TABLE OF CONTENTS

1. FERRITIC/MARTENSITIC STEEL DEVELOPMENT

See also contributions 2.6, 7.3, 7.4, 8.3, 8.4, and 8.5.

1.1 Development of Advanced Reduced Activation Ferritic/Martensitic Steels — L. Tan (Oak Ridge National Laboratory) **1**

A new RAFM steel has been designed to favor the formation of MC (M = metal) carbides because a recent study has shown superior stability of TaC over TaN and VN nanoprecipitates under thermal aging, creep testing, and Fe^{2+} ion irradiation at 500°C. A lab-scale heat of the new alloy has been fabricated in conventional normalization and tempering conditions. Tensile results for test temperatures up to 800°C exhibited yield strength significantly greater than P92 steel with decent total elongation. Four different TMT conditions have been developed on Grade 92 samples. One of the conditions with warm rolling after normalization followed by 2-step tempering was identified as having the best results in terms of tensile and Charpy impact properties; these conditions will be applied to the new alloy. Additionally, preliminary microstructural characterization of the high dose Fe^{2+}-irradiated TaC samples has produced some new observations.

1.2 Fracture Testing and Evaluation Procedures for Miniature F82H DCT Specimens – T. S. Byun (Oak Ridge National Laboratory) and D. Hamaguchi (Japan Atomic Energy Agency) **4**

Fracture toughness testing in high radiation areas using miniaturized specimens has become a major challenge in the evaluation of highly radioactive materials as it requires high precision recording of load-displacement data, including loading-unloading cycles, often in vacuum or controlled environments. A new testing and analysis procedure was established to test small disk compact tension (DCT) fracture specimens irradiated to high doses. This report summarizes the major components of the new procedure: a simplified testing technique to obtain minimum datasets needed for analysis and a simplified normalization method for evaluating crack resistance (J-R) data. In application, two sets of fracture test data obtained from 4.72 and 3.56 mm thick DCT specimens of nonirradiated low-activation ferritic-martensitic steels (F82H steels) were analyzed and the results are discussed focusing on the effect of side grooves and on the recommendation for data validity.

1.3 Disassembly of HFIR JP28&29 Tensile Holders and Vickers Hardness Results on F82H Irradiated at 573 K— M. Ando, D. Hamaguchi and H. Tanigawa (Japan Atomic Energy Agency), R. G. Bowman, G. C. Morris, J. P. Robertson and Y. Katoh (Oak Ridge National Laboratory) **15**

Ten tensile specimen holders from HFIR irradiation experiments JP28 and JP29 were successfully disassembled in the ORNL 3025E hot cell facility. Some holders needed to be cut along corners of the holder because specimens could not be easily pushed out of the holder. All tensile specimens from the disassembled holders were recovered and identified. The surfaces of the specimens irradiated at 673 and 773 K were oxidized during the irradiation and cannot be hardness tested without polishing. Vickers hardness was measured on some of the tensile specimens irradiated at 573 K.

TABLE OF CONTENTS

1.4 **Analytical TEM Characterization of Modified F82H and 14YW under Simultaneous Helium and Neutron Irradiation Compared to Only Neutrons At 500°C** - H.J. Jung, D. J. Edwards, B. Yao, R. J. Kurtz (Pacific Northwest National Laboratory), G. R. Odette, T. Yamamoto, Y. Wu (University of California Santa Barbara) **19**

An RAFM steel and an ODS ferritic alloy (F82H.mod3+CW and 14YW, respectively) were irradiated as part of the HFIR-JP27 irradiation experiment conducted in the High Flux Isotope Reactor to explore He effects in structural alloys. The *in situ* He injection (ISHI) technique is used to implant He up to 9 µm below the surface of a NiAl coated sample at He/dpa levels up to ~50. This report summarizes the current status of TEM characterization of the two irradiated alloys. The He-implanted side of the RAFM alloy exhibited significant swelling due to bubble and void formation - within the matrix, on pre-existing dislocations, and at interfaces within the material. The 14YW alloy exhibited significant swelling even in the absence of implanted He, primarily through large voids that formed on the ODS particles. In addition, significant radiation-induced segregation of the Cr was observed around oxide particles and on lath boundaries and visible α′ particles could be detected via elemental mapping of the matrix of the 14YW alloy.

2. **ODS AND NANOCOMPOSITED ALLOY DEVELOPMENT**

See also contributions 1.4 and 8.7.

