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Amono-metallic V-4Cr-4Ti thermal convection loop was operated in vacuum (~10-5Pa) at a maximum Li temperature of 700°C for 2,355h and Li flow rate of 2-3cm/s. Two-layer, physical vapor deposited Y2O3-vanadium, electrically-insulating coatings on V-4Cr-4Ti substrates as well as uncoated tensile and sheet specimens were located in the flow path in the hot and cold legs. After exposure, specimens at the top of the hot leg showed a maximum mass loss equivalent to ~1.3μm of uniform metal loss. Elsewhere, small mass gains were observed on the majority of specimens that also showed an increase in hardness and room temperature yield stress and a decrease in ductility consistent with interstitial uptake. Specimens that lost mass showed a decrease in yield stress and hardness. Profilometry showed no significant thickness loss from the coatings.

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2.1 DIMENSIONAL AND MICROSTRUCTURAL STABILITY OF 3C-SiC IN HIGH TEMPERATURE IRRADIATION CONDITIONS— S. Kondo, Y. Katoh, L. L. Snead (Oak Ridge National Laboratory) **11**

Microstructural analysis of 3C-SiC following neutron-irradiation at high temperatures provided quantitatively reliable data of temperature and fluence dependence of cavity swelling and dislocation evolution. Post-irradiation annealing effects on microstructural defects were also studied. Cavities were observed for all irradiation conditions (1050-1460°C, up to 9.6 dpa) except for 1050°C, 1.4 dpa. However, the magnitude of cavity swelling was very small below ~1300°C: the largest cavity swelling observed below that temperature was only ~0.01% at 1300°C, 9.3dpa. The temperature dependent increase in the cavity swelling was observed clearly above ~1400°C. Fluence dependent swelling became plainly visible above ~1400°C, and the maximum value observed in this work was 0.25% at 1460°C, 9.6 dpa. The dominating dislocation structure in the high temperature regime is Frank faulted loop. Minor black spots and small loop populations, which dominated the defect microstructure in lower temperature regime, were still coexisted with the Frank loops up to ~1150°C. Defect number density decreased and the size increased with increasing temperature. Significant decrease in the number density and increase in the size was observed at 1300-1460°C.

2.2 EFFECT OF NEUTRON IRRADIATION ON DC ELECTRICAL CONDUCTIVITY OF SILICON CARBIDE CERAMICS AND COMPOSITES FOR FUSION FLOW CHANNEL INSERT APPLICATIONS—Y. Katoh, S. Kondo, L. L. Snead (Oak Ridge National Laboratory) **18**

The objective of this work is to help addressing the electrical conductivity issue for the silicon carbide-based flow channel insert in lead-lithium blanket of fusion breeding reactors; specifically to establish control schemes for electrical conductivity of SiC composites by identifying the conduction mechanism in composite structures and to address neutron irradiation effect

on electrical conductivity in SiC composites and constituents. SUMMARY High purity chemically vapor-deposited silicon carbide (SiC) and 2D continuous SiC fiber, chemically vapor-infiltrated SiC matrix composites with pyrocarbon interphases were examined for temperature dependent (RT to 800ºC) electrical conductivity and the influence of neutron irradiation on it. In the 2D composites, trans-thickness electrical conductivity was dominated by bypass conduction via interphase network at relatively low temperatures, whereas conduction through SiC constituents dominated at higher temperatures. The Influence of neutron irradiation on electrical properties appeared very strong for SiC, resulting typically in by orders lower ambient conductivity and steeper temperature dependency. Through-thickness electrical conductivity of neutron-irradiated 2D SiC composites with thin PyC interphase will likely in the order of 10 S/m in the typical operating temperature range for flow channel inserts. Mechanisms of electrical conduction in the composites and irradiation-induced modification of electrical conductivity of the composites and their constituents are discussed.

