Virtual Laboratory for Technology
FES FY18 First Quarter Report

Phil Ferguson
for the VLT members

VLT
Virtual Laboratory for Technology
For Fusion Energy Science

Director's Corner

- FY18 is off to a busy start for the VLT. The FESAC Transformative Enabling Capabilities report is wrapping up, we were well represented at the APS meeting in Milwaukee, and a second community workshop was held in Austin.
- Bi-monthly teleconferences are continuing with good representation. Additional teleconferences are held as needed to prepare for whitepaper submissions, presentation discussions, etc. Larry Baylor and Rajesh Maingi have presented recent technical presentations to the VLT.
- Following information from FES program managers, the VLT is preparing for a set of reviews for the Materials, Fusion Nuclear Science, and Enabling R&D budget elements in preparation for the upcoming FES Committee of Visitors. 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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Transmutation Effects on 3C-SiC Structure Using $^{25}Mg^{+}$ Ion Implantation

Science Objective

Investigate precipitation of Mg transmutants in cubic phase silicon carbide (3C-SiC) and its structural effects by parameter-controlled ion implantation and thermal annealing

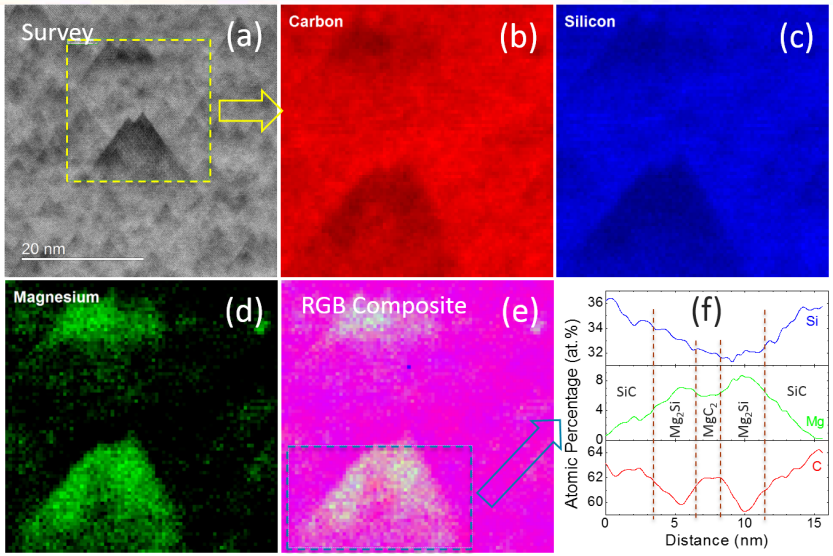
Significance and Impact

Transmutation of Si in 3C-SiC due to high-energy neutron irradiation in a fusion environment leads to a significant production of magnesium. The presence and interactions of the transmutants and irradiation-induced defects in 3C-SiC are expected to affect its chemical and thermomechanical properties

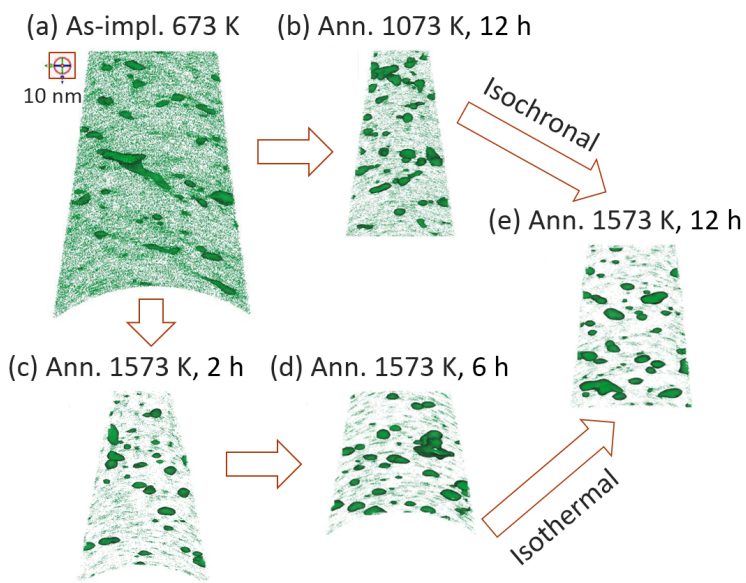
Research Details

Unidirectionally aligned tetrahedral precipitates of core (MgC_2)-shell (Mg_2Si) are likely formed in 3C-SiC implanted with $^{25}Mg^{+}$ ions and annealed at 1573 K. ^{25}Mg segregation is dominated by small atomic clusters with local ^{25}Mg concentrations up to 85 at.%

(a) HAADF-STEM micrograph of 3C-SiC implanted to 9.6×10^{16} $^{25}Mg^{+}/cm^{2}$ at 673 K and annealed at 1573 K for 12 h in Ar. STEM-EELS maps of (b) carbon, (c) silicon, (d) magnesium, and (e) all the elements. (f) Elemental profiles across a selected region.



Isoconcentration surfaces at 10 at.% ^{25}Mg in 3C-SiC (a) implanted to 9.6×10^{16} $^{25}Mg^{+}/cm^{2}$ at 673 K and annealed at (b) 1073 K, 12 h, (c) 1573 K, 2 h, (d) 1573 K, 6 h, and (e) 1573 K, 12 h in Ar.



W. Jiang *et al.*, Journal of Nuclear Materials 498 (2018) 321
https://doi.org/10.1016/j.jnucmat.2017.10.046

A Multiscale Microstructural Approach to Ductile-Phase Toughened Tungsten for PFMs

Science Objective

Increasing fracture toughness and decreasing the ductile-brittle transition temperature of a tungsten-alloy has been shown to be feasible by ductile-phase toughening (DPT) of tungsten. This research models the deformation behavior of DPT tungsten for plasma-facing materials (PFMs) by a multiscale microstructural approach

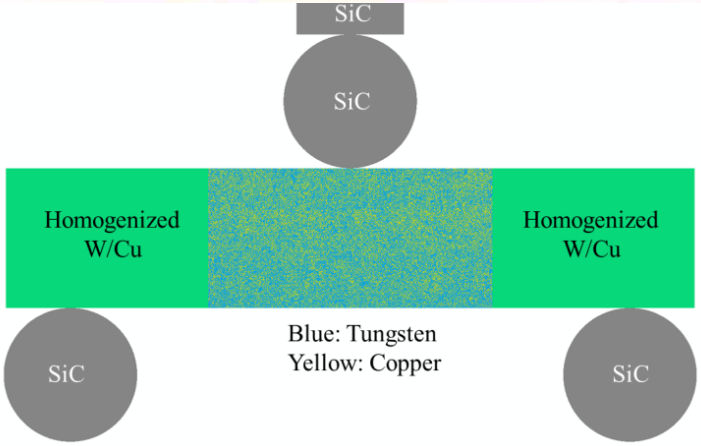
Significance and Impact

Different modeling scales from the micron scale at the grain level to the macroscale of the structure are bridged effectively. The model is able to capture the crack bridging mechanism allowing very good predictions of damage and fracture patterns as well as load-displacement responses that agree with the corresponding experimental results

