Engineered Metallic Nanostructures Laboratory

Stony Brook University

Enhancing the Performance of PFMs through Solute-stabilized Nanostructured Tungsten Alloys

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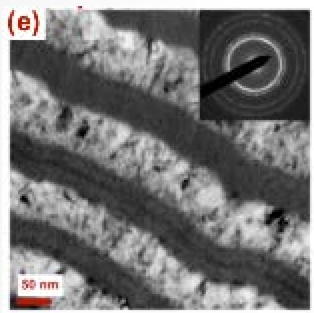
Support for preliminary work acknowledged from the National Science Foundation through awards DMR-1410941 and CMMI-1401662 and the Brookhaven National Lab Seed Grant Program

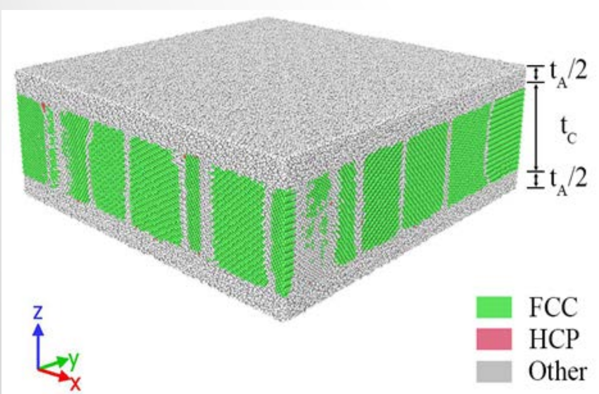
My expertise and areas of interest

Interface-dominated materials explored through a range of *in situ* and analytical characterization techniques coupled with atomistic simulations

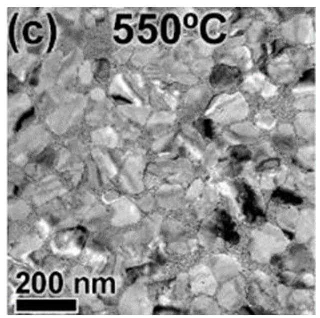
- *Solute stabilization and its implications for interfacial properties*
- *Mechanistic insights into mechanical behavior of stabilized materials*
- *Radiation damage mechanisms and implications for mechanical behavior*

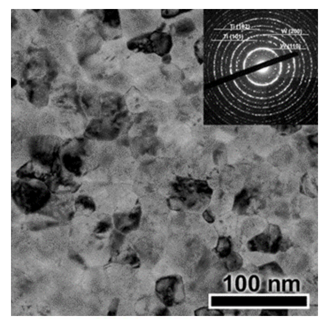
Grain size modulated nanostructures

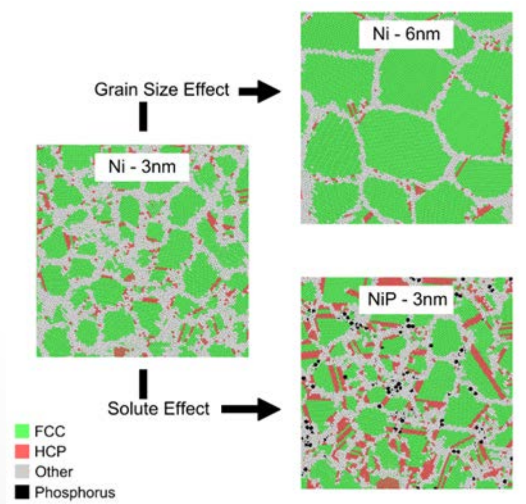




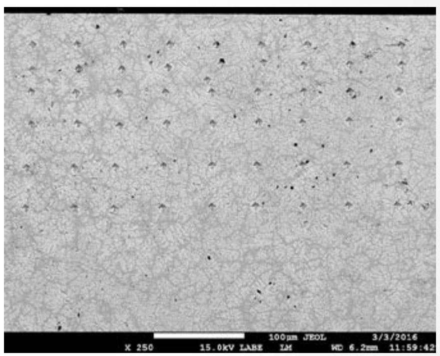
Solute stabilized nanocrystalline alloys

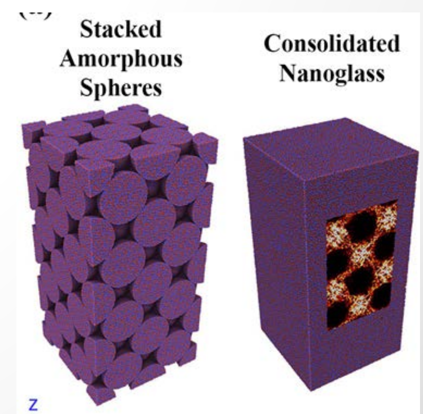






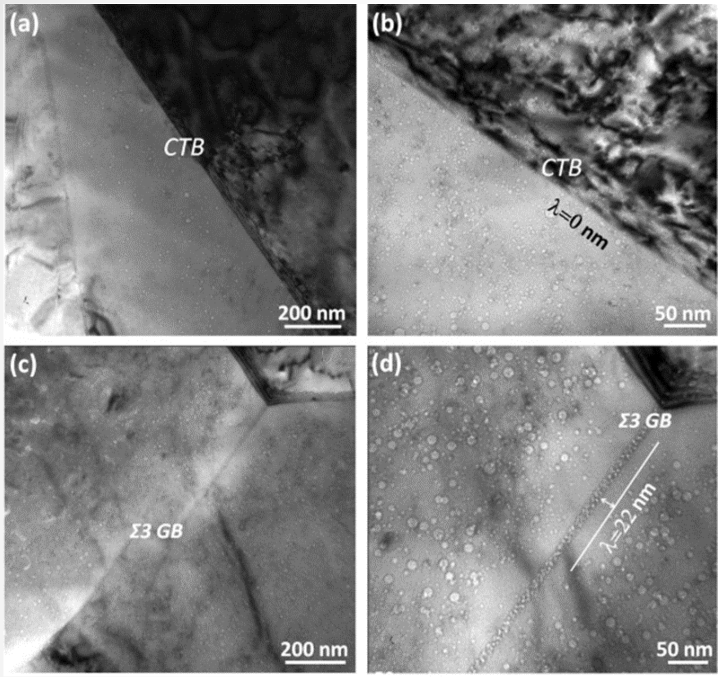
Amorphous composites and nanoglasses





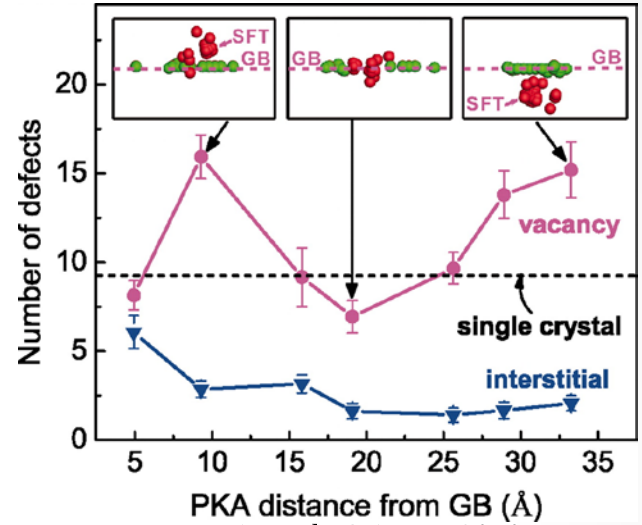
Evidence for self-healing near grain boundaries