2.1 **Development of ODS FeCrAl for Fusion Reactor Applications** — D. T. Hoelzer, K. A. Unocic, S. Dryepondt, and B. A. Pint (Oak Ridge National Laboratory) **31**

Four 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, Y_2O_3 + HfO_2 and Y_2O_3 + TiO_2. Characterization of the as-extruded and aged microstructures are in progress and are compared to a commercial ODS FeCrAl alloy, PM2000. An initial Pb-Li compatibility evaluation was performed at 700°C on the first three alloys. The fourth alloy with TiO_2 was recently produced and tensile properties have been measured from 25° to 800°C. This alloy had high strength but low ductility at 25° and 400°C consistent with its high hardness. Initial creep testing has begun on the alloy with HfO_2 at 800°C and 100 MPa.

2.2 **A New Scandium-Based Nanostructured Ferritic Alloy** – T. Stan, S. Pun, N. J. Cunningham, Y. Wu and G. R. Odette (University of California Santa Barbara) **40**

A new Sc-based nanostructured ferritic alloy (NFA) was processed by ball milling gas atomized Fe alloy and Sc_2O_3 powders. Replacing Y with Sc was motivated by the fact that the latter has a much higher solubility in Fe compared to Y, possibly providing a melt processing path for producing Sc-based NFA. The milled powders were subject to four heat treatments: aging at both 850°C; aging at 1000°C; consolidation by spark plasma sintering (SPS) at a peak temperature of 1100°C; and SPS consolidation followed by annealing at 850°C for 3 hrs. Electron backscatter diffraction (EBSD) measurements showed fine grain sizes in both the 850°C and 1000°C aged powder conditions. Transmission electron microscopy (TEM) and atom probe tomography (APT) show that similar populations of $Sc_2Ti_2O_7$ complex oxide nano-features (NFs) also form at both aging temperatures. The microhardness was high for three conditions, and similar to that typically observed in Y-based NFA. However, the microhardness was much lower in the 1000°C powder aged condition. The reason for the low hardness is not yet understood.

TABLE OF CONTENTS

2.3 **SEM and EBSD Characterization of Fe - {110} $Y_2Ti_2O_7$ INTERFACES** – T. Stan, Y. Wu, G. R. Odette (University of California Santa Barbara) **45**

Nanostructured ferritic alloys (NFAs) are dispersion strengthened by a high density of 2-3 nm fcc pyrochlore $Y_2Ti_2O_7$ nano features (NFs). The interface between the bcc ferrite matrix and the $Y_2Ti_2O_7$ plays critical role in the radiation damage resistance of NFAs. However, details about the interfaces are difficult to determine from the nm-scale features themselves. To partially overcome this obstacle, and to complement other characterization studies of the actual NFs themselves, mesoscopic interfaces were created by electron beam deposition of Fe onto {110} oriented $Y_2Ti_2O_7$ bulk single crystal surfaces. We report characterization of Fe – {110}$Y_2Ti_2O_7$ interfaces using the Scanning Electron Microscopy (SEM) and Electron Backscatter Diffraction (EBSD) techniques. The polycrystalline Fe films had grains with three distinct orientation relationships (ORs). Notably, one 10 µm Fe grain had the favored {100}Fe||{110}$Y_2Ti_2O_7$ and <100>Fe||<100>$Y_2Ti_2O_7$ OR which is found in matrix embedded NFs. This work is continuing and while the mesoscopic interfaces may differ from those of the embedded NFs, the former will facilitate characterization of controlled interfaces, such as interactions with point defects and helium.

2.4 **Fracture Behavior of Advanced ODS Alloy 9YWTV –** T. S. Byun, D. T. Hoelzer (Oak Ridge National Laboratory), J. H. Yoon (Korea Atomic Energy Research Institute), and S. A. Maloy (Los Alamos National Laboratory) **50**

Latest studies on the high temperature fracture of nanostructured ferritic alloys (NFAs) have indicated that the microcracks formed within the alloys propagate by a low energy boundary decohesion mechanism and therefore resulted in low fracture toughness. A 9Cr NFA with improved fracture toughness was successfully developed by applying thermo-mechanical treatments (TMTs) designed to enhance grain boundary bonding. This article focuses on the static fracture behaviors of the newly developed 9Cr NFAs. Fracture mode and cracking resistance were compared among the materials treated through different controlled rolling (CR) routes. Optimal TMTs resulted in high fracture toughness at room temperature (> 250 MPa√m) and in retaining higher than 100 MPa√m over the wide temperature range 22–700°C. Significant differences were found in the fracture resistance (J-R) curves among the low and high fracture toughness NFAs.

