

Recent Advances in Radiation Materials Science from the US Fusion Reactor Materials Program

R. E. Stoller¹, D. W. Clark², N. M. Ghoniem³, Y. Katoh¹, R. J. Kurtz⁴, J. Marian³, G. R. Odette⁵, B. D. Wirth^{1,6}, T. Yamamoto⁵, and S. J. Zinkle^{1,6}

¹Oak Ridge National Laboratory (rkn@ornl.gov), USA, ²Office of Fusion Energy Sciences, Department of Energy, USA, ³University of CA, Los Angeles, USA, ⁴Pacific Northwest National Laboratory, USA, ⁵University of CA, Santa Barbara, USA, ⁶University of TN, Knoxville, USA

E-mail contact of main author: stollerre@ornl.gov

Abstract. In addition to the engineering challenges associated with building and operating any complex facility, a range of critical materials issues must be addressed in order to make fusion power commercially viable. These include: (1) developing structural materials with suitably long lifetimes, (2) obtaining a plasma-facing material with sufficient ductility and low tritium retention, and (3) verifying the performance of functional materials such as electrical insulators, optical fibers, and tritium breeding materials. The US fusion reactor materials program (FRM) has a well-developed focus on radiation effects in candidate structural materials and tungsten as a plasma-facing material. This includes both computational materials science and an extensive irradiation program. Recent results from the US FRM program are discussed with an emphasis on advanced ferritic-martensitic steels, including the oxide-dispersion-strengthened and castable nanostructured alloy variants; SiC composites; and tungsten. This program of computational and experimental research is particularly concerned with the effects of helium produced by nuclear transmutation. In both the structural materials and tungsten, helium may increase tritium retention which has implications for operational safety in the event of an accident and for the successful recovery of tritium for use as fuel. In addition, low energy helium ions may degrade the surface of tungsten components with the potential for increasing the amount of radioactive dust and plasma contamination.

1. Introduction

The objective of international fusion energy research is to provide the scientific and engineering basis that will enable the use nuclear fusion as a practical energy resource. In recent years, research in plasma physics that looks ahead to the era of ITER has seen substantial advances in our understanding of plasma heating and confinement. The anticipation of obtaining a successful burning plasma in ITER, brings a new urgency to other research that is necessary to make the step from a large-scale plasma physics experiment to the development of a fusion reactor capable of providing cost-effective electricity to the grid. Among these research needs are a number of critical materials performance issues. These include: (1) developing structural materials with suitable properties that will be maintained under the extreme fusion irradiation environment to high doses, (2) identifying a plasma-facing material with sufficient thermal and mechanical properties to withstand fusion's high heat loads while not contaminating the plasma or retaining significant levels of tritium, and (3) verifying the performance of functional materials such as superconducting materials for magnets, electrical insulators, optical fibers, and tritium breeding materials.

The US fusion reactor materials program (FRM) is addressing many of these feasibility issues in a broad-based effort that includes several US national laboratories and universities as well as extensive international collaborations. Because of the limitations of space, this paper will focus on FRM program research on the effects of radiation on candidate structural materials and tungsten as a plasma-facing material. The research includes both computational theory and modeling, and an extensive irradiation program utilizing the High Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory (ORNL). Many of the HFIR irradiation experiments have been collaborative efforts involving colleagues from Japan. Research on structural materials emphasizes advanced ferritic-martensitic (FM) steels, including the oxide-

dispersion-strengthened (ODS) and castable nanostructured alloy (CNA) variants, and silicon carbide (SiC) composites. Tungsten is the prime candidate material for plasma-facing applications. The computational and experimental research is particularly concerned with the synergistic effects of neutron irradiation with helium and tritium produced by nuclear transmutation in the structural materials. In addition, the impact of the relatively low-energy He that can be implanted in the plasma-facing tungsten components is being addressed. In both the structural materials and tungsten, helium may increase tritium retention which has implications for operational safety in the event of an accident and for the successful recovery of tritium for use as fuel. In addition, it has been shown that low energy helium ions from the plasma may degrade the surface of tungsten components with the potential for increasing the amount of radioactive dust and plasma contamination.

