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**FUSION MATERIALS
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FOREWORD

This is the thirty-ninth in a series of semiannual technical progress reports on fusion materials science activities supported by the Fusion Energy Sciences Program of the U.S. Department of Energy. This report focuses on research addressing the effects on materials properties and performance from exposure to the neutronic, thermal, and chemical environments anticipated in the chambers of fusion experiments and energy systems. This research is a major element of the national effort to establish the materials knowledge base of an economically and environmentally attractive fusion energy source. Research activities on issues related to the interaction of materials with plasmas are reported separately.

The results reported are the product of a national effort involving a number of national laboratories and universities. A large fraction of this work, particularly in relation to fission reactor irradiations, is carried out collaboratively with partners in Japan, Russia, and the European Union. The purpose of this series of reports is to provide a working technical record for the use of program participants, and to provide a means of communicating the efforts of fusion materials scientists to the broader fusion community, both nationally and worldwide.

This report has been compiled and edited under the guidance of R. L. Klueh and Teresa Roe, Oak Ridge National Laboratory. Their efforts, and the efforts of the many persons who made technical contributions, are gratefully acknowledged.

G. R. Nardella
Research Division
Office of Fusion Energy Sciences

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Fiber push-out test results indicate that neutron irradiation decreased both the interfacial debond shear strength and interfacial friction stress. The mechanism of interphase property decrease for the multilayer interphase composite is due primarily to the changing interfacial cracking path. The primary crack propagated within PyC before irradiation provided a very rough fiber surface, resulting in high interfacial shear properties. In contrast, the cracking at the comparatively smooth fiber/PyC interface upon irradiation significantly decreased the interfacial shear properties. The effects of irradiation-induced dimensional change, associated with microstructure and mechanical property changes, and irradiation creep need to be further investigated.

2.6 COATINGS AND JOINING FOR SiC/SiC COMPOSITES FOR NUCLEAR ENERGY SYSTEMS—C. H. Henager, Jr., and Y. Shin (Pacific Northwest National Laboratory), Y. Blum (SRI), L. A. Giannuzzi (FEI Company), and S. M. Schwarz (University of Central Florida and NanoSpective, Inc.) **57**

Coatings and joining materials for SiC/SiC composites for nuclear energy systems are being developed using preceramic polymers filled with reactive and inert powders, and using solid-state reactions with no polymers. Polymer-filled joints and coatings start with a poly(hydridomethylsiloxane) precursor, such that mixtures of Al/Al₂O₃/polymer form a hard oxide coating, coatings made with Al/SiC mixtures form a mixed oxide-carbide coating, while coatings made with SiC/polymer form a porous, hard carbide coating. Joints made from such mixtures have shear strengths range from 15 to 50 MPa depending on the applied pressure and joint composition. The strongest joints were obtained using tape cast ribbons of Si/TiC powders such that a solid state displacement reaction at 1473K using 30 MPa applied pressure resulted in shear strengths of 200 MPa, which exceeds the shear strength of SiC/SiC composite materials.

2.7 SWELLING AND TIME-DEPENDENT CRACK GROWTH IN SiC/SiC COMPOSITES—C. H. Henager, Jr. (Pacific Northwest National Laboratory) **61**

Pacific Northwest National Laboratory (PNNL) was among the first to identify and study time-dependent bridging in ceramic composites [6–8] and we have proposed a crack growth mechanism map based on available experimental data as a function of temperature and oxygen partial pressure for continuous fiber composites with carbon interphases [4]. Once a relationship between crack-opening displacement and bridging tractions from crack-bridging elements is determined, a governing integral equation is obtained that relates the total crack opening, and the bridging tractions, to the applied load. The solution of this equation gives the force on the crack-bridges and the crack-opening displacement everywhere along the crack face [3]. This relation is rendered time-dependent by including appropriate bridging fiber creep laws and interface removal kinetics, if oxidation is an issue. For fusion environments, both thermal and irradiation-induced fiber creep are included but oxidation is not considered here. Since the frictional sliding stress, τ , is an input parameter for this dynamic model the results from our 4-cylinder model allow τ to be dose-dependent. The bridging model can be used to determine the effects of pyrocarbon type on composite mechanical properties in radiation environments.