2.5 **Mechanical Properties Characterization of a Larger Best Practice Heat of 14YWT NFA1** – M.E. Alam, N. J. Cunningham, D. Gragg, K. Fields, G. R. Odette (UCSB), D. T. Hoelzer (ORNL) and S. A. Maloy (LANL) **63**

A new larger heat of best practice nanostructured ferritic alloy (NFA), designated FCRD NFA1, was produced by ball milling argon atomized Fe-14Cr-3W-0.4Ti-0.2Y (wt.%) and FeO powders followed by consolidation and thermo mechanical processing sequence of extrusion (850°C), annealing and cross-rolling (1000°C) steps. The microhardness of NFA1 averaged ≈ 376 ± 18 (kg/mm^2). The corresponding uniaxial tensile yield stress and ductility from 22 to 800°C are high at >1000 MPa at 22°C to >500 MPa at 600°C and 15-25%, respectively. K_{Jc}(T) fracture toughness curves were also measured from -196 to 22°C using pre-cracked 3-point bend (3PB) specimens. NFA1 manifests an exceptionally low fracture toughness transition temperature of ≈ -175°C in both LT and TL orientations. These results represent an *extraordinary combination* of strength and toughness. Extensive fractography provided insight on key fracture mechanisms.

2.6 **Friction Stir Welding of ODS Steels and Advanced Ferritic Structural Steels** — Z. Feng, X. Yu, W. Tang, D. Hoelzer, and L.T. Tan (Oak Ridge National Laboratory) **70**

Our research during this reporting period focused on (1) understanding the effects of post-weld heat treatment (PWHT) on the microstructure and property variations in friction stir welds of RAFM

TABLE OF CONTENTS

steels, (2) developing the PWHT schedule to homogenize and restore the weld properties to match these of base metal, and (3) understanding the effect of the extreme thermal and deformation conditions associated with FSW on the nano oxide strengthening particles in MA956 ODS alloy. Major findings included the development of a PWHT schedule to produce uniform microstructure and a homogeneous hardness distribution in the weld region that is identical to base metal. Initial atom probe maps of FSWed MA956 revealed complete dissolution of the nano oxide particles, which has major implications on the fundamental understanding the stability of nano-oxide particles under extreme thermal-mechanical process conditions, as well as potential solutions to restore the creep strength of the weld region.

3. CERAMIC COMPOSITE STRUCTURAL MATERIAL DEVELOPMENT

See also Contributions 7.2, 8.9, and 8.10.

3.1 Low Activation Joining of SiC/SiC Composites for Fusion Applications: Modeling Miniature Torsion Tests—C.H. Henager, Jr., B.N. Nguyen, R.J. Kurtz, T. Roosendaal, and B. Borlaug (Pacific Northwest National Laboratory, Richland, WA, USA); M. Ferraris and A. Ventrella (Politecnico di Torino, Torino, Italy); and Y. Katoh (Oak Ridge National Laboratory, Oak Ridge, TN, USA) **79**

The use of SiC and SiC-composites in fission or fusion environments appears to require joining methods for assembling systems. The international fusion community has designed miniature torsion specimens for joint testing and for irradiation in HFIR. Therefore, miniature torsion joints were fabricated using displacement reactions between Si and TiC to produce Ti_3SiC_2 + SiC joints with CVD-SiC that were tested in shear prior to and after HFIR irradiation. However, these torsion specimens fail out-of-plane, which causes difficulties in determining shear strength for the joints or for comparing unirradiated and irradiated joints. A finite element damage model has been developed that indicates fracture is likely to occur within the joined pieces to cause out-of-plane failures for miniature torsion specimens when a certain modulus and strength ratio between the joint material and the joined material exists. The implications for torsion shear joint data based on this sample design are discussed.

3.2 Process Development and Optimization for Silicon Carbide Joining and Irradiation Studies-IV— Takaaki Koyanagi, James Kiggans, Chunghao Shih, Yutai Katoh (Oak Ridge National Laboratory) **94**

Processing and characterization of SiC ceramics joined by the pressureless transient eutectic-phase (PL-TEP) method were conducted. Apparent shear strengths of ~100 MPa was demonstrated by torsion test on the PL-TEP joint formed with SiC nano-powder, oxide additives, and organic agents. The fracture behavior was typical of robust joints. In addition, the joints are expected to have high densities based on sintered densities of monolithic SiC representing the PL-TEP joint layer. Irradiation of SiC joints made with different bonding materials is being conducted in HFIR.