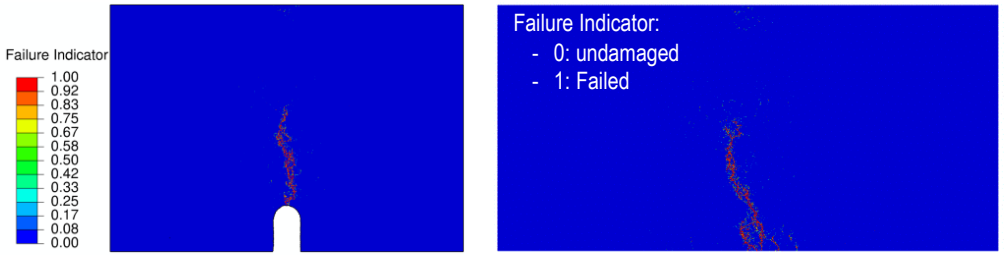
Research Details

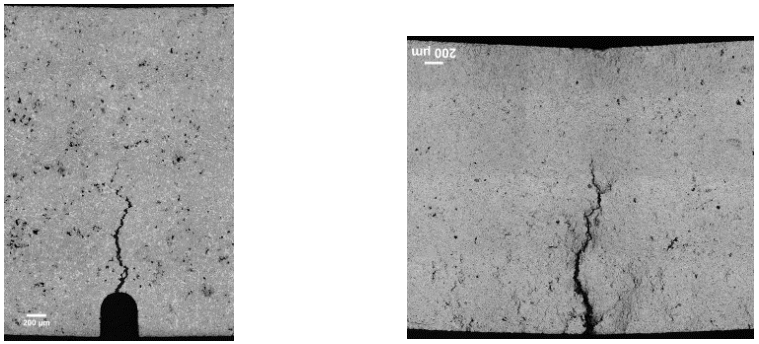
A microstructural dual-phase (copper-tungsten) region is finely discretized using the OOF2 software and is described by a continuum damage mechanics model. This region is connected to the adjacent homogenized elastic regions to form a macroscopic structure such as a test specimen subjected to three-point bending and analyzed by ABAQUS

B.N. Nguyen, C.H. Henager, Jr., N.R. Overman, R.J. Kurtz (2018). "A Multiscale Microstructural Approach to Ductile-Phase Toughened Tungsten for Plasma-Facing Materials" prepared for submission to Journal of Nuclear Materials.



The FE mesh of the un-notched Cu-W three-point bend bar (16 mm x 3.24 mm x 1.55 mm). Damage and fracture are modeled in the finely discretized microstructural region





Predicted damage distributions and crack patterns compared to experiments in the microstructural regions of the Cu-W SENB and un-notched specimens

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Pacific Northwest NATIONAL LABORATORY

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Advanced Materials Modeling Used to Understand/ Improve Tungsten Recrystallization Limit

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.

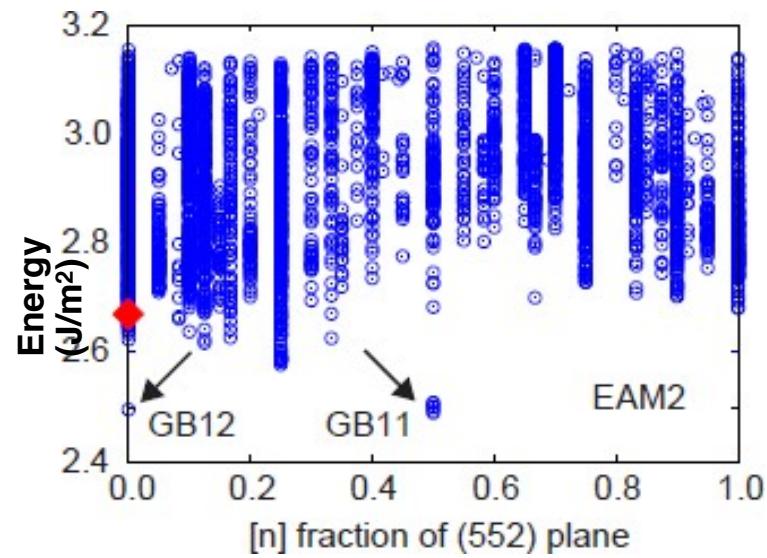
Achievement

We predicted for the first time phase transformations in tungsten grain boundaries (GB) at high temperature. This quarter we have expanded the search, identifying new grain boundary structures.

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.

New Low-Energy Grain Boundaries in Tungsten



An evolutionary algorithm is used to generate a large collection of grain boundaries, allowing for point defect diffusion such as due to radiation damage. The scatter plot shows the grain boundary energies vs. excess atomic density. New low-energy grain boundary structures are found.

"Configurational multiplicity of grain boundary phases in bcc metals," T. Frolov et al., submitted to the journal *Nanoscale*.

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

LLNL-PRES-744820

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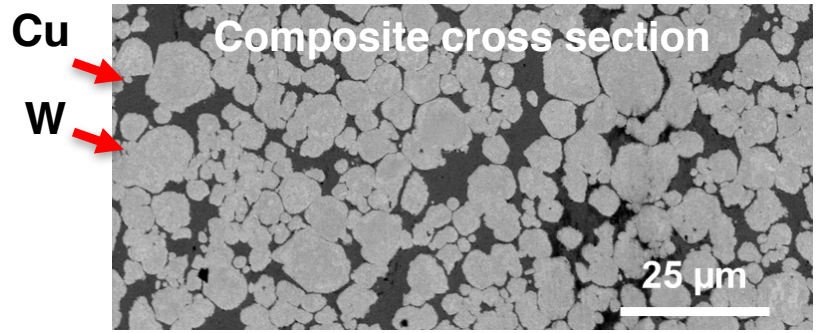
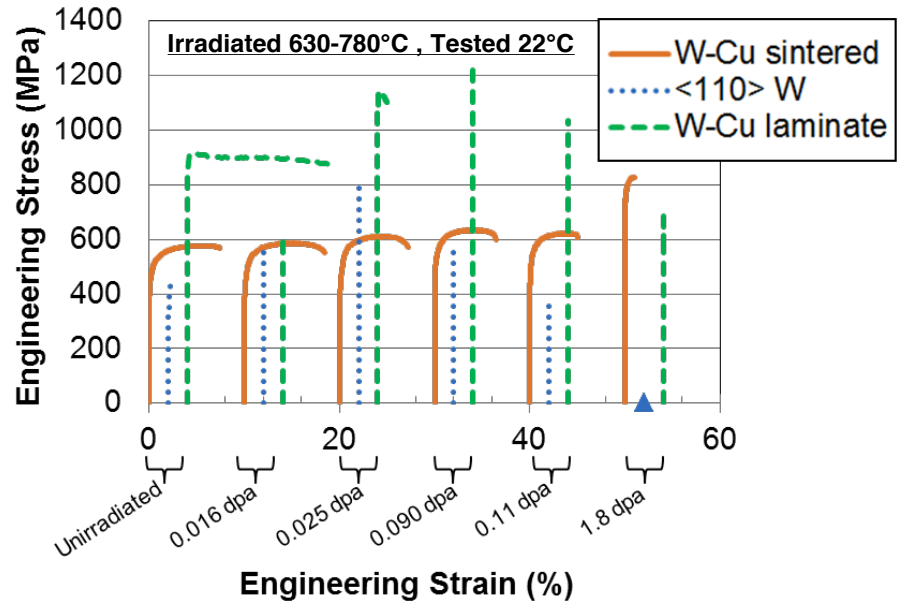
A sintered tungsten-copper composite was more ductile than other irradiated tungsten materials

The need is for a tungsten composite that performs better than tungsten in fusion conditions

- A 75 wt.% W and 25 wt.% Cu sintered powder composite produced by Mi-Tech Metals Inc. was irradiated in HFIR
- The irradiated sintered composite had greater elongation and lower strength than either single crystal tungsten or a W-Cu laminate composite
- The sintered W-Cu composite may be useful as a divertor structural material or as an interlayer between unalloyed W and a structural material





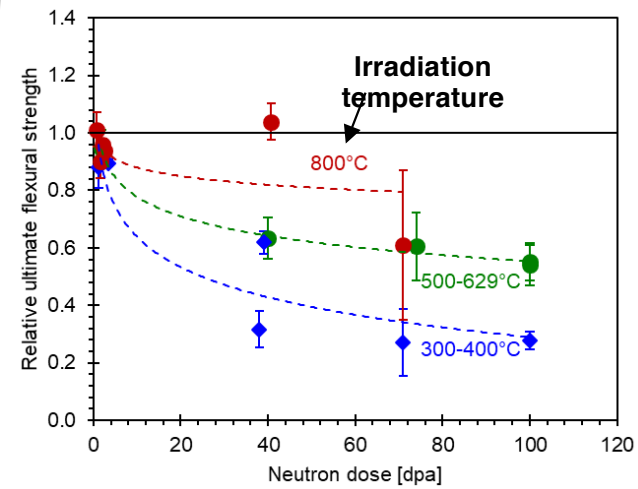
Tensile tests after neutron irradiation show more consistent behavior of W-Cu sintered composite.

