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FOREWORD

This is the thirty-third 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 Ron Klueh and Renetta Godfrey, Oak Ridge National Laboratory. Their efforts, and the efforts of the many persons who made technical contributions, are gratefully acknowledged.

S. E. Berk
Facilities and Enabling Technologies Division
Office of Fusion Energy Sciences

TABLE OF CONTENTS

1.0 VANADIUM ALLOYS ***1***

1.1 STRONGLY NON-ARRHENIUS INTERSTITIAL DIFFUSION IN VANADIUM – S. Han, R. Car, D. J. Srolovitz (Princeton University), and L. A. Zepeda-Ruiz (LLNL) **2**

We perform molecular dynamics simulation to study the diffusion of SIAs in vanadium. The interatomic potentials employed were developed by fitting to first-principle, quantum mechanical results on SIA structure and energetics. The present results demonstrate that the SIA in vanadium exists in a <111>- dumbbell configuration and migrates along <111> directions, in agreement with first-principles calculations. At low and intermediate T, the diffusion is one-dimensional, but at higher temperatures, the dumbbell can rotate into other <111> directions, resulting in three-dimensional at high T. The apparent activation energy for migration increases with temperature as a result of a complex correlation effect even at temperatures before significant dumbbell reorientation occurs.

1.2 FABRICATION OF CREEP TUBING FROM THE US AND NIFS HEATS OF V-4Cr-4Ti – A. F. Rowcliffe, (ORNL), W.R. Johnson (Rocket Science & Materials Engr. Services), D. T. Hoelzer (ORNL) **7**

Commercial-scale fabrication of thin-walled tubing for thermal and irradiation creep testing of V4Cr- 4Ti has been initiated at Century Tubes Inc, San Diego. In an effort to minimize the occurrence of the surface flaws and cracks which characterized the previous batch of tubing, the technical specifications have been extensively modified. In particular improvements have been made in the cleaning procedures and in the control of the vacuum during all stages of the annealing cycle; the levels of cold work applied during the final stages have been substantially reduced. Both the US program heat and the Japanese NIFS-HEAT-2 are being processed; interim examination shows significant increases in oxygen content for both heats in spite of the added precautions introduced. Surface defects similar to those observed in the previous batch of tubing were detected in one section of tubing from the US heat after 4 draw cycles while the NIFS heat was relatively free of surface defects.

2.0 CERAMIC COMPOSITE MATERIALS ***22***

2.1 THERMAL DIFFUSIVITY/CONDUCTIVITY OF IRRADIATED SYLRAMIC 2D-SIC$_F$/SIC COMPOSITE G. E. Youngblood, D. J. Senor, and R. H. Jones (PNNL) **23**

A 2D-SiC$_f$/SiC composite was made by Hypertherm with an ICVI-SiC matrix and with multilayer C/SiC coatings on high thermal conductivity Sylramic fibers woven into 5HS fabric layers. Thermal diffusivity measurements were made on representative samples of this Sylramic composite before and after irradiations in the HFIR reactor as part of the JUPITER 14J test series. The irradiations took place at about 290 and 800°C to equivalent doses of 4.2 and 7.0 dpa-SiC, respectively. The ratios of the transverse thermal conductivity after-to-before irradiation (K_{irr}/K_o) determined at the irradiation temperature were estimated from thermal diffusivity measurements to be about 0.12 and 0.37 at 290 and 800°C, respectively. However, the measured thermal diffusivity values of the unirradiated Sylramic• composite with multilayer C/SiC fiber coatings were about 40% less than values predicted by the H2L model for this composite. This observation could be explained if the net interface conductance of the C/SiC multilayer was less than 0.1 of the interface conductance of a single layer PyC fiber coating.