3.3 Diffusion of Magnesium and Microstructures in Mg^+ Implanted Silicon Carbide— W. Jiang, D. J. Edwards, H J. Jung, Z. Wang, Z. Zhu, T. J. Roosendaal, S. Hu, C. H. Henager, Jr., R. J. Kurtz (Pacific Northwest National Laboratory), and Y. Wang (Los Alamos National Laboratory) **103**

Following our previous reports, further isochronal annealing (2 hrs.) of the monocrystalline 6H-SiC and polycrystalline CVD 3C-SiC was performed at 1573 and 1673 K in Ar environment. SIMS data

TABLE OF CONTENTS

indicate that observable Mg diffusion in 6H-SiC starts and a more rapid diffusion in CVD 3C-SiC occurs at 1573 K. The implanted Mg atoms tend to diffuse deeper into the undamaged CVD 3C-SiC. The microstructure with Mg inclusions in the as-implanted SiC has been initially examined using high-resolution STEM. The presence of Mg in the TEM specimen has been confirmed based on EDS mapping. Additional monocrystalline 3C-SiC samples have been implanted at 673 K to ion fluence 3 times higher than the previous one. RBS/C analysis has been performed before and after thermal annealing at 1573 K for 12 hrs. Isothermal annealing at 1573 K is being carried out and Mg depth profiles being measured. Microstructures in both the as-implanted and annealed samples are also being examined using STEM.

3.4 **Irradiation Creep of Near-Stoichiometric Silicon Carbide Fibers —** T. Koyanagi, K. Ozawa (Oak Ridge National Laboratory), T. Hinoki (Kyoto University), L.L. Snead, Y. Katoh (Oak Ridge National Laboratory) **109**

The neutron irradiation creep of near-stoichiometric SiC fibers was evaluated by bend stress relaxation (BSR) tests. The results indicate that the apparent stress exponent of the irradiation creep of the SiC fibers is near unity at ~500°C. The instantaneous creep compliance of the SiC fibers, which is the creep strain normalized to the applied stress and neutron flux, was estimated to be ~1×10^{-7} [MPa^{-1} dpa^{-1}] at ~6 dpa. The creep compliance values are orders of magnitude smaller than previously reported from light ion irradiation experiments. Quality of the fibers slightly affected the creep behavior: Hi-Nicalon™ Type S fiber showed more creep than other fibers, including Tyranno™ SA3, isotopically-controlled Sylramic™ and Sylramic™ iBN fibers at ~500°C to ~1 dpa.

3.5 **High Dose Neutron Irradiation of Hi-Nicalon Type S Silicon Carbide Composites, Part 1: Microstructural Evaluations** - A. G. Perez-Bergquist, T. Nozawa, C. Shih, K. J. Leonard, L. L. Snead, Y. Katoh (Oak Ridge National Laboratory) **116**

Extended abstract of a paper accepted by the Journal of Nuclear Materials.

4. **HIGH HEAT FLUX MATERIALS AND COMPONENT TESTING**

See also Section 4.3.

4.1 **Recent Progress in the Development of Ductile-Phase Toughened Tungsten for Plasma-Facing Materials –** C. H. Henager, Jr., R. J. Kurtz, T. J. Roosendaal, B. A. Borlaug, W. Setyawan, and K. B. Wagner (Pacific Northwest National Laboratory), G. R. Odette, K. H. Cunningham, K. Fields, D. Gragg, and F. W. Zok (University of California, Santa Barbara) **117**

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 crack bridging. To examine the prospect of DPT, W-Cu three-point bend samples were deformed at several strain rates and temperatures. Data from these tests are used for the calibration of a dynamic crack-bridging model that can effectively predict elevated temperature crack growth in W-composites. The development and initial testing of a Cu-ligament bridging model based on a micromechanical flow stress model of Cu is discussed. Good agreement with the 3-point bend testing data is demonstrated along with future plans to improve the model.

TABLE OF CONTENTS

4.2 **Recent Progress in the Fabrication and Characterization of Ductile-Phase-Toughened Tungsten Composites for Plasma-Facing Materials** –K. H. Cunningham, G. R. Odette, K. Fields, D. Gragg, and F. W. Zok (University of California, Santa Barbara), C. H. Henager, Jr., R. J. Kurtz, T. J. Roosendaal, and B. A. Borlaug (Pacific Northwest National Laboratory) **126**

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 crack propagation by bridging. Composite specimens were fabricated by two methods: 1) sintering W powders together with carburized W wires, and 2) hot pressing W and Cu foils together with W wires. These composites were tested in tension and three-point bending.

4.3 **Specimen Preparations for Mechanical Testing and Hydrogen Permeation of Nano W-1Ti-0.5TiC —** X. Wang and Z. Zak Fang (University of Utah) **132**

During the last reporting period, processing for making nano W with grain size near 100 nm was developed. The ongoing work in this reporting period is focused on evaluating mechanical properties and hydrogen permeation of the nano W alloys. So far, the specimen preparation for testing is being really difficult due to cracking problems during pressing and sintering, which originated from the special characteristics of the high energy milled nano W powders made in this project. Attempts have been made to make crack-free specimens for property evaluations of Nano W.