Void denuded zones near GBs

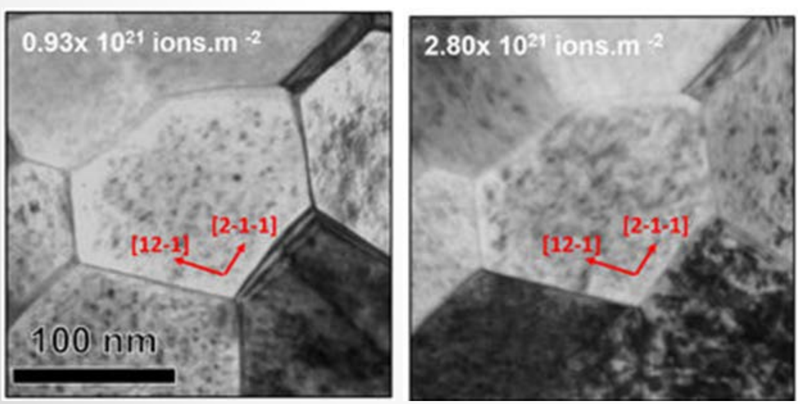


Han, et al., Acta Mat, 2012

Defect recombination at GBs

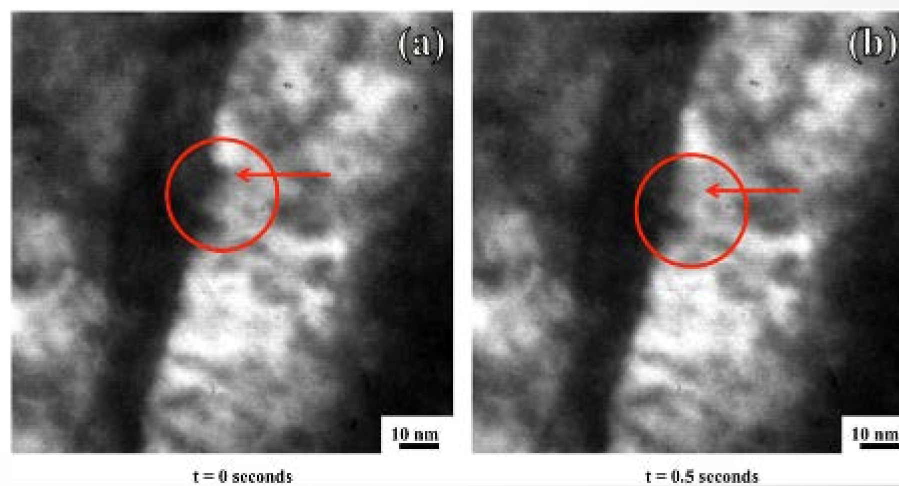


Bai, et al., Science, 2010



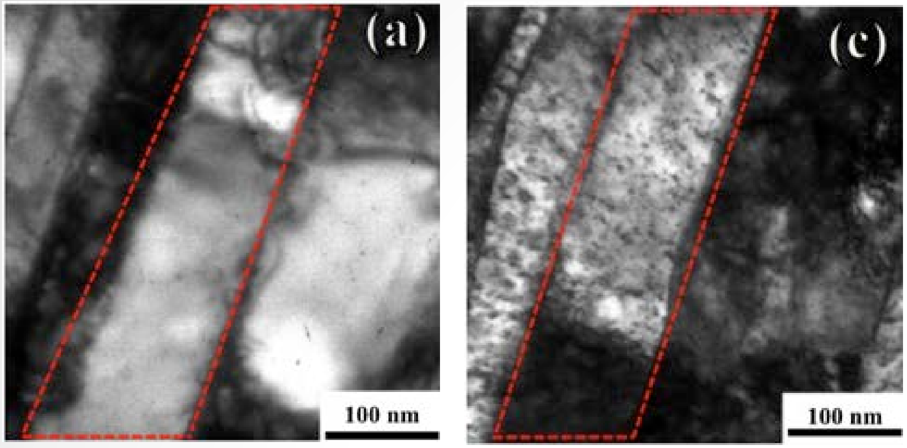
El-Atwani, et al., Sci Rep, 2017

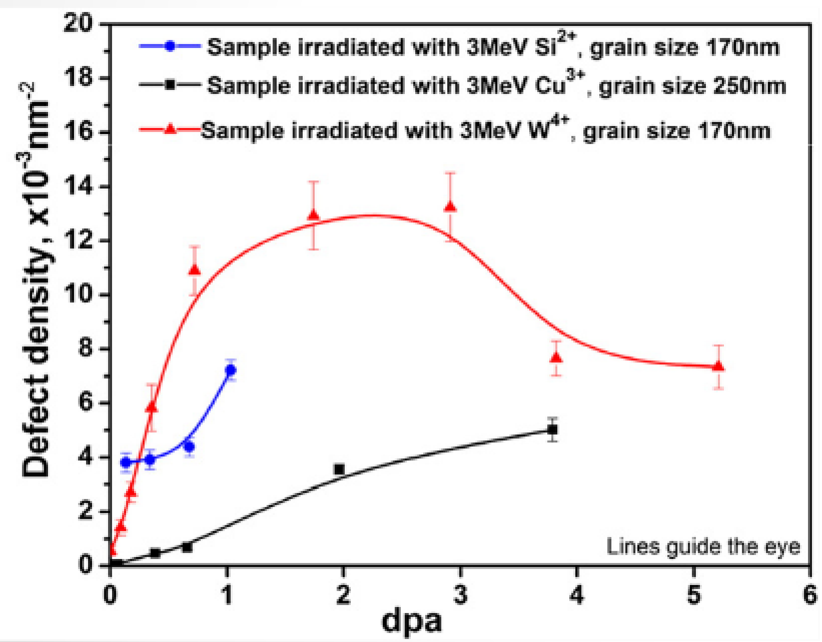
GB induced recombination in tugnsten



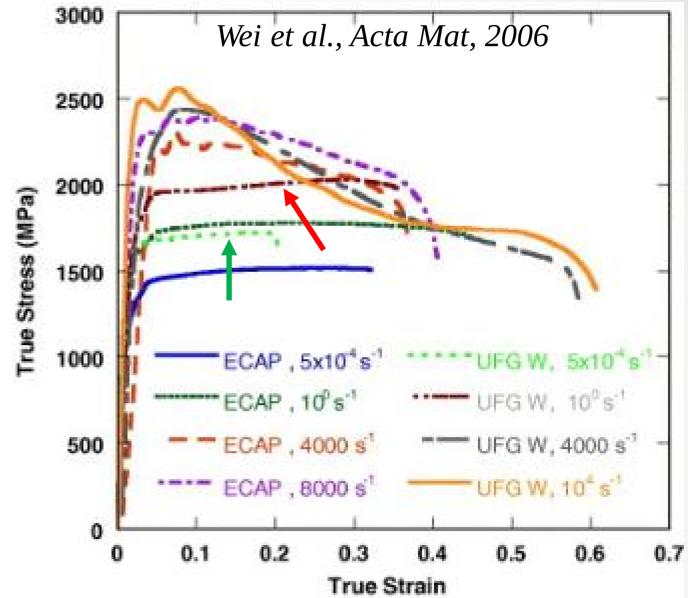
El-Atwani et al., Mat Char, 2015

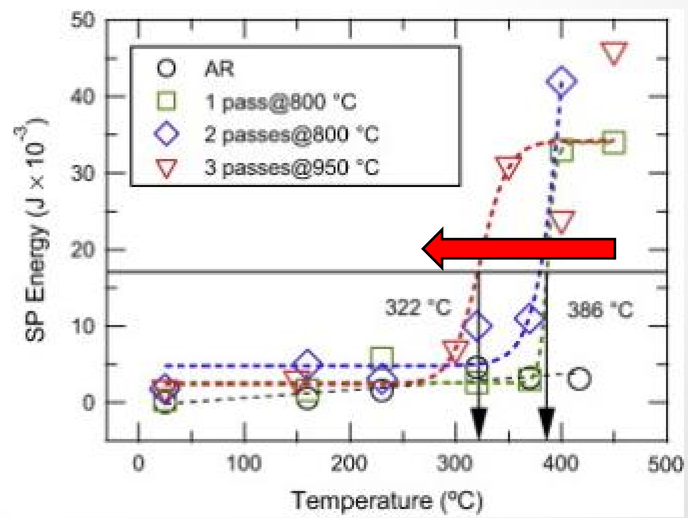
A number of potential benefits for tungsten





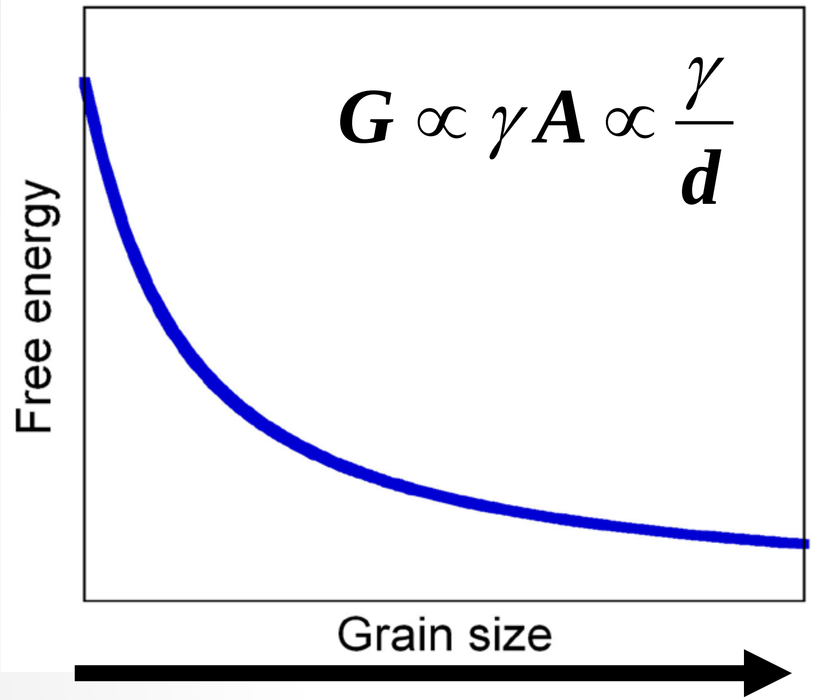
El-Atwani et al., Mat Char, 2015

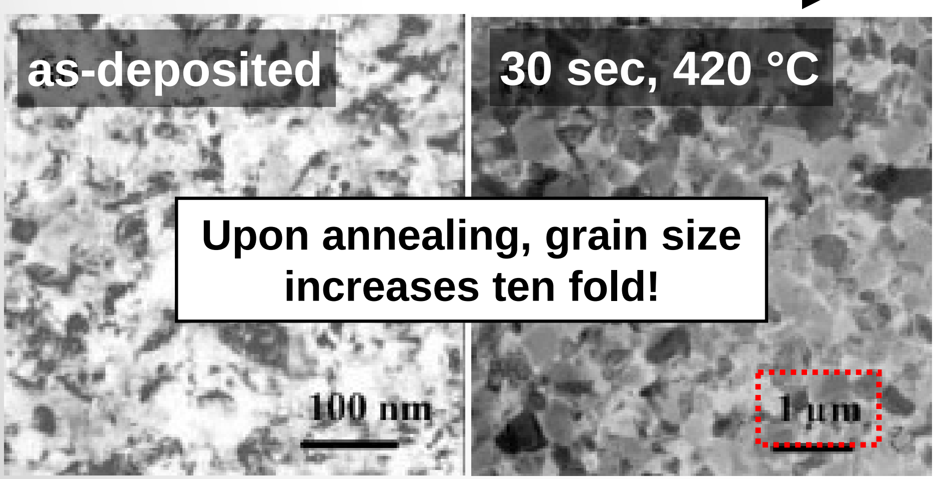




Hao et al., JNM 2014

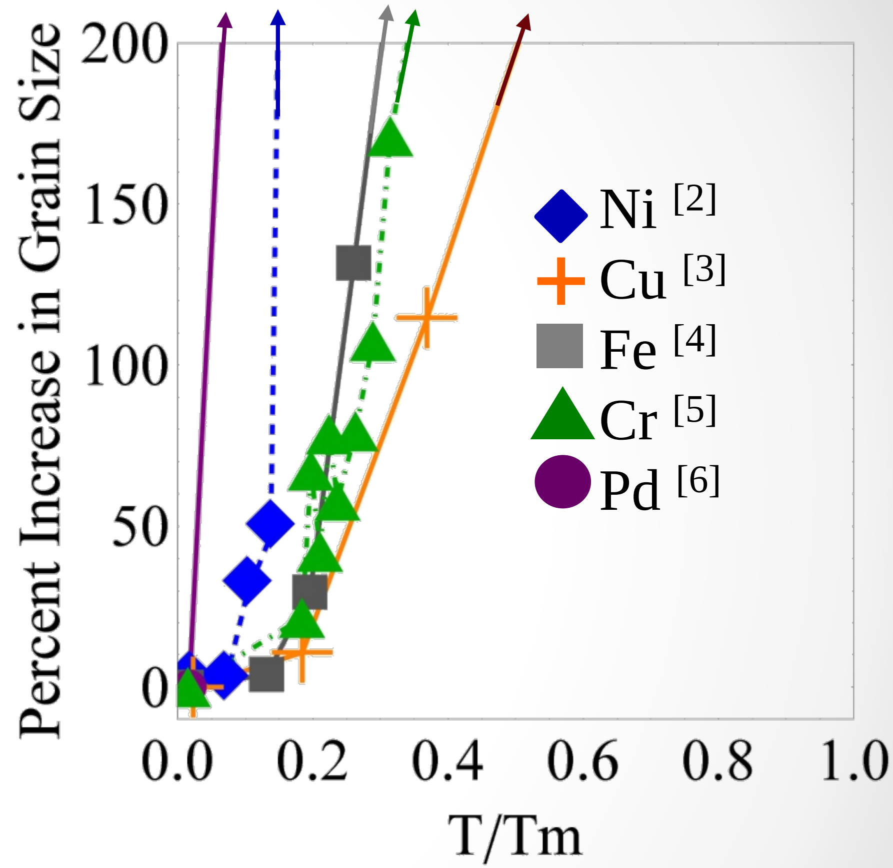
Nanomaterials are intrinsically unstable…