Key computational results include the development of a He-Fe interatomic potential that was used to develop a new equation of state for He in Fe and has been applied in a range of atomistic simulations to investigate the impact of helium on cavity evolution in irradiated steels. The potential also enabled a detailed study of matrix hardening induced by bubbles and the effect of He/dpa ratio on the calculated hardening. A detailed rate theory based model describing the behavior of helium has been developed and integrated with atomistic sub-models and experiments to predict swelling and embrittlement in FM steels and their ODS variants. The use of discrete dislocation dynamics in concert with micro-pillar testing has been used to improve our understanding of plasticity in bcc metals. A new computational approach to model integration has been developed to investigate near-surface segregation of implanted helium and hydrogen in plasma-facing tungsten components, provided new insights into the mechanisms responsible for “fuzz” formation on tungsten surfaces and on the trapping of hydrogen by He-vacancy clusters. Finally, a newly integrated modeling approach has been applied to the design and evaluation of fusion reactor components.

2. Advanced Steels for Structural Applications

The consideration of ferritic-martensitic steels is driven by a number of factors: (1) they have higher thermal conductivity than the austenitic stainless steels (SS) that were initially considered by the fusion and fast fission reactor programs, (2) they swell significantly less than the SS, (3) they have good strength at intermediate temperatures of interest, and (4) the level of long-lived induced radioactivity is lower. However, because they have a body-centered cubic structure, they undergo a ductile to brittle transition at low temperatures and this transition temperature tends to increase with irradiation. They also lose strength at high temperatures which limits the maximum thermodynamic efficiency of the fusion power system. The properties of these steels and their application to fusion are reviewed elsewhere [1-3]. The composition of candidate FM steels such as F82H and EUROFER97 is Fe with ~7.5 to 10 weight-percent (wt%) Cr, ~0.1 wt% C, ~0.1 to 0.6 wt% Mn, 0.15 to 0.25 wt% V, ~0.1 wt% Ta and up to 2 wt% W [4-6]. The CNA have similar Cr levels but minor alloying elements have been adjusted to provide stable, fine-scale precipitate structures [7]. The ODS variants typically have somewhat higher Cr, 12 to 14 wt%, and include ~0.25 wt% Y_2O_3 which is ultimately distributed in a fine, high-density distribution of stable 2 to 5 nm sized oxide clusters [8,9].

Swelling in the candidate ferritic-martensitic steels has been found to be strongly correlated with the He/dpa ratio. Different He/dpa ratios were obtained using dual ion irradiations (6 MeV Fe and He) in the DuET facility at Kyoto University and *in situ* helium implantation (ISHI) in the HFIR. Data from these experiments for several He/dpa ratios are shown in Fig. 1 as a function of an effective dose ($dpa_i \approx 90 - 1.64 \cdot \text{He/dpa}$) to account for the effect of He/dpa ratio on incubation. The void volume fraction, f_v , or swelling is noticeably lower in the ODS MA957 than in F82H at a given He/dpa ratio. This is attributed to He trapping by the interfacial sink strength associated with the oxide particles; these same particles act as recombination sites for vacancies and interstitials which may reduce radiation-induced microstructural evolution.

An example of the mechanical performance of the new CNA is shown in Fig. 2. The CNA yield strength is higher by 100 to 300 MPa than other candidate alloys such as EUROFER97, F82H, or P91, and it extends to higher temperatures. This increase in strength is associated with only a modest reduction in ductility as characterized by total elongation. Longer high temperature creep lifetime was also observed in the CNA compared to EUROFER97 and F82H.

3. Silicon Carbide and Silicon Carbide Composites

Silicon carbide and SiC/SiC composites have a number of desirable properties that make them attractive for fusion energy applications. These include: (1) excellent high temperature strength, (2) resistance to radiation-induced embrittlement, (3) low levels of induced radioactivity and decay heat, and (4) small neutron absorption cross sections. Although large-scale industrial use of these materials is relatively new, the industrial base and applications are maturing rapidly, notably with commercial aircraft applications.