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The HFIR JP26 irradiation experiment contained a series of transmission electron microscopy (TEM) disks intended to study helium effects in ferritic/martensitic steels [1,2]. Table 1 lists specimens from that experiment chosen for examination. The Eurofer-97 disks were prepared with thin NiAl coatings so that irradiation would produce He by transmutation of the Ni and deposit that He uniformly in a thin layer ~ 6 to 8 μ m thick adjacent to the coating. Yamamoto et al. [3] give details of the specimen design and preparation. Following irradiation, samples were prepared for TEM using a cross-section technique to show He effects in the implanted layer near the NiAl coating. The procedure involved mounting the TEM disk between two half cylinders of Cu wire with thermal setting epoxy and slicing the composite wire using a slow speed saw equipped with a diamond-impregnated blade to produce 3 mm disks, with the TEM slice supported

between the half-cylinders of Cu. Each composite disk was then dimple ground to a central thickness of $\sim 100 \mu\text{m}$, and ion milled using a Gatan Precision Ion Polishing System. Ion milling was performed with 5 KV Ar ions to perforation so that the hole grew into the area of interest, followed by ion polishing at 2 KV for up to 1800 s to minimize Ar ion damage near the surface. Microstructural examinations were performed on a JEOL 2010F operating at 200 KeV in transmission with images recorded digitally.

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Tensile and Charpy specimens of normalized-and-tempered ORNL 9Cr-2WVTa reduced-activation steel and that steel composition containing 2% Ni (9Cr-2WVTa-2Ni) were irradiated at 376–405°C in the Experimental Breeder Reactor (EBR-II) to 23–33 dpa. Steels were irradiated in two tempered conditions: 1 hr at 700°C and 1 h at 750°C. The mechanical properties before and after irradiation of the 9Cr-2WVTa-2Ni steel were quite similar to those of the 9Cr-2WVTa steel, indicating no adverse effect of the nickel. Neither of the steels showed excessive hardening or a large increase in ductile-brittle transition temperature.

3.3 NEW NANO-PARTICLE-STRENGTHENED FERRITIC/MARTENSITIC STEELS BY CONVENTIONAL THERMOMECHANICAL TREATMENT—R. L. Klueh and N. Hashimoto (Oak Ridge National Laboratory) 77

Martensitic steels are considered for structural applications for fusion power plants, but they are limited by strength to temperatures of 550–600°C. For increased plant efficiency, steels for operation at 650°C and higher are sought. Based on the science of precipitate strengthening, a thermo-mechanical treatment (TMT) was developed that increased the strength from room temperature to 700°C of commercial nitrogen-containing steels and new steels designed for the TMT. At 700°C an increase in yield stress of 80 and 200% was observed for a commercial steel and a new steel, respectively, compared to commercial steels after a conventional heat treatment. Creep-rupture strength was similarly improved. Depending on the TMT, precipitates in the steels were up to eight-times smaller at a number density four orders of magnitude greater than those in a normalized-and-tempered steel.

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Experimental investigations have demonstrated that neutron irradiation of prime aged CuCrZr at temperatures below $\sim 473\text{K}$ leads to a substantial increase in strength, formation of a tensile instability, and a severe loss of work hardening ability and uniform elongation [1, 2]. The precipitates in this alloy are unable to inhibit localized deformation via dislocation channeling in the irradiated materials, namely because the precipitates are small Guinier-Preston (G-P) zones too weak to effectively prevent or hinder dislocation motion once dislocations become mobile at stress concentrations. It was therefore decided to coarsen the precipitate microstructure by annealing the prime aged CuCrZr so that larger and hopefully stronger precipitates, albeit in lower density, might prove more effective at preventing the initiation of plastic flow localization by resisting dislocation motion. As a starting point, we hoped to achieve a precipitate microstructure in the over-aged CuCrZr that was coarsened to a level near that of the GlidCop Al25, that is, particles with an average size of $\sim 7\text{--}8 \text{ nm}$ with a density of $\sim 1022 \text{ particles per m}^{-3}$.

