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1. FERRITIC/MARTENSITIC STEEL DEVELOPMENT

See also Sections 2.5, 8.4, and 8.5.

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

The radiation resistance of TaC, TaN, and VN MX-type nanoprecipitates is being evaluated using Fe^{2+} ion irradiation at 500°C for nominal doses of ~20 and ~200 dpa. A parallel study using neutron irradiation at 300, 500, and 650°C for up to about 20 dpa is also in progress. The characterization and analyses of the low dose (~20 dpa) Fe^{2+} ion irradiated samples have been completed. The results indicate that the irradiation did not alter the crystalline nature of the nanoprecipitates. Particle dissolution, growth, and reprecipitation in different levels were observed after the irradiation. The radiation resistance of the carbide was much stronger than the nitrides in declined order TaC, VN, and TaN. TaC nanoprecipitates were observed to be much more resistant to irradiation than reported for a study using similar irradiation conditions. Post-irradiation examination of the high dose (~200 dpa) Fe^{2+} ion-irradiated and neutron-irradiated samples will be conducted and compared to the current observations.

1.2 Recent Observations of Helium Effects on Cavity Evolution in Tempered Martensitic Steels — 6
T. Yamamoto, Y. Wu, G. R. Odette, (University of California, Santa Barbara); S. Kondo, and A. Kimura (Kyoto University)

New dual ion (Fe^{3+} and He^{+}) beam irradiations (DII) were performed at 500°C on a group of ferritic alloys up to nominal dpa and He levels of 26 dpa and 390 appm, respectively, at a He (appm)/dpa ratio of ≈ 15 using the DuET facility at Kyoto University in Japan. The actual dpa, He and He/dpa vary with depth in the sample. The alloys studied include normalized and tempered martensitic steels, (TMS) F82H IEA in as-tempered and cold-worked conditions as well as F82H mod.3, and a nanostructured ferritic alloy (NFA), MA957. To date, TEM observations have been performed for F82H mod.3 at depths from 0.1 to 1.7 mm. In the F82H mod.3, the number density of the cavities (N) ranged from 1 to 9 x $10^{21}/m^3$ while average diameter (<d>) of all the cavities ranged from 2.4 to 5.5 nm. The N are significantly smaller than that for higher ≈ 47 appm He/dpa in previous study, while the <d> are similar.

2. ODS AND NANOCOMPOSITED ALLOY DEVELOPMENT

See also Sections 7.3 and 7.4.

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2.1 Characterization of a Larger Best Practice Heat of 14YWT in Annealed Powder, HIP Consolidated and Extruded Forms — 15

N. J. Cunningham, Y. Wu, G. R. Odette, (University of California, Santa Barbara); D. T. Hoelzer, (Oak Ridge National Laboratory); and S. A. Maloy (Los Alamos National Laboratory)

We describe the characterization of new 14YWT heats from gas atomized and mechanically alloyed powder using an alternative processing method that incorporates Y during the gas atomization process. Post mechanically alloying processes included annealing the powder at 850ºC and 1150ºC, HIP consolidation at 850ºC and 1150ºC, and consolidation by hot extrusion at 850ºC, annealing for 1 h at 1000ºC, and then cross-rolling to 50% thickness at 1000ºC; the latter has been dubbed FCRD-NFA1. In all cases a high number density of nm-sized features were observed using a combination of atom probe tomography, transmission electron microscopy, and small angle neutron scattering. The 850ºC lower temperature annealing and HIP consolidation resulted in smaller precipitates compared to the 1150ºC processing temperature. However, after annealing at 1200ºC for 48 h the precipitate size and number density were similar in the two cases. The FCRD-NFA1 had a microstructure and NF distribution similar to a previously reported alloy, PM2. However, the extruded samples also had a large number of large (>20 nm) Ti-rich precipitates. These larger precipitates may affect the mechanical properties, which are currently under investigation.

