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1. FERRITIC/MARTENSITIC STEEL DEVELOPMENT

See also Sections 6.1, 7.5, 8.2, 8.3, 8.4, and 8.5.

1.1 Stability of MX-Type Nanoprecipitates in Fe-Base Model Alloys — 1
L. Tan, Y. Katoh, L. L. Snead (Oak Ridge National Laboratory)

The stability of MX-type nanoprecipitates TaC, TaN, and VN has been evaluated using thermal aging at 600 and 700°C for up to 5000 h, creep testing at 600°C, and Fe^{2+} ion irradiation at 500°C and up to ~49 dpa. Transmission electron microscopy (TEM) has been primarily used to characterize the evolution of the nanoprecipitates. The results indicate different levels of stability of the nanoprecipitates under the three types of experimental conditions. Selected particle degradation modes, e.g., dissolution, growth, re-precipitation, and fragmentation, were observed on the nanoprecipitates. The results are being reported and compared to literature data in our recent papers. A parallel experiment using neutron irradiation at 300, 500, and 650°C for up to about 20 dpa has been completed recently. Post-irradiation examination (PIE) of the neutron-irradiated samples will be conducted to compare them with the Fe^{2+} ion irradiated results.

2. ODS AND NANOCOMPOSITED ALLOY DEVELOPMENT

See also Sections 6.1, 7.5, and 8.4.

2.1 Development of ODS FeCrAl for Fusion Reactor Applications — 5
D. T. Hoelzer, K. A. Unocic, S. Dryepondt, and B. A. Pint (Oak Ridge National Laboratory)

Three experimental ODS FeCrAl heats of composition Fe-12Cr-5Al were prepared by mechanical alloying with additions of Y_2O_3, Y_2O_3 + ZrO_2 and Y_2O_3 + HfO_2. The as-extruded microstructure showed smaller grain size with the co-additions of ZrO_2 or HfO_2 and high concentrations of nano-size (<5 nm diameter) oxide particles within the grains. In the alloy with Y_2O_3 + HfO_2, either a bimodal or trimodal particle size distribution was observed. Tensile testing was performed at 25° up to 800°C and the higher oxide contents with ZrO_2 or HfO_2 resulted in higher yield and ultimate strengths but lower ductility compared to the alloy with only Y_2O_3.

3.0 CERAMIC COMPOSITE STRUCTURAL MATERIAL DEVELOPMENT

See also Sections 8.6 and 8.7.

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3.1 Process Development and Optimization for Silicon Carbide Joining and Irradiation Studies-III — 11
T. Koyanagi, J. Kiggans, C. Shih, Y. Katoh (Oak Ridge National Laboratory)

Two robust pressureless joining methods for SiC ceramics proved to be promising. A Ti-Si-C MAX phase displacement reaction bonding using commercial bonding formula demonstrated dense microstructures and apparent shear strength of ~150 MPa. A pressureless transient eutectic-phase (TEP) process was newly developed to demonstrate promising properties. An experimental plan for the neutron irradiation effects study was developed.

3.2 Low Activation Joining of SiC/SiC Composites for Fusion Applications: Tape Casting TiC+Si Powders — 23
C. H. Henager, Jr., R. J. Kurtz, N. L. Canfield, Y. Shin, W. G. Luscher, J. T. Mansurov, T. J. Roosendaal, and B. A. Borlaug (Pacific Northwest National Laboratory)

The use of SiC composites in fusion environments likely requires joining two plates using reactive joining or brazing. One promising reactive joining method uses solid-state displacement reactions between Si and TiC to produce Ti_3SiC_2 + SiC. We continue to explore the processing envelope for these joints to produce optimal joints to undergo irradiation studies in the High Flux Isotope Reactor (HFIR). One noted feature of the older joints, produced with tape-calendared powders of TiC + Si, were the large, unavoidable void regions they contained. Although the joints were very strong, voids are undesirable. In addition, the tapes made for these joints were produced approximately 20 years ago and had aged. Therefore, we embarked on an effort to produce new tape-cast powders of TiC and Si that can replace our aged tape-calendared materials.