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- Low carbon arc cast (LCAC) molybdenum was neutron irradiated at 80°C in the high flux isotope reactor (HFIR) to fluences between 2×10^{21} and 8×10^{24} n/m² ($E > 0.1$ MeV), corresponding to nominal displacement doses of 7.2×10^{-5} , 7.2×10^{-4} , 7.2×10^{-3} , 7.2×10^{-2} , and 0.28 dpa. Tensile tests were performed on unirradiated and irradiated specimens at 100, 22, -25, and -50°C at a strain rate of 1.1×10^{-3} s⁻¹. The fracture surfaces of tensile-tested specimens were examined by scanning electron microscopy. The paper examined the temperature and dose dependence of yield stress, post-yield strain hardening and tensile ductility. The fracture modes of irradiated Mo were also discussed.
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- In several recently published studies conducted on a Soviet analog of AISI 321 stainless steel irradiated in either fast reactors or light water reactors, it was shown that the void swelling phenomenon extended to temperatures as low as $\sim 300^\circ\text{C}$ or less, when produced by neutron irradiation at dpa rates in the range 10^{-7} to 10^{-8} dpa/sec. Other studies yielded similar results for AISI 316 and the Russian analog of AISI 316. In the current study a blanket duct assembly from BN-350, constructed from the Soviet analog of AISI 321, also exhibits swelling at dpa rates on the order of 10^{-8} dpa/sec, with voids seen as low as 281°C and only 0.65 dpa. It appears that low-temperature swelling occurs at low dpa rates in 300 series stainless steels in general, and also occurs during irradiations conducted in either fast or mixed spectrum reactors. Therefore it is expected that a similar behavior will be observed in fusion devices as well.
- 6.2 MICROSTRUCTURE AND MECHANICAL PROPERTIES OF AUSTENITIC STAINLESS STEEL 12X18H9T AFTER NEUTRON IRRADIATION IN THE PRESSURE VESSEL OF BR-10 FAST REACTOR AT VERY LOW DOSE RATES—S. I. Porollo, A. M. Dvoriashin, Yu. V. Konobeev, A. A. Ivanov, and S. V. Shulepin (Institute of Physics and Power Engineering) and F. A. Garner (Pacific Northwest National Laboratory) 115**
- The internal components of various Russian reactors such as VVER-440 and VVER-1000 pressurized water reactors and the BN-600 fast reactor are usually made of Russian designation 18Cr-9Ni or 18Cr-10Ni-Ti austenitic stainless steel. In Western PWRs and BWRs, the AISI Type 304 steel with composition similar to 18Cr-9Ni steel is used for this purpose. Currently, the issue of reactor life extension is very important for both Russian and Western reactors of the PWR type. It has also been recognized that some problems encountered in PWRs, especially those associated with changes in dimension and mechanical properties, can also be expected to occur in water-cooled fusion devices.
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Multi-layer coatings are being investigated to reduce the MHD pressure drop in a lithium-cooled blanket. As the fabrication process is improved, the performance of the coatings is improving with adequate as-deposited and in-situ resistance, and good compatibility being demonstrated in a recent capsule test. The compatibility of a thin (10-100 μ m) vanadium overlayer is now critical to coating durability. Initial experiments showed no dissolution of V-4Cr-4Ti after 1,000h at 800°C although the specimens were embrittled after exposure. A planned monometallic loop experiment will help verify the compatibility of V-4Cr-4Ti in Li at 700°C. New insulating ceramic materials are being investigated with Y2Ti2O7 showing some promise for this application.

7.2 INVESTIGATION OF Pb-Li COMPATIBILITY FOR THE DUAL COOLANT TEST BLANKET MODULE—B. A. Pint, J. L. Moser, and P. F. Tortorelli (Oak Ridge National Laboratory, USA) 134

Static Pb-17Li capsule tests were performed on monolithic SiC specimens and Al-containing alloys. Both systems showed little or no dissolution in Pb-Li likely due to the formation of a protective surface oxide which was expected to be stable based on thermodynamic evaluations. For SiC, Si was detected in the Pb-Li only at the highest test temperatures (2,000h at 1100°C and 1000h at 1200°C). The addition of Al to Fe- or Ni-base alloys resulted in a significant decrease in the amount of dissolution after 1000h at 700°C and 800°C compared to type 316 stainless steel. Chemical vapor deposited (CVD) aluminide coatings on type 316 substrates significantly reduced the dissolution rate at 800°C. With or without pre-oxidation, Al-containing alloys or coatings formed an Al₂O₃ surface layer. These results demonstrate that aluminide coatings could protect a conventional Fe- or Ni-base tubing alloy to carry Pb-Li between the first wall and the heat exchanger. Future work will need to include testing in a flowing system with a thermal gradient to fully determine the compatibility of these materials.