2.2 Development of ODS FeCrAl for Fusion Reactor Applications — 27

B. A. Pint, D. T. Hoelzer, and K. A. Unocic (Oak Ridge National Laboratory)

Several additional isothermal Pb-Li capsule tests of cast FeCrAlY specimens were completed at 700°C in order to further guide alloy selection. Characterization of specimens after exposure indicated that the Cr and Al contents remain relatively constant near the exposed surface and that LiAlO2 formed on the surface of all of the exposed alloys. In general, the results suggest that the Al content needs to be near 5 wt.% for excellent Pb-Li compatibility. Based on this information, several powder compositions were procured and have now been received and analyzed. These powders are now being milled to produce the first batches of ODS FeCrAl for evaluation.

2.3 TEM Characterization of a Simultaneously Neutron-Irradiated and Helium-Injected PM2000 ODS Alloy — 31

H. J. Jung, D. J. Edwards, R. J. Kurtz, (Pacific Northwest National Laboratory); G. R. Odette, and T. Yamamoto (University of California, Santa Barbara)

TEM examination of a simultaneously neutron-irradiated and He-injected PM2000 ODS alloy was performed. The He implanted region had a high density of <2 nm He bubbles largely associated with matrix dislocation loops. Nearly all ODS particles had a single faceted void attached to them that was from 5 to 15 nm. On the non-implanted side, no He bubbles were seen, and faceted voids were found on ~10% of the ODS particles. The He-implanted side has both <100>{100} and ½<111>{111} dislocation loops and a low density of line dislocations, while the un-implanted side has mostly line dislocations and a lower

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density of dislocation loops. In both regions, nanoscale fcc precipitates having a cube-on-cube orientation relationship with the matrix were observed. EDS measurements indicate this phase is rich in Al and Ti. Substantial Cr segregation occurs around the dislocation loops, concurrent with Fe depletion. The precipitates do not appear to be associated with the loops or line dislocations. The ODS particles, which are all amorphous, contain >20 at% Al, and show Cr segregation/Fe-depletion at their periphery.

2.4 **The Association Relationships Among Bubbles, Precipitates, and Grain Boundaries in Dual Beam Irradiated Nano-Structured Ferritic Alloys —** **42**
Y. Wu, T. Yamamoto, N. Cunningham, G. R. Odette, (University of California, Santa Barbara); S. Kondo, and A. Kimura (University of Kyoto, Japan)

Transmission electron microscopy (TEM) was used to characterize the associations between various microstructural features, including helium bubbles, in nanostructured ferritic alloys, following dual ion irradiations at 650°C. Almost all of the nm-scale oxide precipitates are associated with one and, in some cases a few, interface bubbles. The distribution of precipitates and bubbles along dislocations and small angle grain boundaries are not significantly different than in the matrix. However, the precipitates on large angle grain boundaries are larger and often associated with more bubbles.

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2.5 **Friction Stir Welding of ODS Steels and Advanced Ferritic Structural Steels** —
Z. Feng, Z. Yu, D. Hoelzer, M. A. Sokolov, and L. T. Tan (Oak Ridge National Laboratory)

Initial friction stir trial welds were made on ODS alloy MA965, RAFM steels EUROFER97 and F82H, and between MA956 and EUROFER97 (dissimilar weld). Defect-free similar and dissimilar welds were obtained. The microstructure of the welded region was characterized using optical microscopy (OM) and small-angle neutron scattering (SANS). OM examination showed that the microstructures in the stir zone (SZ), thermo-mechanically affected zone (TMAZ) and heat affect zone (HAZ) were significantly different from these in the base metal (BM). Small angle neutron scattering measurements were performed in the base metal and welded region to characterize the changes in nano-scale oxide features. Aggregation of the fine nano-scale particles was observed in the SZ. Micro-hardness mapping on the cross section of welds clearly revealed the effects of FSW.

3. **CERAMIC COMPOSITE STRUCTURAL MATERIAL DEVELOPMENT**

See also Sections 8.2 and 8.3.