4.4 **Properties of Irradiated Tungsten and Recovery on Annealing** - L. Garrison, X. Hu (Oak Ridge National Laboratory), and M. Fukuda (Tohoku University, Japan) **136**

Samples of (110) single crystal tungsten (SCW) were irradiated in HFIR at 70 to 900°C and fast neutron fluences of 0.01 to 20 $\times 10^{25}$ n/m^2 at E>0.1 MeV. A subset of eleven samples from this group with fluences up to 7×10^{25} n/m^2 have been selected for the annealing study within the PHENIX collaboration. Hardness testing and positron annihilation spectroscopy (PAS) have been completed on unirradiated control samples. The irradiated samples are being polished in preparation for the upcoming tests.

4.5 **Mechanical Properties of Neutron Irradiated Tungsten** —L. L. Snead, L. M. Garrison, N.A.P. Kiran Kumar, T. S. Byun, M. R. McAlister, and W. D. Lewis (Oak Ridge National Lab) **140**

Tungsten samples of types [110] single crystal tungsten (SCW), [100] SCW, wrought tungsten foils, and annealed tungsten foils 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. Samples that were irradiated at 2×10^{25} n/m^2 and below were previously tensile and hardness tested at 300°C and below. In this period samples irradiated at 2×10^{25} n/m^2 and below at temperatures between 300 and 650°C were tensile tested at high temperatures. Annealed and wrought tungsten foils were hardness tested. A sample irradiated to a dose of 2.2dpa at 725°C was analyzed in the TEM.

4.6 **High-Heat Flux Testing of Low-Level Irradiated Materials Using Plasma Arc Lamps** — A.S. Sabau, E.K. Ohriner, Y. Katoh, and L.L. Snead (Oak Ridge National Laboratory) **146**

In this reporting period high-heat flux testing of six samples, which were supplied by the Japanese collaborators in the PHENIX program, was conducted at ORNL in collaboration with Dr. Kazutoshi Tokunaga of Kyushu University, Japan. As part of the joint US/Japan PHENIX program, Dr. Tokunaga was on assignment at ORNL for four weeks. During this high-heat flux testing, several fixtures for specimen clamping were evaluated for their performance.

TABLE OF CONTENTS

4.7 **Characterization of Thermomechanical Damage on Tungsten Surfaces During Long-Duration Plasma Transients** - D. Rivera, A. Sheng, T. Crosby, N.M. Ghoniem (University of California, Los Angeles) **156**

Extended Abstract of an ICFRM-16 paper accepted for J. Nucl. Mater.

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** - K.J. Leonard, T. Aytug, Fred. A List III, Yanwen Zhang (Oak Ridge National Laboratory),A. Perez-Bergquist, W.J. Weber (University of Tennessee), A. Gapud, N.T. Greenwood, J.A. Alexander and A. Khan (University of South Alabama) **159**

During this reporting period, electrical characterization work was completed on the ion irradiated superconducting films. Detailed electrical characterization of the materials response was performed at the University of South Alabama. This contribution highlights results of a forthcoming paper concluding the electrical characterization of the ion irradiated materials. Based on this work, the Zr-doped (Y,Gd)$Ba_2Cu_3O_{7-x}$ and (Dy,Y)$Ba_2Cu_3O_{7-x}$ (DyBCO) materials were selected for neutron irradiation studies. Ion irradiation results for the $GdBa_2Cu_3O_{7-x}$ conductor did not show a significant improvement over second-generation YBCO materials in terms of J_c improvement with irradiation. However, irradiated T_c remained higher than for YBCO. The neutron irradiation exposures are being planned for the July-August 2014 cycle at HFIR. Information on the irradiation capsules and preliminary results will be included in the next semi-annual report.

5.2 **Irradiation Effects on Microstructure and Optical Performance of Multilayered Dielectric Mirrors -** N.A.P. Kiran Kumar, K.J. Leonard, G.E. Jellison and L.L. Snead (*Oak Ridge National Laboratory)* **168**

Specifically engineered Al_2O_3/SiO_2 and HfO_2/SiO_2 dielectric mirrors grown on sapphire substrates and exposed to neutron doses of 1 and 4 dpa at 458±10 K in the High Flux Isotope Reactor (HFIR), resulted in reductions in optical reflectance, indicating a failure of the multilayer coating. HfO_2/SiO_2 mirrors failed completely when exposed to 1 dpa, whereas the reflectivity of Al_2O_3/SiO_2 mirror reduced to 50%, eventually failing at 4 dpa. Transmission electron microscopy (TEM) observation of the Al_2O_3/SiO_2 specimens showed defects increase in size with irradiation dose from 1 to 4 dpa. Heavy interdiffusion leading to formation of Al-Si rich phase and cracking of some of Al_2O_3 layers was observed across the Al_2O_3/SiO_2 mirrors; however the interdiffusion is less evident in HfO_2/SiO_2 mirrors. Delamination at the interface between the substrate and first layer was typically observed in both 1 and 4 dpa HfO_2/SiO_2 specimens, where buckling type delamination was a major observation at all doses.