Recent results illustrating the radiation stability of SiC/SiC composites are shown in Fig. 3. Specimens fabricated from a Hi-Nicalon, Type-S, First Generation Nuclear Grade SiC/SiC were irradiated to about 100 dpa in the HFIR at a range of temperatures. The figure shows the volumetric swelling, change in thermal conductivity, and change in ultimate flexural strength as a function dose. Both the swelling and the change in thermal conductivity are relatively modest and appear to saturate by about 1 dpa. The loss of strength (shown as the ratio to the initial strength) at the higher temperatures of most interest was also small. Although the data are not shown, the first available data on radiation creep up to a dose of 30 dpa also indicate a near saturation of creep by about 1 dpa for temperatures up to 1073K. In spite of these positive results, further work is needed to address the issue of apparent fiber instability at high

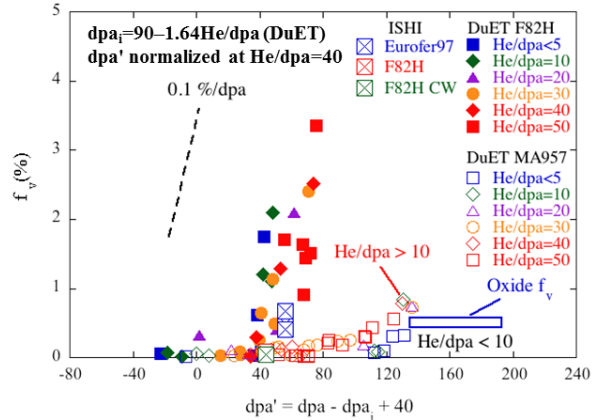


FIG. 1. Dose dependence of void volume fraction, f_v , in F82H and MA957 at different He/dpa ratios under neutron (ISHI) and ion irradiation (DuET).

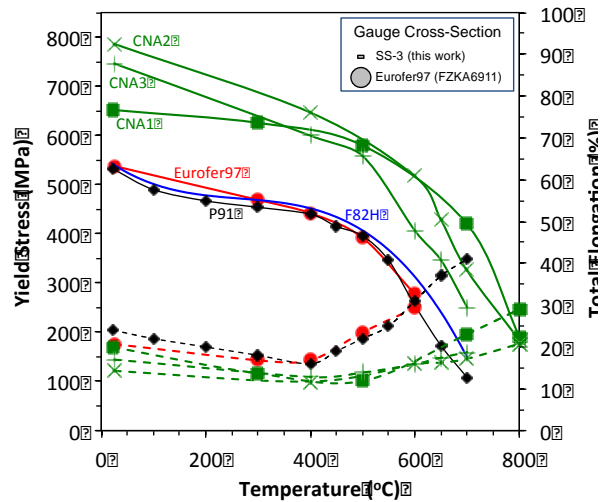


FIG. 2. Comparison of yield strength and uniform elongation measured for CNA compared to conventional ferritic-martensitic steels.

does. This can lead to fiber shrinkage and separation from the matrix. In addition, the limited data on the effects of helium on α -SiC indicate a tendency for anisotropic growth at higher helium levels [10].