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3.1 Swelling and X-Ray Peak Broadening of High Dose Neutron Irradiated SiC Composites — 61

C. Shih, R. Meisner, Y. Katoh, and L. L. Snead (Oak Ridge National Laboratory)

The lattice parameter changes in high dose (up to ~70 dpa) neutron irradiated nuclear grade SiC/SiC composites were studied with room temperature powder XRD and compared with macroscopic dimensional changes at nominal irradiation temperatures of 300, 500 and 800°C. The results show no lattice parameter change for all high dose neutron irradiated SiC/SiC composites while macroscopic volume swelling is observed. This observation agrees with the very limited literature data on XRD studies of high dose CVD SiC and high dose hot pressed SiC. The lattice parameter changes disagree with macroscopic dimensional changes, suggesting progressive evolution of microstructures involving transition of ultra-fine interstitial clusters into larger interstitial loops as the very high irradiation doses are achieved. However, the errors in lattice parameter measurements caused by high surface roughness of the unpolished composites remains an issue and need to be further studied.

3.2 Properties of Defects and Implants in Mg^+ Implanted Silicon Carbide — 70

W. Jiang, Z. Zhu, T. Varga, M. E. Bowden, S. Manandhar, T. Roosendaal, S. Y. Hu, C. H. Henager, Jr., R. J. Kurtz, (Pacific Northwest National Laboratory); and Y. Wang (Los Alamos National Laboratory)

Implantation of 3C-SiC, 6H-SiC and CVD-SiC has been performed with 200 keV Mg^+ ions to fluences up to 3.2×10^{16} ions/cm^2 at 773 K. Rutherford backscattering analyses of the as-produced damage states along multiaxial channeling directions indicate that there are interstitial-type defect configurations that are well aligned with the <100> axis, such as Si-Si <100> interstitial splits. The depth profile of the as-implanted Mg exhibits a Gaussian-like distribution without evidence of considerable diffusion-driven mass transport during implantation. A post implantation thermal annealing study shows that there is a significant recovery of the structural defects with essentially immobile Mg in SiC up to 1473 K. Further annealing at higher temperatures is currently in progress with intent to recover implantation damage to the maximum extent possible while retaining Mg implants in the sample. Characterizations will follow using spectroscopy and microscopy to study microstructure and Mg behavior in SiC.

3.3 EMTA Thermal Conductivity Predictions for Unirradiated and Irradiated SiC/SiC Composites — 76

B. N. Nguyen, C. H. Henager, Jr., and R. J. Kurtz (Pacific Northwest National Laboratory)

This study first applied an Eshelby-Mori-Tanaka approach implemented in PNNL's EMTA software to predict thermal conductivities of unirradiated 2D SiC/SiC composites. The EMTA homogenization method is structured in three steps to capture the effects of the constituent materials including the pyrolytic carbon (PyC) fiber coating on the thermal conductivities of as-formed composites. EMTA also applies an iterative reverse engineering procedure to identify an unknown constituent material thermal conductivity.

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EMTA reverse engineering was shown to be efficient and accurate to compute the thermal conductivities of the SiC matrix and of the fiber coating as functions of temperature, and consequently, to achieve better agreement between the predicted and experimental thermal conductivities for the composites. Next, a new method that builds on EMTA to estimate the thermal conductivity of SiC/SiC composites subjected to neutron irradiation at elevated temperature up to a dose of 10 dpa was developed. This method considers the irradiation-induced conductivity degradation behavior of chemical vapor deposited (CVD) SiC and defines an equivalent CVD-SiC material with an equivalent pore content to estimate the thermal conductivity of a SiC/isothermal-chemical-vapor-infiltration (ICVI)-SiC composite. It was shown that the proposed method effectively mimics the irradiation effect that induces the reduction of composite thermal conductivity.

3.4 Process Development and Optimization for Silicon Carbide Joining and Irradiation Studies-II — **81**
T. Koyanagi, J. O. Kiggans, T. Cheng, and Y. Katoh (Oak Ridge National Laboratory)

The candidate joining methods for SiC ceramics and composites in the ongoing work to develop and optimize performance in neutron irradiation environments include chemically vapor-deposited (CVD) SiC bonded by the NITE (nano-infiltration and transient eutectic-phase) – like processes, diffusion bonding utilizing active titanium or molybdenum inserts, and transient eutectic-phase-assisted bonding with yttria-alumina-garnet (YAG) solder. In previous work the optimal processing conditions for Ti foil joining have been established. During the present reporting period, joint specimens with high shear strength were successfully produced through the active Mo metal insert methods, and then evaluated for as-fabricated properties.