6. **FUSION CORROSION AND COMPATIBILITY SCIENCE**

6.1 **Liquid Metal Compatibility** — S. J. Pawel (Oak Ridge National Laboratory) **178**

Operation of the first thermal convection loop (TCL) using dispersion strengthened FeCrAl (Kanthal APMT) tubing and specimens was completed in this reporting period. The working fluid in the TCL was eutectic Pb-17at%Li, and the peak temperature (550˚) and temperature gradient (116˚C) was maintained without interruption for 1000 h. When operation was terminated, a problem with

TABLE OF CONTENTS

complete draining of the Pb-Li from the loop was encountered, which delayed retrieval of specimens exposed in the hot leg of the TCL; however, analysis of specimens from the cold leg has been initiated.

7. MECHANISMS AND ANALYSIS

7.1 Effects of Ion Irradiation on BAM-11 Bulk Metallic Glass – A. G. Perez-Bergquist[1,2], J. Brechtl[2], H. Bei[1], Y. Zhang[1,2] and S. J. Zinkle[1,2] (*[1]Oak Ridge National Laboratory, [2]University of Tennessee)* **184**

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. Microstructural and mechanical property evaluations have been performed on as-cast and heat-treated $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ bulk metallic glass (BAM-11) irradiated with 3 MeV Ni^+ ions to 1 and 10 dpa. TEM showed no evidence of radiation damage or crystallization following ion irradiation, and changes in hardness and Young's modulus were 10-15%. In addition, irradiation-induced damage was seen to saturate at or below the 1 dpa dose level.

7.2 Effects of Neutron Irradiation on Ti-Si-C Max-Phase Ceramic Microstructures – A. G. Perez-Bergquist[1,2], Y. Katoh[1], C. Shih[1], and S. J. Zinkle[1,2] (*[1]Oak Ridge National Laboratory, [2]University of Tennessee)* **189**

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 samples containing MAX phase Ti_3SiC_2 after neutron irradiation to 3.4 and 5.0 dpa at temperatures of 500 and 800°C. Ti_3SiC_2 in the 500°C sample appeared to decompose into TiC under irradiation, whereas the Ti_3SiC_2 in the 800°C sample did not. Limited radiation damage was visible in the 800°C sample.

7.3 Effects of Helium-DPA Interactions on Cavity Evolution in Tempered Martensitic Steels Under Dual Ion-Beam Irradiation - Takuya Yamamoto, Yuan Wu, G. Robert Odette (University of California Santa Barbara), Sosuke Kondo, Akihiko Kimura (Kyoto University) **194**

Cavity evolution in normalized and tempered martensitic steel (TMS) F82H under Fe^{3+} and He^+ dual ion beam irradiation (DII) at 500°C was characterized over a wide range of dpa, He and He/dpa. Transmission electron microscopy (TEM) showed that DII up to ≈ 60 dpa and ≈ 2400 appm He produced a significant population of non-uniformly distributed cavities with bimodal sizes, ranging from ≈ 1 nm He bubbles to ≈ 20 nm faceted voids, resulting in observed swelling of up more than 3%. The incubation dpa for the onset of void swelling decreased linearly with increasing He/dpa in both IEA and mod.3 heats of F82H.

7.4 Effects of Helium Atoms on the Strength of BCC Fe Grain Boundaries – Xiaoxun Zhang, Jiansha Ji, Fang Ma (Shanghai University of Engineering Science), G. R. Odette (University of California Santa Barbara), R. J. Kurtz, F. Gao (Pacific Northwest National Laboratory) **201**

The effects of helium atoms and the formation of helium clusters on Σ3 <110> {111}, Σ3 <110> {112} and Σ5 <100> {310} symmetric tilt GBs in bcc iron were studied by the molecular dynamics simulation method. We found that helium atoms are deeply trapped at the GBs during annealing at 300 K, and that two or more helium atoms aggregate to form a small helium clusters. The helium

TABLE OF CONTENTS

atom and small clusters act as a failure initiation site under uniaxial straining. We show that helium atoms decreases cohesive strength and ductility of all the grain boundaries in bcc Fe that were studied.

