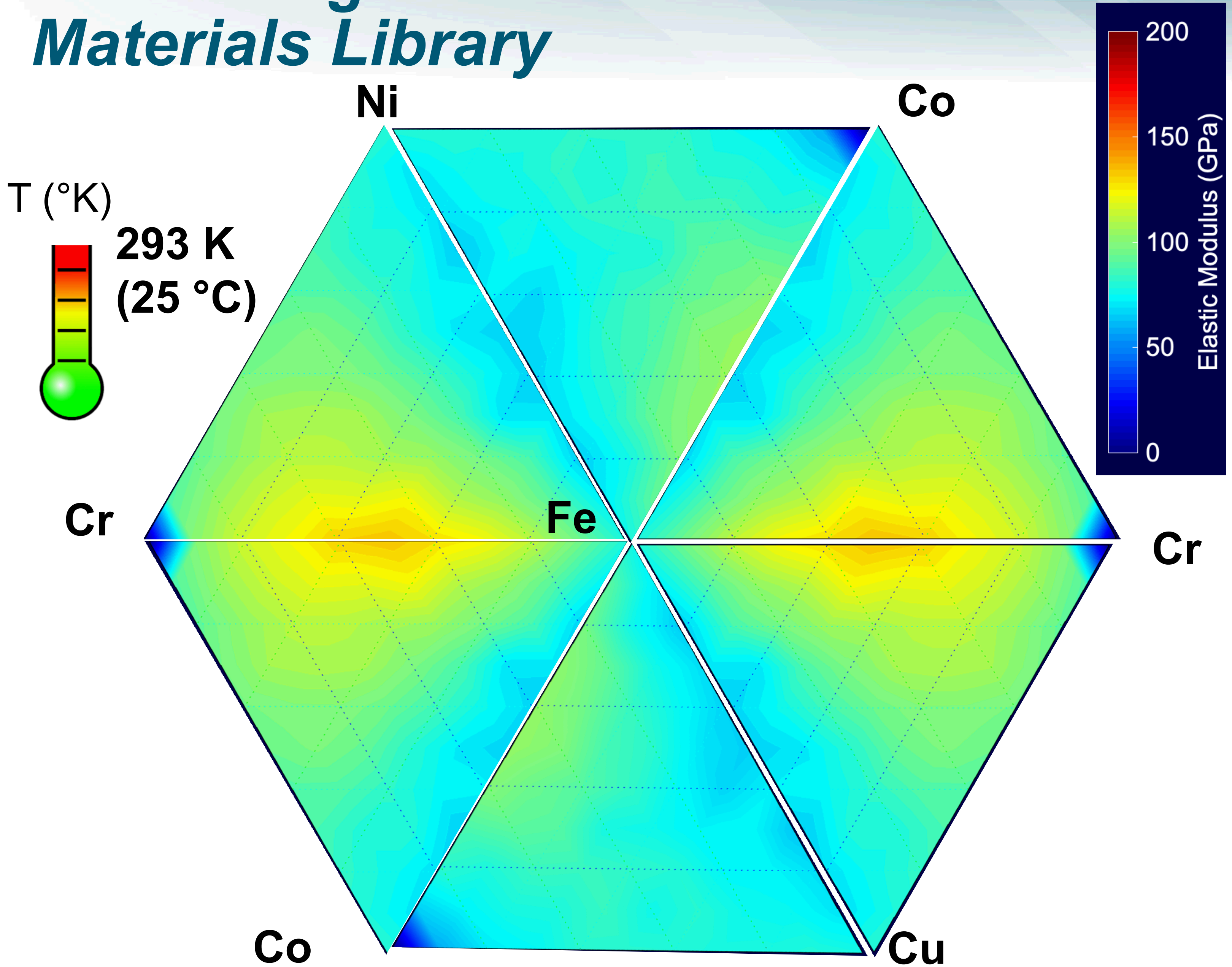
Visualizing Materials Library

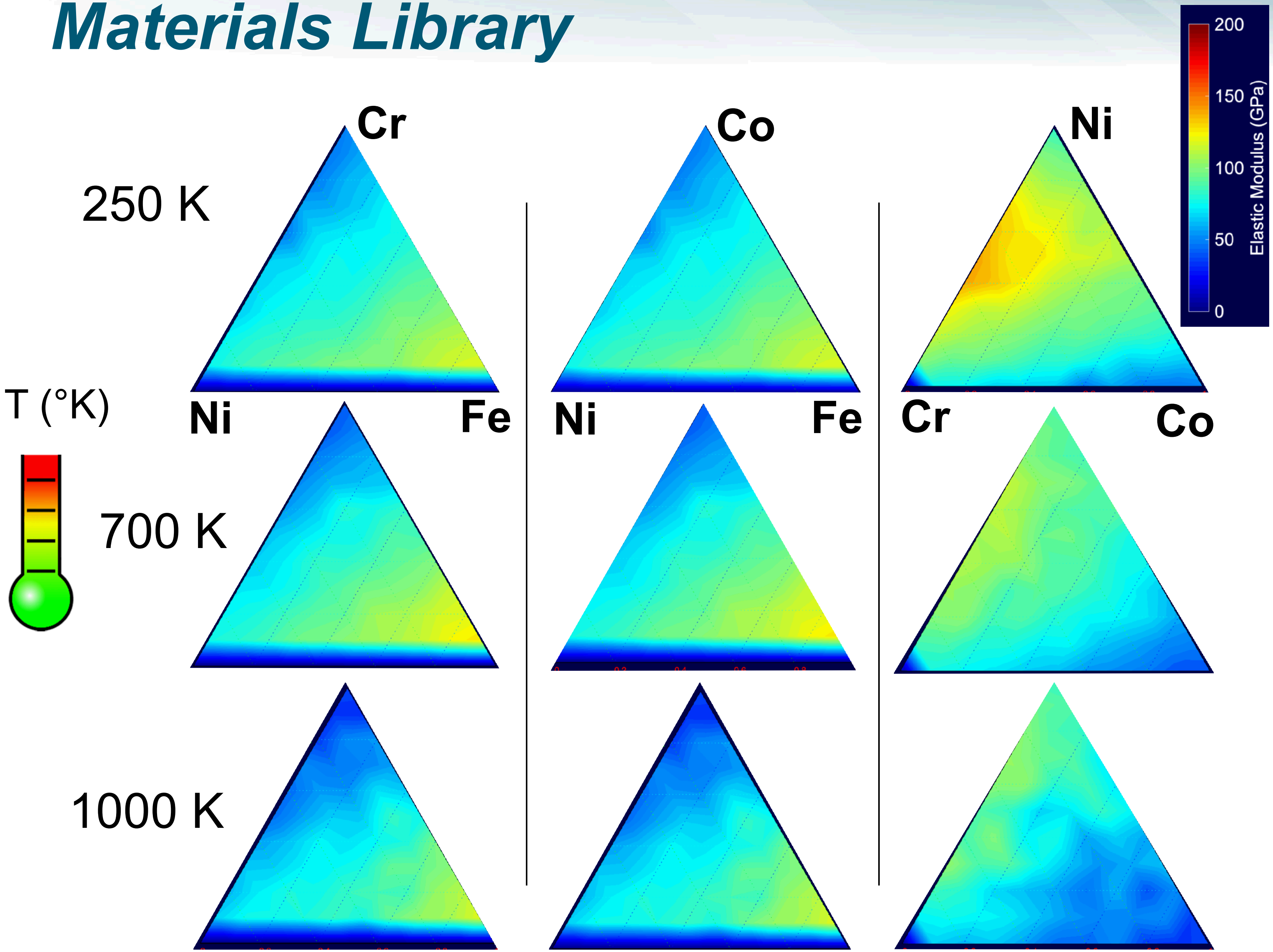


Tracking Properties (and others) with varying <u>composition</u> and <u>temperature.</u>

Changes elastic moduli are visualized with composition and temperature.

Visualizing the relative changes in either elastic modulus, tensile strength, or other is starting point for our data analytics approaches

Visualizing Materials Library



Tracking Properties (and others) with varying <u>composition</u> and <u>temperature.</u>