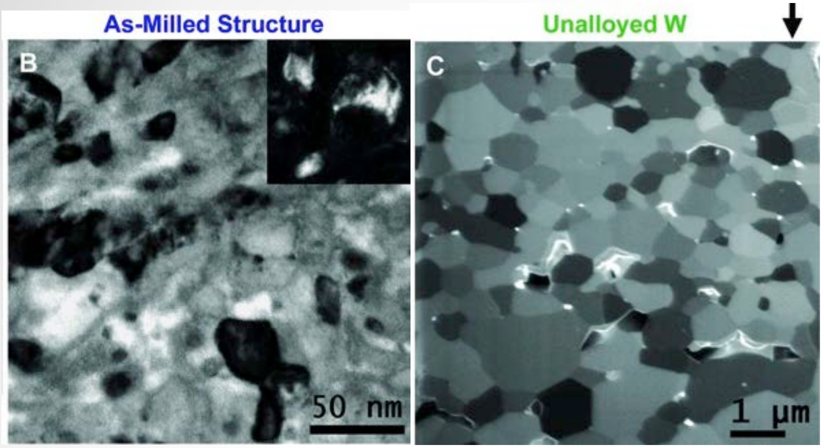
[1] Hibbard et al., Scripta Mater (2002)

Pure nc-metals annealed for 1 hr



[2] Natter H. et. al. J. of Mater. Rsrch. 1998. v13 p1186
[3] Mula S. et. al. 2012. Mat. Sci. Eng. A. v539
[4] Moelle CH, Fecht HJ. 1995. Nano. Mater. v6 p421
[5] Chojnowski G. et. al. J. of Phys. Chem. 2007 v11
[6] Wurschum R. et al. 1997 Nanostruct. Mater. v9 p615
[7] Pantleon K, Somers MAJ. 2010. Mat Sci Eng A. 528 p65
[8] Ames, M et al. 2008 Acta Mater. v56 p4255
[9] Haber, JA, Buhro, WE 1998 J. of ACS v120 p10847

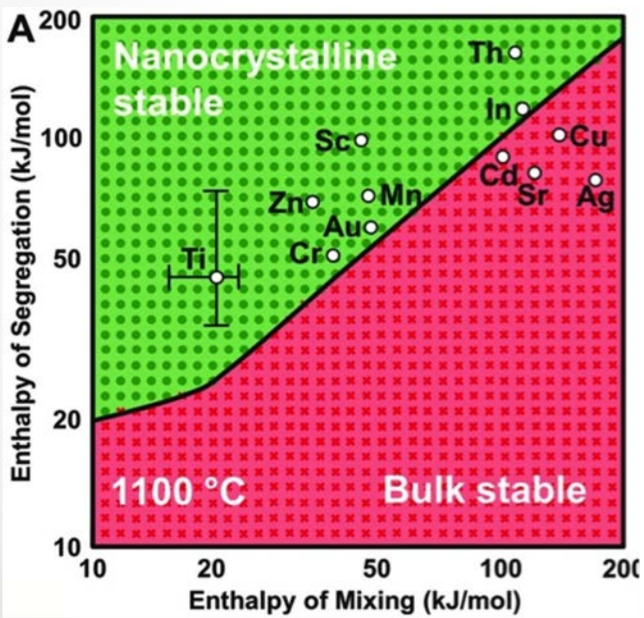
Mitigating instabilities via "alloying by design"

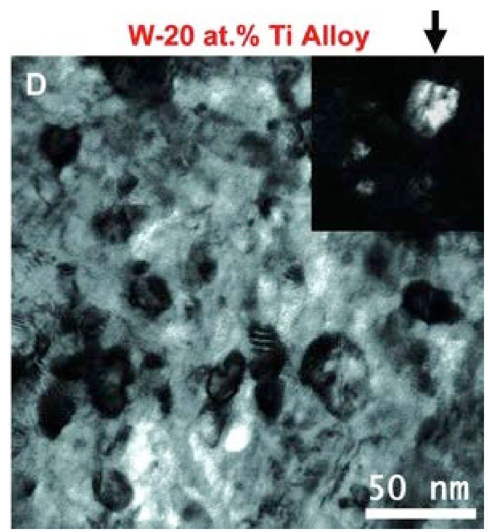


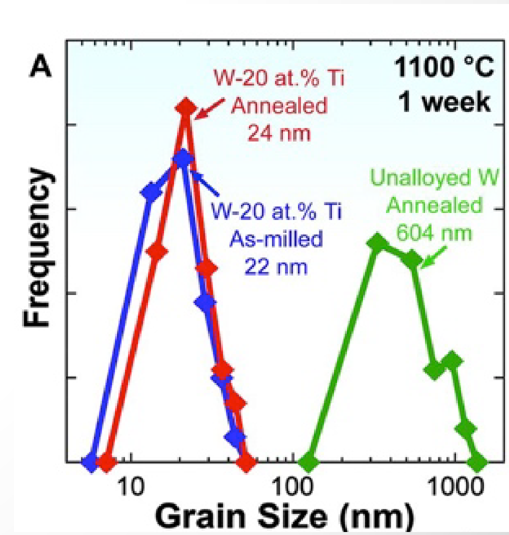
Thermodynamics capturing grain boundary energetics can be used to design stable nanocrystalline alloys

- In W, Ti identified as a stabilizing element and alloys synthesized via high energy ball milling

➔ *Grain size of 20 – 25 nm remained stable after annealing at 1100 °C for 1*







Enhancing the performance of W for PFMs

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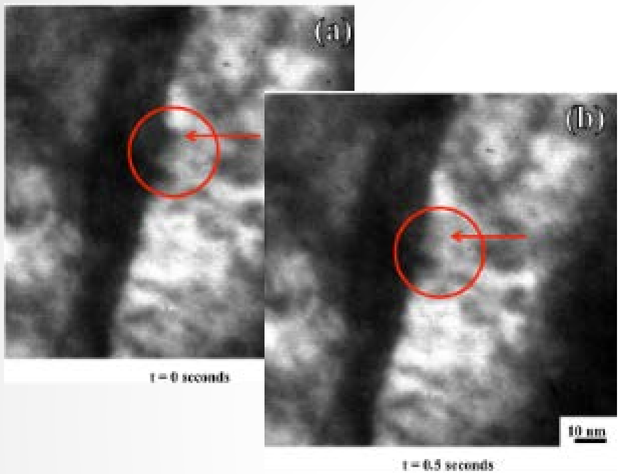
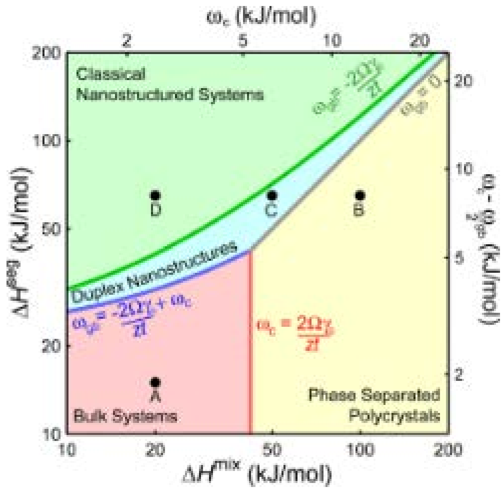
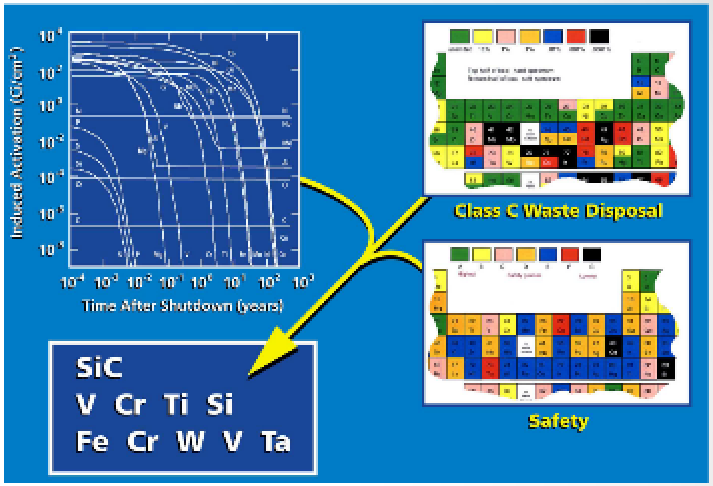
Benefits of Nanograins for Damage Tolerance	+	**Stabilization via Alloying**	+	**Alloy Element Selection for Reduced Activation**



El-Atwani et al., Mat Char, 2015



Chookajorn, PRB, 2014



Zinkle, FST, 2013

Overarching research aim: Explore solute stabilized nanostructured tungsten alloys for stabilization against recrystallization and improving ductility and DBTT collectively with radiation tolerance.