3.5 Low Activation Joining of SiC/SiC Composites for Fusion Applications: Tape Casting TiC+Si Powders — **91**
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 of 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 this joint for the TITAN collaboration in order to produce optimal joints to undergo irradiation studies in HFIR. One noted feature of the joints produced using tape-calendared powders of TiC+Si has been the large void regions that have been apparently unavoidable. Although the produced joints are very strong, these voids are undesirable. In addition, the tapes that were made for this joining was produced about 20 years ago and was aging. Therefore, we embarked on an effort to produce some new tape cast powders of TiC and Si that could replace our aging tape calendared materials.

4.0 HIGH HEAT FLUX MATERIALS AND COMPONENT TESTING

See also Sections 8.6, 8.7, and 8.8.

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4.1 Recent Progress in the Development of Ductile-Phase Toughened Tungsten for Plasma-Facing Materials — 95
K. H. Cunningham, K. Fields, D. Gragg, F. W. Zok, (University of California, Santa Barbara); C. Henager, R. Kurtz, and T. Roosendaal (Pacific Northwest National Laboratory)

Fracture testing was performed on notched and pre-cracked specimens of a W - 28w% Cu plate at room temperature and at 679K, as a follow-up to previous work. An order-of-magnitude toughness increase from that of monolithic tungsten was observed as a result of ductile Cu bridging. Pure W samples were consolidated from elemental powder using spark plasma sintering, achieving a maximum of 95.2% of the theoretical density. Commercially available tungsten wire was tested in tension, showing significant ductility and strength. The tungsten wire was plated with copper using electrodeposition, and continuing research will investigate methods of incorporating the Cu-coated W wire into a consolidated W matrix using spark plasma sintering. We expect the addition of ductile W wire to provide significant toughening compared to monolithic W, with the Cu coating preventing the wire from strongly bonding to the matrix.

4.2 Effect of Green Density and Fast Sintering on Grain Growth of Nano W — 108
X. Wang and Z. Z. Fang (University of Utah)

Two novel processing techniques were developed for inhibiting the grain growth of W during sintering of nano W and W alloy powders; one of which is a hot-pressing green compaction technique for increasing the relative density of green compacts of the nano powders. The second is a fast sintering technique for applying a combination of rapid heating and high pressure during sintering. Nano W and W-TiC powders were used to investigate the effect of green density and fast sintering on grain growth. The following preliminary results were obtained:

(1) The maximum obtainable green density of cold-pressed samples was 38% of the theoretical full density at 800 MPa, while the hot-pressed sample exhibited an 18% increase in green density (56% TD).
(2) Higher green density enabled the samples to be fully sintered at lower temperature.
(3) Near fully dense bodies with a grain size smaller than 300 nm were obtained via fast sintering.

4.3 Electron –Beam Additive Manufacturing of Tungsten Materials for Fusion — 114
E. K. Ohriner, R. Dehoff, and L. L. Snead (Oak Ridge National Laboratory)

Initial experiments were performed with the ARCAM A2 electron beam additive manufacturing unit using standard beam deflection conditions. Local regions were observed with the desired microstructure of a solid tungsten surface layer and a liquid phase sintered boundary layer of tungsten particles in a steel matrix. A new ARCAM unit is currently being installed for use in future experiments.

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4.4 High-Heat Flux Testing of Low-Level Irradiated Materials Using Plasma Arc Lamps — 117
A. S. Sabau, E. K. Ohriner, Y. Katoh and L. L. Snead (Oak Ridge National Laboratory)

The Research Safety Summary (RSS) was approved for high-heat flux testing of irradiated specimens. The radiation safety during high-heat flux testing was enhanced by the installation of a digital flow meter on the outlet part of the rod cooling circuit in order to monitor the flow rate during high-heat flux testing. One of the most difficult tasks is the measurement of sample temperature. The best data on sample temperature was obtained using a thermocouple welded to the sample during the high-heat flux testing. A pyrometer was used to measure the surface temperatures on either the specimen holder or the specimen. It was found that at high IR energies the pyrometer data is affected by the infrared energy from the PAL. Thus calibration runs are needed in order to enhance the accuracy of the pyrometer data.

