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1. VANADIUM ALLOYS

1.1 ADDITIONAL CHARACTERIZATION OF V-4Cr-4Ti EXPOSED TO FLOWING Li **1**
B. A. Pint (Oak Ridge National Laboratory)

In order to clarify prior results, more Li-exposed V-4Cr-4Ti specimens were evaluated at 500°C in vacuum with a strain rate of 10-3s-1. These specimens confirmed prior results that exposure in the loop increased strength and slightly decreased ductility. However, while the increase in strength decreased with exposure temperature, the ductility effect was minor and more variable. The specimens exposed at lower temperatures in the loop showed the highest tensile strength, lowest ductility and least dynamic strain aging. More microstructural characterization is needed to complete this study.

2. CERAMIC COMPOSITE MATERIALS

2.1 THE EFFECTS OF NEUTRON IRRADIATION ON DIMENSIONAL CHANGE IN ADVANCED SILICON CARBIDE COMPOSITES—K. Ozawa, Y. Katoh, L.L. Snead (Oak Ridge National Laboratory), T. Nozawa (Japan Atomic Energy Agency), T. Hinoki (Kyoto University), and A. Hasegawa (Tohoku University) **4**

The dimensional change and elastic modulus of advanced silicon carbide (SiC) fibers reinforced silicon carbide matrix (SiC/SiC) composites included in the HFIR-18J irradiation experiment were measured and the data collected in the past five years were summarized. The excellent dimensional stability of the advanced SiC/SiC composites was confirmed after neutron irradiation to 7.0×10^{25} n/m^2. The stability is superior to composites reinforced with the earlier generation SiC fibers. The swelling of the advanced composites was measured to be ~0.7% for a dose of ~7.0×10^{25} n/m^2 at 800°C (nominal). This corresponds to the swelling behavior of chemically vapor deposited (CVD) SiC.

3. FERRITIC/MARTENSITIC STEELS

See also contribution 12.2

3.1 A REVIEW OF RECENT WORK ON FATIGUE RESPONSE IN FERRITIC/ MARTENSITIC STEELS – D. S. Gelles (Pacific Northwest National Laboratory) **16**

The recent literature on fatigue and creep-fatigue response of ferritic/martensitic steels has been reviewed with particular emphasis on that of interest to the fusion materials community. A range of alloys has been studied including low activation martensitic steels developed in Japan and Europe as well as some work on ODS steels of interest. The results show that all these martensitic steels behave similarly, that ODS steels provide improvement, that irradiation tends to reduce fatigue lifetimes, and that simultaneous helium and hydrogen injection can be very deleterious. Work done on 9Cr-1Mo in support of Gen VI demonstrates that creep-fatigue lifetimes will be controlled by cracking of surface oxides. It may be necessary to test in a fusion environment in order to accurately predict ferritic/martensitic steel fatigue response for a fusion machine.

3.2 CHARACTERIZATION OF THE COMPOSITION AND STRUCTURE OF Y-TI-O RICH PRECIPITATES IN NANOSTRUCTURED FERRITIC ALLOY MA957 BY TRANSMISSION ELECTRON MICROSCOPY AND ATOM PROBE TOMOGRAPHY -

N. J. Cunningham, Y. Wu, E. Haney and G. R. Odette (University of California Santa Barbara)

Nano-dispersion strengthened ferrite alloys (NFA) show great promise for structural applications in severe fusion reactor environments. NFA contain an ultra high density of Y-Ti-O enriched nanofeatures (NF) that, along with fine grains and high dislocation densities, provide high tensile, creep and fatigue strength. The NF are remarkably thermally stable and trap He in fine scale bubbles, thereby suppressing fast fracture embrittlement at lower temperatures, void swelling at intermediate temperatures and degradation of creep rupture properties at high temperatures. However, the precise characteristics of various NF are not yet well understood. They appear to range from coherent solute enriched GP-type zones to near stoichiometric complex oxides, such as Y_2TiO_5 and $Y_2Ti_2O_7$. Here we summarize a recent effort to clarify the characteristics of NF for a reference NFA, MA957, based on the application of several complementary micro-analytical characterization techniques. High-resolution transmission electron microscopy (HRTEM)-Fast Fourier Transform (FFT) power spectra diffraction patterns indicate that the larger features (> 10 nm) are primarily Y_2TiO_5. Limited diffraction data show the smaller features (≈5 nm) are not consistent with known oxide phases. Energy dispersive x-ray (EDX) measurements yield average feature compositions of Y/Ti/O ≈ 27/20/53 for both larger and smaller features. In contrast, atom probe tomography data show average solute compositions of Y/Ti/O = 14/41/45 and Y/Ti/O = 20/32/48 for the smaller and larger features, respectively. The APT data also suggest that even the larger particles contain significant quantities of Fe, and to a lesser extent Cr, which are not observed in the EDX measurements.