L. M. Garrison (garrisonlm@ornl.gov) and Y. Katoh

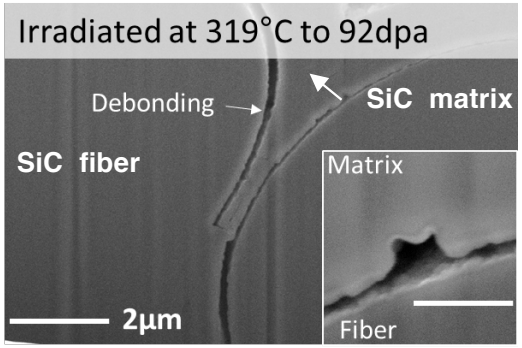
Response of SiC composites to neutron irradiation points the direction for further improvement

SiC composites require resistance to high-dose neutron irradiation for fusion reactor service

- Irradiation of SiC in HFIR to ~100 displacements per atom (dpa) has been achieved for SiC composites
- Degradation of mechanical properties was moderate for irradiation at ~800°C, but significant at <~600°C
- Microstructural examination showed interfacial degradation (debonding)
- Further development of the composites will focus on improved composite interphases



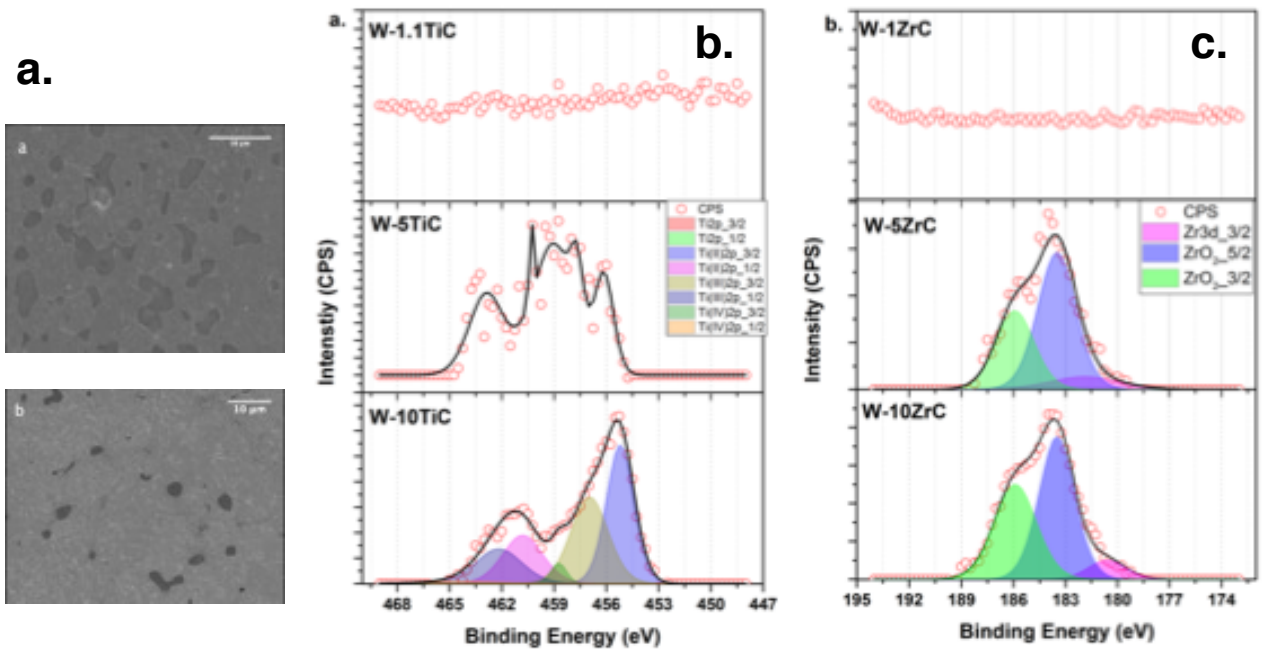
Neutron-dose dependence of 22°C strength of irradiated SiC composite, showing composite is promising at higher temperature, but the degradation is significant at lower temperature.



Interfacial debonding in the irradiated composite explains mechanical degradation.

Koyanagi, T., Nozawa, T., Katoh, Y., & Snead, L. L. (2017). Mechanical property degradation of high crystalline SiC fiber–reinforced SiC matrix composite neutron irradiated to~ 100 displacements per atom. Journal of the European Ceramic Society (in press).

Microstructure and composition of carbide-strengthened tungsten alloys via spark plasma sintering



a) SEM micrographs of W samples strengthened with 10wt.% ZrC and 1.1wt.% TiC showing dispersed second phase particles b) XPS spectra of Ti_2p and Zr_3d regions demonstrating formation of titanium and zirconium oxide phases

- Exposures to low energy D/He ions at Magnum PSI in April 2018
- Tensile tests and recrystallization behavior of alloys at ORNL in Spring 2018
- E. Lang, et al. "Microstructural and compositional effects of transition metal carbide additions on dispersion-strengthened W alloys fabricated via spark plasma sintering." *Int. J. Refractory Metals and Hard Mater.* Submitted Jan. 2018.

Scientific Achievement

- This work focuses on the development of novel carbide-strengthened tungsten alloys.

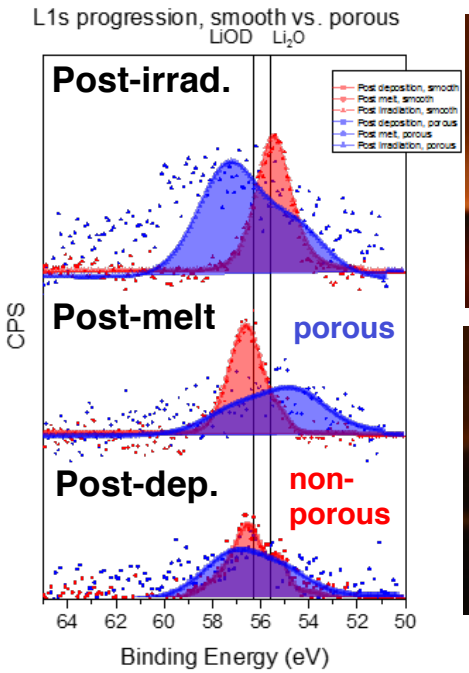
Significance and Impact

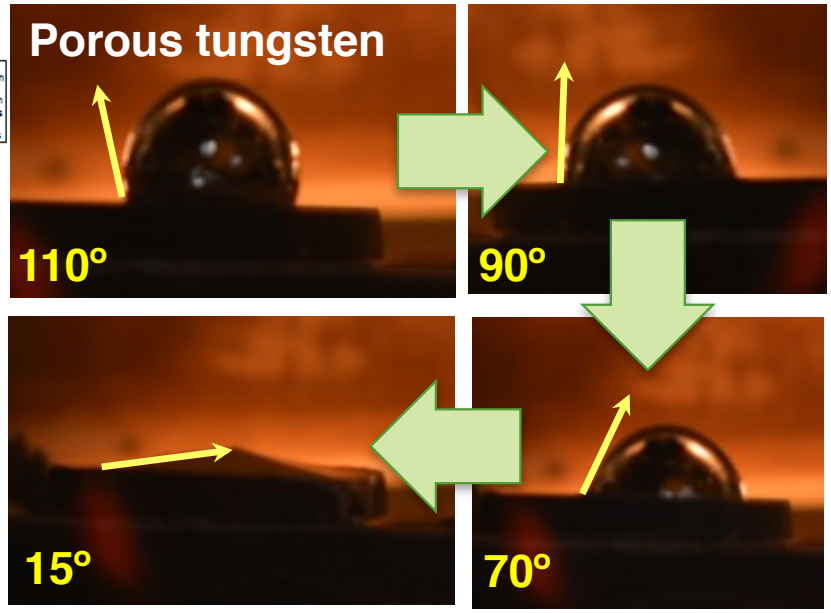
- In this work we explore the impact different carbide dispersoids (ZrC, TiC, TaC) have on the microstructure and mechanical properties of tungsten. We seek to demonstrate how these micro-alloyed materials behave under ion irradiations.