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 — 125
K. J. Leonard, T. Aytug, F. A. List III, (Oak Ridge National Laboratory); A. Perez-Bergquist, W. J. Weber, (University of Tennessee); and A. Gapud (University of South Alabama)

The irradiated superconducting properties of Zr-doped $(Y,Gd)Ba_2Cu_3O_{7-x}$, $(Dy,Y)Ba_2Cu_3O_{7-x}$ and $Gd_2Ba_2Cu_3O_{7-x}$ are being evaluated for 5 MeV Ni, and 25 MeV Au irradiations to fluences between 10^{11} and 10^{12} ions/cm^2. For low fluence irradiations, small decreases were observed in the critical current for a-b pinning in both the $GdBa_2Cu_3O_{7-x}$ and $(Dy,Y)Ba_2Cu_3O_{7-x}$ conductors, but increased pinning at other angular orientations, decreasing angular field isotropy. The 10^{12} cm^{-2} 25 MeV Au irradiated $(Dy,Y)Ba_2Cu_3O_{7-x}$ did show a reduction in critical current, J_c, for externally applied magnetic fields of less than 7 Tesla for tests conducted at 77 K. However, at higher field strengths the irradiated J_c values exceed that of the unirradiated material. Properties of the Zr-doped $(Y,Gd)Ba_2Cu_3O_{7-x}$ conductor also show positive results following low fluence 5 MeV Ni and 25 MeV Au irradiation, where increases in a-b pinning are observed over the control samples.

5.2 High Neutron Dose Irradiation of Dielectric Mirrors — 135
K. L. Leonard, G. E. Jellison, Jr., N. A. P. Kiran Kumar, and L. L. Snead (Oak Ridge National Laboratory)

HfO_2/SiO_2 and Al_2O_3/SiO_2 dielectric mirrors show impressive resistance to neutron irradiation to 0.1 dpa. However, for the HfO_2/SiO_2 mirror the neutron dose causes crystallinity changes in the film layers of the mirrors and substrate resulting in decreases in reflectivity of the HfO_2/SiO_2 mirror following post irradiation annealing. Cooling following annealing resulted in delamination. Al_2O_3/SiO_2 mirrors appear to have added stability with little microstructural and optical property changes in samples irradiated up to 0.1 dpa and

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annealed to 673 K. However significant Si and Al interdiffusion cause compositional variation that will eventually result in the formation of aluminum-silicate structures on the layer interface, disrupting the optical properties.

Optical tests of samples irradiated to 1 and 4 dpa during the first half of 2013 confirmed that both the HfO_2/SiO_2 and Al_2O_3/SiO_2 do not survive exposure to 4 dpa, resulting in film delamination. Microstructural evaluations of the 4-dpa samples are now being performed to verify and build upon the low dose results.

6. FUSION CORROSION AND COMPATIBILITY SCIENCE

See also Section 2.2.

6.1 Liquid Metal Compatibility – A Thermal Convection Loop for Pb-Li Compatibility Testing — **142**
S. J. Pawel, A. W. Willoughby, M. S Stephens, Z. M. Burns, B. A. Pint, and J. D. McNabb (Oak Ridge National Laboratory)

Fabrication of the first Pb-Li thermal convection loop has been completed. The loop was fabricated using dispersion strengthened FeCrAl (Kanthal APMT) tubing. This alloy is known for high strength and creep resistance at elevated temperature, and based on capsule testing, it is also anticipated to have excellent resistance to Pb-Li.