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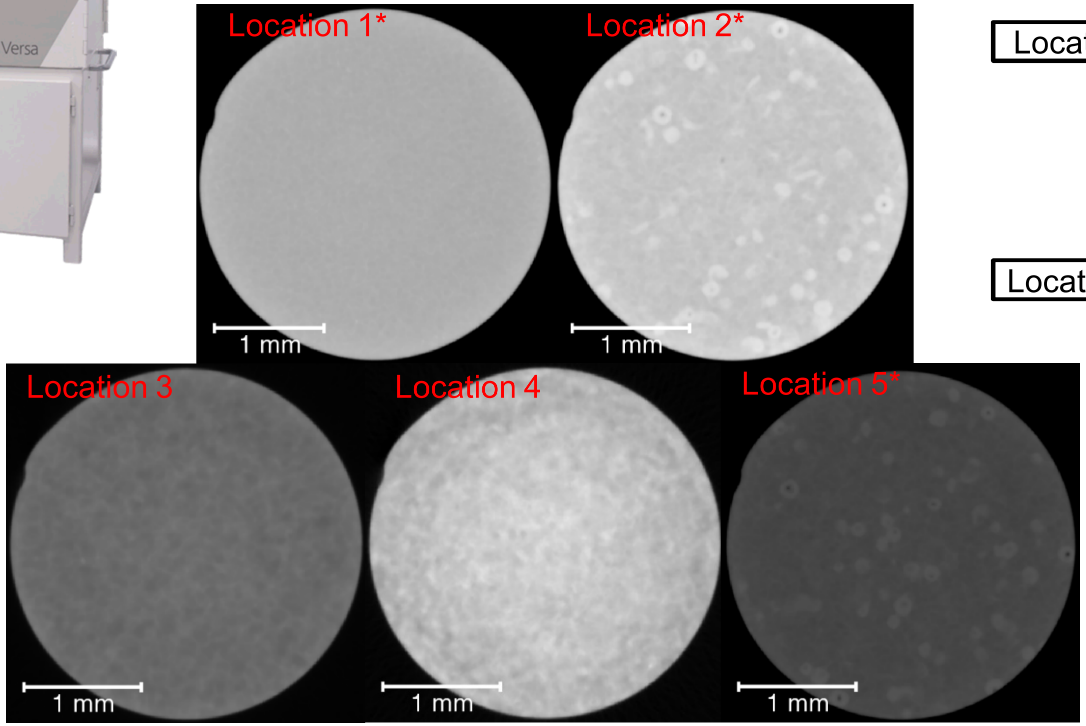
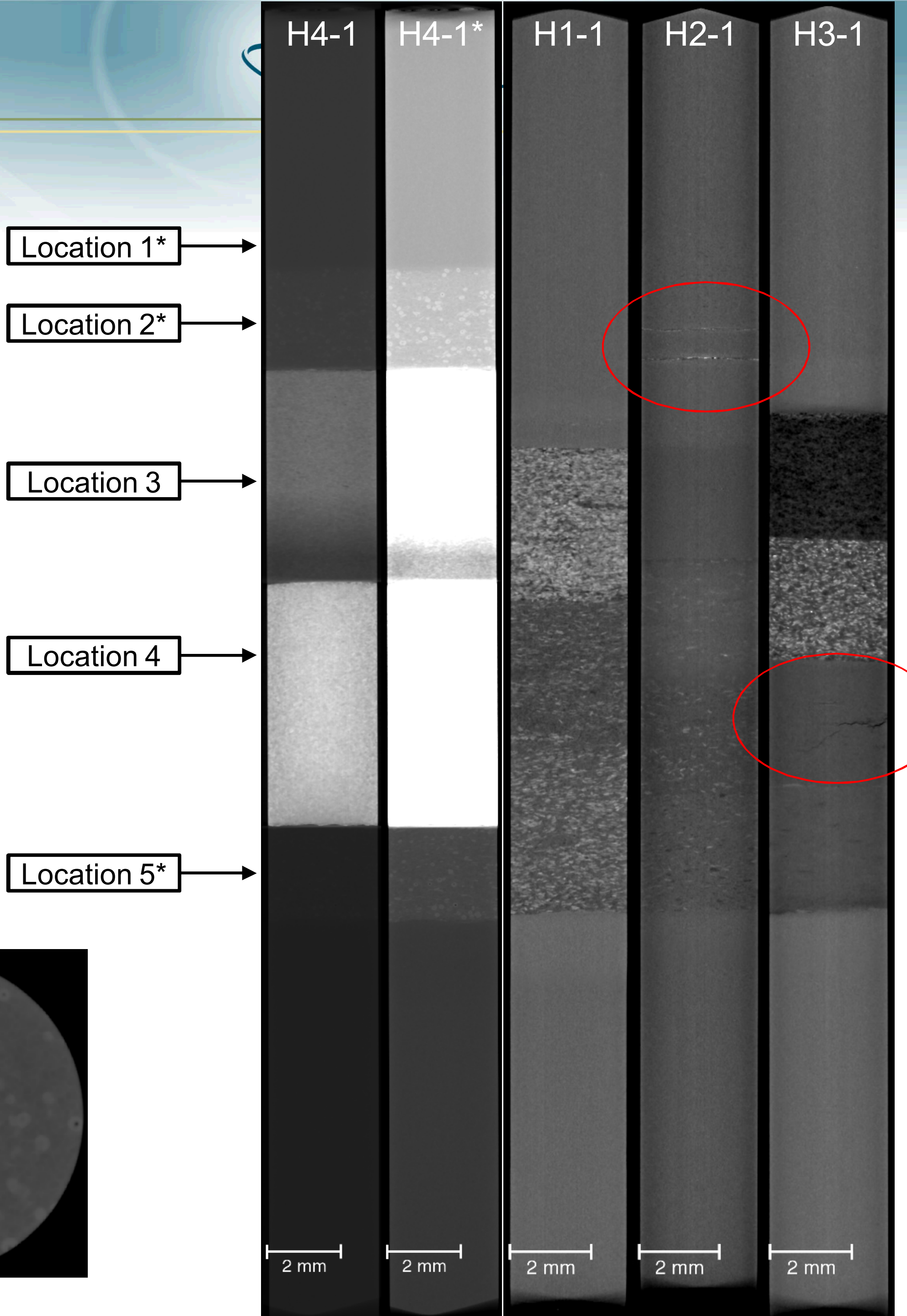
Advanced Microscopy QA – XRCT