2.3 MICROSTRUCTURES OF CHEMICALLY VAPOR-DEPOSITED SILICON CARBIDE AFTER IRRADIATION CREEP DEFORMATION—Y. Katoh, S. Kondo, L. L. Snead (Oak Ridge National Laboratory) 26

Microstructures of silicon carbide were examined by transmission electron microscopy (TEM) after creep deformation under neutron irradiation. Thin strip specimens of polycrystalline and monocrystalline, chemically vapor-deposited, beta-phase silicon carbide were irradiated in High Flux Isotope Reactor to 0.7 - 4.2 dpa at nominal temperatures 640 - 1080ºC in an elastically pre-strained bend stress relaxation configuration with the initial stress of ~100 MPa. Irradiation creep caused permanent strains of 0.6 to 2.3 x 10-4. Tensile-loaded near-surface portions of the crept specimens were examined by TEM. The main microstructural features observed were dislocation loops in all samples, and appeared similar to those observed in samples irradiated in non-stressed conditions. Slight but statistically significant anisotropy in dislocation loop microstructure was observed in one irradiation condition, and accounted for at least a fraction of the creep strain derived from the stress relaxation. The estimated total volume of loops accounted for 10 - 45% of the estimated total swelling. The results imply that the early irradiation creep deformation of SiC observed in this work was driven by anisotropic evolutions of extrinsic dislocation loops and matrix defects with undetectable sizes.

2.4 MODELING SiC/SiC COMPOSITES WITH OFF-AXIS FIBERS – C. H. Henager, Jr. (Pacific Northwest National Laboratory) 38

A time-dependent fiber-bridging model that accounts for fiber orientation has been developed and its predictions are compared to strength and crack growth data for a braided weave composite. The level of agreement suggests that existing models of off-axis bridging fibers are not adequate for fusion reactor designs using SiC/SiC composites in off-axis orientations.

2.5 JOINING SiC/SiC COMPOSITES FOR FUSION APPLICATIONS – C. H. Henager, Jr. (Pacific Northwest National Laboratory) 44

The use of SiC composites in fusion environments may require joining of plates using non-mechanical joints, such as reactive joining or brazing. One promising joining method is the use of solid-state displacement reactions between Si and TiC to produce Ti3SiC2 + SiC. Such joints, while stronger

than the SiC-composite interlaminar shear strength, which is a critical metric for joint performance, requires pressure and bonding at elevated temperatures. We are exploring the processing envelope for this joint in advance of the US-Japan TITAN collaboration so that we can produce viable joints to undergo irradiation studies in HFIR. Joining pressure appears to require almost 30 MPa at 1673K in order to produce strong and dense joints.

2.6 COMPATIBILITY OF INTERFACES AND FIBERS FOR SIC-COMPOSITES IN FUSION ENVIRONMENTS – C. H. Henager, Jr. and R. J. Kurtz (Pacific Northwest National Laboratory) 48

The use of SiC composites in fusion environments is predicated on stability under neutron irradiation, on outstanding high-temperature mechanical properties, and on chemical inertness and corrosion resistance. However, SiC is susceptible to many forms of corrosion in water and in water vapor where silica formation is required as a protective layer because silica forms stable hydroxides that are volatile, even at low temperatures. SiC composites have an additional concern that fine-grained fibers and weak interfaces provide the required fracture toughness, but these components may also exhibit susceptibility to corrosion that can compromise material properties. In this work we examine and review the compatibility of fibers and interfaces, as well as the SiC matrix, in proposed fusion environments including first wall, tritium breeding, and blanket modules and module coolants.

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3.1 ON THE ROLE OF ALLOY COMPOSITION AND PROCESSING PARAMETERS IN NANOCLUSTER FORMATION AND DISPERSION STRENGTHENING IN NANOSTRUCTURED FERRITIC ALLOYS - M. J. Alinger and G. R. Odette (University of California Santa Barbara) and D. T. Hoelzer (Oak Ridge National Laboratory) 57

