SUMMARY REPORT ON THE US/JAPAN JUPITER COLLABORATION INTEGRATED FOCUS ON FUNDAMENTAL STUDIES - VANADIUM INITIATIVE – H.L. Heinisch (Pacific Northwest National Laboratory*) and N. Sekimura (University of Tokyo)

OBJECTIVE

The objective of the Integrated Focus on Fundamental Studies, Vanadium Initiative (IFFS-VI) was to foster direct collaborations, integration of efforts, and joint utilization of resources by the US and Japan under the JUPITER Fusion Materials Collaboration agreement. The basic concept of IFFS-VI was to integrate theory, modeling and experiments, as well as the efforts of Japanese and US participants, toward a common focus on a specific technological problem in Fusion Materials research.

SUMMARY

IFFS-VI was initiated by the participants in the JUPITER Workshop on Theory and Modeling for Fusion Materials held October 30, 1997, during ICFRM-8 in Sendai, Japan. The original initiative is described, participants and collaborations are identified, and progress is summarized.

PROGRESS AND STATUS

Introduction

At the JUPITER Workshop on Theory and Modeling for Fusion Materials held October 30, 1997, in Sendai, the IFFS-VI program was devised and embraced by both sides of the JUPITER collaboration as a means of focusing our individual and joint efforts on the fundamental aspects of radiation effects in fusion materials. IFFS-VI was a program of theory, modeling, simulation and experiments focused on the specific problem of understanding and predicting the effects of temperature variation during fission reactor irradiation on the microstructure development and property changes of V-4Cr-4Ti. This problem was chosen because it aimed our theory and modeling programs at the prime candidate material that has received the least attention in that regard so far. However, it was not our intention that activities under IFFS-VI would preclude further work on advancing the fundamental understanding of irradiation effects in general.

The primary temperature variation experiments to be performed had been planned as a major JUPITER irradiation in HFIR before IFFS-VI was started. They were to provide experimental information on defect accumulation and property changes under well-controlled and monitored conditions. The temperature variation experiments were envisioned as a good comparative data base against which to evaluate the theories and models in V alloys, as well as in general. V-4Cr-4Ti, other V alloys of interest and some pure metals were among the materials included in the experiments. Separate low-dose irradiations were performed in the JMTR reactor and with heavy ions in Japan.

IFFS-VI was expected to continue throughout the remainder of the JUPITER collaboration and become a strong basis upon which to build future Japan/US collaborations on theory, modeling and experiments.

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IFFS-VI Tasks

The IFFS-VI theory and modeling tasks fall into the broad categories of Interatomic Potentials, Defect Properties, Cascade Generation, Annealing Simulation and Comparison with Experiments. A more detailed breakdown of the tasks outlined in Sendai is indicated below. It was never anticipated that sufficient resources would exist for the completion of all the tasks during the JUPITER collaboration. However, the task lists serves as an important instrument for focussing and integrating the activities of both sides. The experimental tasks associated with the neutron irradiations in HFIR and JMTR were planned and performed independent of IFFS-VI.

1. Interatomic Potentials

    a) Design and evaluate interatomic potentials for V, Ti, Cr and their interactions among themselves and with He (and O?).

    b) Evaluate applicability and feasibility of Tight Binding molecular dynamics (MD) for defect simulations.

2. Defect Properties

    a.) Calculate properties of defects in vanadium

        i.) Formation energies, binding energies
            Vacancy clusters, loops ,SFT, voids
            SIA clusters, loops
        ii.) Migration energies, diffusivities
            Vacancies, vacancy clusters
            SIAs, SIA clusters, SIA loops

    b.) Determine alloy and impurity properties

        i.) Binding energies of Ti atoms to point defects and clusters
        ii.) Binding energies of Cr atoms to point defects and clusters

    c.) Simulate defect interactions

        i.) V point defect – dislocation interactions
        ii.) Loop – dislocation interactions
        iii.) Role of Ti, Cr near dislocations
        iv.) Oxide precipitate formation

    d.) Evaluate helium interactions

        i.) He diffusivity in V
        ii.) He binding energies to defects, impurities
        iii.) He at grain boundaries

3.. Cascade Generation

    a.) Create data base of cascades in vanadium for relevant recoil energy spectra
    b.) Examine effects of Ti and Cr alloying elements on defect production

c.) Examine effects of cascade overlap

4. Monte Carlo and Analytical Simulations of Microstructural Evolution

   a.) Determine the fractions of surviving defects for individual cascades as a function of temperature and energy

   b.) Simulate damage accumulation in bulk as a function of temperature and recoil spectrum

   c.) Determine the effects of temperature variation on damage accumulation

   d.) Examine the role of grain boundaries on damage accumulation and He accumulation

5. Comparison with Experiments

The Varying Temperature Irradiation Experiment in HFIR will subject test specimens to cyclic changes in temperature during irradiation. Each cycle will consist of 0.05 dpa at a lower temperature, followed by 0.45 dpa at a higher temperature. Ten temperature cycles are planned for each of two low-high temperature pairs (200-350 C and 300-500 C). TEM specimens and mini-tensile, -Charpy and -bend bar specimens will be irradiated. Materials include ferritic and austenitic steels, refractory alloys, copper alloys and vanadium alloys. The vanadium alloys include pure vanadium, binary and ternary alloys, as well as the V-4Cr-4Ti alloy that is the subject of IFFS-VI. Pure Fe, Cu, Mo and W are also included in the experiment matrix.