Research Details

- Dense tungsten alloys fabricated via Spark Plasma Sintering
- Compositional analysis via XPS and XRD indicate formation of tungsten-metal-carbon-oxygen complexes dispersed throughout tungsten matrix
- Increasing dispersoid concentration refines W grains and increases hardness

Innovating adaptive PMI with porous refractory metals combined with liquid-metals for a hybrid composite





a) *Left picture shows the progression of the Li1s XPS peak on lithiated porous W (blue) and lithiated smooth W (red) from deposition of Li (bottom), Li melt on surface (middle) and post irradiation with D_2^+ at 250 eV/amu*

b) *Right set of pictures show the progression of lithium percolation after Li droplets is placed on porous W at 350°C, within ~10s. Wetting angles as Li percolates labeled. Wetting also observed as low as 250°C*

E. Lang, A.Kapat, J.P. Allain, *Deciphering surface behavior and deuterium retention in tin-lithium-coated fuzzy tungsten substrates,* 12 (2017) 1352

Scientific Achievement

- This work examined Li metal mixing with a porous surface for possible hybrid PFC

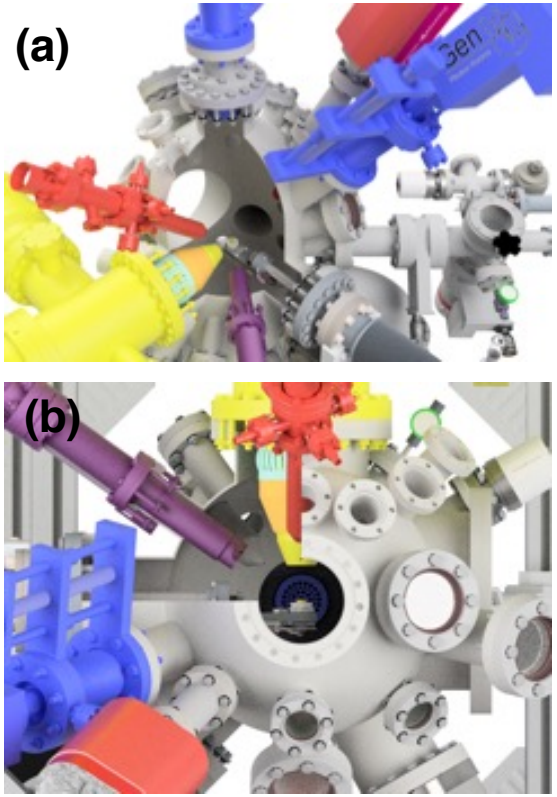
Significance and Impact

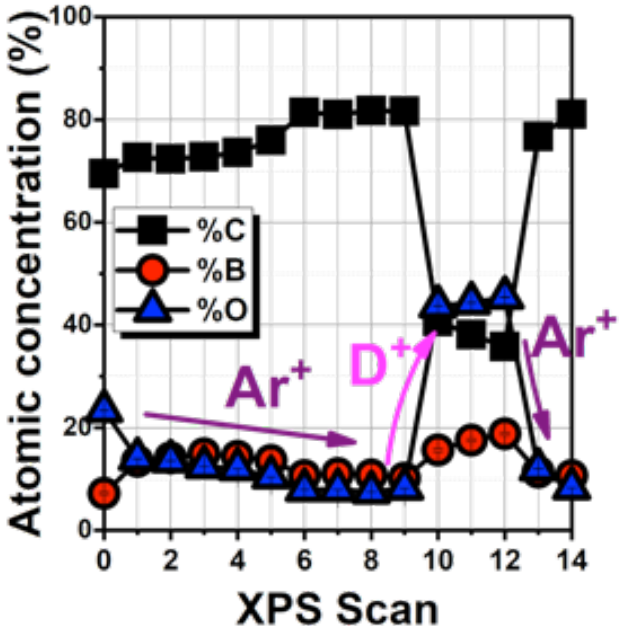
- This work demonstrated that liquid Li metal more readily wets and percolates into porous W, compared to traditional, "smooth" W. Additionally, different chemical complexes in Li have been observed on porous W compared to smooth W.

Research Details

- Lithium droplets on heated spark-plasma-sintered porous W samples
  - Observed wetting at much lower temperature than for smooth W
- *In-vacuo* XPS of lithiated porous W vs. lithiated smooth W irradiated with D_2^+
  - Lithiated porous W more likely to form Li-O-D complex compared to lithiated smooth W

Deciphering role of oxygen in dynamic in-situ D+ irradiations of boronized and lithiumized graphite plasma-material interaction





- *(a, b) Side and top image of the IGNIS in-situ facility at UIUC to study synergistic He and D particle interactions on W-based materials at high gas pressures of order mTorr and high temperatures. In-situ XPS used to study surface chemistry.*
- *(right) Atomic concentrations of B, C and O in boronized graphite with each point was obtained after an irradiation.*

Scientific Achievement

This work examined the role of the surface chemistry in boronized graphite surfaces exposed to NSTX-U plasmas on retention of deuterium.

Significance and Impact

In-situ and *in-operando* testing identified the dynamic enhancement of oxygen near the boronized graphite surface found responsible for D retention under cumulative D exposures in NSTX-U

Research Details

- Samples exposed to NSTX-U plasmas are currently being characterized and studied to understand the role of surface chemistry in D retention
- *In-situ* and *in-operando* experiments in IGNIS prepares samples to expose them to simulated, controlled conditions to explore the variation of surface chemistry *during* exposure to D ions

Novel SiC and MAX phase materials prove robust under DIII-D divertor plasma loading

Scientific Achievement

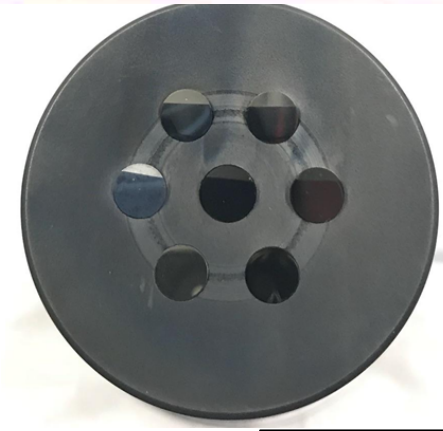
Silicon carbide and MAX phase ceramic materials were exposed to DIII-D divertor heat fluxes of 5-10 MW/m^2 with no macroscopic damage, but some material erosion occurred likely to due physical sputtering.

Research Details

- Novel SiC and MAX phase (TiC_3SiC_2) ceramics exposed to L-mode and H-mode divertor plasmas via DIII-D/DiMES.
- Some samples were flat and others were angled at ~15° with respect to the toroidal field to induce additional heat flux.
- No chipping/cracking of flat or angled samples visible during post-mortem Scanning Electron Microscopy (SEM) analysis.
- Net surface erosion in 'micro-trenches' measured via SEM to be 0.8 μm for SiC and 0.2 μm for Ti_3SiC_2
- Estimated average particle impact angles measured from shadowed region in trenches was ~30° from horizontal.