2.2 THERMAL DIFFUSIVITY/CONDUCTIVITY OF IRRADIATED MONOLITHIC CVD-SIC 27
- G. E. Youngblood, D. J. Senor, and R. H. Jones (PNNL)

Several thermal diffusivity disc samples of high purity CVD-SiC were neutron-irradiated to equivalent doses of about 5-8 dpa-SiC at temperatures from 252 up to 800°C. For this temperature range, the degradation in the thermal diffusivity ranged from about 95% down to 89%, respectively. The reciprocal thermal diffusivity method was used to estimate the phonon mean free paths and defect concentrations before and after the irradiations for these materials. Even though the CVD-SiC material is an excellent monitor of certain neutron irradiation effects, the degradation in the thermal diffusivity (conductivity) appears to be more than a factor of two greater than predicted by recent theoretical model simulations.

2.3 EVALUATION OF TRANSTHICKNESS TENSILE STRENGTH OF SiC/SiC COMPOSITES - T. Hinoki, E. Lara-Curzio, and L. L. Snead (ORNL) 34

The transthickness tensile strength (TTS) of 2-D CVI-SiC/SiC composites reinforced with Tyranno SA fibers was evaluated by the diametral compression test. The effects of specimen size and specimen shape on the magnitude of the TTS were studied and the results were analyzed using an analysis of variance (ANOVA) and Weibull statistics.
Specimens failed along an interlaminar plane adjacent to the line of action of the applied load and fractographic analyses revealed that the crack had propagated through matrix pores and along interfaces between the fiber, fiber coating and matrix. The magnitude of the TTS was found to be independent of specimen size or shape for the range of specimen dimensions investigated, although the amount of scatter was largest for the results obtained from the evaluation of the smallest specimens. The characteristic value of the TTS and the Weibull modulus for the distribution of TTS values were 24.9 MPa and 6.48, respectively.

2.4 DEVELOPMENT OF REFRACTORY ARMORED SILICON CARBIDE - T. Hinoki, L.L. Snead, C.A. Blue, M.L. Santella, D.C. Harper and N. Hashimoto (ORNL), H. Kishimoto (Kyoto University) 39

A uniform strong W coating was successfully formed. Tungsten vapor deposition and pre-heating at 5.2 MW/m^2 made for a refractory layer containing no cracks which propagated into the SiC substrate. This layer was formed without the thick reaction layer (WC and W_5Si_3) reported in previous studies. Moreover the thinner interface transition layer and armor avoid coefficient of thermal expansion (CTE) mismatch driven failure previously reported. For this study, small W_xC_y grains were observed adjacent to interface. Silicon carbide grains and W_xSi_y grains were observed within W coating. By contrast, Mo was not successfully formed. Most of Mo coating debonded at reaction layer due to too much absorbed energy for Mo and larger CTE mismatch than that of W and SiC. Further study at lower absorbed powers would be required to carry the Mo coating further.

2.5 TOTAL DPA CROSS SECTIONS FOR SIC AS A FUNCTION OF NEUTRON ENERGY - H. L. Heinisch, L. R. Greenwood, W. J. Weber, and R. E. Williford (PNNL) 44

Total DPA cross sections for SiC as a function of neutron energy have been calculated using the latest and best knowledge about damage production in SiC. We encourage the adoption of these cross sections as the standard to be used for calculating radiation damage production in DPA for all neutronirradiated SiC samples, including those in past irradiations.

2.6 STRENGTH OF NEUTRON IRRADIATED SILICON CARBIDE AND SILICON CARBIDE COMPOSITE - L. L. Snead and T. Hinoki (ORNL) and Y. Katoh (Kyoto University) **49**

Specimens of monolithic SiC and SiC composite have been irradiated with fission neutrons in the temperature and dose range of 90-1000°C and 1.1- 7.7 x 1025 n/m2 (E>0.1 dpa), respectively. Materials included stoichiometric chemically vapor deposited SiC and composites containing SiC-based fibers chemicaly vapor infiltrated with SiC. For the case of the monolithic SiC and the composite containing the near-zero oxygen content fibers, no degradation in bend strength was observed. Composite materials containing the higher oxygen content fibers exibited significant degradation. These results are compared with data from the literature on the irradiation effects on the properties of stoichiometric and non-stoichiometric SiC-based materials.