8. MODELING PROCESSES IN FUSION SYSTEM MATERIALS

8.1 Influence of Mass on Displacement Threshold—W. Setyawan, A. P. Selby, G. Nandipati, K. J. Roche, R.J. Kurtz (Pacific Northwest National Laboratory, Richland, WA 99352) and B. D. Wirth (University of Tennessee, Knoxville, TN 37996) **209**

Molecular dynamics simulations are performed to investigate the effect of mass on displacement threshold energy in Cr, Mo, Fe and W. For each interatomic potential, the mass of the atoms is varied among those metals for a total of 16 combinations. The average threshold energy over all crystal directions is calculated within the irreducible crystal directions using appropriate weighting factors. The weighting factors account for the different number of equivalent directions among the grid points and the different solid angle coverage of each grid point. The grid points are constructed with a Miller index increment of 1/24 for a total of 325 points. For each direction, 10 simulations each with a different primary-knock-on atom are performed. The results show that for each interatomic potential, the average threshold energy is insensitive to the mass; i.e., the values are the same within the standard error. In the future, the effect of mass on high-energy cascades for a given interatomic potential will be investigated.

8.2 Implementation of First-Passage Time Approach for Object Kinetic Monte Carlo Simulations of Irradiation—G. Nandipati, W. Setyawan, H. L. Heinisch, K. J. Roche, R. J. Kurtz (Pacific Northwest National Laboratory) and B. D. Wirth (University of Tennessee) **213**

This is a work in progress and in this report we present basic implementation details of the first-passage time (FPT) approach to deal with very fast 1D diffusing SIA clusters in *KSOME* (kinetic simulations of microstructural evolution) and the status of its development.

8.3 An Initial Atomistic-Based Equation of State for Helium in Iron - R. E. Stoller and Y. N. Osetskiy (Oak Ridge National Laboratory) **217**

An equation of state that accurately reproduces the pressure-volume relationship of helium is necessary to understand and predict the behavior of He-vacancy defects in irradiated materials. We have used *ab initio* calculations to determine the energetics of helium-vacancy clusters and applied the results to develop a new three-body interatomic potential that describes the behavior of helium in iron. The potential was employed in molecular dynamics simulations to determine the conditions for mechanical equilibrium between small helium-stabilized bubbles and an iron matrix, and to systematically map the pressure-volume relationship for the bubbles at a range of temperatures. These atomistic results are compared to an existing equation of state and a modification is proposed for bubbles with high helium densities.

8.4 A Stochastic Nonlinear Differential Equations Approach to the Solution of the Helium Bubble Size Distribution in Irradiated Metals - D. Seif (University of California, Los Angeles), N.M. Ghoniem (University of California, Los Angeles) **224**

Extended Abstract of an ICFRM-16 paper submitted to J. Nucl. Mater.

TABLE OF CONTENTS

8.5 **Atomistic Studies of Growth of Helium Bubbles in α-Fe—**F. Gao, L. Yang, and R. J. Kurtz (Pacific Northwest National Laboratory) **226**

Experimental results and atomistic simulations demonstrate that nucleation and growth of He bubbles in α-Fe will contribute to embrittlement and is a significant material problem for development of fusion power. Understanding the nucleation growth of He bubbles in steels is one of the most important issues in nuclear fusion technology. In order to understand the formation and evolution of self-interstitials (SIAs) caused by He bubble growth under He-rich/vacancy-poor conditions, the clustering of He and growth of He bubbles in bulk Fe is currently being investigated by inserting He atoms one by one into one or two He clusters. We find that a 1/2 <111> dislocation loop is formed and eventually punched out by a single He cluster, but when two He clusters are present the configuration of the SIA loop formed depends on the distance between the two He clusters. A <100> cluster is created when the distance between the He clusters is less than about $6a_0$ and eventually grows into a <100>{100} dislocation loop.

8.6 **Relative Stability of Helium and Hydrogen in Nano-Structured Ferritic Alloys** – B. Tsuchiya, T. Yamamoto, G. R. Odette, (University of California, Santa Barbara); K. Ohsawa (Kyushu University) **232**

First principle calculations were carried out for tetrahedral- and octahedral-interstitial sites in $Y_2Ti_2O_7$, and tetrahedral- and octahedral-interstitial as well as substitutional sites in Fe, in order to assess the energetics of He and H in Fe containing $Y_2Ti_2O_7$. The formation energies of He at tetrahedral- and octahedral-interstitial sites in $Y_2Ti_2O_7$ were 1.59 and 1.02 eV, respectively, which were much lower than the corresponding energies (4.47, 4.67, and 2.23 eV) in tetrahedral-, octahedral-interstitial and substitutional sites in Fe. On the other hand, the formation energies of H at tetrahedral- and octahedral-interstitial sites in $Y_2Ti_2O_7$ were 2.87 and 3.01 eV, respectively, which are much higher than the corresponding energies (0.11, 0.24, and 0.41 eV) at tetrahedral-, octahedral-interstitial and substitutional sites in Fe. Thus He and H in NFAs partition to the oxide and Fe, respectively.