1. Design alloys by combining nanostructure stability models leveraging thin film deposition techniques for rapid alloy assessment and optimization
2. Scale chemistries to produce bulk alloys through powder metallurgy and field assisted sintering techniques for bulk mechanical property measurements

Early Career Award Research Activities

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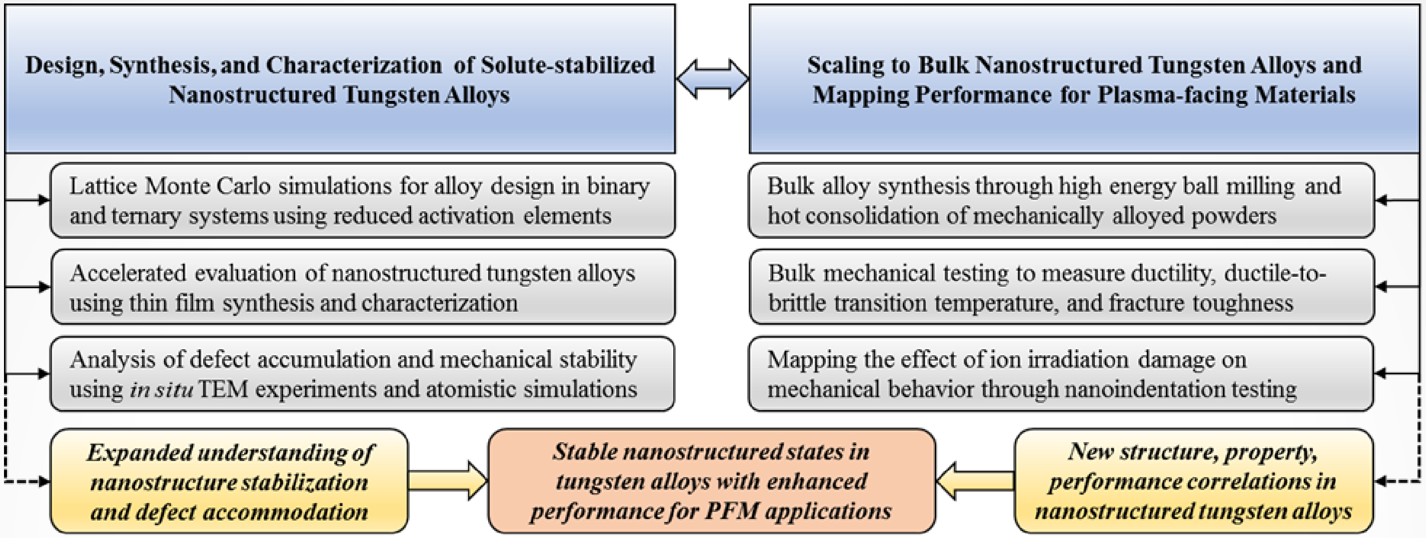

Research Tasks

1. Design, synthesis, and characterization of nanostructured tungsten alloys
   i. Lattice Monte Carlo modeling for alloy design
   ii. Accelerated alloy synthesis and characterization using thin film techniques
2. Analysis of defect formation and mechanical stability
   i. *In situ* ion irradiation of nanostructured tungsten alloy thin films
   ii. Nanomechanical testing on pristine and ion irradiated alloys
   iii. Understanding mechanisms through atomistic simulations

   Coupled radiation effects and mechanical behavior
3. Bulk nanostructured tungsten alloy synthesis and property mapping
   i. Powder metallurgy synthesis and bulk alloy consolidation
   ii. Structural characterization and mechanical testing

Lattice Monte Carlo Modeling for Alloy Design

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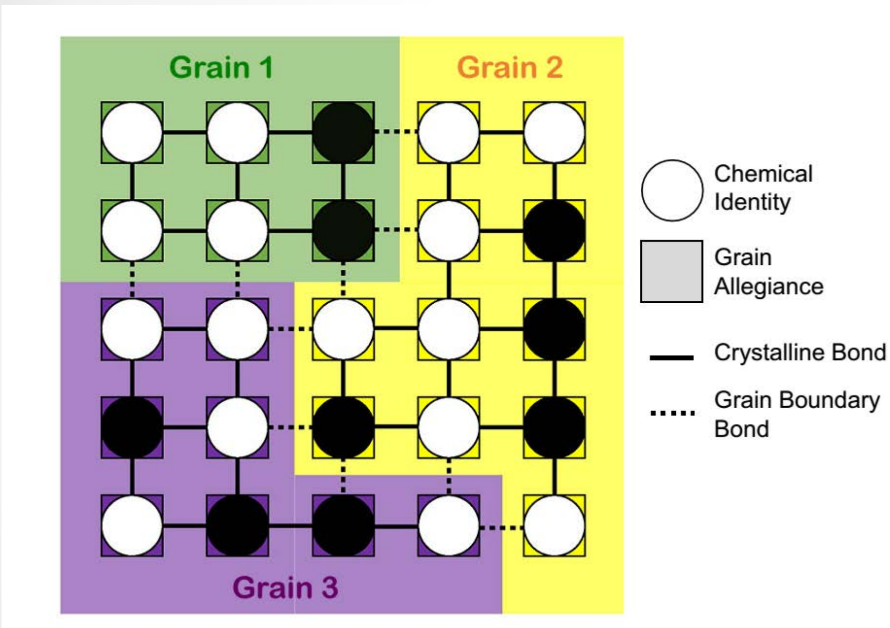
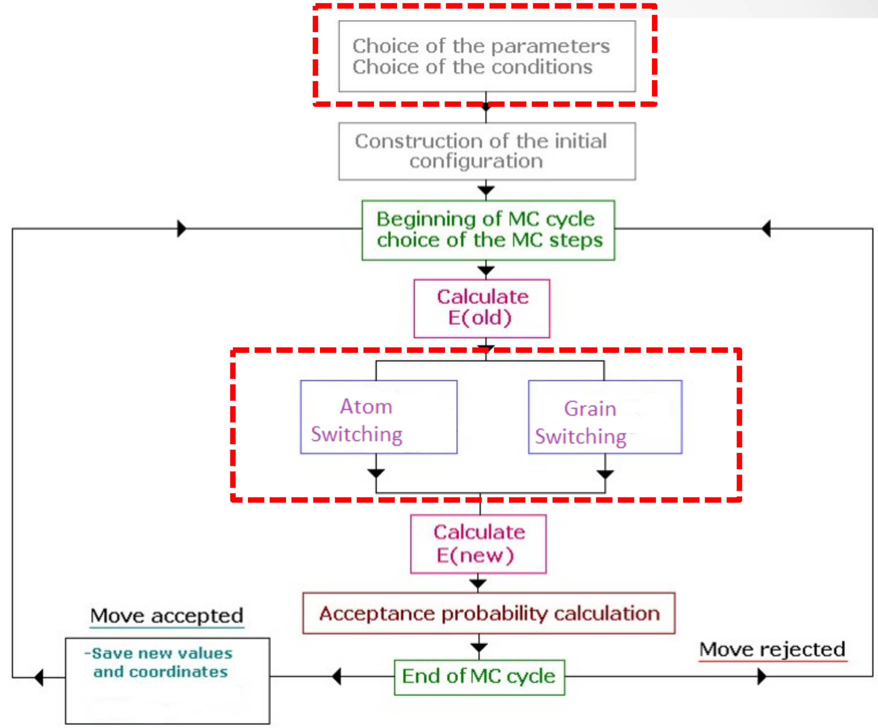
Task Aim: Nanostructure stability maps from LMC simulations for binary and ternary tungsten alloys using reduced activation elements and other relevant solute additions

Model Framework





Energy Parameterization

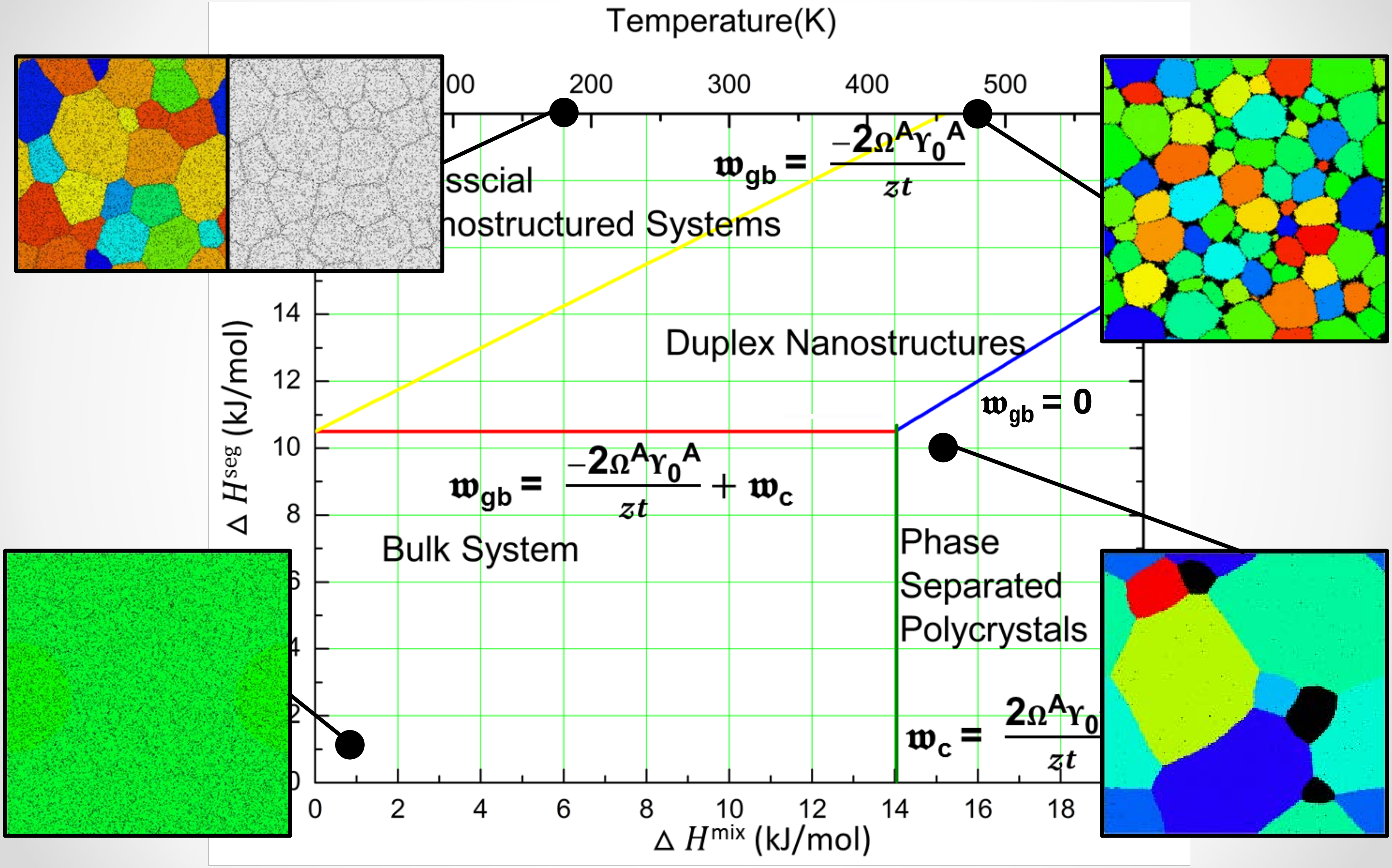
$$U = \sum_{\text{all bonds}} \left[\left(N_c^{AA} E_c^{AA} + N_c^{BB} E_c^{BB} + N_c^{AB} E_c^{AB} \right) + \left(N_{gb}^{AA} E_{gb}^{AA} + N_{gb}^{BB} E_{gb}^{BB} + N_{gb}^{AB} E_{gb}^{AB} \right) \right],$$