3.0 FERRITIC MARTENSITIC STEELS ***58***

3.1 FRACTURE TOUGHNESS CHARACTERIZATION OF THE IRRADIATED F82H IN THE TRANSITION REGION - M. A. Sokolov, R. L. Klueh (ORNL), G. R. Odette (UCSB), K. Shiba, and H. Tanigawa (JAERI) **59**

The ferritic-martensitic steel F82H is a primary candidate low-activation material for fusion applications, and it is being investigated in the joint U.S. Department of Energy-Japan Atomic Energy Research Institute collaboration program. As part of this program, two capsules containing a variety of specimen designs were irradiated at two different temperatures in the Oak Ridge National Laboratory (ORNL) High Flux Isotope Reactor. The bottom and top parts of these capsules were loaded with disk-shaped compact tension [DC(T)] specimens that were used for fracture toughness characterization. This small (12.5 mm in diameter with thickness of 4.6 mm) DC(T) specimen was developed at ORNL for testing irradiated materials. Six specimens were irradiated in each “low-“ and “high-“ irradiation temperature capsule up to ~3.8 dpa. Irradiation temperatures were measured by thermocouples. In the low-temperature capsule, three specimens were irradiated at an average temperature of 261°C and another three at 240°C; temperature variation during irradiation was within ±19°C for a given specimen. In the high temperature capsule, all six specimens were irradiated at an average temperature of 377°C in the bottom part of the capsule; temperature variation during irradiation was within ±30°C for a given specimen. All irradiated specimens failed by cleavage instability. From these data, fracture toughness transition temperatures were evaluated for irradiated F82H steel and compared to unirradiated values. Specimens irradiated at the higher temperature exhibited a relatively modest shift of the fracture toughness transition temperature of ~57°C. However, the shift of fracture toughness transition temperature of specimens irradiated at 250°C was much larger, ~191°C. These results are compared with available tensile and impact Charpy data for this material.

3.2 CHARPY IMPACT PROPERTIES OF REDUCED-ACTIVATION FERRITIC/ MARTENSITIC STEELS IRRADIATED IN HFIR UP TO 20 DPA — H. Tanigawa (JAERI) M. A. Sokolov (ORNL), K. Shiba (JAERI), and R. L. Klueh (ORNL) **66**

The effects of irradiation up to 20 dpa on the Charpy impact properties of reduced-activation ferritic/martensitic steels (RAFs) were investigated. The ductile-brittle transition temperature (DBTT) of F82H-IEA shifted up to around 50°C. TIG weldments of F82H showed a fairly small variation on their impact properties. A finer prior austenite grain size in F82H-IEA after a different heat treatment resulted in a 20°C lower DBTT compared to F82H-IEA after the standard heat treatment, and that effect was maintained even after irradiation. Helium effects were investigated utilizing Ni-doped F82H, but no obvious evidence of helium effects was obtained. ORNL9Cr-2WVTa and JLF-1 steels showed smaller DBTT shifts compared to F82H-IEA.

3.3 DEFORMATION MICROSTRUCTURE OF A REDUCED-ACTIVATION FERRITIC/MARTENSITIC STEEL IRRADIATED IN HFIR - N. Hashimoto (ORNL), M. Ando, H. Tanigawa, T. Sawai, K. Shiba (JAERI), and R. L. Klueh (ORNL) **73**

In order to determine the contributions of different microstructural features to strength and to deformation mode, the microstructures of deformed flat tensile specimens of irradiated reduced activation F82H (IEA heat) base metal (BM) and its tungsten inert-gas (TIG) weldments (weld metal and weld joint) were investigated by transmission electron microscopy (TEM), following fracture surface examination by scanning electron microscopy (SEM). After irradiation, the fracture surfaces of F82H BM and TIG weldment showed a martensitic mixed quasi-cleavage and ductile-dimple fracture. The microstructure of the deformed region of irradiated F82H BM contained dislocation channels. This suggests that dislocation channeling could be the dominant deformation mechanism in this steel, resulting in the loss of strain-hardening capacity. While, the necked region of the irradiated F82H TIG, which showed less hardening than F82H BM, showed deformation bands only. From these results, it is suggested that the pre-irradiation microstructure, especially the dislocation density, could affect the post-irradiation deformation mode.