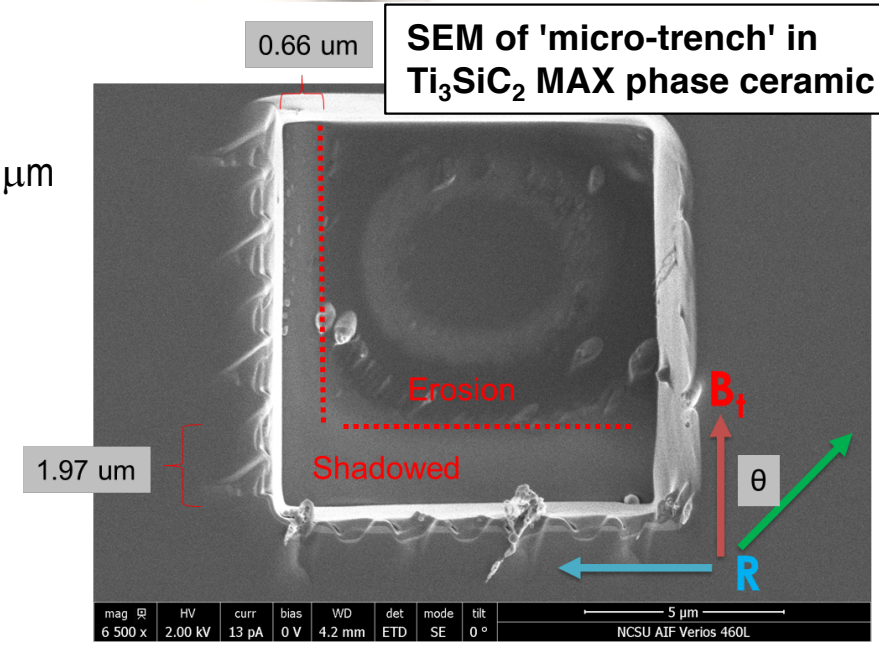
Significance and Impact

High-temperature ceramics such as SiC and MAX phase materials are candidate plasma facing materials due to their neutron damage resistance, low activation, and low T permeation, but limited testing has been performed on tokamaks. The tests suggest that these materials are robust to divertor plasma heat fluxes of 5-10 MW/m^2, contributing to building the database of tokamak exposures on these materials.



Ceramic DiMES samples after plasma exposure

SEM of 'micro-trench' in Ti_3SiC_2 MAX phase ceramic

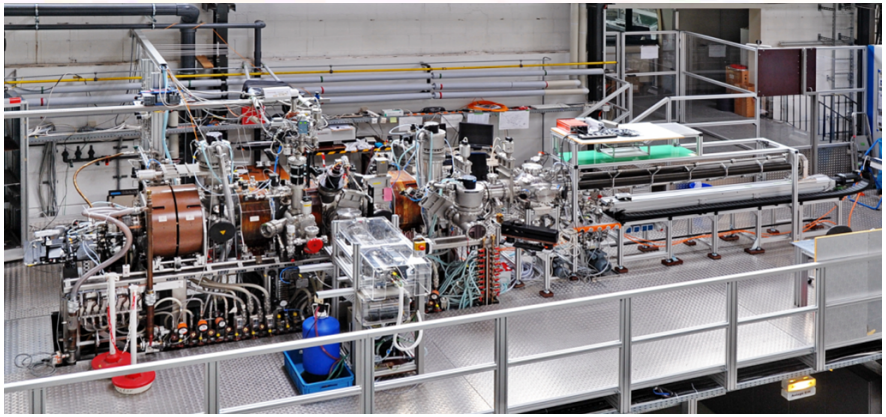


J. Coburn, J. Barton, T. Abrams, E. Unterberg, D. Rudakov
J. Coburn et al., PSI-2018 Conference (upcoming)

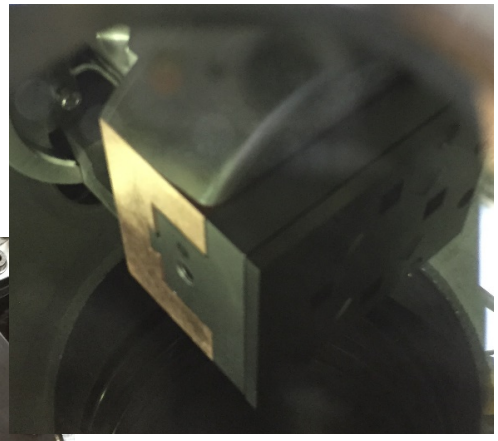
DIII-D NATIONAL FUSION FACILITY · GENERAL ATOMICS · NC STATE UNIVERSITY · VLT Virtual Laboratory for Technology For Fusion Energy Science

First Plasma Exposure of Graphite Foam

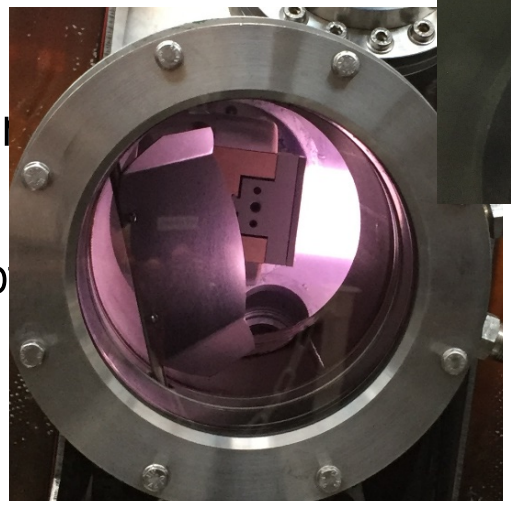
- ORNL's graphite foam has the potential to serve as a light-weight, low-Z armor with the isotropic thermal conductivity of copper
  - First time ever: armor will have thermal conductivity comparable to that of the heat sink!
  - Better heat transfer = lower surface temperatures
  - Thicker armor leads to longer erosion lifetime
  - Reduced thermal stress in joint owing to reduced temperature gradient
- First test of Compatibility of graphite foam with a relevant plasma flux
- Four foam samples were placed in the PSI-2 linear plasma facility in Jülich, Germany
  - exposed to a deuterium plasma with an ion energy of 100 eV and fluence of 5×10^{25} m^{-2}
  - No cracking or ablation was observed
  - On average, about 39 µm was eroded from the surface or about 5 mg per sample



PSI-2 Linear Plasma Facility, Jülich, Germany



Sample holder, mask with four graphite foam samples



Side view of plasma exposure

Dennis Youchison and Arnie Lumsdaine

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Improved Measurement of Elliptical Polarization in ECH Transmission Lines

Scientific Achievement

Improved low power measurements were done on motorized miter-bend polarizers used for converting a linearly polarized microwave beam into an arbitrary elliptically polarized beam for Electron Cyclotron Heating in ITER.

Significance and Impact

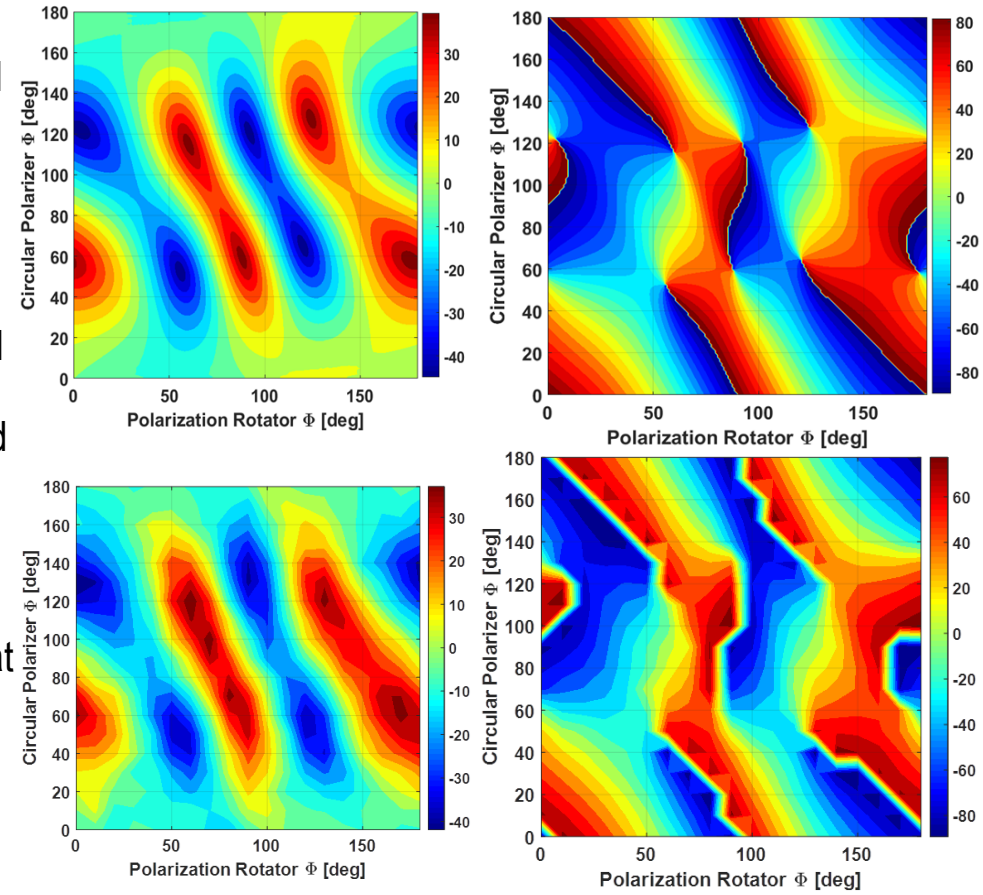
ECH power, transported through highly oversized corrugated metallic waveguides, must achieve a specific elliptical polarization in order to be launched and absorbed as needed in ITER. These new results greatly expand our confidence in our ability to achieve the necessary desired polarization.