4. HIGH HEAT FLUX MATERIALS AND COMPONENT TESTING

See also Sections 8.8 and 8.9.

4.1 Recent Progress in the Development of Ductile-Phase Toughened Tungsten for Plasma-Facing Materials — 29
C. H. Henager, Jr., R. J. Kurtz, T. J. Roosendaal, and B. A. Borlaug (Pacific Northwest National Laboratory), G. R. Odette, K. H. Cunningham, K. Fields, D. Gragg, and F. W. Zok (University of California, Santa Barbara)

Tungsten (W) and W-alloys are the leading candidates for plasma-facing components in nuclear fusion reactor designs because of their high melting point, strength at high temperatures, and low sputtering yield. However, tungsten is brittle and does not exhibit the required fracture toughness for nuclear applications. The ductile-brittle transition temperature (DBTT) for unirradiated W-alloys ranges from 300-1000ºC and radiation hardening further elevates this range. A promising approach to increasing fracture toughness and decreasing the DBTT of a W-alloy is by ductile-phase toughening (DPT). In this method, a ductile phase is included in a brittle matrix to prevent fracture propagation by

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crack bridging. To examine the prospect of DPT, W-Cu and W-Ni-Fe three-point bend samples were deformed at several strain rates and temperatures. Data from these tests will be used for time-dependent crack bridging studies and the calibration of a crack-bridging model that can effectively predict elevated temperature crack growth in W-composites. A study of fabricating W-wire-reinforced W-matrix composites by spark plasma sintering (SPS) was initiated. W-wires coated with Cu or tungsten carbide (WC) was consolidated in a W matrix. Characterization of these composites is ongoing.

4.2 Evaluation of Mechanical Properties of Tungsten After Neutron Irradiation — **40**
L. L. Snead, L. M. Garrison, T. S. Byun, N. A. P. K. Kumar, and W. D. Lewis (Oak Ridge National Laboratory)

A total of 440 tungsten samples were irradiated in HFIR at temperatures from 70 to 900°C and fast neutron fluences of 0.01 to 20 $\times 10^{25}$ n/m^2 at E>0.1 MeV over the last year. Types of tungsten included were [110] single crystal tungsten, [100] single crystal tungsten, wrought tungsten foils, annealed tungsten foils, and tungsten-copper laminate. Samples that were irradiated at 2×10^{25} n/m^2 and below have been tensile and hardness tested at 300°C and below. The defect structure of selected low dose samples has been investigated in the TEM. The analysis of the lower dose samples is ongoing, and analysis of the higher dose samples will follow.

4.3 High-Heat Flux Testing of Low-Level Irradiated Materials Using Plasma Arc Lamps — **48**
A. S. Sabau, E. K. Ohriner, Y. Katoh, and L. L. Snead (Oak Ridge National Laboratory)

A neutron-irradiated tungsten specimen was successfully tested at ITER-relevant high-heat flux conditions using Plasma Arc Lamp at ORNL on Aug. 14, 2013, without any contamination outside the testing box, ensuring the readiness of the new facility for irradiated samples. For thin specimens, often used for studies of neutron irradiation effects, one of the main challenges to the PAL systems is the measurement of the sample temperature.