3.4 CRACK TIP MICROSTRUCTURES IN F82H ON THE LOWER SHELF - D. S. Gelles (PNNL), G. R. Odette (UCSB) and P. Spätig (École Polytechnique Fédérale de Lausanne, – Centre de Recherches en Physique des Plasma, Villigen PSI, Switzerland) **79**

Dislocation microstructures have been examined near the crack tip of a compact tension specimen of unirradiated F82H loaded to 25.6 MPa $m^{1/2}$ at –196°C after fatigue precracking. A specimen was prepared by sectioning, dimple grinding and ion milling in order to produce electron transparency just behind the crack tip. The tip was found to have trifurcated with moderate dislocation densities ahead and to the side of each tip extending at least 4 to 5 μm, but regions adjacent to the fatigue crack but back from the tip displayed only minor dislocation rearrangement of lath boundaries.

3.5 IRRADIATION EFFECTS ON IMPACT TOUGHNESS OF HIGH-CHROMIUM FERRITIC/MARTENSITIC STEELS - R. L. Klueh and M. A. Sokolov (ORNL) 85

Charpy specimens of four ferritic/martensitic steels were irradiated at 376-405ºC in the Experimental Breeder Reactor (EBR-II) to 23-33 dpa. The steels were the ORNL reduced-activation 9Cr-2WVTa and that steel containing 2% Ni (9Cr-2WVTa-2Ni), modified 9Cr-1Mo, and Sandvik HT9 (12Cr-1MoVW). The steels were normalized and then the 9Cr-2WVTa and 9Cr-2WVTa-Ni were irradiated after tempering 1 hr at 700ºC and after tempering 1 h at 750ºC; the 9Cr-1MoVNb and 12Cr-1MoVW were tempered 1 h at 760ºC. Based on the change in ductile-brittle transition temperature and the upper-shelf energy, the results again demonstrated the superiority of the 9Cr-2WVTa steel over the two commercial steels, which were replaced by the reduced-activation steels. The Charpy properties of the 9Cr-2WVTa-2Ni steel were similar to those of the 9Cr-2WVTa steel for both heat treatments, indicating no adverse effect of the nickel on the properties after irradiation.

3.6 MICROSTRUCTURE AND HARDNESS VARIATION IN A TIG WELDMENT OF IRRADIATED F82H — H. Tanigawa (JAERI), N. Hashimoto (ORNL), M. Ando, T. Sawai, K. Shiba (JAERI), R.L. Klueh (ORNL) 92

Previous work reported that a TIG weld joint of F82H exhibited low irradiation hardening in a tensile test, compared to the base metal. Microhardness tests and microstructure observation on the neutron-irradiated TIG weld joint of F82H revealed that the over-tempered zone in the heat-affected zone (HAZ) exhibited this good performance. The region in the HAZ where the prior austenite grain became very fine during welding also exhibited lower irradiation hardening. Hypotheses for these low-hardening mechanisms were proposed based on the phase diagram and grain orientation.

3.7 NEUTRON-INDUCED SWELLING OF Fe-Cr BINARY ALLOYS IN FFTF at ~400°C - F. A. Garner and L. R. Greenwood (PNNL), T. Okita and N. Sekimura (U. of Tokyo) and W. G. Wolfer (LLNL) 99

Contrary to the behavior of swelling of model fcc Fe-Cr-Ni alloys irradiated in the same FFTF-MOTA experiment, model bcc Fe-Cr alloys do not exhibit a dependence of swelling on dpa rate at ~400°C. This is surprising in that an apparent flux-sensitivity was observed in an earlier comparative irradiation of Fe-Cr binaries conducted in EBR-II and FFTF. The difference in behavior is ascribed to the higher helium generation rates of Fe-Cr alloys in EBR-II compared to that of FFTF, and also the fact that lower dpa rates in FFTF are accompanied by progressively lower helium generation rates.