An extensive experimental study to characterize the sequence-of-events that lead to the formation of a very high density of Y-Ti-O solute nanoclusters (NFs) in mechanically alloyed (MA), hot isostatically pressed (HIPed) ferritic stainless steels is reported. Yttria and O dissolve in the Fe-14Cr3W(0.4Ti) powders during MA. The dissolved Y and O, and when present Ti, subsequently precipitate during hot consolidation. The number densities and volume fractions of the NF decrease, and their radii increase, with increasing consolidation temperature. The NF form at 850 and 1000°C in both attritor and higher energy SPEX milled alloys containing Y, both with and without Ti additions. SPEX milling produces higher volume fractions of NFs and higher hardness in these cases. The presence of Ti refines the NFs, and both Ti and high milling energy (SPEX versus attritor) are necessary for the formation NFs at the highest consolidation temperatures of 1150°C. Microhardness trends closely mirror the effects of the compositional and processing variables on the NFs. However, the precise structure and composition of the NFs are not well understood. Indeed, their character varies, depending on the alloy composition and processing variables. The NFs appear to range from coherent solute enriched zones, or sub-oxides, to complex oxide phases.

3.2 EMBRITTLEMENT OF IRRADIATED F82H IN THE ABSENCE OF IRRADIATION HARDENING—R. L. Klueh (Oak Ridge National Laboratory), K. Shiba (Japan Atomic Energy Agency), and M. A. Sokolov (Oak Ridge National Laboratory) 80

Neutron irradiation of 7-12% Cr ferritic/martensitic steels below 425–450ºC produces microstructural defects and precipitation that cause an increase in yield stress. This irradiation hardening causes embrittlement, which is observed in a Charpy impact or fracture toughness test as an increase in the ductile-brittle transition temperature. Based on observations that show little change in strength in steels irradiated above 425–450ºC, the general conclusion has been that no embrittlement occurs above these temperatures. In a recent study of F82H steel, significant embrittlement was observed after irradiation at 500ºC. This embrittlement is apparently due to irradiation-accelerated Laves-phase precipitation. Observations of the embrittlement in the absence of hardening has been examined and analyzed with thermal-aging studies and computational thermodynamics calculations to illuminate and understand the effect.

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5.1 THE INFLUENCE OF NEUTRON IRRADIATION AND TRANSMUTATION IN FFTF ON THE MICROSTRUCTURAL AND MICROCHEMICAL DEVELOPMENT OF Mo-41Re AT 470-730ºC – D. J. Edwards and F. A. Garner (Pacific Northwest National Laboratory) 88

Specimens of Mo-41 wt% Re irradiated in the Fast Flux Test Facility (FFTF) experience significant and non-monotonic changes in density that arise first from radiation-induced segregation, leading to non-equilibrium phase separation, and second by progressive transmutation of Re to Os. As a consequence the density of Mo-41Re initially decreases and then increases thereafter. Beginning as a single-phase solid solution of Re and Mo, irradiation of Mo-41 wt% Re over a range of temperatures (470-730ºC) to 28-96 dpa produces a high density of thin platelets of a hexagonal close-packed phase identified as a solid solution of Re, Os and possibly a small amount of Mo. These hcp precipitates are thought to form in the alloy matrix as a consequence of strong radiation-induced segregation to Frank loops. Grain boundaries also segregate Re to form the hcp phase, but the precipitates are much bigger and more equiaxed in shape. Although not formed at lower dose, continued irradiation at 730º C leads to the co-formation of late-forming Chi–phase, an equilibrium phase that then competes with the preexisting hcp phase for rhenium.

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6.1 THE CONFLICTING ROLES OF BORON ON THE RADIATION RESPONSE OF PRECIPITATE-FORMING AUSTENITIC ALLOYS - T. Okita, N. Sekimura (Department of Quantum Engineering and Systems Science, University of Tokyo) and F. A. Garner (Pacific Northwest National Laboratory) **104**

The behavior of void swelling at 400ºC of model f.c.c. alloy Fe-15Cr-16Ti-0.25Ti-0.05C doped with boron was examined in the FFTF-MOTA. Boron additions modify the neutron-induced swelling of Fe-15Cr-16Ni-0.25Ti-0.05C somewhat, but the changes appear to arise primarily from the influence of boron as a chemical species rather than as a source of helium. Boron additions initially depress swelling strongly, but the effect saturates by 100 appm. The reduction in swelling is thought to arise from boron's influence on distribution and precipitation of carbon. As the boron level is raised to significantly larger levels swelling then swelling begins to increase, but at a slower rate per boron atom. This subsequent increase is thought to reflect the higher He/dpa ratio generated by the boron, overwhelming the helium produced by (n,) reactions with nickel.