5. MAGNET AND DIAGNOSTIC SYSTEM MATERIALS

5.1 Irradiation Response of Next Generation High Temperature Superconducting Rare Earth and Nanoparticle-Doped $YBa_2Cu_3O_{7-x}$ Coated Conductors for Fusion Energy Applications — **54**
K. J. Leonard, T. Aytug, Fred. A List III, Yanwen Zhang (Oak Ridge National Laboratory), A. Perez-Bergquist, W. J. Weber (University of Tennessee), and A. Gapud (University of South Alabama)

During this semiannual reporting period, electrical characterization work was completed on the irradiated superconducting films, and two presentations were made at conferences. The first, “Irradiation Response of Next Generation High Temperature Superconductors for Fusion Energy Applications” was presented at the International Conference of Fusion

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Reactor Materials in Beijing, China. This presentation introduced the fusion materials community to the advances that have been made in coated conductor technology and the potential for use in nuclear application. The second presentation "Irradiation of Commercial, High-T_c Superconducting Tape for Potential Fusion Application: Electromagnetic Transport Properties," was presented in November at the Southeastern Section American Physical Society Meeting in Bowling Green, KY. This detailed the electrical property characterizations of the conductors and is summarized in this report.

5.2 High Neutron Dose Irradiation of Dielectric Mirrors — **63**
K. J. Leonard, G. E. Jellison Jr., N. A. P. K. Kumar and L. L. Snead (Oak Ridge National Laboratory)

During this semiannual reporting period, work was completed on low dose (0.001 to 0.1 dpa) examinations culminating in the presentation of data at the Radiation Effects in Insulators conference in Helsinki, Finland in July 2013. Publication of the paper "The role of microstructure on the optical performance of neutron irradiated dielectric mirrors" has been confirmed for the Journal of Nuclear Materials in 2014, volume 445, pages 281-290. The optical property characterization of the 1 and 4 dpa-irradiated mirrors has also been completed, with data presented in poster form at the International Conference of Fusion Reactor Materials in Beijing, China in October. This semiannual contribution briefly summarizes the low dose results, which are presented in more detail in the previous contributions, as well as the optical property data for the high dose samples.

6. FUSION CORROSION AND COMPATIBILITY SCIENCE

6.1 Liquid Metal Compatibility — **67**
S. J. Pawel (Oak Ridge National Laboratory)

Fabrication of the first thermal convection loop (TCL) using dispersion strengthened FeCrAl (Kanthal APMT) tubing was completed in the previous reporting period. This alloy is known for high strength and creep resistance at elevated temperature and, based on capsule testing, it is anticipated to have excellent resistance to Pb-Li. Recent accomplishments include initial refurbishment of suitable laboratory space in which to operate the TCL, acquisition and chemical analysis of the Pb-17at%Li that will be used as a working fluid, and preparation of the Kanthal APMT test coupons that will be used in the specimen chains that will be inserted into each vertical leg of the TCL.

7. MECHANISMS AND ANALYSIS

7.1 Microstructural Stability and Mechanical Behavior of FeMnNiCr High Entropy Alloy Under Ion Irradiation — **70**
N. A. P. K. Kumar[1,2], K. J. Leonard[1], H. Bei[1], Y. Zhang[1,2] and S. J. Zinkle[1] (Oak Ridge National Laboratory[1], University of Tennessee[2])

Abstract of paper to be submitted.

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7.2 Effects of Ion Irradiation on BAM-11 Bulk Metallic Glass — 71
A. G. Perez-Bergquist[1,2], H. Bei[1], Y. Zhang[1,2], and S. J. Zinkle[1,2] (Oak Ridge National Laboratory[1], University of Tennessee[2])

Bulk metallic glasses are intriguing candidates for structural applications in nuclear environments due to their good mechanical properties along with their inherent amorphous nature, but their radiation response is largely unknown due to the relatively recent nature of innovations in bulk metallic glass fabrication. Here, microstructural and mechanical property evaluations have been performed on a $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ bulk metallic glass (BAM-11) irradiated with 3 MeV Ni^+ ions to 0.1 and 1.0 dpa at room temperature and 200°C. Transmission electron microscopy showed no evidence of radiation damage or crystallization following ion irradiation, and changes in hardness and Young's modulus were typically <10%, with slight softening following irradiation at room temperature and no significant changes at 200°C. These results suggest that the BAM-11 bulk metallic glass may be useful for certain applications in nuclear environments.