$$\Delta H^{mix} = z\omega_c X(1-X),\quad \Delta H^{seg} = z\left[\omega_c - \frac{\omega_{gb}}{2} - \frac{1}{2zt}\left(\Omega^B \gamma_0^B - \Omega^A \gamma_0^A \right) \right],\quad \gamma_0^A = \frac{zt}{2\Omega^A}\left(E_{gb}^{AA} - E_c^{AA} \right),$$

GB segregation: Ti, Cr, Cu, Zr
SS effects: V, Si, Fe, Ta, K
Transmutation products Re & Os

Trelewicz and Schuh, PRB (2014)
Chookajorn and Schuh, PRB (2014); Kalidindi et al. JOM (2015)

General approach (demonstrated for Al Alloys)



Accelerated Alloy Synthesis and Characterization

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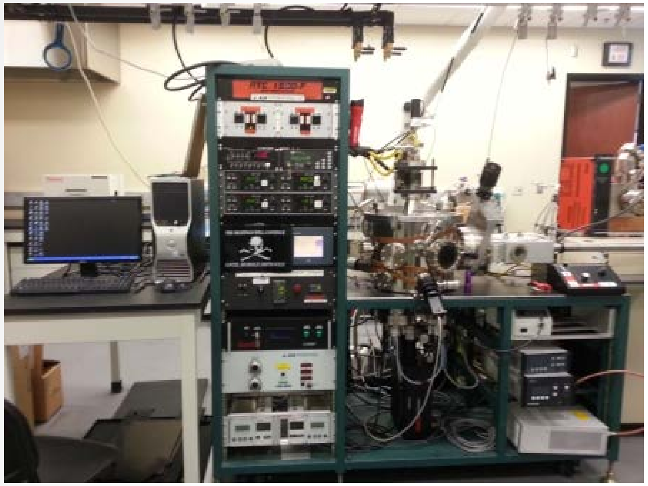
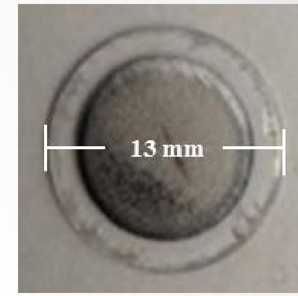
Task Aim: Verification of alloy stability against grain growth and recrystallization at temperatures up to 1500 °C in the systems identified from LMC simulations.

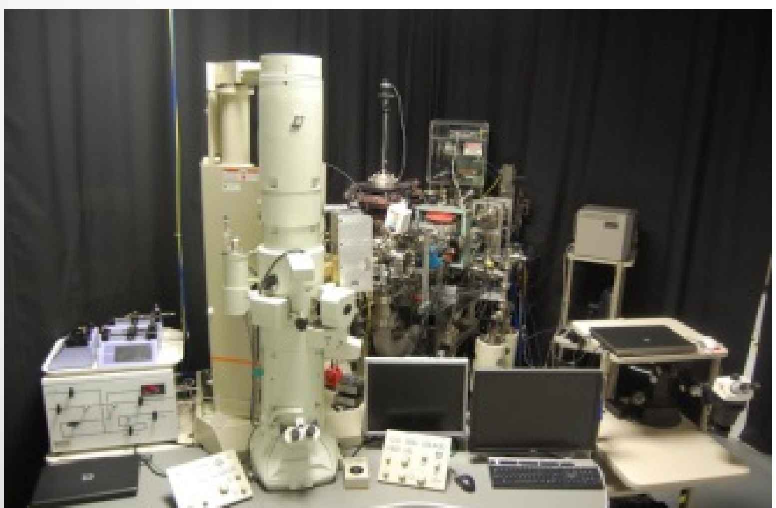


Sample Preparation

- Films deposited to ~20 nm thick onto 13 mm diameter NaCl
- ~3 mm squares for TEM samples

AJA Sputtering Tool
University of Alabama





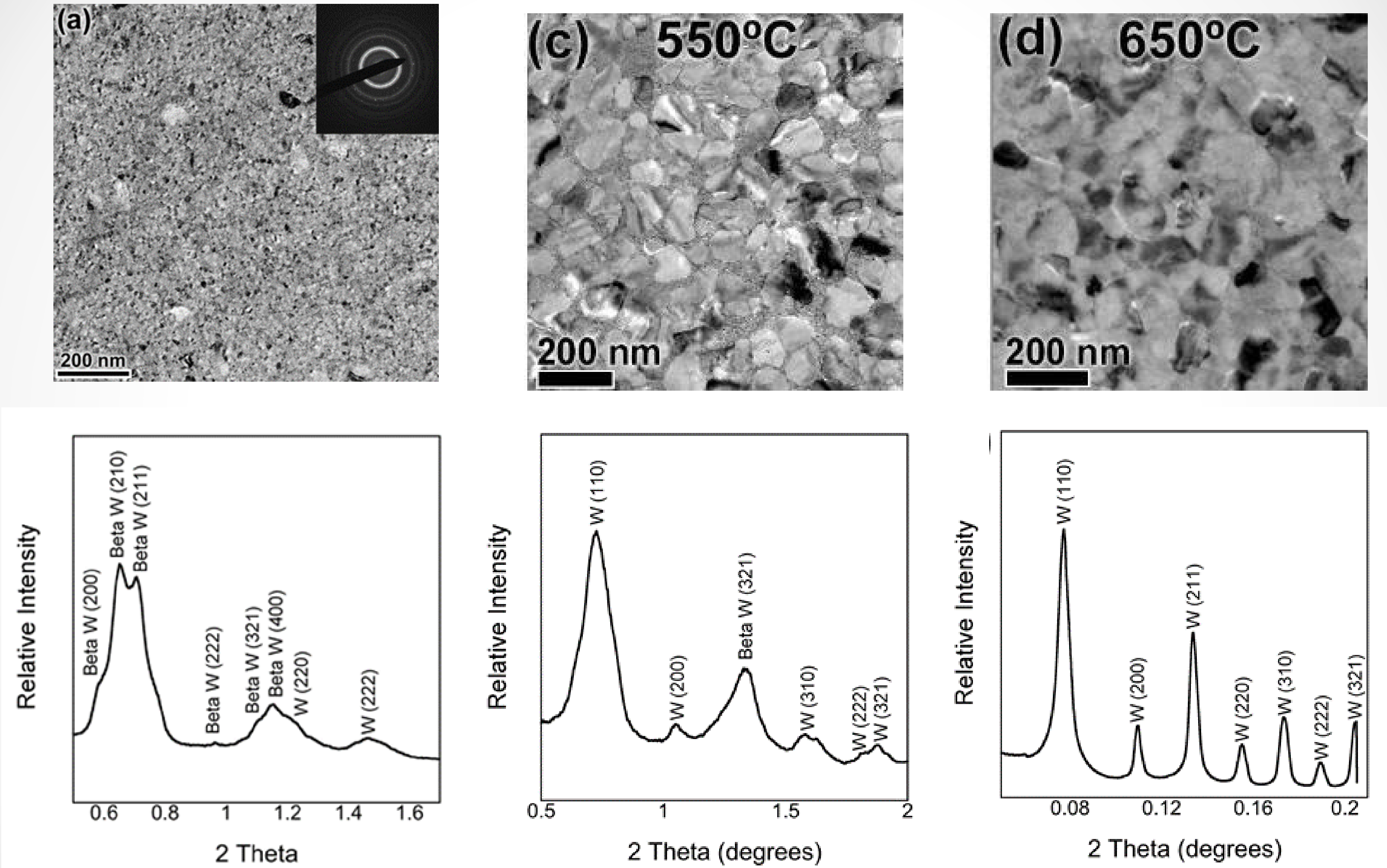
In situ annealing:

- Gatan heating holder in the Philips CM-30 300kV TEM for up to 1000 ºC
- Capable of coupled ion irradiation

Ex situ annealing:

- MTI vacuum furnace for annealing up to 1600 ºC (10^{-7} Torr)

Coupled microstructural and phase evolution



➔ ***Abnormal grain growth coupled to the transformation of the metastable β-phase to BCC α-tungsten, which produced severe microstructural instabilities***