3.8 ON THE EFFECTS OF PRECRACKING TECHNIQUE ON TRANSITION FRACTURE TOUGHNESS VALUES DERIVED FROM SMALL 3-POINT BEND SPECIMENS — M. A. Sokolov (ORNL) and H. Tanigawa (JAERI) 105

Small 3-point bend specimens of F82H steel were precracked using the “plate-precracking” and traditional “specimen-precracking” techniques. The “plate-precracking” technique guarantees crack front that is straight and practically perpendicular to the sides for all specimens in the group. The results suggest that the plate-precracked specimens were in higher constraint during the fracture toughness test than in the "specimen-precracked" specimen. However, difference in T0 value is within statistical scatter of fracture toughness. Additional testing on different materials is needed to validate the effects.

4.0 COPPER ALLOYS ***110***

4.1 STATUS OF COLLABORATIVE RESEARCH PROGRAM BETWEEN PNNL AND RISØ NATIONAL LABORATORY - D. J. Edwards (PNNL) and B. N. Singh (Risø National Laboratory, Denmark) **111**

PNNL and Risø have been collaborating since 1994 on a series of irradiation experiments on pure copper and various alloys of interest to the fusion materials community. The collaboration has been of great benefit to both institutes by sharing resources and experience. Past research has concentrated on examining the microstructural evolution during neutron irradiation and the influence this microstructural change exerts on the deformation response. Post-irradiation annealing experiments of both irradiated pure copper and CuCrZr yielded unique insights into the relationship between the microstructure and the deformation response. The results of that experiment also raised further questions regarding the stability and structure of the small defects produced during irradiation, particularly regarding the stability of these defects during annealing and how they interact with mobile dislocations. The focus of ongoing work has now shifted to examining the issues of defect stability in irradiated materials, dislocation generation from stress concentrations at interfaces in irradiated materials, and a new experiment on in-situ straining during irradiation and how this affects microstructural evolution and the relationship to mechanical properties.

5.0 REFRACTORY METALS AND ALLOYS ***120***

No contributions

6.0 AUSTENITIC STAINLESS STEELS ***121***

6.1 INFLUENCE OF CARBON AND DPA RATE ON NEUTRON-INDUCED SWELLING OF Fe-15Cr-16Ni- 0.25Ti IN FFTF at ~400°C - T. Okita and N. Sekimura (U. of Tokyo), F. A. Garner (PNNL) and W. G. Wolfer (LLNL) **122**

Contrary to the swelling behavior of fcc Fe-15Cr-16Ni and Fe-15Cr-16Ni-0.25Ti alloys irradiated in the same FFTF-MOTA experiment, Fe-15Cr-16Ni-0.25Ti-0.04C does not exhibit a dependence of swelling on dpa rate at ~400°C. The transient regime of swelling is prolonged by carbon addition, however.

7.0 MHD INSULATORS, INSULATING CERAMICS AND OPTICAL MATERIALS ***128***

7.1 STUDY OF THE LONG-TERM STABILITY OF Y_2O_3 MHD COATINGS FOR FUSION REACTOR APPLICATIONS -- B. A. Pint and L. D. Chitwood (ORNL) **129**

Two batches of Y2O3 coatings (12.5μm thick) were formed on V-4Cr-4Ti substrates using electronbeam assisted, physical vapor deposition (EB-PVD). The performance of the first batch of coatings was previously reported1 and was promising. However, additional results on the second batch showed spallation after extended capsule exposures in Li at 700° and 800°C. These observations may be the result of an incompatibility between Y2O3 and Li, problems with the processing technique, or batch to batch variation in coating performance. A vacuum rig has been built to measure coating electrical resistance up to 800°C.