7. MECHANISMS AND ANALYSIS

7.1 Ion Irradiation Effects on High Entropy Alloy— **145**
N. A. P. Kiran Kumar[1,2*], K. J. Leonard [1], H. Bei[1], T. S. Byun[1], Y. Zhang[1,2], and S. J. Zinkle[1]
(Oak Ridge National Laboratory[1], University of Tennessee[2])

Preliminary microstructural and nanoindentation examinations have been performed on Fe-28%Ni-27%Mn-18%Cr high entropy alloy specimens irradiated with 3 MeV Ni ions at room temperature to 0.1 and 1 dpa and at 500°C to 1 and 10 dpa. The hardness in the ion irradiated region of the crystalline face centered cubic HEA samples increased rapidly with increasing dose at room temperature, from ~40% higher than the unirradiated value at 0.1 dpa to approximately double the unirradiated hardness at 1 dpa. The increase in the irradiated hardness was less pronounced for irradiations at 500°C, with values of 15-20% increase at 1 dpa and ~20% increase at 10 dpa. Microstructural characterization of the irradiated HEA specimens found small defect clusters after room temperature irradiation and larger defect clusters after 500°C irradiation; voids were not observed at any irradiation condition in the preliminary examination. After irradiation at 500°C, evidence of significant solute segregation was observed at grain boundaries and discrete precipitates were observed; precipitation was not observed in the room temperature irradiated samples. The grain boundary precipitates were highly enriched in Cr and Mn. Overall, the behavior of the high entropy alloy following irradiation at 500°C appears to be significantly different from the behavior observed in irradiated Fe-Cr-Ni austenitic alloys.

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7.2 Effects of Ion Irradiation on BAM-11 Bulk Metallic Glass — 154

A. G. Perez-Bergquist[1,2], H. Bei[1], Y. Zhang[1,2], and S. J. Zinkle[1] *([1]Oak Ridge National Laboratory, [2]University of Tennessee)*

Preliminary microstructural and nanoindentation examinations have been performed on BAM-11 (Zr-17.9%Cu-14.6%Ni-10%Al-5%Ti) bulk metallic glass (BMG) irradiated with 3 MeV Ni^+ ions to 0.1 and 1 dpa at room temperature and 200°C. Transmission electron microscopy (TEM) examination indicated the unirradiated and irradiated BMG samples were all fully amorphous with no evidence of nanoscale crystals. The hardness in the ion irradiated region of the BMG samples decreased by nearly 20% after irradiation at room temperature to 0.1 and 1 dpa, and decreased by ~25% and ~10%, respectively after irradiation at 200°C to 0.1 and 1 dpa. The elastic modulus of the irradiated samples decreased by ~10% after irradiation at room temperature to 0.1 and 1 dpa, and increased by ~10% and ~5%, respectively after irradiation at 200°C to 0.1 and 1 dpa. These results suggest that the BAM-11 bulk metallic glass may not have high intrinsic resistance to radiation-induced atomic rearrangements, i.e., the glass may not be in an optimized short-range order configuration for radiation damage stability.

7.3 The Effect of Deposition Rate, Miscut Angle and Orientation on $FeY_2Ti_2O_7$ Interfaces: Implications to the Development and Optimization of Nanostructured Ferritic Alloys — 162

T. Stan, Y. Wu, and G. R. Odette (University of California, Santa Barbara)

The smallest 2-3 nm features in nanostructured ferritic alloys (NFA) are $Y_2Ti_2O_7$ complex oxide cubic pyrochlore phase. The interface between the bcc Fe-Cr ferrite matrix and the fcc $Y_2Ti_2O_7$ plays a critical role in the stability, strength and damage tolerance of NFA. To complement other characterization studies of the actual nano-features, mesoscopic interfaces were created by electron beam deposition of a thin Fe layer onto {111} and {100} $Y_2Ti_2O_7$ bulk single crystal surfaces. Cross-section high resolution TEM was used to characterize details of the interfaces, which ranged from being atomically sharp to more diffuse interface zones that, in some cases, included a thin metallic oxide MO_x layer. The fast deposited polycrystalline Fe layer on the 5 degree miscut {111} $Y_2Ti_2O_7$ sample has the Nishiyama-Wasserman orientation relationship: $\{110\}_{Fe}||\{111\}_{Y2Ti2O7}$ and $<001>_{Fe}||<110>_{Y2Ti2O7}$. Fe grains on the well-oriented {111} $Y_2Ti_2O_7$ sample have nano-grains at the interface. The grains on the {100} $Y_2Ti_2O_7$ sample were {110} textured but had no in-plane orientation relationship with the sample. We recognize that the mesoscopic interfaces may differ from those of the embedded NF, but the former will facilitate characterization and investigations of the functionality of controlled interfaces, such as interactions with point defects and helium.