Donaldson, et al., JMR, Invited Feature Article, In Press, 2017

Solute stabilization of nanocrystalline tungsten

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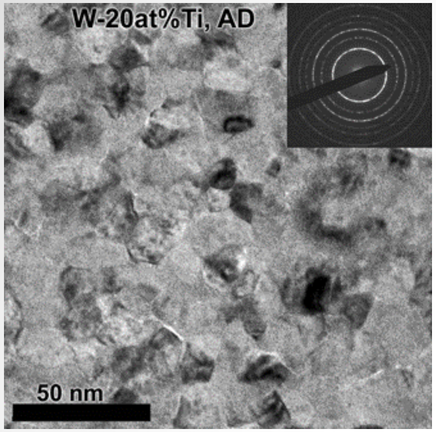
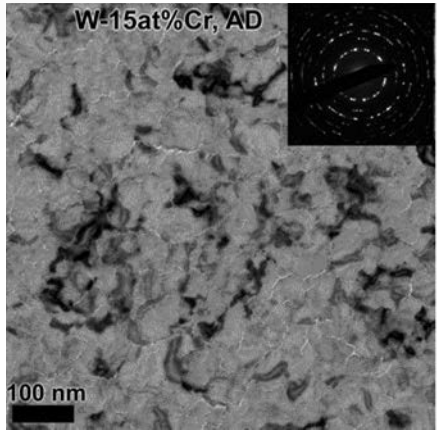
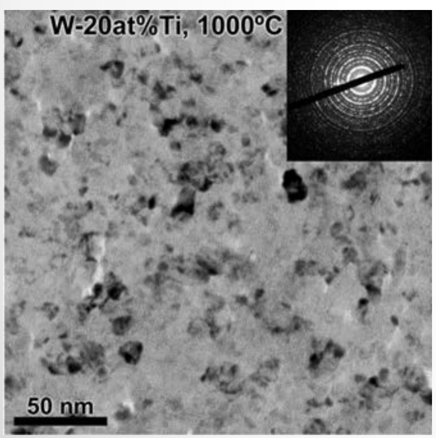
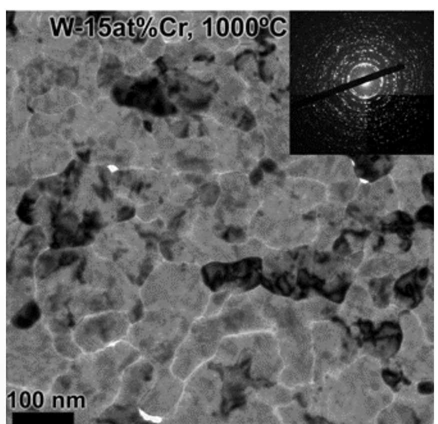
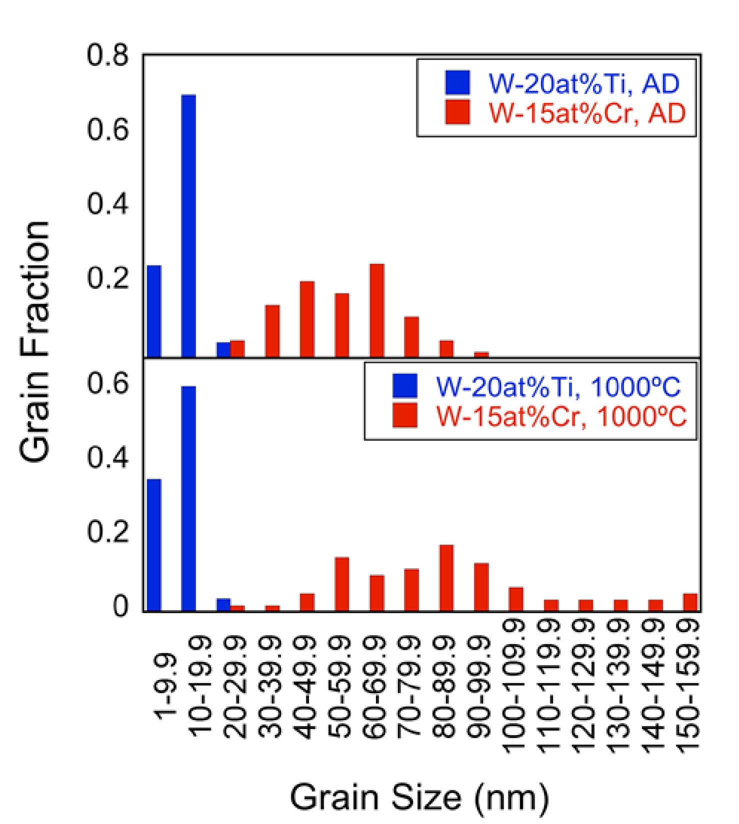




No metastable phase formation and stable through annealing at 1000 ºC







Tungsten alloy films remained nanostructured through annealing

- *Grain size of W-Ti: 14 ➔ 18 nm*
- *Grain size of W-Cr: 55 ➔ 86 nm, corresponding to a 56% increase*

Donaldson, et al., JMR, Invited Feature Article, In Press, 2017

In Situ Ion Irradiation in the TEM

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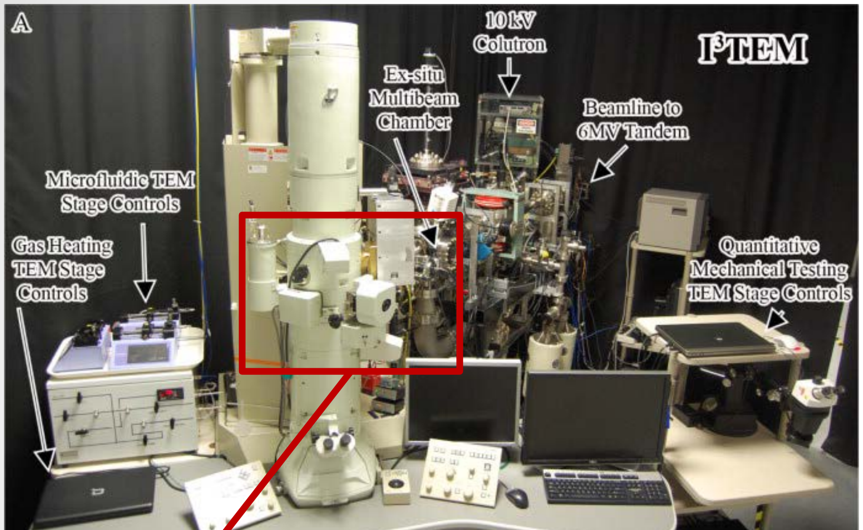
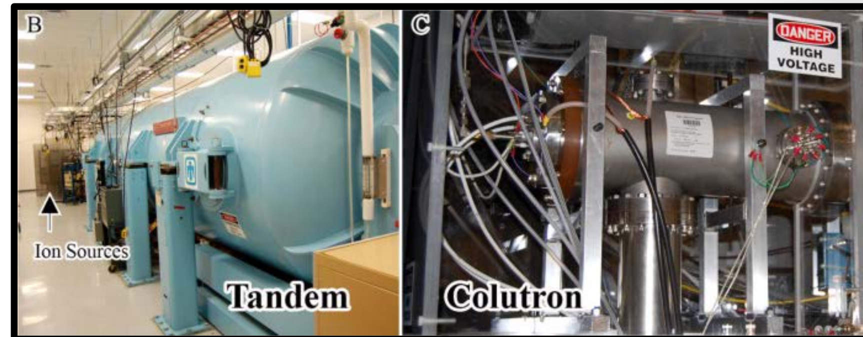
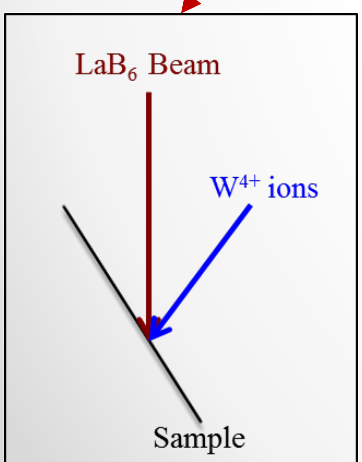
<u>*Task Aim:*</u> Map defect density under coupled ion irradiation as a function of grain size and grain boundary chemistry to determine its implications for alloy stability.

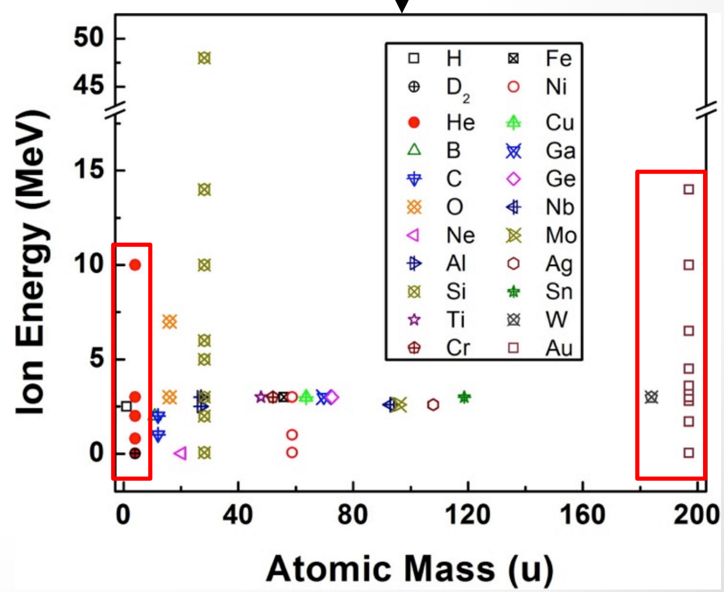






Experimental Analysis

- W/Au/He beams
- 30° tilt relative to incident ion beam
- Imaging/video performed throughout bombardment



