Virtual Laboratory for Technology
FES FY2018 Second Quarter Report

Phil Ferguson
for the VLT members

VLT
Virtual Laboratory for Technology
For Fusion Energy Science

Director's Corner

- The FESAC Transformative Enabling Capabilities report was finalized in February 2018, and the VLT was well represented both on the committee and submitting/presenting whitepapers on concepts. The community viewed this positively, and the VLT is ready to explore these technologies further should the opportunity arise.
- Bi-monthly teleconferences are continuing with good representation. Discussion last month centered around the NAS study and how the VLT could provide additional input on community whitepapers.
- Program reviews for the Materials, Fusion Nuclear Science, and Enabling R&D budget elements in preparation for the upcoming FES Committee of Visitors have started. Consistent with prior COV recommendations, this review process is intended to provide an evaluation of quality and progress of base programs over the last four fiscal years, spanning FY 2014 to FY 2017.
- This and future highlights will continue to cover research highlights from recent VLT publications and the main VLT research areas:
  - Magnet Systems; Heating & Current Drive; Plasma Fueling/ ELM Pacing/Disruption Mitigation
  - Plasma Facing Components; Plasma Materials Interactions; Structural Materials
  - Design/Systems studies; Power Handling; Fusion Safety; Fuel Cycle Research; Blanket Technology; Vacuum System

If you have any questions on the information in this report, please don't hesitate to contact us.

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Solute Stabilization of Nanocrystalline Tungsten Against the Onset of Rapid Abnormal Grain Growth

Scientific Achievement

The addition of titanium and chromium to nanocrystalline tungsten films stabilized the alloys against the formation of the metastable β-phase and in turn, rapid microstructural coarsening through abnormal grain growth.

Significance and Impact

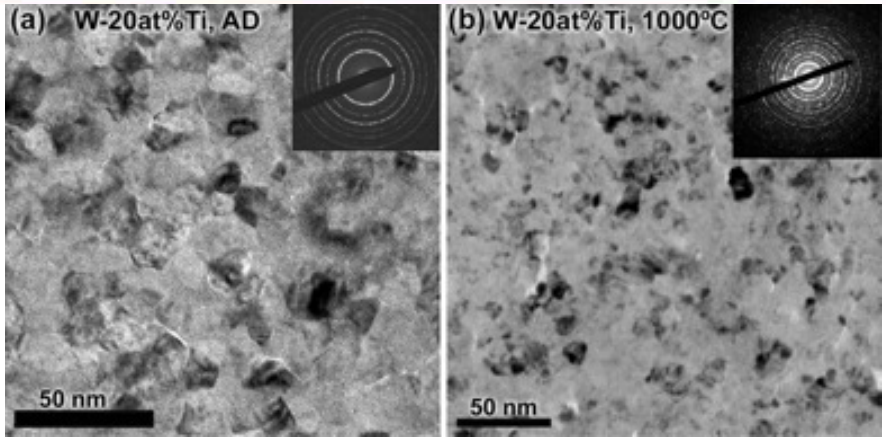
Thermal stability of nanocrystalline tungsten alloy films was demonstrated at temperatures up to 1000°C and attributed to solute enrichment of grain boundaries.

Research Details

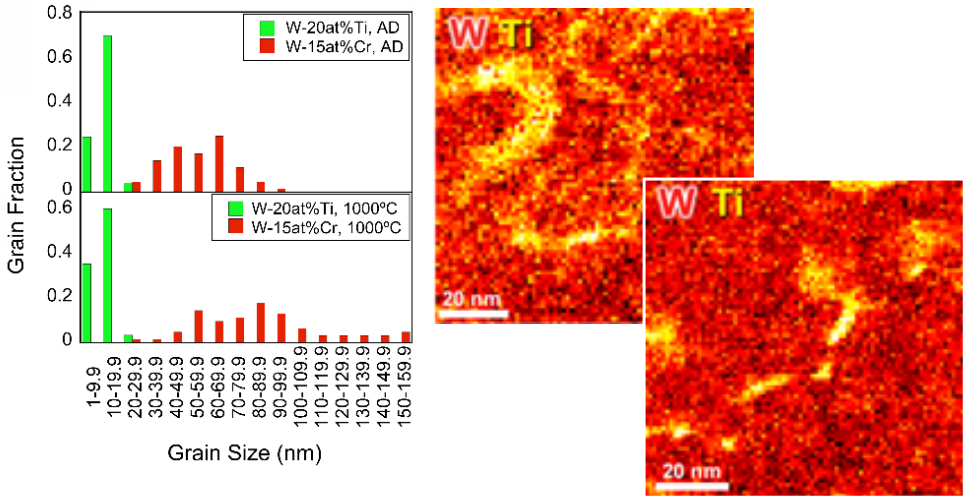
In situ TEM experiments were combined with STEM analysis to correlate nanostructure stability with underlying solute distributions.

Application

These materials have the potential to address stability issues in coarse-grained tungsten for plasma-facing components.



TEM images of nanocrystalline W-20 at.% Ti alloys.



Grain size distributions and EELS maps for W-Ti alloys.

Donaldson, O.K., Hattar, K., Kaub, T., Thompson, G.B., and **Trelewicz, J.R.**, "Solute Stabilization of Nanocrystalline Tungsten Against Abnormal Grain Growth", Early Career Scholars in Materials Science: Invited Feature Article, Journal of Materials Research, 33, 1, 2018

Work sponsored by DOE Office of Fusion Energy Sciences

U.S. DEPARTMENT OF ENERGY | Office of Science

Stony Brook University

Sandia National Laboratories

VLT Virtual Laboratory for Technology For Fusion Energy Science

Advanced Materials Modeling Used to Understand/ Improve Tungsten Recrystallization Limits

Science Objective

Here we use molecular dynamics and multiscale modeling techniques in collaboration with the Marian group at UCLA to develop a predictive model of tungsten recrystallization.

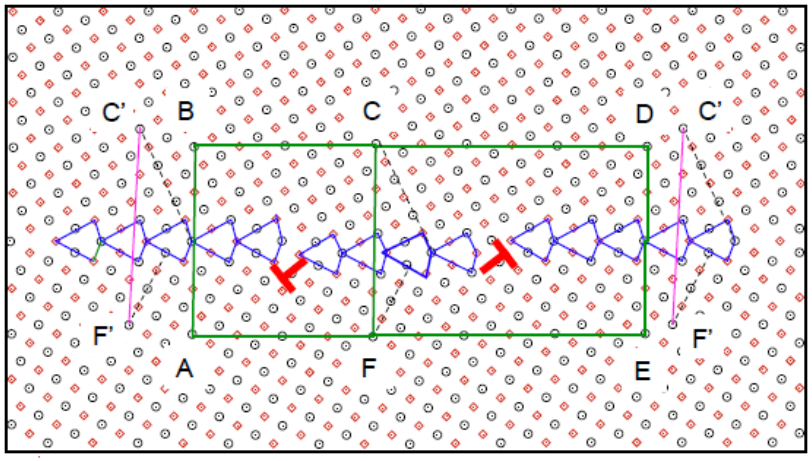
Achievement

We predicted for the first time phase transformations in tungsten grain boundaries (GB) at high temperature. This quarter we have determined new tilt boundary properties and discovered mechanisms of GB transition induced by point defect flux such as arising from radiation damage.

Why it Matters

Recrystallization limits the operating temperature for tungsten in plasma facing components in tokamaks. Recrystallization involves the movement of grain boundaries in damaged metals at high temperature. It is crucial that calculations of GB properties that affect recrystallization start with the correct GB structure, something that has not been possible previously.