8.7 **Strengthening Due to Hard Obstacles in Ferritic Alloys-** Y. N. Osetskiy and R. E. Stoller (Oak Ridge National Laboratory) **238**

We have developed a molecular dynamics (MD) based model to simulated dislocation dynamics in the presence of rigid, impenetrable inclusions. These inclusions simulate rigid oxide particles as obstacles to dislocation motion. Interactions between a moving edge dislocation ½<111> {110} and rigid inclusions was modeled over a wide range of parameters such as inclusion size, temperature, strain rate and interaction geometry. It was found that the interaction mechanism depends strongly on the inclusion size and interaction geometry. Some new mechanisms were observed and are now under detailed investigation.

8.8 **Simulation of Triple Ion-Beam Irradiation in Fe Single Crystals Using Stochastic Cluster Dynamics** - Jaime Marian, Tuan Hoang (Lawrence Livermore National Laboratory) **242**

Helium and hydrogen are produced at rates of about 10 and 40 appm per dpa during fusion reactor operation. Although, the effects of He and H on microstructure are more or less well understood independently, their combined action under irradiation has not been established yet and the experimental evidence obtained over three decades of research is inconclusive. In recent years, electronic structure calculations have shed some light on the joint effect of He and H on defect cluster stability, and the associated energetics has begun to be used in long-term models of damage accumulation. In this work, we present stochastic cluster dynamics (SCD) simulations of triple (Fe/He/H) ion beam irradiations of pure single crystal Fe. With SCD we can perform

TABLE OF CONTENTS

simulations of multiple damage species up to doses beyond the 1-dpa limit. We calculate the amount of swelling as a function of temperature and point to the limitations of the He/H interaction model by comparing and discussing the experimental data.

8.9 **Molecular Dynamics Modeling of Atomic Displacement Cascades in 3C-SiC** – G. D. Samolyuk, Y. N. Osetskiy and R. E. Stoller (Oak Ridge National Laboratory) **252**

We demonstrated that the most commonly used interatomic potentials are inconsistent with *ab initio* calculations of defect energetics. Both the Tersoff potential used in this work and an alternate modified embedded atom method potential reveal a barrier to recombination which is much higher than the density functional theory (DFT) results. The barrier obtained with a newer potential by Gao and Weber is closer to the DFT result but the overall energy landscape is significantly different. This difference results in a significant difference in the cascade production of points defects. We have completed both 10 keV and 50 keV pka energy cascade simulations in SiC at temperatures equal to 300, 600, 900 and 1200 K. Results were obtained for the number of stable point defects using the Tersoff/ZBL and Gao-Weber/ZBL (GW) interatomic potentials. In a contrast to Tersoff potential, the GW potential produces almost twice as many C vacancies and interstitials at the time of maximum disorder (~0.2 ps) but only about 25% more stable defects at the end of the simulation. Only about 20% of the carbon defects produced with the Tersoff potential recombine during the in-cascade annealing phase, while about 60% recombine with the GW potential. The GW potential appears to give a more realistic description of cascade dynamics in SiC, but still has some shortcomings when the defect migration barriers are compared to the *ab initio* results.

8.10 **First-Principles Calculations of Charge States and Formation Energies of Mg, Al, and Be Transmutants in 3C-SiC** – S.Y. Hu, W. Setyawan, W. Jiang, C. H. Henager, Jr. and R. J. Kurtz (Pacific Northwest National Laboratory) **258**

The Vienna Ab-initio Simulation Package (VASP) is employed to calculate charge states and the formation energies of Mg, Al and Be transmutants at different lattice sites in 3C-SiC. The results provide important information on the dependence of the most stable charge state and formation energy of Mg, Al, Be and vacancies on electron potentials.

9. **IRRADIATION METHODS, EXPERIMENTS, AND SCHEDULES**

9.1 **Fusion Materials Irradiation Test Station (FMITS) at SNS** – Mark Wendel, Phil Ferguson (ORNL) **262**

FMITS irradiations at SNS would occur on samples welded inside an 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.

The deliverables for the FY14 funding from OFES have all been met:

1. A review of the 30% design for FMITS was conducted on June 2-3,
2. The feasibility study report was completed July 1, 2014, and
3. The preliminary safety assessment was completed July 1, 2014.

The 30%-design review committee found that the FMITS design was feasible in that all of the

TABLE OF CONTENTS

technical and safety issues were addressed at a level appropriate for a 30% design. Specific recommendations were addressed in the feasibility study report appendices.

Other highlights of the FMITS 30% design progress during the past 6 months include a completed preliminary seal mock-up test, improved remote handling tooling and procedures, and a completed project resource-loaded schedule and contingency analysis.

9.2 HFIR Irradiation Experiments – June 30, 2014 **265**