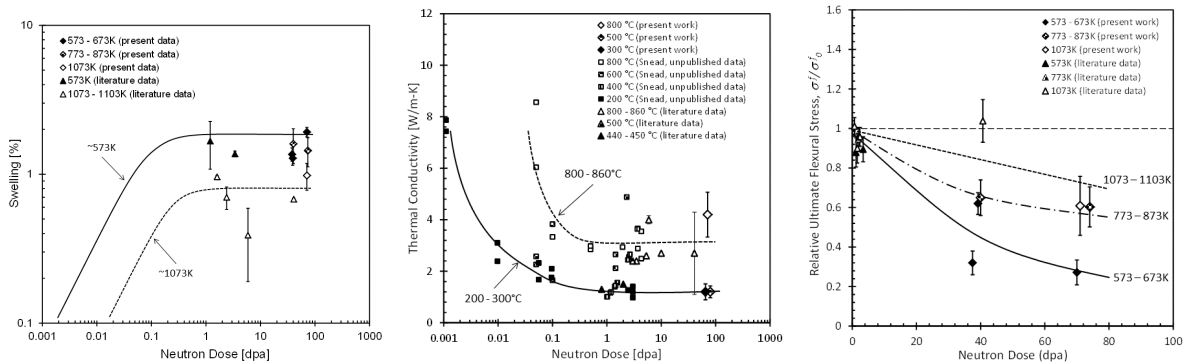


FIG. 3. Radiation-induced property changes in Hi-Nicalon, Type-S, First Generation Nuclear Grade SiC/SiC after irradiation in the HFIR up to 100 dpa: (a) swelling, (b) thermal conductivity, and (c) ultimate flexural strength.

The ability to provide high-integrity joints will be critical to the use of SiC/SiC composites in fusion blanket structures such as flow channel inserts. The US FRM program, in concert with international collaborators have developed new radiation-resistant joints for SiC and SiC/SiC. The experimental component of the program devised both joining methods and developed test methods to evaluate the strength of the joints. The torsional shear test method that has been developed is in the process of becoming an ASTM standard test method for ceramics adhesive joints under the guidance of a Task Group in ASTM Committee C28 on Advanced Ceramics. The program has included irradiation of the joint specimens in the HFIR at several temperatures to doses up to 10 dpa. s methods to irradiate and test joints for fusion and fission applications. The joint torsional strength was little effected by irradiation [11].

A 3D finite element model has been developed that implements elastic and elastic-plastic damage models for predicting failure initiation and propagation. The model has been applied to investigate failure mechanisms in different joints [12]. The results shown in Fig. 4 demonstrate that the model correctly predicts the generic response of joint failures with strong effects of the modulus and explains torsion specimen failure modes. In-plane and out-of-plane failures were captured by the finite element elastic-plastic damage models. However, internal joint microstructure plays a role in joint failure and the model does not currently address joint microstructure.

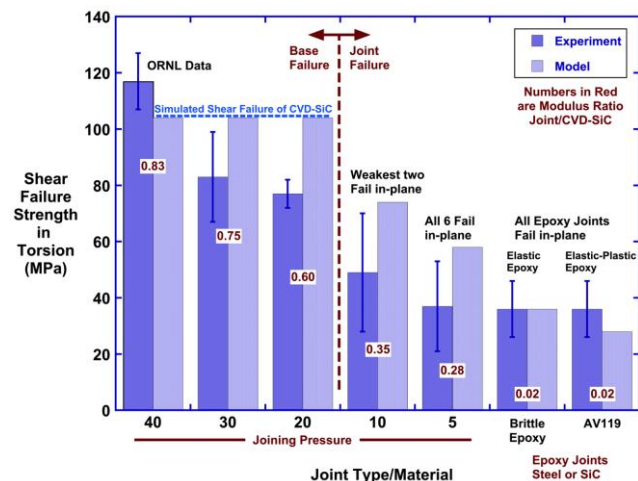


FIG. 4. Comparison of 3D finite element model and experimental measurements of shear failure strength in torsion for SiC joints with different joining parameters

4. Tungsten as a Plasma-facing Material

The attributes of tungsten that make it the current prime candidate for a plasma facing material include: a very high melting point, good thermal conductivity, low sputtering yield

and low activation properties in terms of long-term waste disposal. Unfortunately it is also characterized by a very low fracture toughness which severely restricts the useful operating temperature window and also creates a range of fabrication difficulties. Even its best, for temperatures above the ductile-to-brittle transition temperature, the fracture toughness of pure tungsten is comparable to that observed on the lower shelf of the fracture toughness curve for advanced FM steels. In spite of this, the primary development approach for divertor components involves a combination of inventive design solutions to accommodate the brittle behavior of W coupled with the development of either tungsten alloys or tungsten composites with improved toughness [13]. The discovery of nanometer-scale "fuzz" growing on the surface of tungsten components exposed to low energy helium raised a new concern [14]. Such structures are potentially large sources of plasma contamination by high-Z dust, could contribute to a significant level of tritium retention, and could substantially degrade the thermal properties of the plasma-facing surface.