Point Defect Induced Grain Boundary Reconstruction

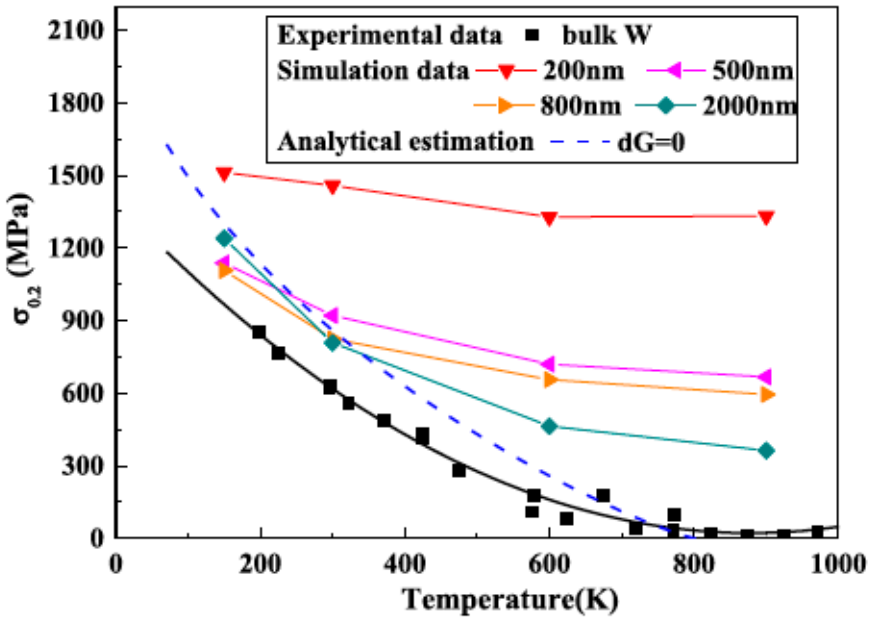


An evolutionary algorithm was applied to find new tilt grain boundary structures in tungsten. High-temperature MD simulations revealed mechanisms of GB transformations, including the mechanism shown above in which point defects induced a GB transition that ultimately reconstructs into a dislocation loop.

"Grain boundary phases in bcc metals," T. Frolov et al., *Nanoscale (2018) accepted;*
"Structures and transitions in bcc tungsten grain boundaries and their role absorption of point defects," T. Frolov et al, submitted *Acta Mater*

Robert E. Rudd and Tim Frolov (LLNL FWP SCW0458)

Temperature insensitivity of the flow stress in body-centered cubic micropillar crystals



The dependence of the flow (yield) stress on temperature for various sample sizes. Note the insensitivity of the flow stress to test temperature when the sample size is small (e.g. 200 nm).

*Cui, Yinan, Giacomo Po, and Nasr Ghoniem. "Temperature insensitivity of the flow stress in body-centered cubic micropillar crystals." Acta Materialia **108** (2016): 128-137.*

Scientific Achievement

Plasticity of body-centered cubic (bcc) crystals is known to have a strong dependence on temperature, as a direct consequence of the thermally-activated process of kink pair nucleation and migration with a high energy (Peierls) barrier. Here we demonstrate that, in the sub-micron size scale, such strong temperature dependence of the flow stress must disappear

Significance and Impact

This finding opens the door to materials-by-design of nano-grained BCC metals (e,g, tungsten and iron" that do not show strong DBTT behavior.

Research Details

We explore the flow stress and hardening behavior of micro-pillar sizes in the range 200e2000 nm at temperatures of 150e900 K. Discrete Dislocation Dynamics (DDD) simulations reveal that the weak temperature sensitivity can be rationalized in terms of the weak role of screw dislocations in controlling plasticity; unique to small crystals of finite size. It is shown that finite, sub-micron samples have limited ability to store screw dislocations. The necessity of applying high stress in sub-micron crystals is demonstrated to greatly enhance the mobility of screw dislocations, rendering it close to that of edge dislocations. This leads to a transition of the dislocation mobility mechanism from being thermal-activated kink dominated to being phonon-drag dominated. Thus, the flow stress gradually becomes not governed by the mobility of screw dislocations (as determined by the critical resolved shear stress), giving rise to the weak temperature sensitivity of the flow stress. A dislocation mechanism map in the temperature-size space is proposed to further illustrate this phenomenon in tungsten micropillars.

A Tungsten-Rhenium Interatomic Potential for Point Defect Studies

Science Objective

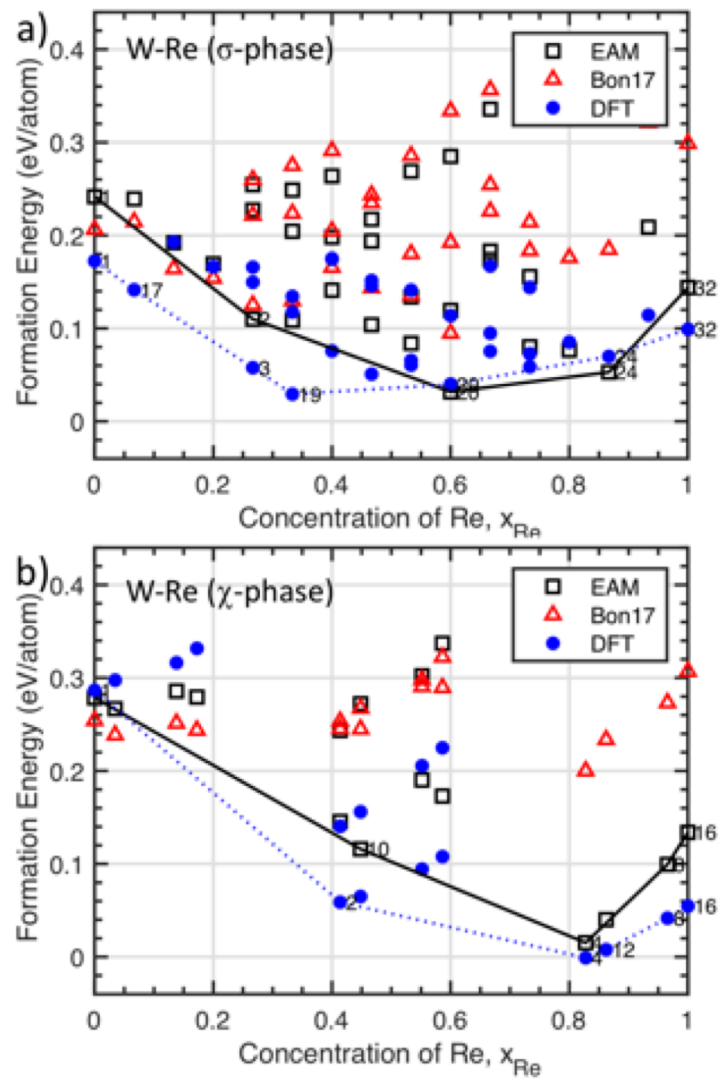
Develop a classical interatomic potential for tungsten-rhenium to enable large-scale computer simulations of the effects of transmutation produced rhenium on microstructure evolution of irradiated tungsten.

Significance and Impact

Transmutation products can be both beneficial and detrimental to defect microstructure evolution and the resulting material properties of tungsten. Much of the exploration of the rich influence of transmutation products has been limited by the absence of adequate classical interatomic potentials.

Research Details

A force-matching method is employed to fit the potential to *ab initio* forces, energies, and stresses. Simulated annealing is combined with a conjugate gradient technique to search for an optimum potential from over 1000 initial trials.



Formation energy of W-Re structures in the a) σ and b) χ phases with respect to body centered cubic tungsten and hexagonal close packed rhenium. The stable structures in each phase are connected with a common-tangent line forming a convex-hull.