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9.1 THE INTERACTION OF HELIUM ATOMS WITH SCREW DISLOCATIONS IN α -Fe—H. L. Heinisch, F. Gao, and R. J. Kurtz (Pacific Northwest National Laboratory) 143

Formation energies, binding energies, and migration energies of interstitial He atoms in and near the core of an $a/2\langle 111 \rangle$ screw dislocation in α -Fe are determined in atomistic simulations using conjugate gradient relaxation and the Dimer method for determining saddle point energies. Results are compared as a function of the proximity of the He to the dislocation core and the excess interstitial volume in regions around the dislocation. Interstitial He atoms have binding energies to the screw dislocation that are about half the magnitude of binding energies to the $a/2\langle 111 \rangle\{110\}$ edge dislocation in α -Fe. Migration energies of interstitial He atoms for diffusion toward the dislocation and for pipe diffusion along the dislocation are about the same magnitude for the screw and edge dislocations, despite a significant difference in their migration mechanisms. Interstitial He atoms diffuse along the dislocation cores with a migration energy of 0.4–0.5 eV.

9.2 KINETIC MONTE CARLO STUDIES OF THE REACTION KINETICS OF CRYSTAL DEFECTS THAT DIFFUSE ONE-DIMENSIONALLY WITH OCCASIONAL TRANSVERSE MIGRATION—H. L. Heinisch (Pacific Northwest National Laboratory), H. Trinkaus (Institute für Festkörperforschung), and B. N. Singh (Risø National Laboratory) 147

The reaction kinetics of the various species of mobile defects in irradiated materials are crucially dependent on the dimensionality of their diffusion processes. Sink strengths for

one-dimensionally (1D) gliding interstitial loops undergoing occasional direction changes have been described analytically and confirmed by kinetic Monte Carlo (KMC) simulations. Here we report on KMC simulations investigating the transition from 1D to 3D diffusion for 1D gliding loops whose 1D migration is interrupted by occasional 2D migration due to conservative climb by dislocation core diffusion within a plane transverse to their 1D glide direction. Their transition from 1D to 3D kinetics is significantly different from that due to direction changes. The KMC results are compared to an analytical description of this diffusion mode in the form of a master curve relating the 1D normalized sink strength to the frequency of disturbance of 1D migration.

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Elemental iron implanted with He at different energies and doses is studied using thermal helium desorption spectrometry (THDS). Currently examined energies and doses include: 100 keV, and 1×10^{11} , 1×10^{13} , and 1×10^{15} He/cm², respectively. While no clear desorption signals have been observed for the two lower dose samples, the present results reveal that for the iron implanted to 1×10^{15} He/cm² the majority of the implanted He atoms desorb at $\sim 1000^\circ\text{C}$ and at $> 1100^\circ\text{C}$. Both conventional reaction model and Johnson-Mehl-Avrami (JMA) transformation model kinetics were utilized to fit the lower temperature ($\sim 1000^\circ\text{C}$) desorption event of the 1×10^{15} He/cm² dosed iron. Surprisingly, single (either 1st or higher) order fits can not adequately describe the event. Excellent fits are obtained when combining a lower ($n \sim 1.1$) order with a higher ($n \sim 5.8$) order JMA fit. Additionally, spurious desorption peaks and certain complex desorption features have been observed which may affect future THDS studies.

9.4 MOLECULAR DYNAMICS SIMULATIONS OF POINT DEFECT INTERACTIONS IN FE-CR ALLOYS—K. L. Wong, J. H. Shim, and B. D. Wirth (University of California, Berkeley) 160

Two different Finnis-Sinclair-type potentials were used to model Fe-1%Cr and Fe-10%Cr alloys, which alternately describe Cr as under- or over-sized in body-centered cubic Fe. In general, the diffusivity of the single interstitials and di- and tri-interstitial clusters was reduced in the Fe-10%Cr alloys, irrespective of interatomic potential, although the underlying mechanism(s) were different. When Cr is undersized, interstitial diffusion is retarded through a trapping mechanism associated with bound Cr-interstitial (mixed dumbbell) complexes, whereas oversized Cr atoms retard interstitial diffusion by enhancing the rotation frequency away from one-dimensionally mobile $\langle 111 \rangle$ interstitial dumbbell configurations.