Research Details

- The polarization is measured using a 170 GHz VNA system at MIT and 63.5 mm waveguides and motorized polarizers built by General Atomics and on loan to MIT from US ITER IPO.
- The theory is calculated using the CST code for the exact shape of the grating grooves.

Application

These results are critical to designing the ITER ECH transmission lines but also apply to all other ECH experiments.



Excellent agreement of calculated polarization results (top) vs. experiment (bottom) for ellipticity magnitude (left, tanβ) and angle (right, α).

MIT: H. Hoffmann, S. Jawla, M. Shapiro and R. Temkin; G. Hanson, ORNL; supported by DOE VLT and US IPO

Tritium Processing Development for Magnetic Fusion

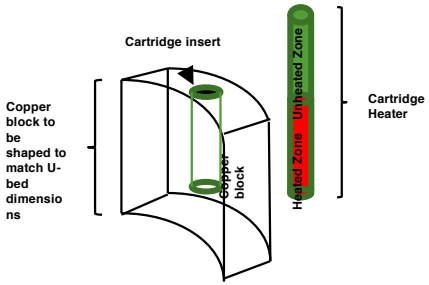
Application

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

Scientific Achievement

Work continuing on upgrades of Hydrogen Processing Laboratory (HPL) test stand and replacement heater design for U-Bed. Continued participation in Liquid metal plasma facing component (LM-PFC) System Study biweekly conference calls.

HPL Line Heater Controller
Replaced 12 individual Variac transformer



Heater Design

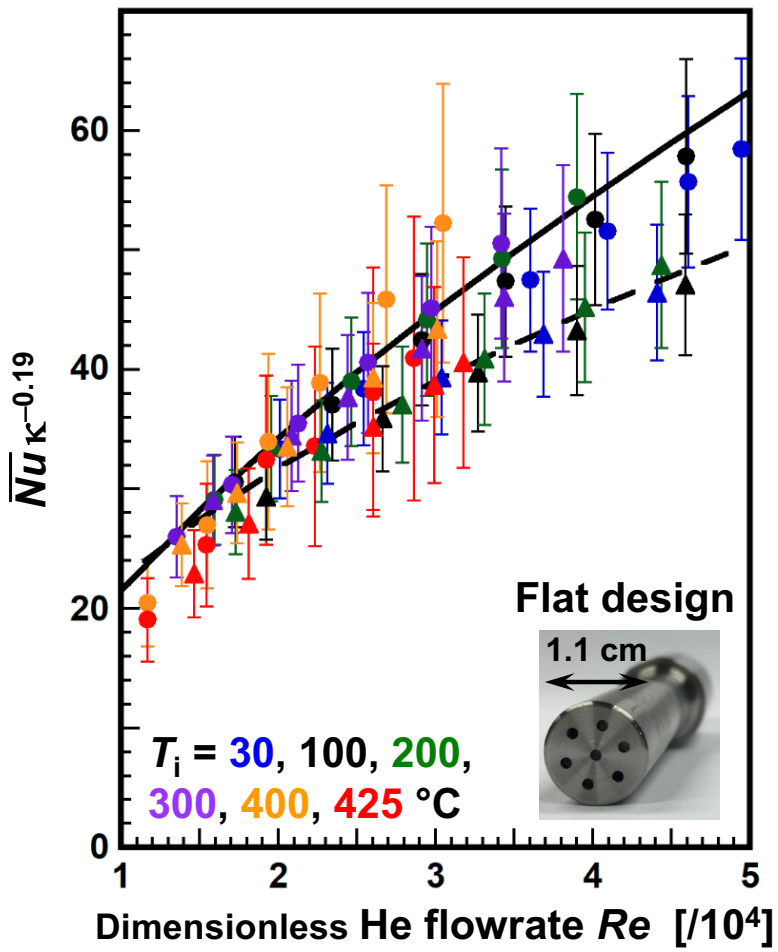
Significance and Impact

- 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

- All materials for HPL upgrades have been received, old wiring has been removed and new instrumentation is being installed. New Line Heater Controller Unit shown (figure on right).
- Proposed design for new heater (vacuum compatible) showed in last quarters update has been eliminated from consideration due to installation and maintenance issues. A new design has been identified (figure on left) that address these concerns based on input from SRNL and other tritium programs at LANL. Final design drawing and material quotes are being collected.
- Completed 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.

Thermal-Hydraulics Experiments on He-Cooled Solid Divertors



Application

Helium-cooled solid divertors leading candidate for solving power and particle exhaust issues in long-pulse fusion magnetic fusion devices

Engineering Achievement

New experiments suggest that the He-cooled modular ("finger") divertor with multiple jets (HEMJ) has improved thermal performance: dimensionless heat transfer coefficient $\overline{Nu}$ increases 18% at prototypical conditions

Significance and Impact

Improved design margins: at prototypical conditions, extrapolations ⇒ HEMJ can withstand 9.9 MW/m^2 on hexagonal tile even at He inlet temperature T_i = 700 °C (*vs.* original 600 °C)

Research Details + Schedule

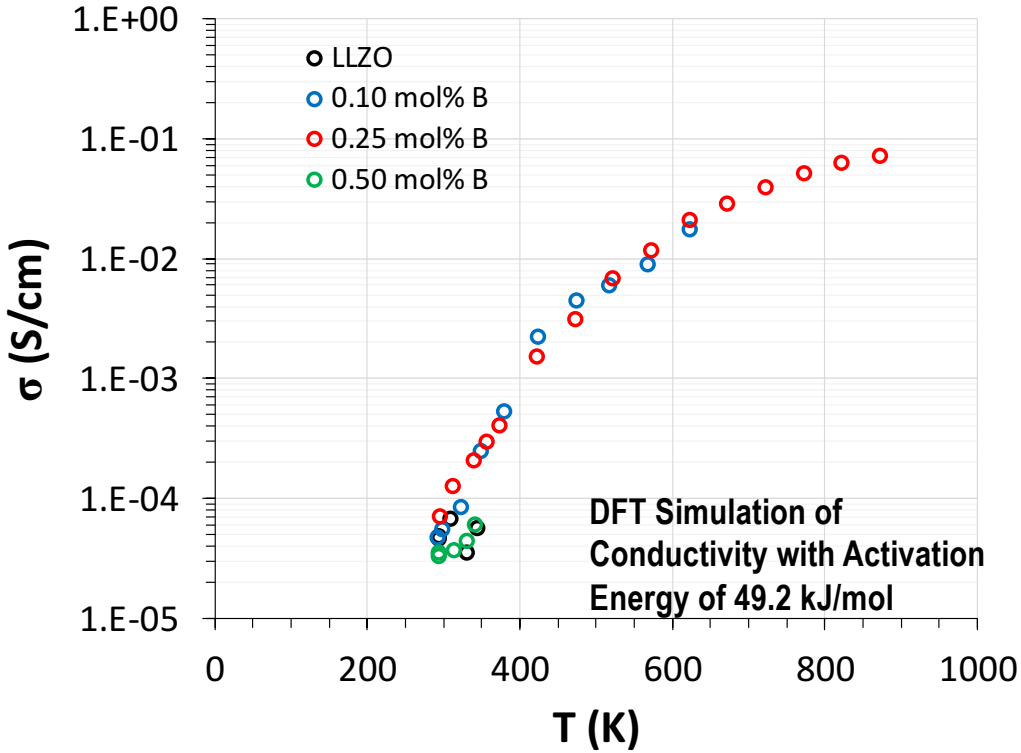
- New data at T_i = 300–425 °C; q''< 3 MW/m^2
  - HEMJ (●) : new correlation gives higher $\overline{Nu}$ (dimensionless heat transfer coefficients): $\overline{Nu} = 0.045\,(Re)^{0.67}\,\kappa^{0.19}$ (——)
  - Flat design (▲): $\overline{Nu}$ 6% lower than HEMJ at prototypical conditions: $\overline{Nu} = 0.216\,(Re)^{0.504}\,\kappa^{0.19}$ (- - -)
- Upgrade of Georgia Tech He loop
  - Enclose test section and RF heater coil in vacuum chamber
  - Modifying chamber to minimize RF coupling to chamber walls and increase incident heat fluxes q'' [ongoing]