7.3 Physical and Thermal Mechanical Characterization of Non-Irradiated MAX Phase Materials (Ti-Si-C and Ti-Al-C Systems) — 78
C. Shih, R. Meisner, W. Porter, Y. Katoh, and S. J. Zinkle (Oak Ridge National Laboratory)

The physical and thermo mechanical properties of two commercially available MAX phase materials have been characterized in the non-irradiated states including: density, X-ray diffraction analysis, microstructure analysis by SEM, coefficient of thermal expansion, thermal diffusivity, thermal conductivity, dynamic Young's modulus, electrical conductivity, and equibiaxial fracture strength (including Weibull modulus). The results show that the materials contain multiple phases. However, predominate phases are hexagonal MAX phases composed of Ti-SiC-C and Ti-Al-C ternary systems. High thermal and electrical conductivity, adequate Young's modulus and equibiaxial fracture strength were observed. All the properties studied agree well with data from the literature.

7.4 Effects of Neutron Irradiation on Ti-Si-C MAX-Phase Ceramic Microstructures — 94
A. G. Perez-Bergquist[1,2], Y. Katoh[1], C. Shih[1], N. A. P. K. Kumar[1,2], and S. J. Zinkle[1,2] (Oak Ridge National Laboratory[1], University of Tennessee[2])

MAX phase ceramics are intriguing candidates for structural applications in nuclear environments due to their unique mixture of metallic and ceramic properties. Specifically, their potential to retain adequate thermal conductivity after high levels of irradiation damage may make them an attractive alternative to SiC in fusion environments. In this study, we investigate the MAX phase ceramic Ti_3SiC_2 after neutron irradiation to 3.4 dpa and 5.0 dpa at temperatures of 500 and 800°C, respectively. Initial results showed large amounts of atomic-scale radiation damage in the material, but minimal loss of strength in selected Ti_3SiC_2/Ti_5Si_3 samples.

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7.5 A Dual Ion Irradiation Study of Helium-DPA Interactions on Cavity Evolution in Tempered Martensitic Steels and Nanostructured Ferritic Alloys — **100**
T. Yamamoto, Y. Wu, G. Robert Odette (University of California Santa Barbara),
K. Yabuuchi, S. Kondo, and A. Kimura (Kyoto University)

Cavity evolutions in a normalized and tempered martensitic steel (TMS) and two nanostructured ferritic alloys (NFA) under Fe^{3+} and He^{+} dual ion beam irradiations (DII) at 500°C and 650°C were characterized over a wide range of dpa, He and He/dpa. Transmission electron microscopy (TEM) showed that DII of a 8Cr TMS, at 500°C to up to 60 dpa and 2100 appm He, produced a moderate density of non-uniformly distributed cavities with bimodal sizes ranging from ≈ 1 nm He bubbles to ≈ 20 nm faceted voids, and swelling ≈ 0.44%. In contrast, the same irradiation conditions produced only small ≈ 1.3 nm diameter bubbles and swelling of ≈ 0.05% in the NFA MA957. Similar bubble distributions were observed in MA957 and a developmental NFA DII at 650°C up to ≈ 80 dpa and ≈ 3900 appm He. These results demonstrate the outstanding He management capability of the oxide nano-features in the NFA. The various data trends are shown as a function of dpa, He, He/dpa and He*dpa.

8. MODELING PROCESSES IN FUSION SYSTEM MATERIALS

8.1 Modeling Concurrent Radiation Damage and Plastic Deformation — **107**
T. Crosby, G. Po, N. Ghoniem (University of California, Los Angeles)

We present here an application of a fundamentally new theoretical framework for description of the simultaneous evolution of radiation damage and plasticity that can describe both in-situ and ex-situ deformation of structural materials. The developed self-consistent framework allows for the determination of the simultaneous evolution of the dislocation microstructure, as well as the spatial distribution of vacancies, interstitials and the temperature diffusion fields. The developed theory is implemented in a new computational code that facilitates the simulation of irradiated and unirradiated materials alike in a consistent fashion. Computer simulations are presented for irradiated fcc metals that address dislocation channel formation in irradiated metals (ex-situ). The simulations, which focus on plastic flow localization in micro-pillars, show that the spatial heterogeneity in the distribution of Stacking Fault Tetrahedra (SFTs) leads to localize plastic deformation and incipient surface fracture of micropillars.