4. COPPER ALLOYS

No contributions this period

5. REFRACTORY METALS AND ALLOYS

No contributions this period

6. AUSTENITIC STAINLESS STEELS

No contributions this period

7. FUNCTIONAL MATERIALS – INCLUDING MHD INSULATORS, COATINGS, INSULATING CERAMICS, AND OPTICAL MATERIALS

7.1 COMPATIBILITY OF MATERIALS EXPOSED TO ISOTHERMAL Pb-Li – 28

B. A. Pint (Oak Ridge National Laboratory, USA)

Two sets of capsules experiments exposed for 1000h at 500°-700°C were completed to determine the effect of various factors on the amount of dissolution in Pb-Li. The first set examined the effects of Al-rich coatings and the characterization has been completed. Thin coatings exposed at 700°C showed significant Al loss with different variations: (1) pre-oxidation, (2) O gettering and (3) exposure in pure Pb without Li. Less Al loss was observed after exposure at 600°C. A second series of capsules were recently completed that explored the effect of Fe and Ni impurities on the dissolution rate and dissimilar metal reactions between Fe and SiC at 600°C. Based on only the mass gain data, there is some indication of a dissimilar metal effect in Pb-Li.

8. BREEDING MATERIALS

No contributions this period

9. RADIATION EFFECTS, MECHANISTIC STUDIES, AND EXPERIMENTAL METHODS

9.1 MODELLING THERMODYNAMICS OF ALLOYS FOR FUSION APPLICATION - 35

A. Caro, P. Erhart, M. Serrano de Caro, B. Sadigh (Lawrence Livermore National Laboratory), S.G. Srinivasan (UNT), A. Stukowski (Germany)

This semester has been very productive in the developments of both tools and algorithms.

- With the visit of a A. Stukowsky, a graduate student from Prof. K. Albe (Germany) we implemented the formalism of the composition dependent embedded atom model (CD-EAM) into Lammps, a freely distributed code for molecular dynamics. We also implemented a ‘variance constrained’ Metropolis Monte Carlo, MMC, algorithm into Lammps.
- We developed a modified version of the CD-EAM, that we call ‘one site’ CD-EAM that significantly improves the performance of a MMC algorithm without affecting the accuracy of the interatomic potential.
- We developed a ternary FeCr-He potential based on data obtained from Prof. K. Nordlund’s group in Finland. We validate this potential against *ab initio* data on He in FeCr obtained from within a collaboration with Chu Chun Fu at CEA-Saclay, France.
- We started simulation of He bubbles in FeCr alloys, determining the pressure versus size relation for the 1He/vacancy ratio

9.2 MODELING OF POINT DEFECT CLUSTER EVOLUTION UNDER PULSED IRRADIATION - S.I. Golubov (Oak Ridge National Laboratory, University of Tennessee), R.E. Stoller (Oak Ridge National Laboratory), A.V. Barashev (The University of Liverpool) **40**

The main results of this work are summarized as follows:

- For the first time point defect (PD) cluster nucleation and growth during different pulsed irradiation regimes has been calculated and compared with that of steady irradiation.
- It is found that PD cluster nucleation is extremely sensitive to the type of irradiation: it is enhanced in the case of pulsed irradiation. The effect increases with decrease of pulse frequency.
- Rate of damage accumulation under pulsed irradiation is larger at small doses and smaller at high doses than that for steady irradiation.
- The calculation results obtained suggest that the pulse structure of MTS and IFMIF may reproduce damage accumulation quite close to that one may expect for steady irradiation whereas it may be very different in the case of SNS irradiation.
- The new method for numerical integration of the Master Equation used provides a valuable tool to link experimental data obtained using different types of irradiations.

9.3 ATOMISTIC STUDIES OF PROPERTIES OF HELIUM IN BCC IRON USING THE NEW HE–FE POTENTIAL—David M. Stewart, Stanislav Golubov (Oak Ridge National Laboratory and the University of Tennessee), Yuri Ostesky, Roger E. Stoller, Tatiana Seletskaia, and Paul Kamenski (Oak Ridge National Laboratory) **52**

In fusion applications, helium caused by transmutation plays an important role in the response of RAFM steels to neutron radiation damage. We have performed atomistic simulations using a new 3-body Fe–He inter-atomic potential combined with the Ackland iron potential. With the ORNL potential, interstitial helium is very mobile and coalesces together to form interstitial clusters. We have investigated the mobility of these clusters. If the He cluster is sufficiently large the cluster can push out an Fe interstitial, creating a Frenkel pair. The resulting helium-vacancy cluster is not mobile. The ejected SIA is mobile, but is weakly trapped by the He–V cluster. If more helium atoms join the He–V cluster, more Fe interstitials can be pushed out, and they combine to form an interstitial dislocation loop. The reverse process is also studied. Multiple helium atoms can be trapped in a single vacancy, and if there are few enough, the vacancy can recombine with an Fe interstitial to create a helium interstitial cluster. These mechanisms are investigated together in larger simulations that examine the nucleation of He defects. Results are compared based on temperature, interatomic potentials used and helium concentration. Helium bubbles of sizes 1-6nm are also studied.