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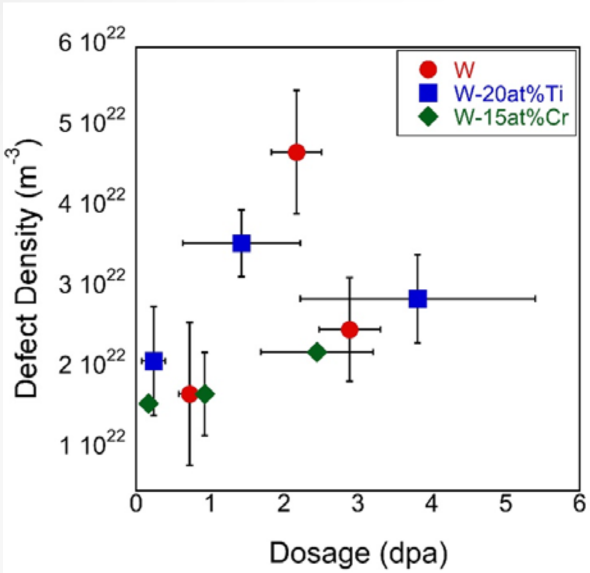
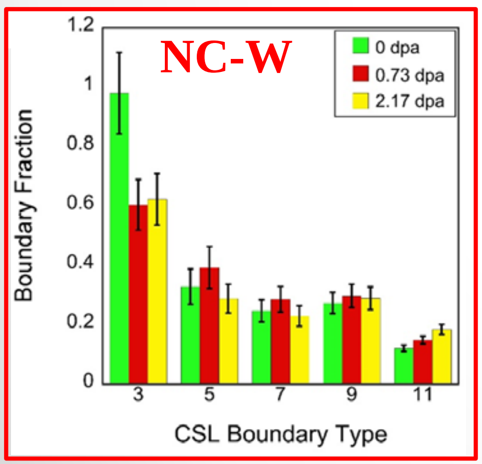
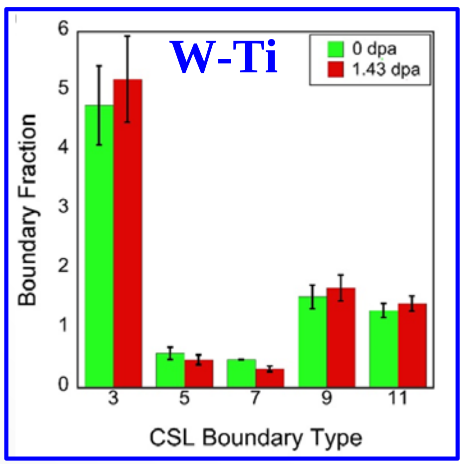
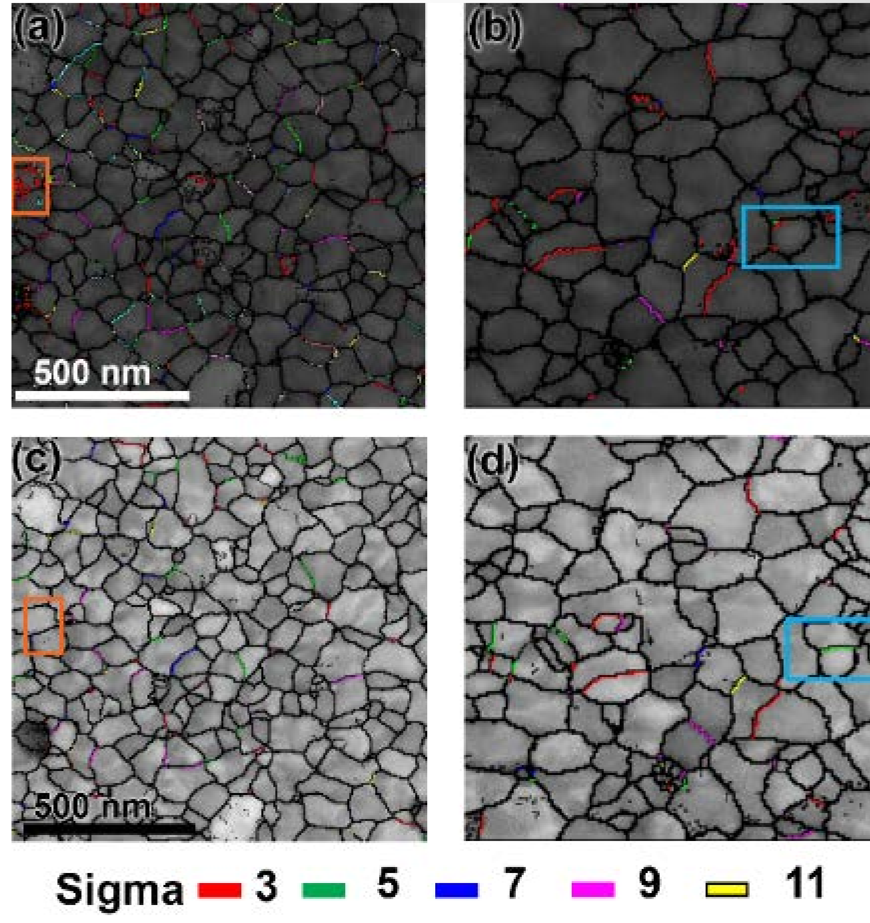
Hattar, et al., Nuclear Instruments and Methods in Physics Review B, 2014

NC-W vs. Stabilized W-Ti and W-Cr









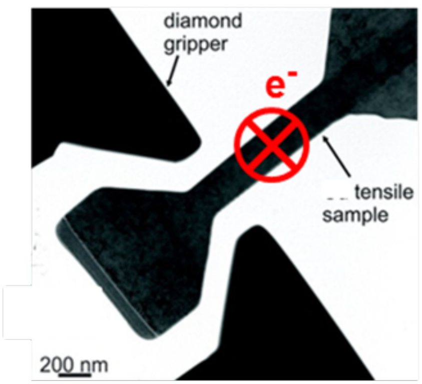
Changes in CSL boundary fractions detected in unalloyed NC-W eliminated through the addition of solute atoms

Donaldson, et al., JNM, in preparation

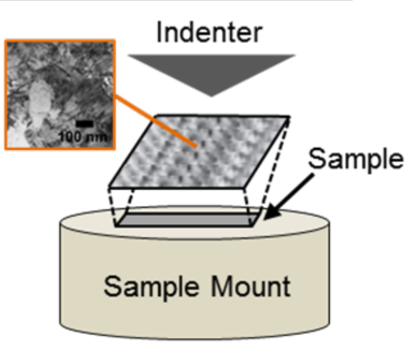
Radiation Effects and Mechanical Behavior

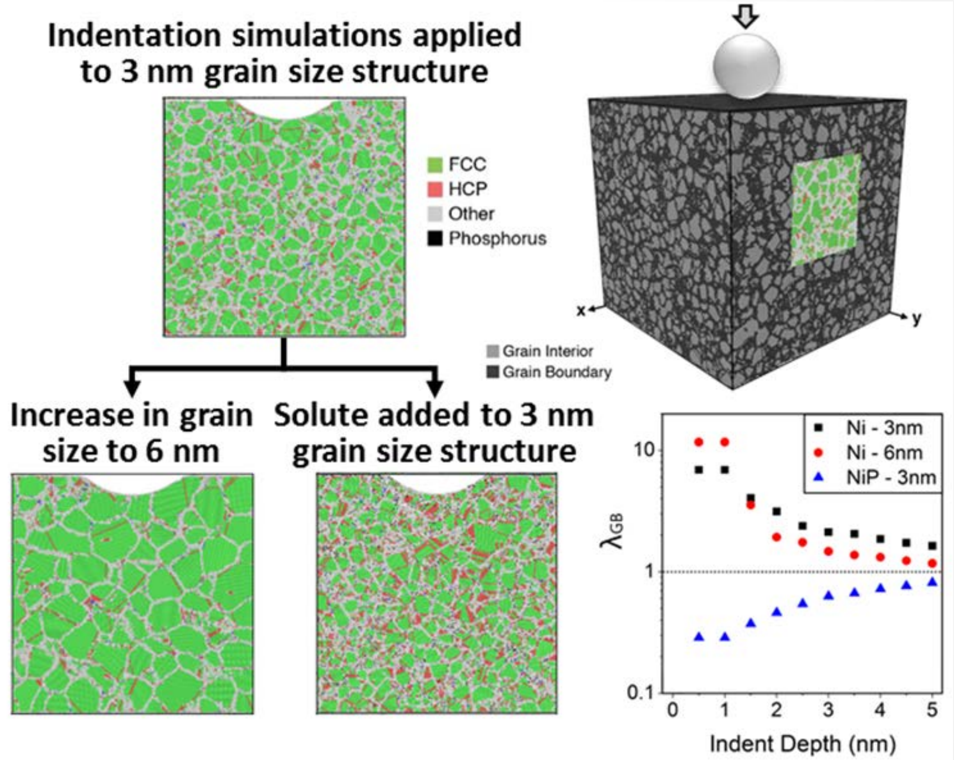
Task Aim: Understand the coupling between radiation effects and mechanical behavior through nanomechanical testing combined with atomistic simulations to bridge measured properties to underlying mechanisms.

(a) ***In situ tensile testing on FIB dogbones in the TEM***



(b) ***Indent samples in top-down or in cross-section***





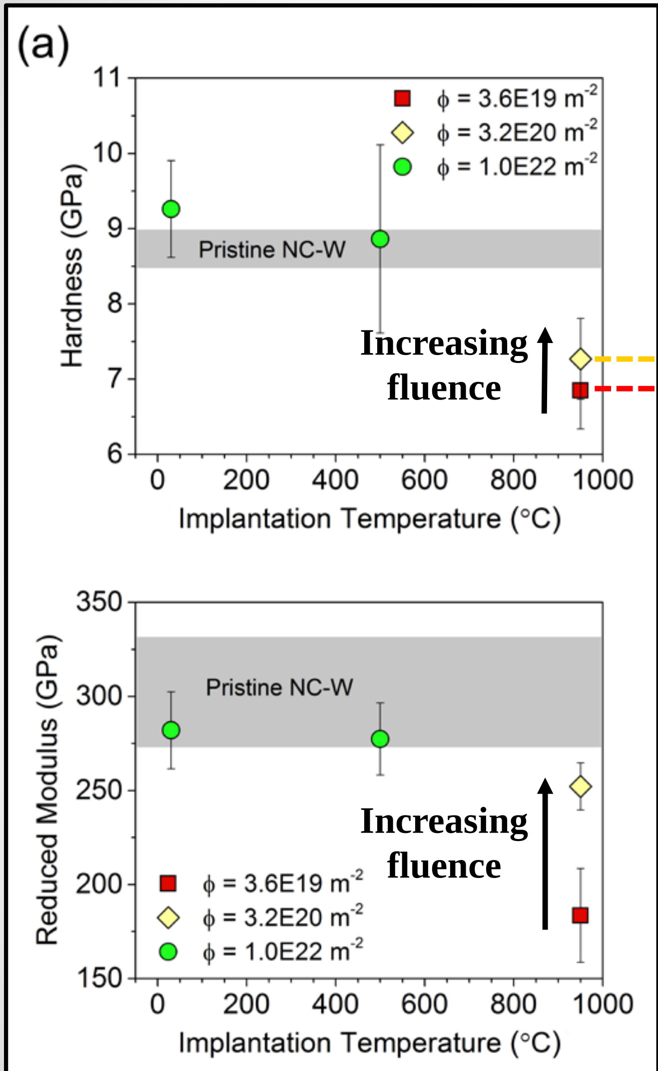
Correlate changes in fundamental GB properties to mechanical behavior with a focus on deformation mechanism shifts as a function of defect state