W. Setyawan, N. Gao, R.J. Kurtz (2018). "A tungsten-rhenium interatomic potential for point defect studies" submitted to J. App. Phys.

Atomistic Simulation of Interstitial Dislocation Loop Evolution under Applied Stresses in BCC Iron

Science Objective

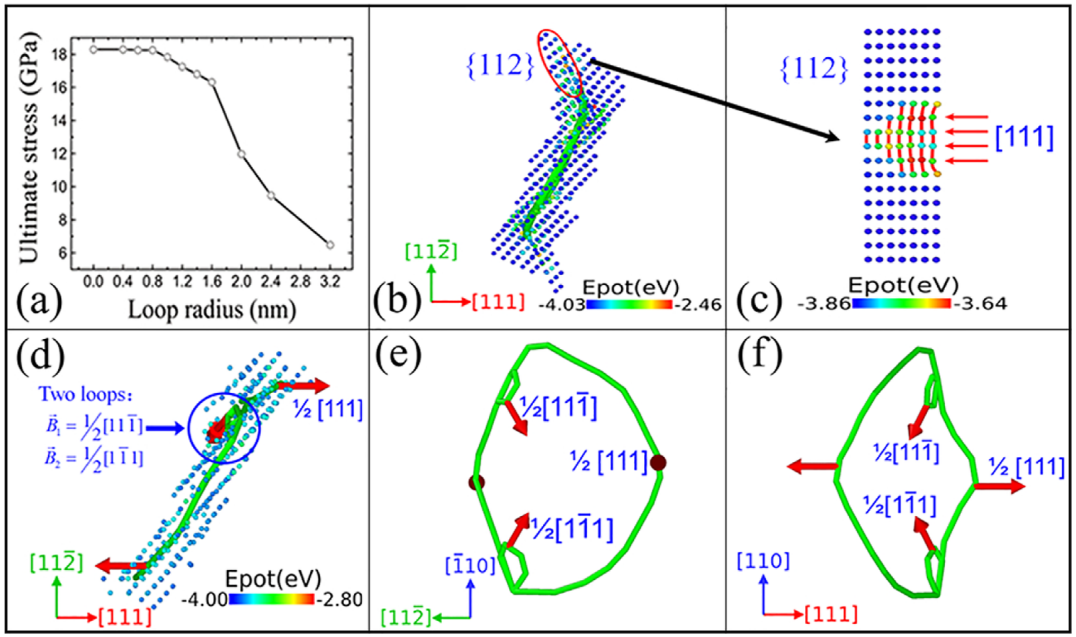
Interstitial dislocation loops are formed directly in displacement cascades or through agglomeration of self-interstitial atoms after a cascade event. Understanding loop evolutions under different applied stresses is needed for mesoscale models of microstructure evolution.

Significance and Impact

Under tensile loading strength decreases rapidly in the presence of a loop with radius ≥ 0.8 nm, which is associated with triggering of slip on a {112} plane. Under shear loading the loop rotates by changing the habit plane from {111} to {100} and by transforming from a prismatic loop to a shear loop. Under torsion a normally observed phase transformation from BCC to FCC and partially to HCP is delayed and a free-surface micro-crack forms.

Research Details

The evolution of interstitial ½<111> dislocation loops under tensile, shear, and torsional stresses was studied using a molecular statics method. Rather than applying a constant strain rate to the computational cell, constant stresses and torsion were used in this work.



- Evolution of ½ <111> dislocation loop under tensile stress

  a) effect of loop size on ultimate tensile strength
  b) and c) the initial stage of slip along <111> on {112}
  d) to f) formation of two small shear loops around initial ½<111> dislocation loop

- The color of each atom is defined according to its potential energy as shown by color bar in the figure

X.H. Long, D. Wang, W. Setyawan, P. Liu, N. Gao, R.J. Kurtz, Z.G Wang, X.L. Wang (2018). "Atomistic simulation of interstitial dislocation loop evolution under applied stresses in BCC iron" Phys. Status Solidi A 215 (2018) 1700494

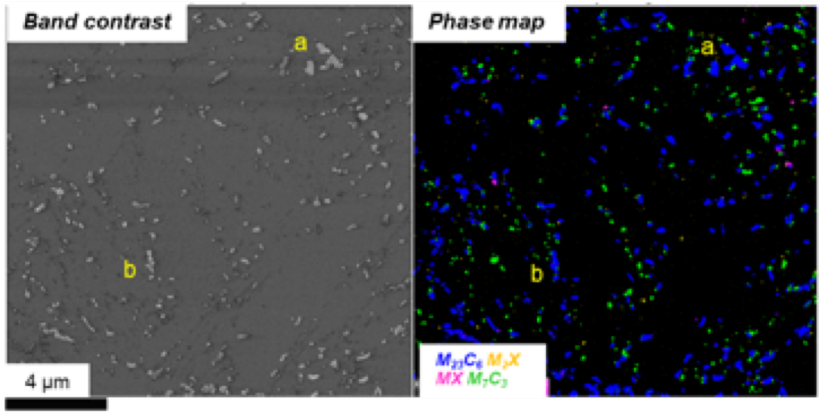
New analysis techniques and old extraction method produces unprecedented precipitate statistics

Analysis of modified EUROFER 97 showed type /distribution of $M_{23}C_6$, M_7C_3, MX and M_2X phases

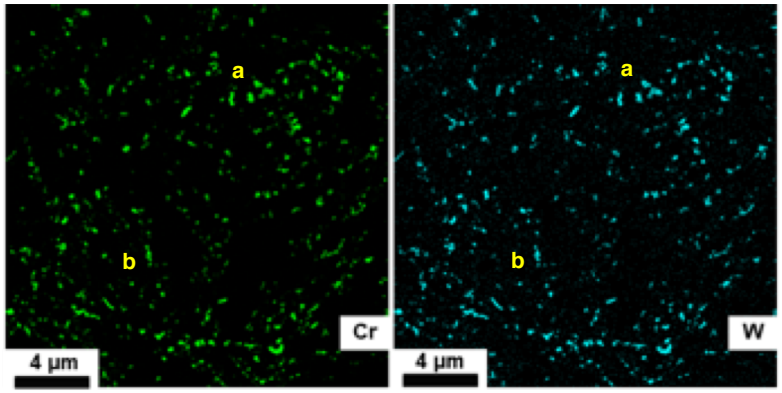
- Extraction Replicas - Etching, deposition of carbon, then dissolution of the sample leaves precipitates suspended in a carbon film
- Transmission Kikuchi diffraction (tKD) identified crystal structure. tKD used the FEI Versa 3D SEM to identify thousands of ppts in single scan.
- Energy Dispersive Xray analysis (EDX) shows the chemistry of the ppts. EDX mapping used the FEI 200X Talos STEM
- Precipitates as small as ~5-10 nm were successfully indexed by tKD.
- tKD identified $M_{23}C_6$, M_7C_3, MX, M_2X phases with unprecedented statistics