7.2 MICROSTRUCTURES OF Y-O, Si-O, AND IN-SITU FORMED CaO COATINGS ON V-4%Cr-4%Ti IN LIQUID 2.8 at. % Ca-Li * - J. -H. Park and K. Natesan (ANL) **133**

In a previous study, we demonstrated the in-situ formation of a CaO insulator coating, generating defects under thermal cycling conditions, and self-healing of defects on V-Cr-Ti alloys in the liquid lithium system.1 We also found that sintered Y2O3 is compatible with liquid Li.2 These encouraging results caused us to investigate O-charged V-4Cr-4Ti with a Y film deposited by means of physical vapor deposition (PVD). We are now investigating the in-situ formation of a CaO layer on a V-4Cr-4Ti surface enriched with Y-O or Si-O. In the study of coatings on the V/Li blanket, the electrical insulation behavior should be maximized to have a thin film with high toughness and thermal conduction. What needs to be eliminated or minimized is V incorporation into the insulator film and in-situ self-healing. In this report we present microstructures for the electrical insulator coating reported previously.3 Also investigated was Si-O addition based on a thermodynamic evaluation. The addition of Si was tested to minimize the V incorporation in the in-situ CaO film. Our previous investigations showed that the incorporation of V into the in-situ-formed CaO was normally 15 to 35 at.%. If V is highly incorporated, the film could be conductive due to the V having a wide range of ionic valence states. Based on the thermodynamic evaluation, we determined that additions of Si could form as Ca-Si-O in the Ca-Li environment. Therefore, we performed surface modification by Cr+Cr2O3 equilibrium inside a vacuumsealed quartz (SiO2) chamber. When the oxygen partial pressure (pO2) is low, such as the level corresponding to Cr+Cr2O3 equilibrium at high temperatures, the quartz becomes the source of the Si, Si- O, and Cr that are incorporated into the V-4Cr-4Ti along with O in the chemical vapor. Based on these concerns, we initiated study of the Y and Si additions to the in-situ CaO films, and we are reporting the results of short exposures.

8.0 BREEDING MATERIALS ***138***

No Contributions.

9.0 RADIATION EFFECTS, MECHANISTIC STUDIES, AND EXPERIMENTAL METHOD ***139***

9.1 MD MODELING OF SCREW DISLOCATION - <100> LOOP IINTERATION IN Fe – J. Marian and B. D. Wirth (LLNL) **140**

Ferritic/martensitic steels considered as candidate first-wall materials for fusion reactors experience significant radiation hardening at temperatures below ~400°C. In this work we describe the motion of screw dislocations, known to control the plastic response of bcc materials to external stress, and their interaction with 100 dislocation loops. MD simulations are used to simulate screw dislocation motion and, following a description of the computational method, we report the main physical mechanisms of the dislocation – loop interaction, including an estimate of the critical bowing angle and a first-order estimation of the induced hardening.

9.2 KINETIC MONTE CARLO SIMULATIONS OF THE EFFECTS OF 1-D DEFECT TRANSPORT ON DEFECT REACTION KINETICS AND VOID LATTICE FORMATION DURING IRRADIATION - H. L. Heinisch (PNNL) and B. N. Singh (Risø National Laboratory, Denmark) **146**

Within the last decade molecular dynamics simulations of displacement cascades have revealed that glissile clusters of self-interstitial crowdions are formed directly in cascades. Also, under various conditions, a crowdion cluster can change its Burgers vector and glide along a different close-packed direction. In order to incorporate the migration properties of crowdion clusters into analytical rate theory models, it is necessary to describe the reaction kinetics of defects that migrate one-dimensionally with occasional changes in their Burgers vector. To meet this requirement, atomic-scale kinetic Monte Carlo (KMC) simulations have been used to study the defect reaction kinetics of one-dimensionally migrating crowdion clusters as a function of the frequency of direction changes, specifically to determine the sink strengths for such one-dimensionally migrating defects. The KMC experiments are used to guide the development of analytical expressions for use in reaction rate theories and especially to test their validity. Excellent agreement is found between the results of KMC experiments and the analytical expressions derived for the transition from one-dimensional to three-dimensional reaction kinetics. Furthermore, KMC simulations have been performed to investigate the significant role of crowdion clusters in the formation and stability of void lattices. The necessity for both one-dimensional migration and Burgers vectors changes for achieving a stable void lattice is demonstrated.