Because of the issues just mentioned, there have been extensive international programs to characterize the exposure conditions that lead to W fuzz formation., see for example [15,16]. However, it has been a challenging problem to computationally investigate the phenomenon of fuzz formation because of the time and length scales involved. It appears to be driven by processes which require atomistic simulation such as molecular dynamics that are limited to very short times, generally less than $\sim 1\mu\text{s}$. However, large scale simulations have identified unit mechanisms which may ultimately lead to fuzz formation. Some of these mechanisms and representative results from MD simulations are shown in Fig. 5. Trap mutation occurs

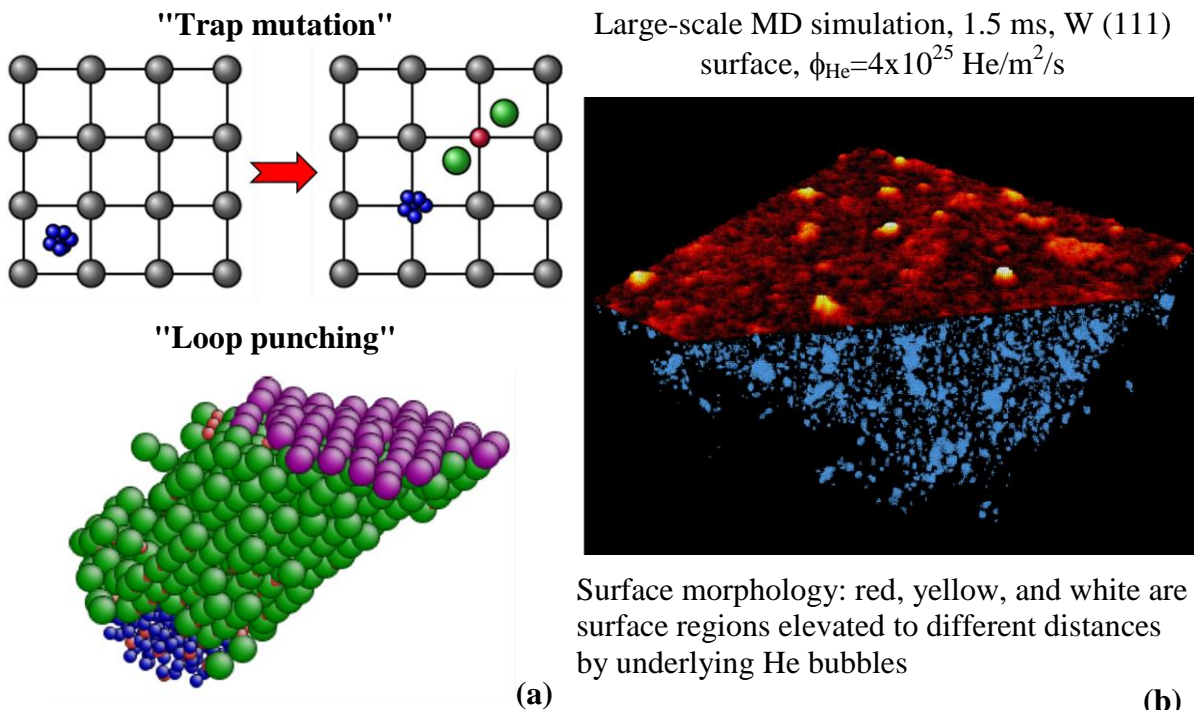


FIG 5. Unit mechanisms in (a) that contribute to (b) surface roughening in tungsten exposed to low-energy He, a possible precursor to fuzz formation.

when a cluster of interstitial He creates a Frenkel pair (a vacancy and an interstitial) to relieve the local pressure. The helium moves into the vacancy and the interstitial is trapped nearby. This process can be repeated as more helium is trapped in the He-vacancy cluster until a small bubble is created. Loop punching involves the creation of multiple Frenkel pair by a pressurized bubble, leading to the formation of an interstitial cluster that can glide to the surface forming a small island of adatoms.