Bailey Zhao: Ph.D. 2017

B. Zhao, S.I. Abdel-Khalik, S.A. Musa and M. Yoda (2018) "Experimental and numerical studies of helium-cooled modular divertors with multiple jets," to appear in *Fusion Eng. Des.*

M. Yoda, S. I. Abdel-Khalik, S. Musa

Demonstration of Direct LiT Electrolysis using an Immersion Cell



Sample	σ (S/cm) 298 K	σ (S/cm) 723 K
LLZO	4.78E-05	
0.10 mol% A - LLZO	2.56E-04	2.27E-01
0.25 mol% A - LLZO	2.04E-04	2.26E-01
0.50 mol% A - LLZO	8.20E-05	1.95E-01
0.10 mol% B - LLZO	5.46E-05	2.32E-03
0.25 mol% B - LLZO	7.07E-05	3.93E-02
0.50 mol% B - LLZO	3.51E-05	

Updated Ionic Conductivity Equivalent Circuit Modeling

Scientific Achievement

- Pellets with additives were synthesized and tested to determine Li-ion conductivity at different temperatures
- Density functional theory calculations have been made to understand the effect of dopants on lithium-ion conductivity through the electrolyte where the activation energy can be varied

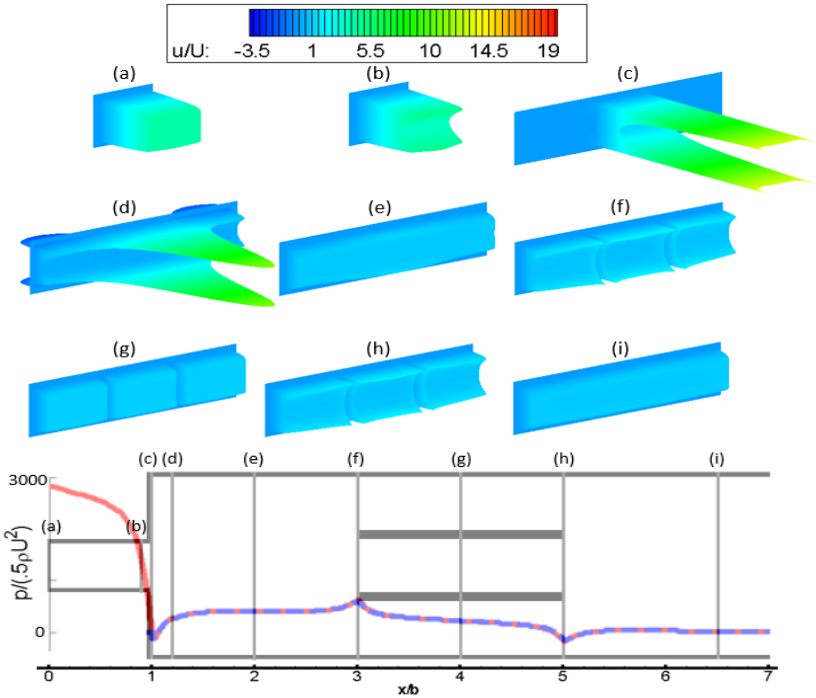
Significance and Impact

- The development of a revised synthesis method allows significant variation of LLZO electrolyte properties and can be used to increase conductivity and strength of the electrolyte

Research Details

- Updated equivalent circuit models were developed to better account for different contributions to the impedance spectra
- Updated equivalent circuit modes show that dopant A is optimal below 0.25 mol%
- Dopant B has higher conductivity at 0.25 mol% compared to 0.1 mol%

Manifold for a LM breeder blanket: flow physics, MHD pressure drop, flow balancing and optimization



(Bottom) Non-dimensional pressure is plotted for the centerlines of the center (solid red) and side (dashed blue) channels over a top-down view of a manifold with r_{exp}=4, L_{exp}/b=2, L_{chan}/b=2, s_c=0.3, and n=3 channels for Ha=1465 and Re=50. The vertical grey lines labeled (a) through (i) correspond to the 9 axial velocity profiles shown above. (Top) Non-dimensional axial component of velocity, u/U, is plotted at 9 locations along the manifold.

Tyler J. Rhodes, Sergey Smolentsev, Mohamed Abdou, *Effect of the Length of the Poloidal Ducts on Flow Balancing in a Liquid Metal Blanket*. Submitted to *Fusion Engineering and Design*, 2017.

Scientific Achievement

Intensive 3D numerical computations for a prototypic inlet manifold of a LM breeder blanket have been performed aiming at characterization of the flow, MHD pressure drop model, analysis of flow balancing and design optimization.

Significance and Impact

3D MHD pressure drop associated with a LM flow in the inlet/outlet manifolds is up to 50% of the entire pressure drop in the blanket. The imbalance of the flow among the parallel channels may result in overheated channels. The numerical data and the developed pressure model can be used to accurately predict the pressure drop and flow distribution among the parallel channels.

Research Details

Associated Hartmann and Reynolds numbers in the computations using the 3D MHD HIMAG code were Ha~10^3 and Re~10^2-10^3. An extension of Ludford layer theory to 3D is shown to agree with a proposed model for pressure drop, which is much more accurate than previous models. Two flow regimes have been identified: inertial-electromagnetic and viscous-electromagnetic. Improved flow balance can be obtained by lengthening distance between the manifold inlet and the entrances of the parallel channels.

Impact of Temperature on Fusion Neutronics Calculations

- Operational material temperature can affect radiation transport calculations
  - **material density**: changes for liquids and solids
    DT=20-100 C: water Dr=4%, steel Dr=0.4%
  - **neutron cross sections**: doppler broadening and thermal scattering treatment
  - **geometry**: thermal expansion of components into gaps
- Modern 3-D CAD based neutronics calculations allow high fidelity nuclear heating data to be passed to thermal analysis software (e.g. ANSYS)

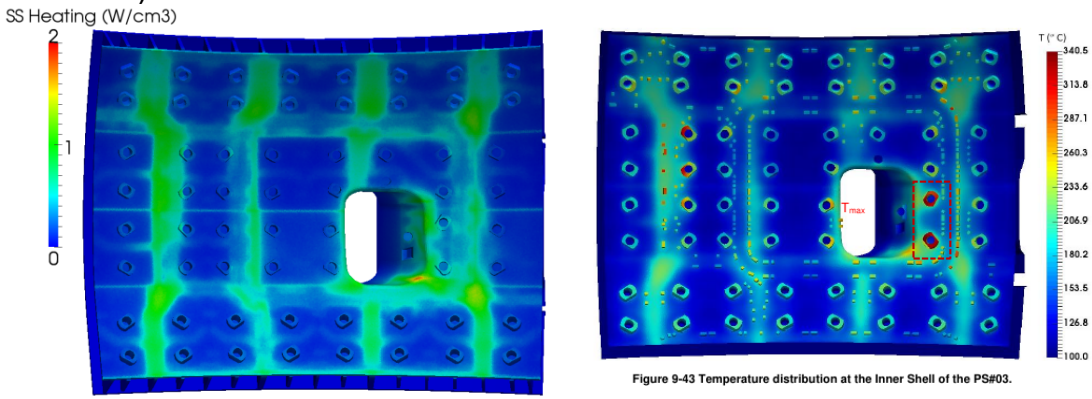
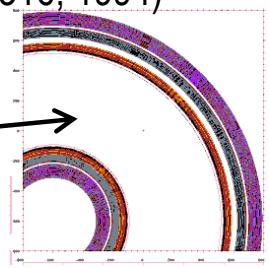


Figure 9-43 Temperature distribution at the Inner Shell of the PS#03.