6.2 VERY HIGH SWELLING AND EMBRITTLEMENT OBSERVED IN A Fe-18Cr-10Ni-Ti HEXAGONAL FUEL WRAPPER IRRADIATED IN THE BOR-60 FAST REACTOR - V. S. Neustroev (Research Institute of Atomic Reactors, Dimitrovgrad, Russia) and F. A. Garner (Pacific Northwest National Laboratory) **109**

The highest void swelling level ever observed in an operating fast reactor component has been found after irradiation in BOR-60 with swelling in Kh18H10T (Fe-18Cr-10Ni-Ti) austenitic steel exceeding 50%. At such high swelling levels the steel has reached a terminal swelling rate of ~1%/dpa after a transient that depends on both dpa rate and irradiation temperature. The transient duration at the higher irradiation temperatures is as small as 10-13 dpa depending on which face was examined. When irradiated in a fast reactor such as BOR-60 with a rather low inlet temperature, most of the swelling occurs above the core center-plane and produces a highly asymmetric swelling loop when plotted vs. dpa. Voids initially harden the alloy but as the swelling level becomes significant the elastic moduli of the alloy decreases strongly with swelling, leading to the consequence that the steel actually softens with increasing swelling. This softening occurs even as the elongation decreases as a result of void linkage during deformation. Finally, the elongation decreases to zero with further increases of swelling. This very brittle failure is known to arise from segregation of nickel to void surfaces which induces a martensitic instability leading to a zero tearing modulus and zero deformation.

6.3 ANOMALOUSLY LARGE DEFORMATION OF 12Cr18Ni10Ti AUSTENITIC STEEL IRRADIATED TO 55 DPA AT 310ºC IN THE BN-350 REACTOR - M. N. Gusev, O. P. Maksimkin, I. S. Osipov (Institute of Nuclear Physics, Kazakhstan) and F. A Garner (Pacific Northwest National Laboratory) **123**

Whereas most previous irradiation studies conducted at lower neutron exposures in the range 100-400ºC have consistently produced strengthening and strongly reduced ductility in stainless steels it now appears possible that higher exposures may lead to a reversal in ductility loss for some steels. A new radiation-induced phenomenon has been observed in 12Cr18Ni10Ti

stainless steel irradiated to 55 dpa. It involves “a moving wave of plastic deformation” at 20ºC that produces “anomalously” high values of engineering ductility, especially when compared to deformation occurring at lower neutron exposures. Using the technique of digital optical extensometry the “true stress σ –true strain ε” curves were obtained. It was shown that a moving wave of plastic deformation occurs as a result of an increase in the intensity of strain hardening, dσ/dε(ε). The increase in strain hardening is thought to arise from an irradiation-induced increase in the propensity of the γ→α martensitic transformation.

6.4 ANISOTROPIC SWELLING OBSERVED DURING STRESS-FREE REIRRADIATION OF AISI 304 TUBES PREVIOUSLY IRRADIATED UNDER STRESS - F. A. Garner (Pacific Northwest National Laboratory), J. E. Flinn, (Argonne National Laboratory, EBR-II Project, [Retired]) and M. M. Hall, (Bechtel Bettis Company) 130

A “history effects” experiment was conducted in EBR-II that involved the reirradiation of AISI 304 cladding and capsule tubes. It is shown that when irradiated tubes had not previously experienced stress, subsequent irradiation led to additional swelling strains that were isotropically distributed. However, when tubes previously irradiated under a 2:1 biaxial stress were reirradiated without stress the additional swelling strains were not isotropically distributed. The tubes retained a memory of the previous stress state that appears to be attempting to distribute strains in the directions dictated by the previous stress state. It is clear, however, that the memory of that stress state is fading as the anisotropic dislocation microstructure developed during irradiation under stress is replaced by an isotropic dislocation microstructure during subsequent exposure in the absence of stress. It is also shown that once the transient regime of swelling nears completion, further changes in stress state or irradiation temperature have no influence on the swelling rate thereafter.