A. Bhattacharya, C.M. Parish, Y. Katoh

Large area tKD scan showing precipitates in replica



STEM-EDX maps on precipitates detected by tKD

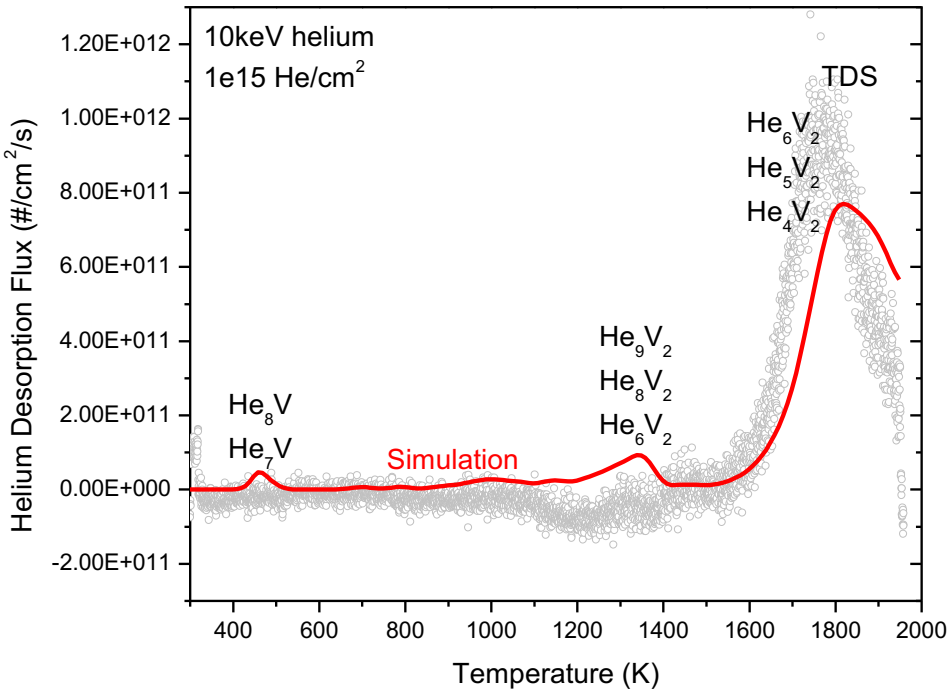


Combining tKD with STEM-EDX mapping opens new pathways in "big data material characterization" applicable to nuclear and non-nuclear materials.

Helium-defect interactions have been modeled in tungsten

Validation of energetic and kinetic parameters describing He-defect interactions in W is critical to predicting He bubble nucleation and growth

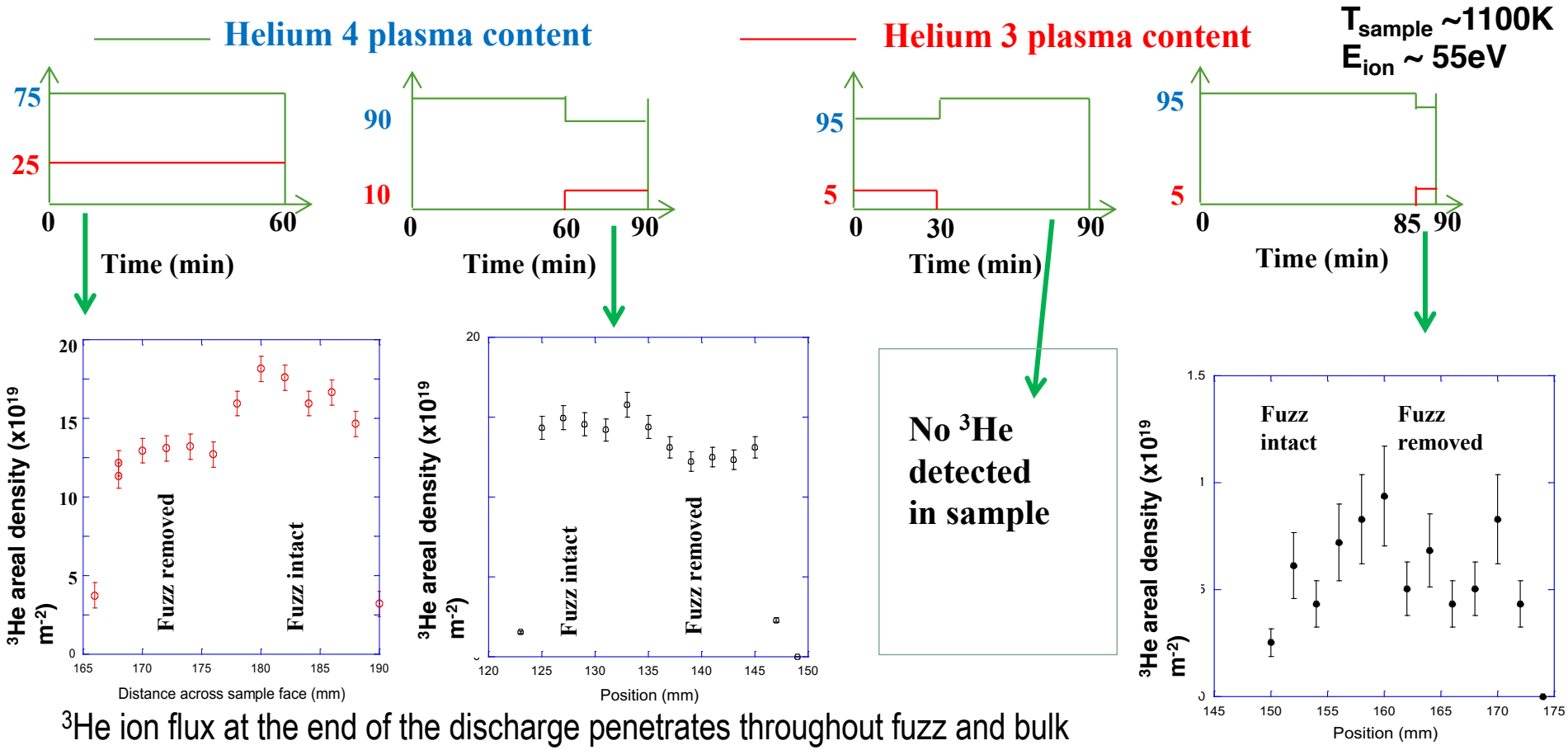
- A cluster dynamics model based on diffusion-reaction rate theory was developed to describe the evolution of He-defect complexes in He ion-implanted tungsten
- Thermal He desorption spectrum from He-implanted W was used to validate the applied migration energies of mobile species and the binding energies of clusters in the model
- The model successfully reproduced the He desorption spectrum and identified the clusters possibly contributing to the desorption peaks



Comparison of experimentally measured thermal helium desorption from tungsten implanted with 10 keV He to a fluence of 10^{15} He/cm^2, with spatially-dependent cluster dynamics model simulation

Xunxiang Hu, Jie Qiu, Brian D. Wirth, Yutai Katoh

He bubbles behave dynamically during W fuzz growth



- ^{3}He ion flux at the end of the discharge penetrates throughout fuzz and bulk
- ^{3}He initially in bubbles throughout the material is removed during subsequent ^{4}He plasma exposure
- Bubbles bursting and reforming throughout fuzz and in the base explains behavior (because a 6-9 eV energy barrier for He to enter W would prevent He from exiting the bubble)
- He content in target is proportional to plasma fluence (implies direct implantation of He into both the tendrils and the base of the structures)

Doerner et al, in press Nucl. Fusion 2018.

New plasma source to enhance ion flux density in Tritium Plasma Experiment

- Challenge in existing linear plasma device is to achieve ITER divertor relevant condition (ion flux density $>10^{23}$ $m^{-2}s^{-1}$) for understanding plasma-surface interaction in burning plasma condition.
- Power supplies were upgraded to produce ITER divertor relevant condition in FY2013.
- New plasma source was designed and fabricated (see Fig.1&2) in FY2017 based on PISCES-A plasma source to increase ion flux density to $>10^{23}$ $m^{-2}s^{-1}$. [collaboration with UCSD PISCES group].
- Initial deuterium discharge was successfully carried out with new plasma source, and the discharge I-V curve showed promising result at low discharge current range (see Fig.3).
- Cooling system was modified for high current discharge operation, and higher discharge current will be tested to achieve ITER divertor relevant condition in FY2018 Q2.