Example: nuclear heating distribution in ITER vacuum vessel (ref. Bohm, ITER_D_NS9KST) and corresponding temperature distribution (ref. IDOM, ITER_D_SSMNC9)

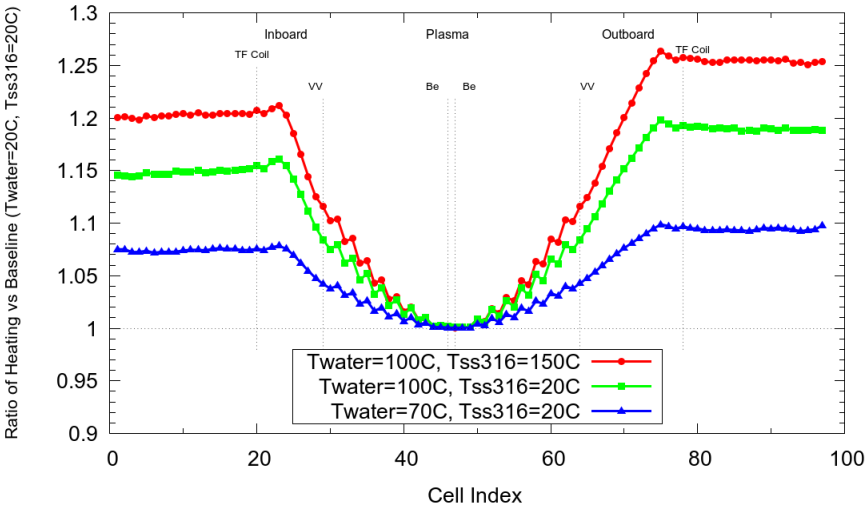
- Traditionally, fusion neutronics calculations are performed at conditions representing some nominal temperature
- Evaluated these temperature effects using a simple, yet realistic 1-D model of ITER (INDC(NDS)-316, 1994)

Plasma region

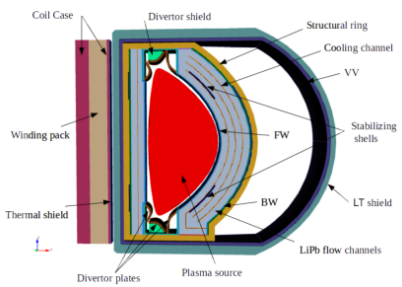


➢ Results show the biggest impact is due to material density changes

- nuclear heating of toroidal field coil increases up to 26% in extreme case and 5% for more typical case



- Future work will examine the impact on FESS-FNSF, and explore the workflow needed to feed thermally expanded CAD models back to neutronics calculations



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IAEA International Atomic Energy Agency

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VLT Virtual Laboratory for Technology For Fusion Energy Science

Modeling SOL Plasma/Neutral Interactions with PFCs in Present-Day Devices Validates Models

Scientific Objective

Develop and validate simulation models of particle and heat fluxes to plasma-facing components (PFCs) on present-day devices and assess innovative divertor designs. Aid physics understanding of data.

Achievement

Continued 4D COGENT simulations of LTX to obtain first kinetic ion distribution at core edge and into the scrape-off layer. Provides details of hot ion distribution function striking walls in low-recycling LTX.

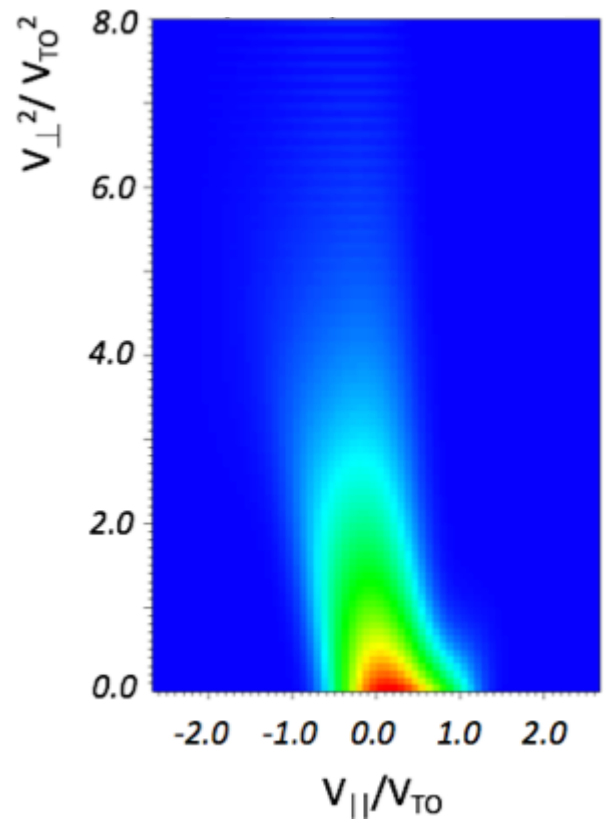
Ion velocity-space anisotropy is large in low-aspect-ratio LTX-like devices. (In plot, isotropic distribution would follow inverted parabola in shape rather than vertically elongation shape shown.) Recently added potential calculation.

Continued support of snowflake divertor simulations for present-day devices including cross-field drifts.

Why it matters

Low-recycling devices utilizing lithium PFCs such as LTX yield edge plasmas with low collisionality resulting in energetic, non-Maxwellian ions impinging of PFCs. Predictive capability of surface heat fluxes for such conditions requires use of a kinetic code like COGENT.

COGENT simulation shows escaping SOL ions are strongly non-Maxwellian in LTX-like geometry



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LLNL-PRES-744820

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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.

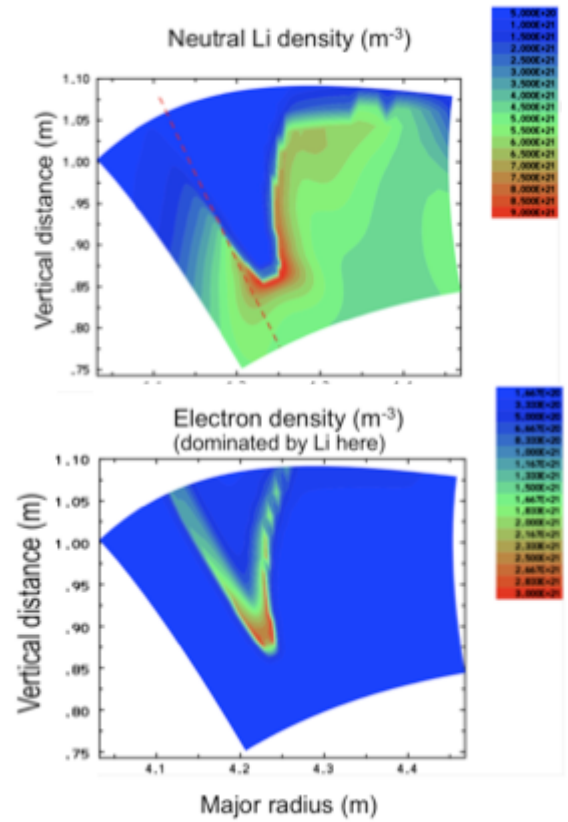
Achievement

Continued analysis of 2D UEDGE simulations for Li divertor in FNSF geometry showing >90% input power radiated by Li in the ionization layer. Provided details of solution to Goldston/Emdee for more detailed vapor-box neutral Li analysis using the SPARTA code. Key issue remaining is Li intrusion to core edge and related DT fuel dilution.

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.

FNSF divertor plasma enveloped by Li gas that is promptly ionizied by incoming hot plasma yielding high electron density layer



T.D. Rognlien, M.E. Rensink, *Fusion Eng. Design,* http://dx.doi.org/10.1016/j.fusengdes.2017.07.024.

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