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7.1 FURTHER CHARACTERIZATION OF THE TRANS-FORMATION OF Al_2O_3 TO $LiAlO_2$ IN Pb-17 Li AT 800°C– B. A. Pint and K. L. More (Oak Ridge National Laboratory, USA) 140

In order to study the compatibility of -Al2O3with Pb-17Li, a FeCrAl substrate was pre-oxidized at 1000°Cto thermally grow an external alumina scale. The specimen was then isothermally exposed to Pb-Li for1000h at 800°C in a Mo capsule. The alumina layer prevented dissolution of the metallic substrate but was found to transform to LiAlO2.The current report includes additional XRD and TEM characterization of the external oxide layer before and after exposure to Pb-Li.

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9.1 MULTISCALE MODELING OF POINT DEFECT INTER-ACTIONS IN BCC FE-CR ALLOYS –K. L. Wong, H.-J. Lee, B. D. Wirth (University of California, Berkeley), J.-H. Shim (Korea Institute of Science and Technology), and B. Sadigh (Lawrence Livermore National Laboratory) 146

Predictive performance models of ferritic/martensitic alloys in fusion neutron irradiation environments require knowledge of point defect interactions with Cr, which can be investigated by a multiscale modeling approach. Molecular dynamics simulations, using Finnis-Sinclair-type potentials, have been used to investigate interstitial diffusion, and the resulting atomic transport of Cr and Fe using interatomic potentials that predict Cr as either an under- or over-sized solute with otherwise constant materials properties. Ab-initio calculations on vacancy–Cr interactions reveal complex electronic and magnetic interactions between Cr and Fe. These values have been used to calculate the ratio of Cr-to-Fe diffusion by a vacancy mechanism using the LeClaire multi-frequency model and a kinetic lattice Monte Carlo model, both of which indicate that Cr diffuses faster than Fe by a vacancy mechanism. The results are discussed in the context of the radiation-induced segregation of Cr at grain boundaries in BCC Fe-Cr alloys.

9.2 MOLECULAR DYNAMICS SIMULATION OF MIXED DISLOCATION INTERACTION WITH STACKING FAULT TETRAHEDRON - H.-J. Lee and B. D. Wirth (University of California, Berkeley) 153

The interaction between a 60 degree mixed dislocation and a stacking fault tetrahedron (SFT) is investigated using molecular dynamics (MD) simulation. The interaction strongly depends on the sense of the dislocation Burgers vector, with un-faulting and stable shear ledge formation occurring in one case, while simple bypass and immediate reconstruction of the SFT is observed for the opposite Burgers vector direction. SFT un-faulting by a mixed dislocation occurs following the constriction of a mixed dislocation on the SFT, which produces a Shockley partial that can glide on the SFT face(s). In particular, when the dislocation intersects the SFT edge side, the SFT base is absorbed into the dislocation core as a super-jog pair. After dislocation bypass, a smaller SFT and vacancy clusters remain behind. When the dislocation glides on the base plane of the SFT, the strong repulsion between the mixed dislocation and the SFT induced SFT collapse.

9.3 MOLECULAR DYNAMICS SIMULATION OF DISLOC-ATION-VOID INTERACTIONS IN BCC MO - H.-J. Lee and B. D. Wirth (University of California, Berkeley) 163

Molecular dynamics (MD) and molecular statics (MS) simulations have been performed to simulate the plastic deformation processes in irradiated body centered cubic (BCC) Mo. Considering the unique non-planar core structures of the screw dislocation in BCC metals, the behavior of screw dislocation motion as a function of temperature and applied shear stress is first discussed. A transition from smooth to rough motion of the screw dislocation is observed with increasing shear stress, as well as a change of dislocation glide plane from {110} to {112} with increasing temperature. The interaction of a screw dislocation with nanometer-sized voids observed in both dynamic and static conditions is then reported. The obstacle strength calculated from MS calculations shows a large increase in critical resolved shear stress for

void diameter larger than about 3 nm. However, the MD results indicate that the screw dislocation interaction with void occurs via a simple shear mechanism.