9.3 FINDING POSSIBLE TRANSITION STATES OF DEFECTS IN SILICON-CARBIDE AND ALPHA-IRON USING THE DIMER METHOD – F. Gao, W. J. Weber, L. R. Corrales (PNNL), G. Henkelman, and H. Jónsson (U. of Washington) **151**

The ‘dimer’ method was employed to search for possible transition states and their saddle point energies for interstitials and small interstitial clusters in SiC and £\-Fe. The dimer method is a technique for finding saddle points in the potential energy surface within a solid, without knowledge of the final state of transition, and without the use of second derivatives of the potential, has been recently developed by Henkelman and Jónsson [1]. In addition to the calculation of activation energies of point defect and cluster migration along the <111> direction in £\-Fe, the activation energies for the directional change of interstitial clusters is investigated. The dimer method, described in detail elsewhere [1], involves two atomic images of the system, separated by a very small 3N-dimensional unit vector. The energy of this dimer and the force on the midpoint, as well as the curvature of the potential at the dimer, can be calculated from the forces acting on the two images. The net force on the dimer is minimized by rotation of the dimer, and the dimer is translated so as to move up the potential surface. Saddle points are located through a series of rotations and translations of the dimer. Upon finding a saddle point, the dimer is returned to the starting configuration, and it is randomly assigned a new orientation as a starting configuration for another saddle point search. In principle, all saddle points surrounding the initial configuration can be found. In practice, the same saddle point or symmetrically equivalent saddle points are often found, and occasionally no saddle points are located after a reasonable expenditure of computer time. Once the saddle point is found, the minimum energy path to the next energy basin can be determined, and the changes in atom positions during the transition can be followed.

9.4 NUCLEATION AND GROWTH OF HELIUM-VACANCY CLUSTERS IN IRRADIATED METALS. PART. I. A GROUP METHOD FOR AN APPROXIMATE SOLUTION OF TWO DIMENSIONAL KINETIC EQUATIONS DESCRIBING EVOLUTION OF POINT DEFECT CLUSTERS - S. I. Golubov, R. E. Stoller, S. J. Zinkle (ORNL). **155**

Nucleation, growth and coarsening of point-defect clusters or secondary phase precipitates are of interest for many applications in solid-state physics. As an example, clusters nucleate and grow from point defects in solids through irradiation. In typical nucleation, growth and coarsening problems, a master equation (ME) is constructed that summarizes the large number of ordinary differential equations (ODE) needed to describe the evolution process. To solve the large number of ODEs in the case when it is one dimensional, e.g. clustering of vacancies and self-interstitial atoms (SIAs) under irradiation in a form of voids or dislocation loops, a grouping method was originally proposed by Kiritani [1] in 1972. In 2001 Golubov et al. [2] have shown that Kiritani's method is not adequate and developed a new grouping method. The gas-assisted nucleation of voids or bubble formation is typical of problems that require solving two-dimensional ME, which has not been subjected to any specific grouping method of the type mentioned. This work intends to fill this gap. In the present work the grouping method proposed by Golubov et al. [2] is generalized for the case of the two-dimensional one. An application of the method to the problem of helium-assisted void/bubble formation under irradiation is presented.

10.0 DOSIMETRY, DAMAGE PARAMETERS, AND ACTIVATION CALCULATIONS ***181***

No contributions

11.0 MATERIALS ENGINEERING AND DESIGN REQUIREMENTS ***182***

No contributions

12.0 IRRADIATION FACILITIES AND TEST MATRICES ***183***

No contributions