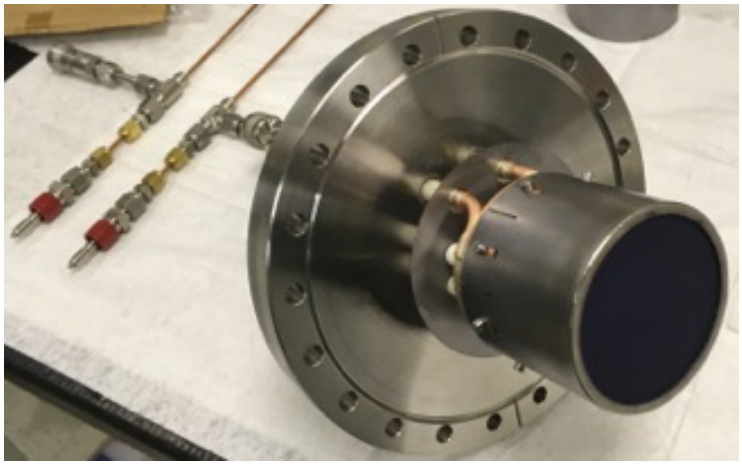


Fig. 1: TPE new source

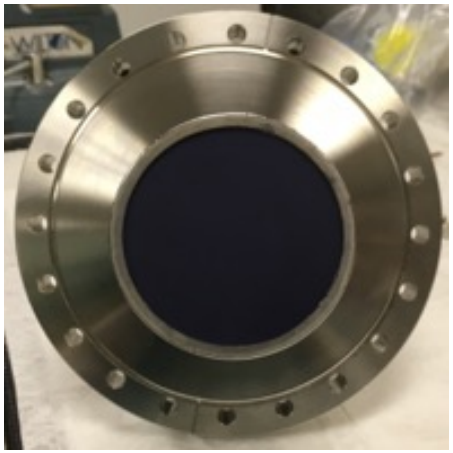


Fig. 2: TPE new source (front view)

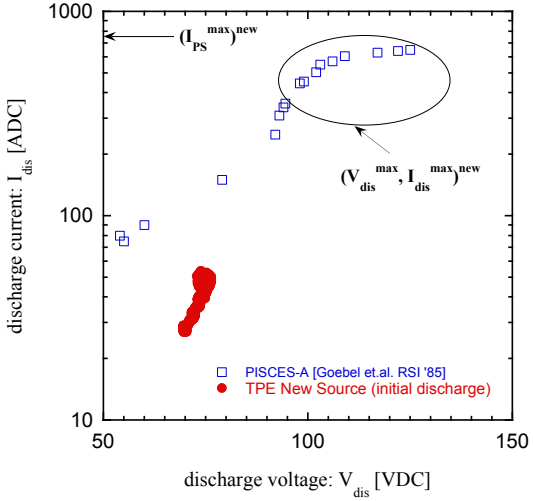


Fig. 3: Discharge I-V characteristic

Toward high-field compact fusion magnets: update #2 on the characterization of electro-mechanical performance of REBCO conductors

Scientific status as of April 2018

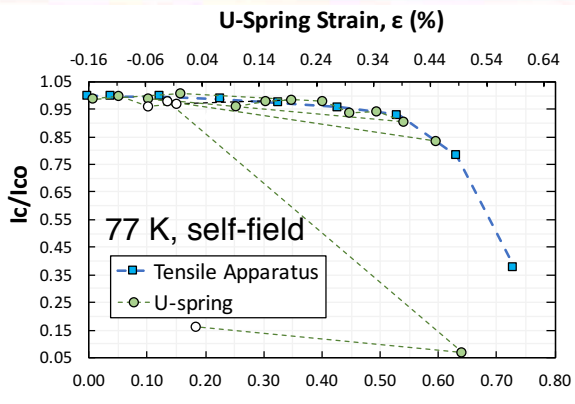
We made first measurements of commercial REBCO tapes at 15 T and various temperatures (4.2 K to 40 K). The new sample holder worked.

Significance and Impact

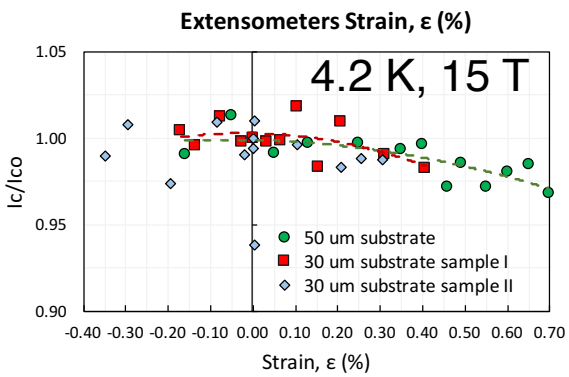
The current-carrying capability of REBCO tapes depends on applied strains. Understanding the strain dependence at high magnetic fields and elevated temperatures (20 – 50 K) will help the design and optimization of high-current REBCO cables for high-field compact fusion reactor magnets. Please see update #1 in Q4 2017 for more details.

Research Details

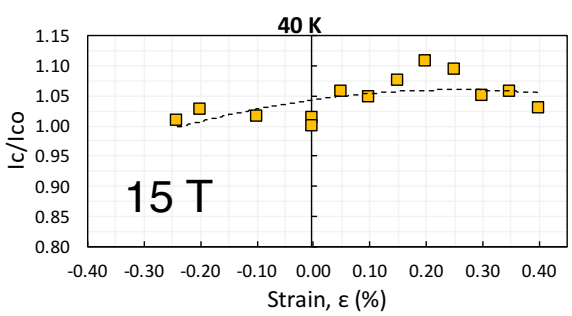
The new U-spring sample holder was validated against an extensometer-based setup at Tufts University. Both setup gave similar tension results at 77 K. Commercial tapes with different substrate thicknesses showed similar strain dependence at 4.2 K, 15 T. A first attempt was made to measure the strain dependence at 20, 30 and 40 K, 15 T. We are planning for a comprehensive test campaign to obtain more statistics on the strain dependence of the current carrying capability for REBCO tapes with different characteristics and made from various vendors.



Cross cablibration at 77 K with a setup at Tufts University.



Tapes of different substrate thicknesses showed similar strain dependence at 4.2 K, 15 T



First attempt to measure the strain dependence at 40 K, 15 T.

F. Pierro, L. Chiesa, H. Higley, S. O. Prestemon, X. Wang

Observation of an unwanted 98 GHz mode in a 110 GHz Gyrotron

Scientific Achievement

- Megawatt power level gyrotrons are a key technology needed for heating and current drive in present day experiments, such as the DIII-D tokamak and ITER, as well as in future experiments. The operation of gyrotrons in unwanted modes can cause failure of the gyrotron and damage to the plasma machine and diagnostics.