8.2 An Atomistic Assessment of Helium Behavior in Iron — **110**
R. E. Stoller and Y. N. Osetskiy (Oak Ridge National Laboratory)

Extended abstract – paper submitted to J. Nucl. Mater. after ICFRM-16.

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8.3 Dynamics of Helium-Loaded Grain Boundaries under Shear Deformation in α-Fe — 112
F. Gao, L. Yang, H. L. Heinisch and R. J. Kurtz (Pacific Northwest National Laboratory)

Helium produced in the fusion nuclear environment will interact with microstructural features in materials, such as GBs and dislocations. At elevated temperatures helium at GBs can significantly influence creep-rupture properties by enhancing cavity formation and lowering GB cohesive energy. Grain boundary sliding can lead to stress concentrations at GB triple junctions and hard precipitates in the GB plane that may be sufficient to nucleate cavities. Here we explore the effects of helium on coupled GB migration and sliding under an applied shear stress. The Σ3 symmetric tilt GB with a <110> rotation axis in bcc iron was selected for study. The method for exploring helium effects on GB motion involved randomly inserting different concentrations of helium atoms around the GB plane and then applying a shear stress parallel to the GB plane at 300 K. We reported previously [1] that, in the absence of helium, the critical stress to induce coupled GB migration and sliding occurred at 300 K was 1.5 GPa. The current simulations show that when helium is present the critical stress for coupled GB motion, and the GB migration velocity are both reduced. When the GB helium concentration is low, most single helium atoms and small helium clusters migrate along with the GB. However, at high helium concentrations clusters easily form that remain behind in the bulk when the GB migrates away from its original position.

8.4 Radiation-Induced Obstacles in Iron and Ferritic Alloys: An Atomic-Scale View — 119
Y. N. Osetskiy and R. E. Stoller (Oak Ridge National Laboratory)

Extended abstract – paper submitted to J. Nucl. Mater. after ICFRM-16, with results on 6nm obstacles added.

8.5 Modeling of Irradiation Hardening of Iron After Low Dose and Low Temperature Neutron Irradiation — 121
X. Hu, D. Xu, B. D. Wirth (University of Tennessee, Knoxville), and T. S. Byun (Oak Ridge National Laboratory)

Irradiation hardening is a prominent low temperature degradation phenomena in materials. In this paper, a reaction-diffusion cluster dynamics model is used to predict the distribution of vacancy and interstitial clusters in iron subject to low temperature (< 373K) and low dose (< 0.1 dpa) neutron irradiation. The predicted microstructure evolutions of high purity iron samples are compared to positron annihilation spectroscopy (PAS) and transmission electron microscopy (TEM) observations and show good agreement for neutron irradiation in this regime. The defect cluster distributions are then coupled to a dispersed barrier hardening model that assumes a strength factor, α, which varies with cluster type and size to compute the yield strength increase, the results of which are compared to the values obtained from tensile tests. A reasonable agreement between modeling and experiments is achieved.

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8.6 Molecular Dynamics Modeling of Atomic Displacement Cascades in 3C-SiC — 147
G. D. Samolyuk, Y. N. Osetskiy and R. E. Stoller (Oak Ridge National Laboratory)

Extended abstract – paper submittefd to J. Nucl. Mater. after ICFRM-16.