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7.4 **An Electron Energy Loss Spectroscopy Study of Helium Bubbles in Nanostructured Ferritic Alloys —** **172**
Y. Wu, R. G. Odette, T. Yamamoto, (University of California, Santa Barbara); J. Ciston, (Lawrence Berkeley National Laboratory); and P. Hosemann (University of California, Berkeley)

Here we compare a measurement of the helium content in bubbles with a model based on the capillary approximation and a high-pressure equation of state. Electron Energy-Loss Spectroscopy (EELS) measurements on bubbles were carried out using the TEAM 0.5 microscope at the National Center for Electron Microscopy and Lawrence Berkeley Laboratory (LBL). The EELS energy shift can be related to the helium atom density. The best estimate of the helium density was ≈ 61±2.8 He atoms/nm^3 for bubbles with radii of ≈ 1.36±0.3 nm. These results are reasonably consistent with a high pressure EOS assuming a simple capillary model and surface energy of 1.8 J/m^2.

8. **MODELING PROCESSES IN FUSION SYSTEM MATERIALS**

8.1 **Object Kinetic Monte Carlo Simulations of Microstructure Evolution —** **179**
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 have developed a flexible lattice-based object KMC code, *KSOME*, to simulate the evolution of point defects in metals created by particle irradiation. In principle, *KSOME* deals with the migration, emission, creation, transformation and recombination of all types of intrinsic point defects and their complexes. In addition, the interaction of these point defects with sinks such as dislocations, grain boundaries and free surfaces is also treated. *KSOME* is designed such that all the necessary information regarding the properties of defects such as type, size, location, orientation etc., and their diffusion-reaction processes, along with simulation parameters regarding the size, temperature and properties of the simulation cell, are provided via text-based input files. This gives *KSOME* the capability to simulate complex systems involving complex processes that have not been possible with previously developed OKMC codes.

8.2 **Molecular Dynamics Modeling of Atomic Displacement Cascades in 3C-SiC —** **184**
G. D. Samolyuk, Y. N. Osetskiy, and R. E. Stoller (Oak Ridge National Laboratory)

A set of atomic displacement cascades was simulated using the Tersoff and Gao-Weber [1] interatomic potentials for SiC. The types of created defects and their dynamics were analyzed. The validity of existing interatomic potentials was investigated by comparing typical point defect formation energies with first principles results.

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8.3 **First-Principles Calculations of Intrinsic Defects and Mg Transmutants in 3C-SiC —** **188**
S. Y. Hu, W. Setyawan, R. M. Van Ginhoven, W. Jiang, C. H. Henager, Jr., and R. J. Kurtz (Pacific Northwest National Laboratory)

This is an extended abstract for a paper submitted for publication in the Journal of Nuclear Materials [1].

8.4 **Molecular Dynamics Investigation of Helium Bubble Equation of State —** **190**
Y. N. Osetskiy and R. E. Stoller (Oak Ridge National Laboratory)

An extensive modeling program was launched earlier to model He-filled bubbles in Fe. We are studying bubbles of radius from 0.25 to 5.0nm with He-to-vacancy ratio from 0.1 to 2.0 over the temperature range 300-1000K. An unexpectedly long simulation time was found to be necessary to accurately determine the equilibrium properties of small bubbles.