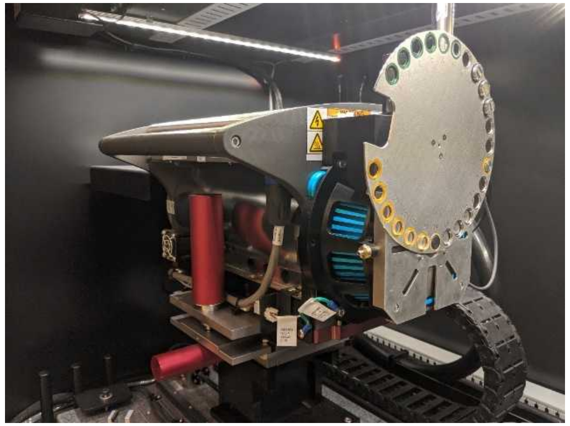
- ZEISS Xradia 520 Versa X-Ray Microscope



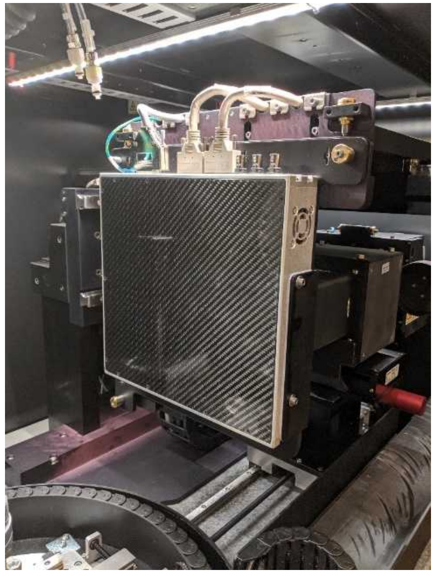


Micro X-ray Computed Tomography of High Entropy Alloy Rods

- ZEISS Xradia 520 Versa X-ray Microscope
- Image Acquisition Parameters
  - X-ray Source
    - 160 kVp accelerating voltage
    - 10 W power
  - Flat Panel Detector (geometric magnification only)
    - 3064 px X 1936 px detector size
    - Detector binning = 1
  - 3201 radiographs per 360° sample rotation
  - 0.04 s exposure per frame
  - 20 frames per radiograph (resulting in ~1 h per tomogram)
  - 4 tomograms per sample* were acquired and digitally stitched using ZEISS software
    - *Sample H4-1 is comprised of 5 tomograms
  - Isotropic voxel size for each tomogram = **6.7 µm**



ZEISS Versa X-ray Source



ZEISS Versa Flat Panel Detector