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The results of He desorption measurements are presented for both poly- (PC) and single-crystalline (SC) iron (>99.99%) using constant rate (1 K/s) heating following room temperature 4He implantations at energies of 5 and 10 keV, and fluences of 1014 and 1015 He/cm2. A sharp desorption peak due to BCC-FCC phase transformation is observed for both PC and SC specimens, which provides precise temperature calibration. Within the BCC structural range, three groups (I: below 300 ºC; II: 300-600 ºC; III: 600-900 ºC) of desorption signal are identified for PC specimens while only two groups (I: below 300 ºC; II: 550-900 ºC) are identified for SC specimens. The low T group appears broader for PC specimens than for SC specimens. PC and SC desorption spectra show similar dependence on implantation energy and fluence, namely that the relative intensity at low and intermediate temperatures decreases with increasing implantation energy or fluence, while the fluence effect is much more pronounced than the energy effect. Simple first order dissociation kinetics are used to estimate the average activation energies associated with all the desorption groups, and these energies range from about 1.1 to 3.4 eV. However, precise identification of the mechanisms controlling each desorption event requires further study by complementary characerization and modeling techniques. The present SC iron data are expected to provide an appropriate experimental reference for future rate-theory or kinetic Monte-Carlo modeling of helium defect evolution in BCC iron.

9.5 INTERACTION OF HenVm CLUSTERS WITH COHERENT AND SEMI-COHERENT Fe/Cu INTERFACES – R. J. Kurtz, H. L. Heinisch, and F. Gao (Pacific Northwest National Laboratory) 175

Previous computational modeling has shown that interstitial and substitutional He as well as He-divacancy clusters are strongly bound to extended defects in Fe such as dislocations, grain boundaries and particle-matrix interfaces. One aspect of the earlier work was the interaction of He with nanometer-scale, coherent particles embedded in an Fe matrix. Our earlier research also established that the core of an edge dislocation strongly traps He. Thus we hypothesized that a semi-coherent interface might be a stronger trap for He than a coherent interface due to the array of misfit dislocations needed to accommodate the lattice parameter mismatch between the particle and the matrix in the semi-coherent case. In the present study we employ atomisitic simulations to compare the binding of HenVm complexes to coherent and semi-coherent bcc Fe/ bcc Cu interfaces. The simulations show that the binding energy of HenVm complexes to a coherent Fe/Cu interface range from 0.35 eV for a single vacancy up to 0.70 eV for a He1V2 complex. A semi-coherent interface was found to be a much stronger trap for He near the core of a misfit dislocation. Binding energies varied from 0.86 eV for a substitutional He atom up to 2.38 eV for a He1V2 complex. These binding energies were found to be significantly larger than the values obtained for simple edge dislocations in Fe. The trend in binding

energies can be rationalized in terms of the spatial dependence of excess atomic volume for each interface.

9.6 INTERACTION OF VACANCIES AND HELIUM ATOMS WITH a/2 <111> SCREW DISLOCATIONS IN α-Fe - H. L. Heinisch, F. Gao, R. J. Kurtz (Pacific Northwest National Laboratory) 182

Migration energies of vacancies and He atoms in and near the core of an a/2<111> screw dislocation in α-Fe were determined in atomistic simulations using conjugate gradient relaxation and the Dimer method for determining saddle point energies. Results for defects in initial positions in and near the screw dislocation core were obtained for migration toward and away from the dislocation line, as well as along the dislocation line direction. For both vacancies and individual interstitial helium atoms migration is favored toward and along the screw dislocation. Vacancies trapped in the dislocation core migrate along the dislocation with a migration energy of about 0.4 eV, which is about half the migration energy of vacancies in the perfect crystal.