8.5 **Dynamics of Defect-Loaded Grain Boundaries Under Shear Deformation in α-Fe —** **193**
L. Yang, F. Gao, H. L. Heinisch, and R. J. Kurtz (Pacific Northwest National Laboratory)

The defects produced in collision cascades will interact with microstructural features in materials, such as GBs and dislocations. The coupled motion of GBs under stress has been widely observed in simulations and experiments. Two symmetric tilt GBs with a common <110> tilt axis (Σ3 and Σ11) in bcc iron are used to investigate the coupled motion of GBs under shear deformation. Also, we have explored the effect of self-interstitial atoms (SIAs) loading on the GB motion, with different concentrations of interstitials randomly inserted around the GB plane. The simulation results show that the interstitial loading reduces the critical stress of the GB coupled motion for the Σ3 GB. Furthermore, the interstitials and vacancies are inserted randomly at the GB plane and at a distance of 1 nm away from the GB plane, respectively, to understand the self-healing mechanism of GBs under stress. The behavior of the defect-loaded GBs depends on the GB structure. The loaded interstitials in the Σ3 GB easily form <111> interstitial clusters that do not move along with the GB. The vacancies in the Σ3 GB impede the GB motion. However, the interstitials move along with the Σ11 GB and annihilate with vacancies when the GB moves into the vacancy-rich region, leading to the self-healing and damage recovery of the Σ11 GB.

8.6 **Displacement Cascade Simulation in Tungsten at 1025 K —** **200**
W. Setyawan, G. Nandipati, K. Roche, H. Heinisch, R. J. Kurtz, (Pacific Northwest National Laboratory) and B. D. Wirth (University of Tennessee, Knoxville)

Molecular dynamics simulation was employed to investigate the irradiation damage properties of bulk tungsten at 1025 K (0.25 melting temperature). A comprehensive data set of primary cascade damage was generated up to primary knock-on atom (PKA) energies 100 keV. The dependence of the number of surviving Frenkel pairs (N_{FP}) on the PKA energy (E) exhibits three different characteristic domains presumably related to the different cascade morphologies that form. The low-energy regime < 0.2 keV is

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characterized by a hit-or-miss type of Frenkel pair (FP) production near the displacement threshold energy of 128 eV. The middle regime 0.3 – 30 keV exhibits a sublinear dependence of log(N_{FP}) vs log(E) associated with compact cascade morphology with a slope of 0.73. Above 30 keV, the cascade morphology consists of complex branches or interconnected damage regions. In this extended morphology, large interstitial clusters form from superposition of interstitials from nearby damage regions. Strong clustering above 30 keV results in a superlinear dependence of log(N_{FP}) vs log(E) with a slope of 1.365. At 100 keV, an interstitial cluster of size 92 and a vacancy cluster of size 114 were observed.

8.7 **A Semi-Phenomenological Model for Dislocation Mobility in Tungsten —** **205**
D. Rivera, G. Po, T. Crosby, and N. Ghoniem (University of California at Los Angeles, UCLA)

The dependence of dislocation velocity in tungsten on the applied stress and temperature is investigated. A brief theoretical overview of the mechanisms of kink pair formation and the relationship to dislocation motion under stress is given. We then discuss the theory of phonon scattering and its influence on damping dislocation motion at stresses higher than a transition value, where kink nucleation ceases to control dislocation mobility. A general phenomenological framework is formulated, where semi-empirical equations for the dislocation velocity in tungsten are given.

8.8 **Helium Effects on Displacement Cascades in Tungsten —** **223**
W. Setyawan, G. Nandipati, K. Roche, H. Heinisch, R. J. Kurtz, (Pacific Northwest National Laboratory); and B. D. Wirth (University of Tennessee)

Molecular dynamics (MD) simulations were performed to investigate He effects on displacement cascades in W. Helium content, proportion of interstitial and substitutional He and temperature were varied to reveal the various effects. The effect of interstitial He on the number of self-interstitial atoms (SIAs) produced during cascade damage appears to be insignificant. However, interstitial He tends to fill a vacancy (V). Nevertheless, this process is less favorable than SIA-V recombination particularly when excess SIAs are present before a cascade. The efficiency of He filling and SIA-V recombination increases as temperature increases due to increased point defect mobility. Likewise, substitutional He is more susceptible to displacement during a collision cascade than W. This susceptibility increases towards higher temperatures. Consequently, the number of surviving V is governed by the interplay between displaced substitutional He and SIA-V recombination. The temperature dependence of these processes results in a minimum number of V reached at an intermediate temperature.

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

9.1 **HFIR Irradiation Experiments —** **228**
Y. Katoh and J. L. McDuffee (Oak Ridge National Laboratory)