9.4 HARDENING DUE TO HE-FILLED BUBBLES IN IRON – Yu. N. Osetskiy, R. E. Stoller and D. Stewart (Oak Ridge National Laboratory) **58**

Gas-filled bubble strengthening is an important radiation effect observed in structural materials subjected to high dose irradiation at moderate temperature. The usual treatment of this effect is based on the continuum approach to estimate the equilibrium state of gas bubbles and simplified estimation of their strengthening on the basis of line tension models. We suggest employing multi-scale computer modeling to investigate such effects. This includes low level Density Functional Theory (DFT) calculations to construct an empirical potential for interatomic interactions in Metal-Gas system. Such calculations need up to a few hundred atoms and their free electrons. Next level includes Molecular Dynamics (MD) technique to investigate the equilibrium state of gas filled bubbles as a function of their size and ambient temperature. The scale covered at this level includes bubble of size up to 10nm in matrix crystals of up to 2-4x10^6 atoms. Finally, MD modeling of interactions between moving dislocations and gas-filled bubbles is the largest scale in this approach considering up to 10^8 atoms modeled over a few nanosecond simulated time. This cutting edge research has started at ORNL and will demand significant computational and intellectual resources over the next few next years. We present here the first few results of a multi-scale study of He-bubbles in Fe obtained during FY 2009.

9.5 VALIDATION OF EQUIBIAXIAL FLEXURAL TEST FOR MINIATURIZED CERAMIC SPECIMENS — S. Kondo, Y. Katoh, J.W. Kim, L.L. Snead (Oak Ridge National Laboratory) **62**

For the purpose of evaluating fracture strength of irradiated ceramic specimens, a miniature disc equibiaxial flexural test technique was developed. It was applied to graphite specimens in a variety of combination of sample thickness and loading ring diameter to investigate the influences on the stress uniformity within the loading ring. Although similar and relatively high Weibull modulus were observed for all conditions ($m \approx 20$), the significant stress concentration associated with the large deflection was observed at the loading location for thinner specimens ($t<0.2$mm). However, the true local fracture stress was successfully estimated from the measured fracture load using finite element analysis. The method for estimating true local fracture stress appear reasonable for evaluating the fracture strength of dense poly-crystalline graphite, and can be used for determination of the statistical parameters for fracture stress of various ceramics.

10. DOSIMETRY, DAMAGE PARAMETERS, AND ACTIVATION CALCULATIONS

No contributions this period

11. MATERIALS ENGINEERING AND DESIGN REQUIREMENTS

No contributions this period

12. IRRADIATION FACILITIES AND TEST MATRICES

12.1 HFIR Irradiation Experiments – F. W. Wiffen, Oak Ridge National Laboratory **71**

The current status of Fusion Materials Program irradiation experiments in the HFIR reactor is tabulated.

12.2 ASSEMBLY OF THE US-JAPAN MFE-RB-15J EXPERIMENT FOR IRRADIATION IN THE HFIR – T. Hirose, M. Ando, H. Tanigawa, N. Okubo (Japan Atomic Energy Agency), J. L. McDuffee, D. W. Heatherly, R. G. Sitterson, R. E. Stoller (Oak Ridge National Laboratory) and T. Yamamoto (University of California, Santa Barbara) **72**

Assembly of the MFE-RB-15J capsule was completed in April, 2008 and installed in HFIR location RB-1A inside a europia thermal neutron shield. Irradiation began with cycle 415, starting June 3, 2008. A detailed specimen loading list for the capsule is provided in this report.

12.3 SUMMARY OF THE USCB ADVANCED TEST REACTOR NATIONAL SCIENTIFIC USERS FACILITY IRRADIATION EXPERIMENT – G. R. Odette, T. Yamamoto, B. Sams, D. Klingensmith, and N. Cunningham (Department of Mechanical Engineering, University of California Santa Barbara); G. Waches, J. I. Cole, and P. E. Murrey (Idaho National Laboratory) **79**

We have designed and prepared a comprehensive Advanced Test Reactor (ATR) irradiation experiment as part of a successful ATR National Scientific Users Facility (NSUF) proposal entitled *Characterization of the Microstructures and Mechanical Properties of Advanced Structural Alloys for Radiation Service: A Comprehensive Library of ATR Irradiated Alloys and Specimen.* A total of about 1400 specimens were fabricated and loaded at UCSB in 33 packets. Each packet has a unique outer profile and insulator design to minimize axial variations set by the Ar-He gas mixture and gap dimension. The packets were assembled at UCSB and subsequently loaded into 11 approximately 11 mm diameter capsule tubes at the Idaho National Laboratory (INL) in July, 2009. The experimental objective is to develop an integrated hardening/softening database from 288 to 750 ºC on 44 steels and model alloys irradiated up to 6 dpa. The experiment will also characterize the irradiation embrittlement of 6 alloys and support the development of small specimen fracture test methods including for interface fracture. The specimens will also support extensive microstructural and mechanism studies, including helium injection and diffusion multiple experiments. The irradiated specimens will form a “lending library” and sustain a number of future collaborations. The irradiation will be initiated in August of 2009 and completed in April of 2010.