9.5 ATOMISTIC MODELING OF THE INTERACTION OF HE WITH NANOCLUSTERS IN FE—R. J. Kurtz, F. Gao, and H. L. Heinisch (Pacific Northwest National Laboratory), B. D. Wirth (University of California, Berkeley), G. R. Odette and T. Yamamoto (University of California, Santa Barbara) 167

Structural materials of a fusion power system will be exposed to high concentrations of He produced from nuclear transmutation reactions. Helium is essentially insoluble in metals so there is a strong tendency for it to form bubbles that can significantly degrade mechanical properties. A strategy to effectively manage He is to provide a high-density of internal interfaces to serve as He bubble nucleation sites and vacancy-interstitial recombination centers. Nanostructured ferritic alloys are being developed to provide improved creep strength and He management capability compared to conventional steels. A key characteristic of these materials is the high-density ($\sim 10^{24} \text{ m}^{-3}$) of nanometer-scale ($\sim 3 \text{ nm}$ diameter) Y-Ti-O clusters. We describe molecular dynamics simulations to assess the interaction of He atoms, vacancies and He-vacancy complexes with coherent Cu nanoclusters in Fe. The potentials employed here were adjusted to explore the effect of nanocluster elastic properties on He trapping efficiency.

- 9.6 DIFFUSION OF He INTERSTITIAL AND SMALL CLUSTERS AT GRAIN BOUNDARIES IN α -Fe—F. Gao, R. J. Kurtz, and H. L. Heinisch, Jr. (Pacific Northwest National Laboratory) 174**
- A systematic molecular dynamics study of the diffusion mechanisms of He interstitial and their small clusters at two representative interfaces, $\Sigma 11$ and $\Sigma 3$, has been carried out in α -Fe. The diffusion coefficient of a He interstitial and the effective migration energies were determined, and the diffusion mechanisms of single interstitials and di-He interstitials are discussed in detail. A di-He interstitial cluster can kick out a self interstitial atom (SIA) at high temperatures, forming a He₂V complex. The SIA migrates rapidly near interfaces, whereas the He₂V complex is immobile at the temperatures considered. This small cluster may serve as a smallest nucleation for the formation of helium bubbles at interfaces.
- 9.7 MODELLING THERMODYNAMICS OF ALLOYS FOR FUSION APPLICATION—A. Caro, B. Sadigh, M. Caro, J. Marian (Lawrence Livermore National Laboratory), E. Lopasso (Centro Atomico Bariloche, Argentine), and D. Crowson (Virginia Polytechnical Institute) 177**
- Atomistic simulations of alloys at the empirical level face the challenge of correctly modeling basic thermodynamic properties. In this work we develop a methodology to generalize many-body classic potentials to incorporate complex formation energy curves. Application to Fe-Cr allows us to predict the implications of the ab initio results of formation energy on the phase diagram of this alloy.
- 10.0 DOSIMETRY, DAMAGE PARAMETERS, AND ACTIVATION CALCULATIONS 183**
- 10.1 ERRATUM to "NEUTRON DOSIMETRY AND DAMAGE CALCULATIONS FOR THE HFIR-MFE-200J-1 IRRADIATION," in Fusion Materials Semiannual Progress Report for Period Ending December 31, 1997, DOE/ER-0313/23, pp. 329–332. 184**
- Table 2 of this report contains an error. The thermal neutron fluence should be 0.35 x 10²² n/cm². The error has been corrected, and a revised version of the report is available on-line in DOE/ER-0313/23. Anyone who downloaded and/or referred the original report is encouraged to obtain the corrected copy.
- 11.0 MATERIALS ENGINEERING AND DESIGN REQUIREMENTS 185**
- No contributions.*
- 12.0 IRRADIATION FACILITIES AND TEST MATRICES 186**
- No contributions.*