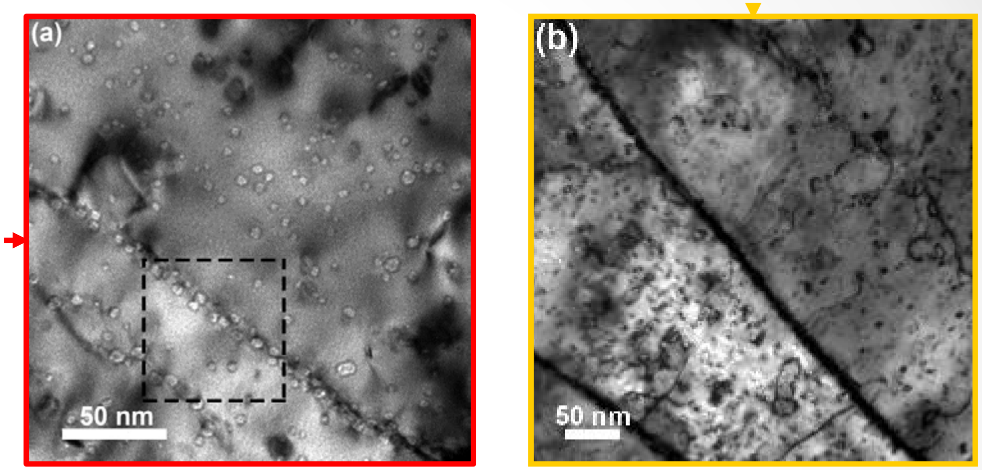
(Example shown for nanoindentation simulations in Ni and Ni-P)

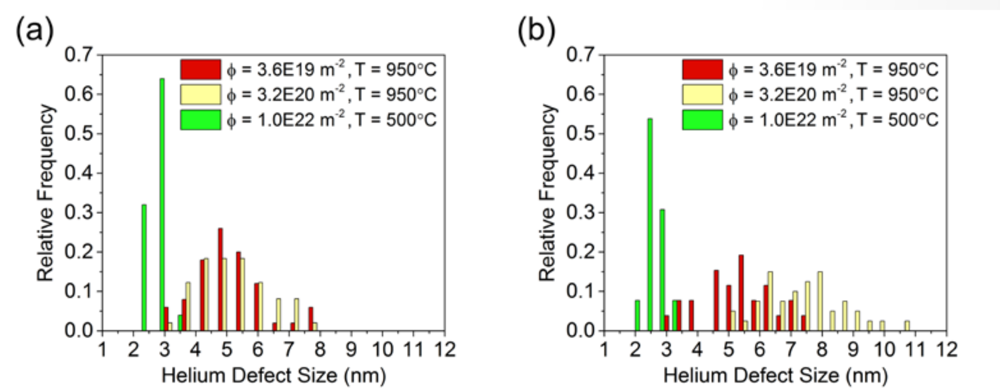
Kiener and Minor, Nano Letters, 2011

Zhang and Trelewicz, Acta Mat, 2017

Radiation Effects and Mechanical Behavior







A confluence of mechanisms places softening due to grain boundary cavity formation in competition with hardening from intragranular defect loop damage

Cunningham, et al., Scientific Reports, Unver Review

Bulk Nanostructured Tungsten Alloys

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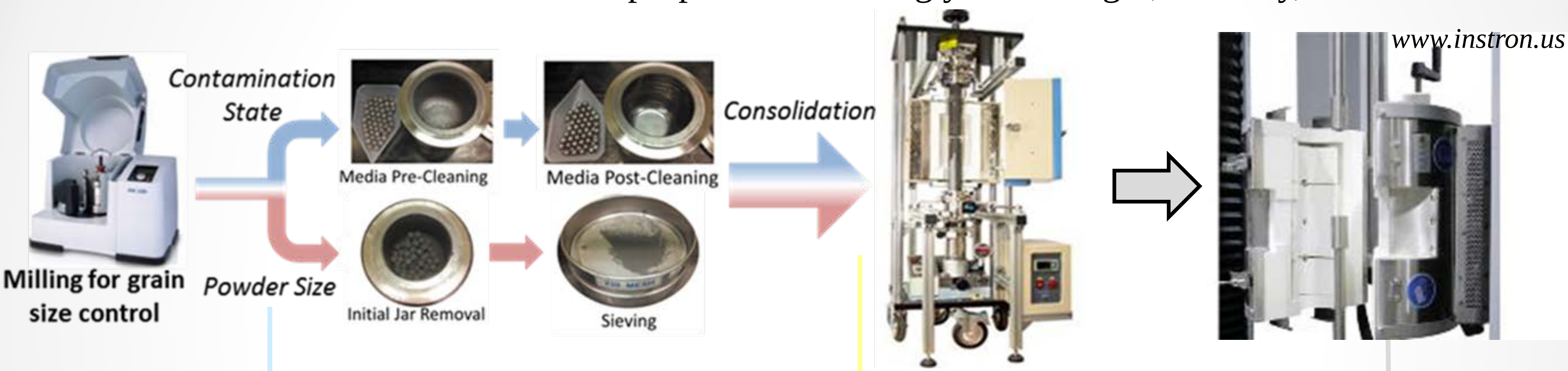
Task Aims:

- Bulk nanostructured tungsten alloys synthesized through ball milling and hot consolidation.
- Grain growth and recrystallization stability maps as a function of composition and grain size.
- Measurement of bulk mechanical properties including yield strength, ductility, and DBTT.



Mechanical Alloying

- Binary and ternary alloys via high energy ball milling
- Vary media-to-powder ratio, milling speed and time

→ *Map minimum achievable grain size vs. impurity content*

Hot Consolidation

- For given temperatures, vary pressure and time
- Compare hot pressing with spark plasma sintering

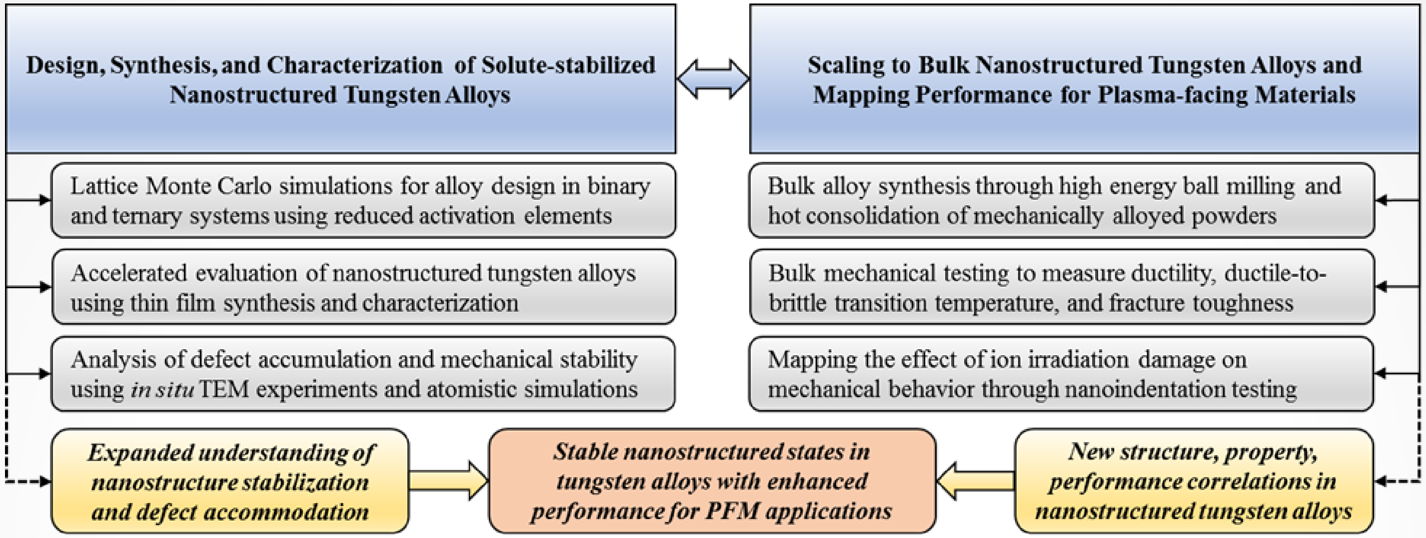
→ *Map density, phases, and grain size as a function of process variables*

Mechanical Testing

- Room and elevated temperature testing (ASTM E8/E21)
- Fracture toughness after ASTM E1820

→ *Strength, ductility, rate sensitivity, and DBTT*

Early Career Award Research Activities



Research Tasks

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   - i. Lattice Monte Carlo modeling for alloy design
   - ii. Accelerated alloy synthesis and characterization using thin film techniques
2. Analysis of defect formation and mechanical stability
   - *i.* *In situ* ion irradiation of nanostructured tungsten alloy thin films
   - ii. Nanomechanical testing on pristine and ion irradiated alloys
   - iii. Understanding mechanisms through atomistic simulations

   } *Coupled radiation effects and mechanical behavior*
3. Bulk nanostructured tungsten alloy synthesis and property mapping
   - i. Powder metallurgy synthesis and bulk alloy consolidation
   - ii. Structural characterization and mechanical testing