Significance and Impact

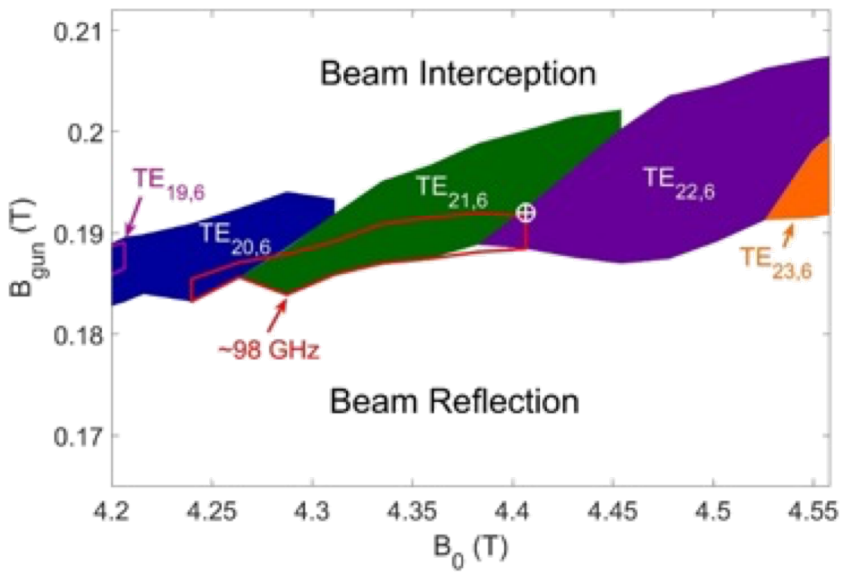
- Recent research by Prof. M. C. Lin of Korea using the codes VORPAL and VSIM has predicted the possibility of the 110 GHz gyrotron switching into an unwanted 98 GHz mode. This prediction has been verified at MIT (see figure).

Research Details

- The MIT gyrotron is operated at 96 kV, 42 A in three microsecond pulses. The modes are measured on a map of main magnetic field vs. magnetic field at the electron gun.
- Mode frequencies are measured by a heterodyne receiver.

Application

- These results help validate modern gyrotron design codes leading to improved gyrotron efficiency and reliability.



Existence of a competing mode at 98 GHz, predicted in recent simulations, is demonstrated on the MIT pulsed 110 GHz gyrotron.

MIT: S. Schaub, S. Jawla, M. Shapiro and R. Temkin; Korea: M. C. Lin; supported by DOE VLT and US IPO

Beginning work on modeling of powder-dropper experiments for wall conditioning

Scientific Objective

Develop and validate simulation models of dust particle dynamics and the resulting flows of impurity ions to PFC. Aid physics understanding of data.

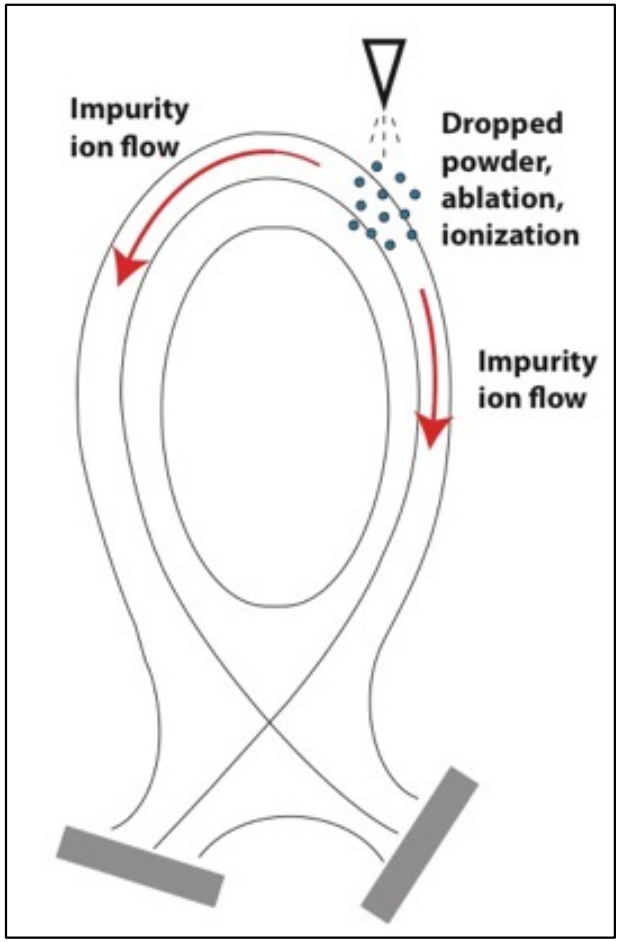
Detailed work plan

- Modeling dynamics of injected dust cloud with DUSTT
- Modeling in UEDGE impurity ion flows in the edge due to ablation of injected dust cloud
- Calculation of impurity ion deposition on PFC in UEDGE
- Collaboration with U. Illinois for calculation of impurity ion flow through the sheath with hPIC, and for dynamics of surface layer of PFC with F-TRIDYN

Why it matters

Powder-dropping is a new, potentially revolutionary, techniques for real-time delivery of impurities into tokamak edge plasma; may allow real-time wall conditioning and advanced ways for maintaining radiative divertor

Schematic of physical processes in the model



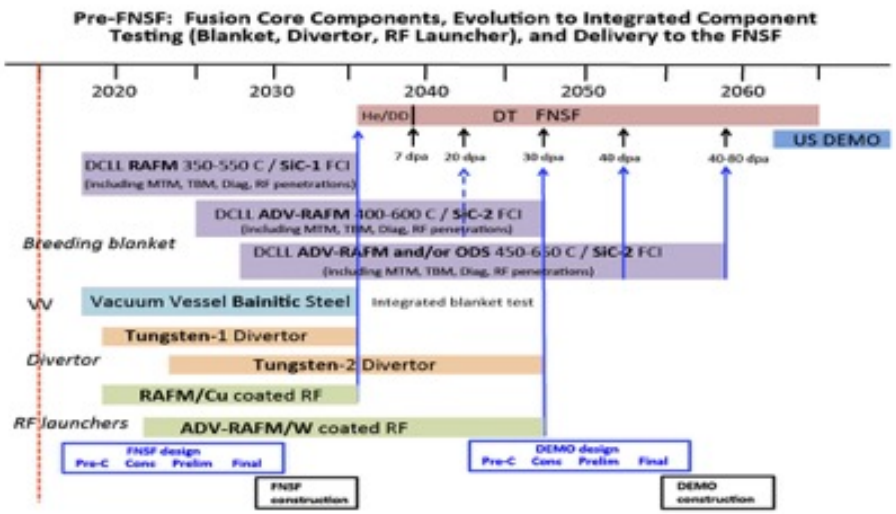
M. Umansky, M. Dorf, T. Rognlien (LLNL FWP SCW0455)

Materials Engineering Support for the FNSF Conceptual Design

The goal is to identify materials solutions for the FNSF power core and other system components

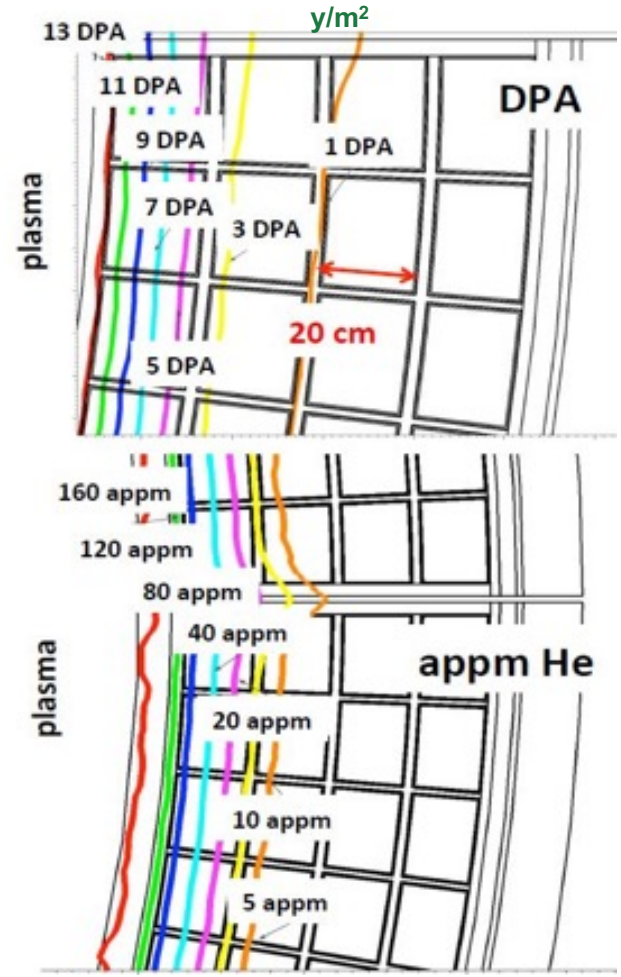
Activities within the Fusion Nuclear Science Facility study have identified candidate materials, established performance limits for these materials, and suggested needed materials improvements