The plastic behavior of body-centered cubic (bcc) crystals typically exhibits significant temperature dependence which is explained in terms of the thermally activated process of kink pair nucleation and migration with a high energy (Peierls) barrier. Here we demonstrate that such strong temperature dependence of the flow stress must disappear on the sub-micron scale. A series of atomistically informed discrete dislocation dynamics simulations were carried out on W micropillar subjected to uniaxial loading [17-19]. We explored the flow stress and hardening behavior of micro-pillar sizes in the range 200-2000 nm at temperatures of 150-900 K. The calculated yield stress at room temperature shows good agreement with experimental data (see Fig. 6) [20]. The calculated yield stresses are summarized in Fig. 7 by averaging over multiple realizations for each size and temperature. The experimental yield stress of bulk tungsten [21] is also given for comparison. This clearly shows that the temperature sensitivity of the yield stress becomes weaker as the sample size decreases; for small pillars, the yield stress almost exhibits no temperature dependence.

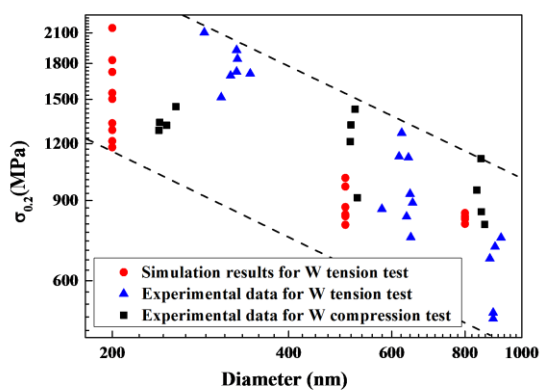


Fig. 6. Comparison of the yield strength of W micropillars with experimental data [18] at room temperature. Note the scatter in the data, which is inherent in the plasticity behavior of small size sample.