9.7 MIGRATION OF VACANCIES, HE INTERSTITIALS AND HE-VACANCY CLUSTERS AT GRAIN BOUNDARIES IN ALPHA-FE – F. Gao, H. L. Heinisch and R. J. Kurtz (Pacific Northwest National Laboratory) 186

The dimer method for searching transition states has been used to systematically study possible migration paths of vacancies, He interstitials and He-vacancy (He/V) clusters at Σ11<110> {323} and Σ3<110> {111} grain boundaries (GBs) in α-Fe. Vacancies trapped at the GBs diffuse along the GBs with migration energies much less than that within the perfect crystal. Long-time dynamics simulations of diffusion pathways reveal that vacancies migrate one-dimensionally along the close-packed rows in the Σ3 GB, and one-dimensionally in zigzag paths within the Σ11 GB. Also, dimer saddle point searches show that He interstitials can diffuse along the GBs with migration energies of 0.4-0.5 eV, similar to those of individual vacancies at the GBs, and the corresponding mechanisms are determined. The rate-controlling activation energy for migration of a He-divacancy cluster in the GBs determined using the dimer method is about 0.9 eV, which is comparable to the migration energy for a He-divacancy cluster in bulk α-Fe.

9.8 MODELLING THERMODYNAMICS OF ALLOYS FOR FUSION APPLICATION - A. Caro, P. Erhart, M. Serrano de Caro, B. Sadigh (Lawrence Livermore National Laboratory), E. Lopasso (Centro Atomico Bariloche, Argentine), D. Farkas (Virginia Polytechnical Institute), S.G. Srinivasan, and C. Jiang (LANL) 192

Computer simulations of processes related to radiation damage have provided deep insight into atomistic processes at the origin of all changes that irradiation produces on mechanical properties of materials. However, as progress continues and more and more complex materials are developed, like the nanostructured Oxide Disperse Strengthened (ODS) ferritic steels, the simulations are confronted with the necessity to capture intricate thermodynamic and kinetic effects. The work reported here is an attempt to bring simulation capabilities to new domains where such effects are accurately described. In this report we present our recent results on the nature of the phase diagram of FeCr in the low Cr region, where finite solubility together with the existence of new intermetallic phases may be at the origin of the explanation of embrittlement and swelling under irradiation, with their intricate dependence on Cr composition. Our work in the last few

years has followed a systematic approach to model this alloy that started with a methodology to generalize many-body classic potentials to incorporate complex formation energy curves. Application to Fe-Cr allowed us to predict the implications of the ab initio results of formation energy on the phase diagram of this alloy and to get a detailed insight into the processes leading to precipitation of α' phase under irradiation. In this period we report on the consequences of the negative heat of formation at low Cr composition on the formation of new phases at low T, in particular ordered intermetallic phases, whose existence have been the subject of speculation in recent years.

9.9 APPLICATION OF DIGITAL MARKER EXTENSOMETRY TO DETERMINE THE TRUE STRESS-STRAIN BEHAVIOR OF IRRADIATED METALS AND ALLOYS - M. N. Gusev, O. P. Maksimkin, I. S. Osipov (Institute of Nuclear Physics, Almaty, Kazakhstan) and F. A. Garner (Pacific Northwest National Laboratory) 198

To study the mechanisms of deformation hardening and flow localization of radioactive materials, a non-contact "digital marker extensometry" technique has been employed. It allows researchers to easily define plasticity parameters and true stresses in experiments where highly radioactive miniature specimens are used. The engineering and "true stress – true local strain" relationships of irradiated metal polycrystals during plastic flow and hardening have been investigated experimentally after irradiation in two reactors in Kazakhstan. The true curves were obtained for copper, nickel, iron, molybdenum, as well as for the Russian stainless steels 08Cr16Ni11Mo3 and 12Cr18Ni10Ti. Describing these curves using the equation $\sigma_i = \sigma_0 + k\sqrt{\varepsilon_i}$ demonstrates that the concept of ultimate stress in highly irradiated materials is an artifact arising from flow localization and is not fully informative of the operating hardening mechanisms.

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No contributions.

11.0 MATERIALS ENGINEERING AND DESIGN REQUIREMENTS 211

No contributions.

12.0 IRRADIATION FACILITIES AND TEST MATRICES 212

No contributions.