The FNSF time line ties materials development to reactor operation



A.F. Rowcliffe, C. E. Kessel, Y. Katoh, L. M. Garrison, L. Tan, Y. Yamamoto, F.W. Wiffen, "Materials-Engineering Challenges for the Fusion Core and Lifetime Components of the Fusion Nuclear Science Facility," accepted for publication in Nuclear Materials and Energy

Radiation response parameters for FNSF outboard blanket at 1 MW-y/m^2



Critical Issues for Liquid PFCs include Managing Power & Particle Fluxes and Shielding Vapor

Scientific Objective

Predict edge-plasma properties that are compatible with manageable heat flux and core plasma operation for FNSF design when using of various liquid walls. Compare results with similar configurations that used solid walls to identify key issues and impact on overall fusion performance.

Achievement

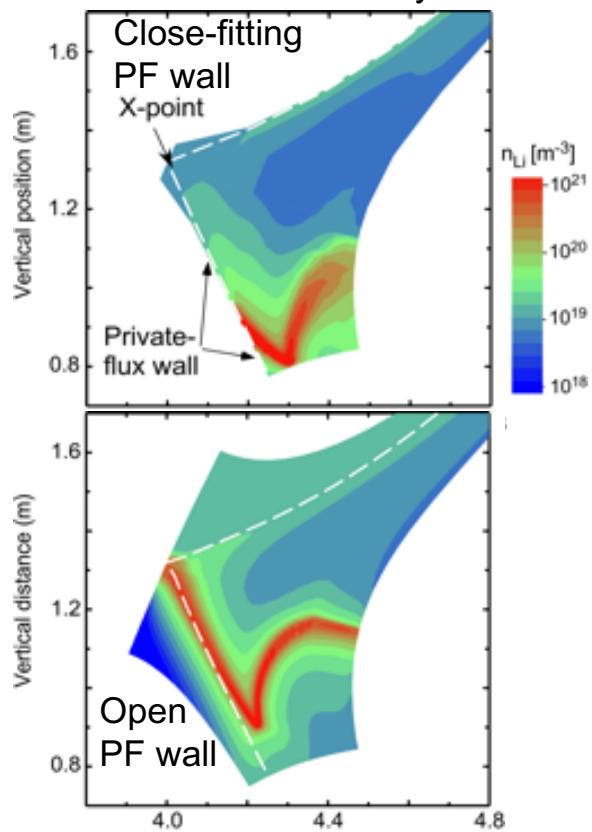
Continued analysis of 2D UEDGE simulations for Li divertor in FNSF geometry to understand if the previous wide private flux region was the cause of substantial Li ion density in the core region. New simulations with a tight-fitting wall in the private-flux region shows reduced Li near the X-point, but very similar midplane values. Next, the outer region of the divertor will be narrows to assess if close-fitting walls on both sides are sufficient to reduce the midplane Li density.

Why it matters

Flowing liquid walls could avoid the issue of wall erosion by ions and neutrals and could also lead to high-performance core operational modes through high-temperature edge conditions.

Confinement of Li ions to the divertor is key to preventing lithium in the core region. A close-fitting private-flux wall reduces Li near X-point, but not substantially near miplane.

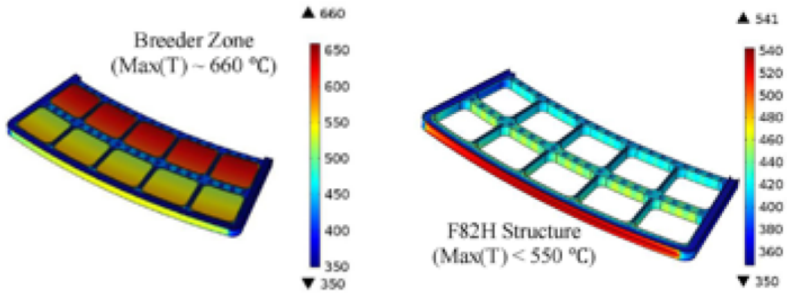
Lithium ion density



Tom Rognlien and Marv Rensink (LLNL FWP SCW1122)

U.S. DEPARTMENT OF ENERGY | Office of Science
VLT Virtual Laboratory for Technology For Fusion Energy Science

Multiphysics-Multiscale Design of Fusion Energy Structures (UCLA) – Jan-March 2018



(a) Breeding zone (b) Blanket structure

Temperature distributions of the global FW/Blanket structure.

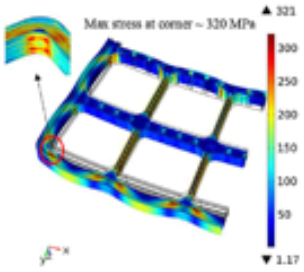
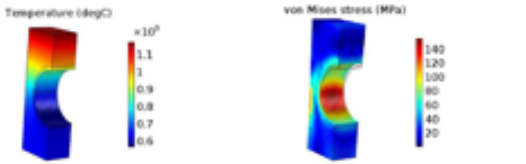


Fig. 11. Primary stress distribution (Von-Mises stress).



(a) Temperature distribution (b) Total stress distribution in deformed structure

Fig. 9. Thermo-mechanical results of optimum geometry for SiC/SiC round pipe.

(1)) Y Huang, MS Tillack, NM Ghoniem, JP Blanchard, LA El-Guebaly, CE Kessel, "Multiphysics modeling of the FW/Blanket of the US fusion nuclear science facility (FNSF***," Fusion Engineering & Design*** Publication date 2017/7/13.

(2) Y Huang, MS Tillack, NM Ghoniem, "Tungsten monoblock concepts for the Fusion Nuclear Science Facility (FNSF) first wall and divertor," ***Fusion Engineering and Design***, Publication date 2017/6/23

Scientific Achievement

The design of fusion energy structures, such as the First Wall (FW), Blanket (B), and Divertor (D) is achieved with a newly-developed two-step approach. In the first step, a multiphysics simulations are used to couple heat transfer, fluid flow, and structural mechanics. In the second step, successively more detailed models of the thermomechanical and radiation response of the structure is achieved with at multiscales, where continuum models are coupled to elastoplasticty and microstructure-baaed representations of the structure.

Significance and Impact

This is a breakthrough in our ability to make computer models of high fidelity including damage phenomena due to neutron irradiation and high heat flux emanating from the plasma. Such detailed models will accelerate the development of fusion energy components without the need for expensive and empirical testing.

Research Details

- ***Multiphysics modeling of the FW/Blanket of FNSF***
  - The dual coolant lead-lithium (DCLL) blanket concept, which is utilized in the Fusion Nuclear Science Facility (FNSF) conceptual design, is based on a helium-cooled first wall and blanket structure with RAFS (Reduced Activation Ferritic Steel) and a self-cooled LiPb breeding zone. We show here that the structural design meets the ITER-ISDC design rules under both normal and off-normal operating conditions, though the safety factors under off-normal condition with 8 MPa helium pressure are
- 2) ***Tungsten monoblock concepts***
  - We analyzed advanced "monoblock" designs using coolants and materials that offer more attractive long-term performance. The results of analysis show that helium-cooled steel can remove up to 5 MW/m^2 of steady-state surface heat flux and helium-cooled SiC/SiC can remove nearly 10 MW/m^2 while satisfying all materials and design requirements.