8.7 First-Principles Calculations of Charge States and Formation Energies of Mg Transmutant in 3C-SiC — 149
S. Y. Hu, W. Setyawan, W. Jiang, C. H. Henager, Jr. and R. J. Kurtz (Pacific Northwest National Laboratory)

We employed density functional theory to study the effect of electron potentials on charge states and the formation energies of Mg transmutant at different lattice sites in 3C-SiC. We found that Mg_C, Mg_{TC} and Mg_{TSi} most likely have charge state +2 while Mg_{Si} prefers charge state -2. The results also show that the substitutional Mg_{Si}^{-2} has much smaller formation energy than that of Mg_C^{+2}, and interstitial Mg_{TC}^{+2} has lower formation energy than that of Mg_{TSi}^{+2}. These results imply that Mg_{Si}^{-2} is the most stable substitutional defect while Mg_{TC}^{+2} is the most stable interstitial defect in 3C-SiC. Since the quadrupole correction due to the spurious interactions between images of charged defects in periodic simulation cells was not taken into account, the calculated formation energies were overestimated. In future work we will examine the effect of quadrupole correction on the formation energies of defects. Additional studies on Al and Be transmutants in 3C-SiC are currently underway.

8.8 Analytical Model of Homogeneous Helium Trap-Mutation Evolution in Tungsten — 154
W. Setyawan, G. Nandipati, K. J. Roche, H. L. Heinisch, R. J. Kurtz (Pacific Northwest National Laboratory) and B. D. Wirth (University of Tennessee, Knoxville)

Homogeneous trap-mutation events in which helium (He) clusters above a minimum size displace tungsten (W) atoms from their lattice sites are simulated with molecular dynamics. Using a He concentration of up to 4600 appm and temperature up to 2050 K (half the absolute melting temperature), analytical models are formulated to describe the evolution of the number of trap-mutation nucleation sites (N_C) and the number of created self-interstitial atoms (N_I) as a function of He concentration and temperature. Consistent time scaling with respect to concentration (linear scaling) and temperature (Arrhenius scaling) is observed in the case of N_C curves. Therefore, a single analytical model can be obtained. On the other hand, while the linear time scaling still applies among the N_I curves, the Arrhenius time scaling holds only during early stages of the evolution due to the temperature-dependence of the saturation value (larger at higher temperatures). Hence, for N_I, a specific model is formulated for each temperature.

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8.9 Object Kinetic Monte Carlo Simulations of Cascade Annealing in Tungsten — 161
G. Nandipati, W. Setyawan, H. L. Heinisch, K. J. Roche, R. J. Kurtz (Pacific Northwest National Laboratory) and B. D. Wirth (University of Tennessee)

We used our recently developed lattice based object kinetic Monte Carlo code; KSOME [1] to carryout simulations of annealing of individual displacement cascades in bulk tungsten that were generated using molecular dynamics (MD) simulations, at temperatures of 300, 1025 and 2050 K and PKA energies up to 100 keV. We find that at smaller PKA energies the fraction of surviving self-interstitial atoms (SIAs) and vacancies decreases with temperature, whereas at higher PKA energies the fraction of surviving defects at first decreases and then increases with temperature.

9. IRRADIATION METHODS, EXPERIMENTS, AND SCHEDULES

9.1 Fusion Material Irradiation Test Station (FMITS) at SNS — 167
Mark Wendel, Phil Ferguson (Oak Ridge National Laboratory)

Highlights of the FMITS Concept Design include safety round-table findings, advances in the mechanical design of the harness and vent-line shield block (through which FMITS utilities pass), improved remote handling procedures and tooling, and refinements of the user science envelope. Samples would be welded inside the FMITS target harness in two horizontal tubes, which project out in front of the mercury target. For these specimen locations, the back-scattering neutron flux spectra should be close to the ITER fusion spectrum. The PKA spectra at the FMITS samples were also compared to those for ITER, and the results show good agreement. Radiation damage rates would be 1.6–5.5 dpa/y for steel, with the range of helium-to-dpa production ratios starting close to those expected in D-T fusion, and increasing toward beam center locations.

9.2 HFIR Irradiation Experiments – December 31, 2013 — 175
Y. Katoh (Oak Ridge National Laboratory)