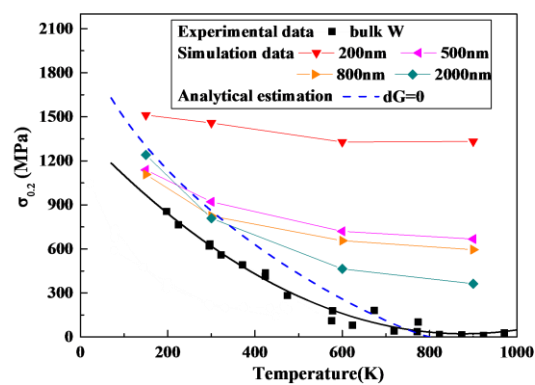


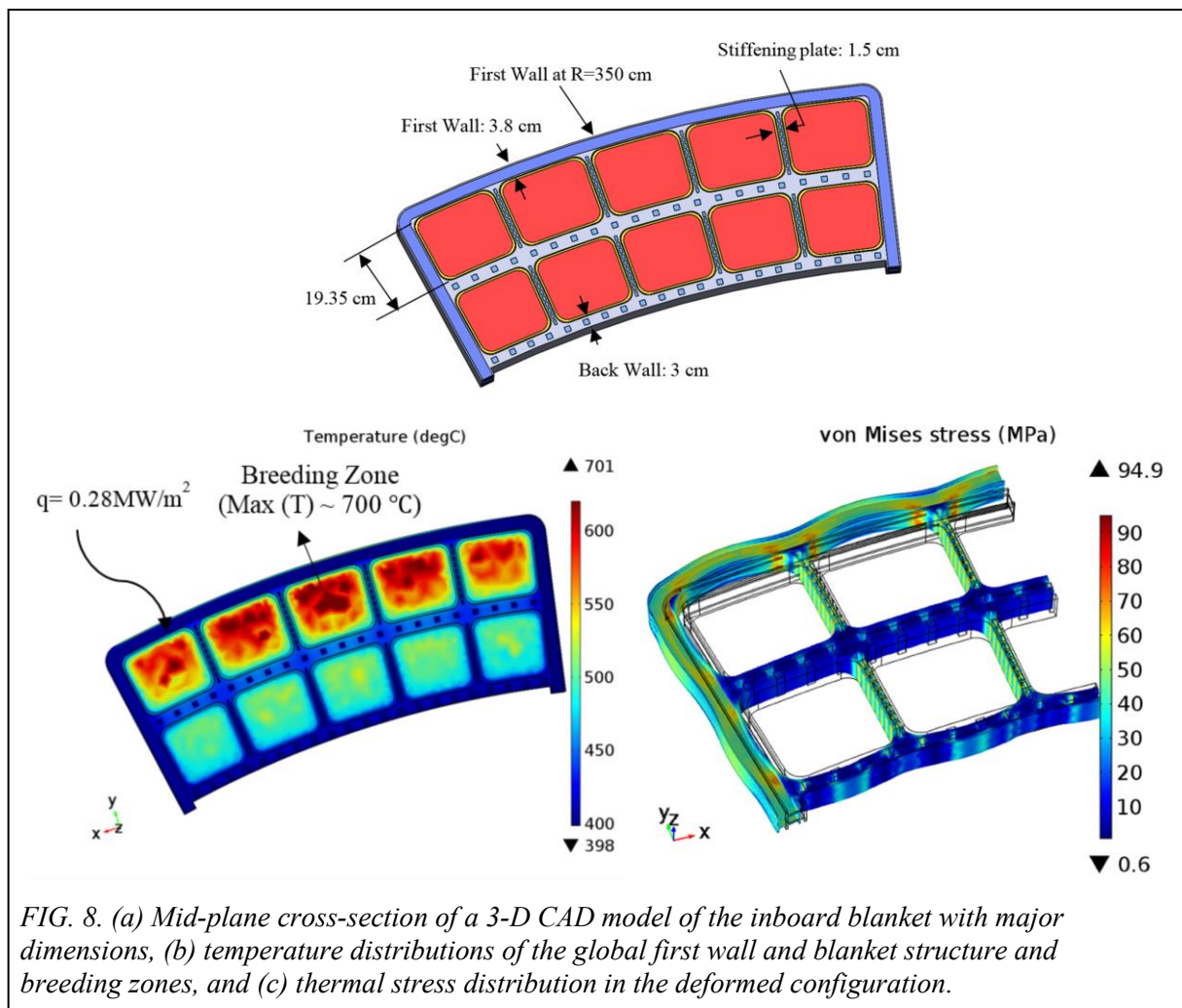
Fig. 7. The dependence of the yield stress on temperature for various sample sizes. Note the insensitivity of the flow stress to test temperature when the sample size is small (e.g. 200 nm).

5. Multi-Scale and Multi-Physics Design of Fusion Reactor Components

A Fusion Nuclear Science Facility (FNSF) has been recently proposed in the U.S. to provide a technical basis for the development of a commercial fusion power plant. Several previous design studies have shown that energy conversion components such as blankets in a fusion power plant will become significantly more complex when they must provide the multiple functions of extracting heat for thermal conversion while breeding tritium for fuel. The structural design of these components must meet strict temperature and stress design limits, have a credibly manufacturable configuration, and provide for maintenance. The dual coolant lead-lithium (DCLL) blanket concept employed in the FNSF conceptual design is based on a helium-cooled first wall and blanket structure with a self-cooled LiPb breeding zone.

A multiscale, multiphysics modeling approach has been developed to optimize the design and achieve long lifetime, maintainability, and high reliability. The commercial software: SOLIDWORKS was employed to provide 3D solid modeling, while 3D finite element modeling of the DCLL first wall and blanket (midplane of one sector) was performed using COMSOL 5.0. The multiphysics aspect of the design is demonstrated by coupling the computational fluid dynamics, heat transfer in solids, and heat transfer in fluids modules

within COMSOL. Both normal and off-normal loading conditions have been analyzed. The results of velocity, pressure, and temperature distributions of helium flow, as well as the primary and thermal stress of the structure were obtained. Then the safety factors were determined along three critical paths based on the ITER Structural Design Criteria for In-vessel Components. The results demonstrate that the optimized structural design meets the ITER design rules under normal operating conditions. However, the design must consider the possibility of plastic damage and fracture under off-normal conditions which will require further plastic and fracture mechanics analyses in critical regions employing a multiscale approach. Future work must consider the effects of radiation on the lifetime and reliability of the design, improvements in the geometric layout of the structure, improvements in heat transfer and fluid flow models, and integration of the plasticity and fracture models. Fig. 8 show examples of solid modeling, temperature distributions and stresses in a blanket and first wall structure.