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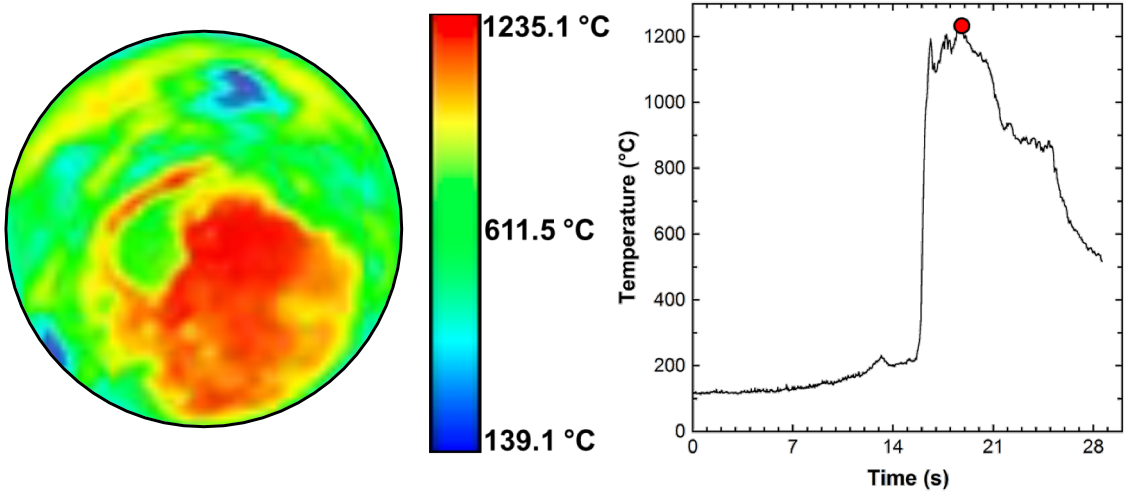
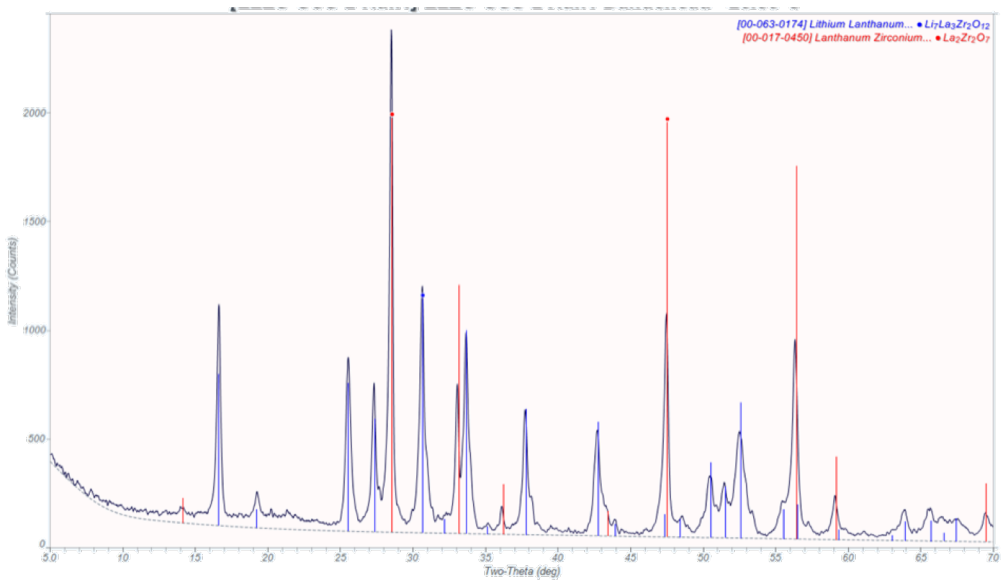
Demonstration of Direct LiT Electrolysis using an Immersion Cell





Scientific Achievement

- **Developed a solution combustion synthesis method that can speed synthesis and lead to greater incorporation of lithium and other dopants while minimizing evaporation losses**

Significance and Impact

The development of a **sol-gel or solution combustion synthesis allows significant variation of LLZO electrolyte properties and can be used to increase conductivity and strength of the electrolyte**

Research Details

- **An initial solution combustion synthesis run was performed to test its viability as a method for producing high quality LLZO materials**
- **Synthesis was mostly successful, but the choice of lithium precursor led to some $La_2Zr_2O_7$ formation**
- **Variations on the reaction utilizing a lithium precursor that mixes better will be attempted to see if this could resolve synthesis issues**
- **SCS could significantly improve options the viability of LLZO synthesis**

Tritium Processing Development for Magnetic Fusion

Application

Development and testing of tritium fuel cycle components and data-mining of TSTA historical documentation.

Scientific Achievement

Work has been completed on the HPL line heater controller and current under electrical safety review/approval. Participation in Liquid metal plasma facing component (LM-PFC) System Study biweekly conference calls and Face to Face meeting at DOE HQ.

Final Wiring for Heater Controllers

Table 3
Comparison of the liquid breeder/coolant performances

Liquid breeder	Li	$Li_{17}Pb_{83}$	Flibe	$Li_{20}Sn_{80}$
Melting point (°C)	180	235	459	320
Density (g/cm^3) (873 K)	0.48 [12]	8.98 [13]	2.0 [14]	6.0 [5]
Li density (g/cm^3) (873 K)	0.48	0.061	0.28	0.09
Breeding property	Good	Fairly good	Neutron multiplier required	Neutron multiplier required
Chemical stability	Active	Middle	Almost stable	Almost stable
Corrosion	Severe	More severe	HF exist, severe	?
Tritium release form	HT, T_2	HT, T_2	HT, T_2, TF	HT, T_2
Tritium solubility (atom frac Pa$^{-0.5}$) (873 K)	Very high 7.49×10^{-3} [8]	Very low 1.93×10^{-8} [15]	Very low for HT/T_2, 1.77×10^{-11} Pa^{-1} [9] for TF, 4.32×10^{-9} Pa^{-1} [10]	Middle 2×10^{-7}–1×10^{-5}
Tritium diffusivity order (m^2/s) (873 K)	Relative high 10^{-9}	Relative high 10^{-9}	Relative high 10^{-9}	Relative high 10^{-9}
Thermal conductivity [16,17]	Li > $Li_{20}Sn_{80}$ > $Li_{17}Pb_{83}$ > Flibe			
Dynamic viscosity [16,17]	Flibe > $Li_{20}Sn_{80}$ ≈ $Li_{17}Pb_{83}$ > Li			

Y. Kang, Moderate tritium properties in lithium-tin alloy as a liquid breeder/coolant, Fusion Engineering and Design, 2006

Significance and Impact

- HPL and U-Bed upgrades will allow for continued engineering design development of tritium fuel cycle for fusion processes
- Integration of fuel cycle design into LM-PFC development will strengthen design options and applications.

Research Details

- Presented literature survey for Li, LiPb, and LiSn and tritium solubility and diffusivity constants to be used in tritium inventory estimates for and liquid metal wall on FNFS to address safety and feasibility studies at Face to Face meeting in March 2018. Summary table to applicable constants to be integrated into calculations shown on left.
- Completed summary report for FNS Panel Review and submitted to FES.

Hollis, W. Kirk, LM PFC Meeting, LM PFC Working Group Meeting. FES Germantown, March 2018

Hollis, W. Kirk, Tritium Processing Development for Magnetic Fusion, Summary Report, March 2018