6. Summary

The US FRM program maintains an emphasis on advanced ferritic-martensitic steels, including the ODS and CNA variants; SiC composites; and tungsten. This program of computational and experimental research is particularly concerned with the effects of helium produced by nuclear transmutation. In both the structural materials and tungsten, helium may increase tritium retention which has implications for operational safety in the event of an accident and for the successful recovery of tritium for use as fuel. In addition, it has been shown that low energy helium ions from the plasma may degrade the surface of tungsten

components with the potential for increasing the amount of radioactive dust and plasma contamination. There has been significant progress on other topics that are critical to the success of fusion energy, these include understanding the effects of neutron irradiation on mechanical properties of tungsten, new insight into the synergism between high heat flux and neutron irradiation in SiC composites, and the development of joining technologies for advanced materials including nanostructured ferritic/martensitic steels and SiC composites, and new computational tools for component design.

Acknowledgement

Research sponsored by the Office of Fusion Energy Sciences, U.S. Department of Energy. The U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

References

- [1] KLUEH, R. L. and HARRIES, D. R., High-Chromium Ferritic and Martensitic Steels for Nuclear Applications, American Society for Testing and Materials, West Conshohocken, PA, 2001.
- [2] MUROGA, T, Gasparotto, M., and ZINKLE, S. J., Fus. Engr. Des. 61-62 (2002) 13-25.
- [3] ZINKLE, S. J., Fus. Engr. Des. 74 (2005) 31-40.
- [4] JITSUKAWA, S., *et al.*, J. Nucl. Mater. 307-311 (2002) 179-196.
- [5] VAN DER SCHAAF, B., *et al.*, Fus. Engr. Des. 69 (2003) 197-203.
- [6] LINDAU, R., *et al.*, Fus. Engr. Des. 75-79 (2005) 989-996.
- [7] TAN, L., SNEAD, L. L., and KATOH, Y., J. Nucl. Mater. 478 (2016) 42-49.
- [8] KIM, I.-S., *et al.*, J. Nucl. Mater. 280 (2000) 264-274.
- [9] HOELZER, D.T., *et al.*, J. Nucl. Mater. 367-370 (2007) 166-72.
- [10] PRAMONO, Y., IMAI, M., and YANO, Y., J. Nucl. Sci.Tech. 40 (2003) 531-536.
- [11] KATOH, Y., *et al.*, J. Nucl. Mater. 455 (2014) 387-397.
- [12] HENAGER, C. H., *et al.*, J. Nucl. Mater. 466 (1015) 253-268.
- [13] NYGREN, R. E., *et al.*, J. Nucl. Mater. 417 (2011) 451-456.
- [14] TAKAMURA, S, *et al.* Plas. Fus. Res. 1 (2006) 051: 1-2.
- [15] BALDWIN, M. J. and DOERNER, R. P., Nucl. Fusion 48 (2008) 035001 (5 pp).
- [16] KAJITA, S., *et al.*, Nucl. Fusion 49 (2009) 095005 (6 pp).
- [17] CUI, Y., PO, G., and GHONIEM, N. M., Acta Mater. 108 (2016) 128-137.
- [18] CUI, Y., PO, G., and GHONIEM, N. M, Phys. Rev. Let. (2016) in press.
- [19] PO, G., *et al.*, Acta Mater. 119 (2016) 123-135.
- [20] SCHNITZEL, R. H., J. Less Comm. Met. 8 (1965) 81-89.
- [21] KIM, J.-Y., JANG, D., GREER, J. R., Acta Mater. 58 (2010) 2355-2363.