Prior to obtaining the results from repeated cycles in HFIR, several irradiations will be carried out in JMTR for conditions identical to one cycle of the HFIR Varying Temperature Irradiation Experiment.

Some irradiation effects data for vanadium, V-4Cr-4Ti and other vanadium alloys already exists, although effects of temperature variation are not included.

IFFS-VI Strategy

It was envisioned that most of the IFFS-VI tasks could be worked on simultaneously and at various levels of physical realism until all the pieces could be fit together with the requisite level of physical reality. It was also expected that many of the developments in theory and modeling of irradiation effects that have been ongoing for many years are directly relevant to IFFS-VI without being developed specifically for V-4Cr-4Ti or pure V or even bcc metals and alloys, especially the development of models over multi-scales dealing with defect accumulation, microstructure evolution and mechanical property changes. These models are being developed in a general way and can be made specific to V-4Cr-4Ti when the necessary fundamental information for that material is available from first principles calculations, MD simulations, etc.

<u>IFFS-VI Progress in Theory, Modeling and Experiments</u>

Only a small fraction of the items on the daunting list of tasks above has been completed, but, given the unofficial nature of the Theory and Modeling Tasks under JUPITER and the limited resources available, IFFS-VI should be considered a success. Several direct collaborations of US and Japanese participants were initiated or sustained in response to the IFFS-VI program. Tools have been developed to investigate issues specific to vanadium as well as to extend our basic knowledge of radiation effects in metals and alloys. Perhaps IFFS-VI even influenced individual program goals and priorities. Specific details of the technical accomplishments under IFFS-VI can be found in the publications listed below.

A progress report on the first year of IFFS-VI was published in the *Fusion Materials Semiannual Progress Report for the Period Ending December 31, 1998* (DOE/ER-0313/25, 1999, p. 254). Progress on IFFS-VI was also reviewed at two JUPITER Collaboration Workshops on Theory and Modeling, held following the ICFRM-9, October 10-15, 1999 in Colorado Springs, and following the Materials Research Society Fall Meeting in Boston, December 1, 2000.

Progress on the Experiments

The Varying Temperature Irradiation Experiment in HFIR ended May 16, 1999, after eight of the planned ten cycles had been completed. A total dose of 4 dpa in the vanadium alloys was achieved. Post-irradiation examination of the specimens began in late 2000.

Lower dose irradiations were also carried out in JMTR under conditions similar to those of the HFIR Varying Temperature Irradiation Experiment but with significantly shorter temperature variation cycles. Ion irradiations with stepwise temperature variation have also been performed. Post-irradiation examination of many specimens has been completed.

IFFS-VI PUBLICATIONS

Below is a list of publications on fundamental studies of radiation damage relevant to IFFS-VI objectives (theory and modeling of damage production, damage accumulation and microstructure evolution; effects of temperature variation; irradiation experiments on vanadium and vanadium alloys and experiments on temperature variation under irradiation) involving US and Japanese JUPITER participants that have been published or submitted during the IFFS-VI program. The list of 36 papers is probably not exhaustive, but it represents well the studies performed in the three categories into which it is organized: Atomistic, Analytical and Experimental studies. Papers listed in **bold** type explicitly involve vanadium or vanadium alloys. Seven of the papers involve direct collaboration of Japanese and US investigators, as indicated by their authorship.

ATOMISTIC

E. Alonso, M. J. Caturla, T. Diaz de la Rubia and J. M. Perlado, Simulation of damage production and accumulation in vanadium, J. Nucl. Mater. 276 (2000) 221.

K. Morishita and T. Diaz de la Rubia, "A Molecular Dynamics Simulation Study of Displacement Cascades in Vanadium", J. Nucl. Mater. 271&272 (1999) 35.

K. Morishita, T. Diaz de la Rubia and A. Kimura, Mobility of self-interstitial atom clusters in vanadium, tantalum and copper, COSIRES

2000, USA, July, 2000, to be published in Nuclear Instruments and Methods in Physics Research B.

T. Morioka, K. Morishita and N. Sekimura, Monte-Carlo Simulation of point-defect behavior in cascades, Nucl. Inst. and Methods B 153 (1999) 130.

Y. Shimomura, I. Mukouda, K. Sugio and P. Zhao, Atomistic processes of damage evolution in neutron-irradiated Cu and Ni at high temperature, Rad. Effects and Defects in Solids, 148 (1999) 127.

Y. Shimomura, I. Mukouda and K. Sugio, Computer simulation on the void formation in neutron-irradiated Cu and Ni at high temperature, J. Nucl. Mater. 271&272 (1999) 225.

M. J. Caturla, N. Soneda, E. Alonso. B. D. Wirth, T. Diaz de la Rubia and J. M. Perlado, Comparative study of irradiation damage accumulation in Cu and Fe, J. Nucl. Mater. 276 (2000) 13.

R. Stoller, The role of cascade energy and temperature in primary defect formation in iron, J. Nucl. Mater. 276 (2000), 22.

Dislocation loop structure, energy and mobility of self-interstitial atom clusters in BCC iron, B. D. Wirth, G. R. Odette, D. Maroudas and G. E. Lucas, J. Nucl. Mater. 276 (2000) 33.

E. Kuramoto, Computer simulation of fundamental behaviors of interstitial clusters in Fe and Ni, J. Nucl. Mater. 276 (2000) 143.

Q. Xu, H. L. Heinisch and T. Yoshiie, Effects of temperature variation during neutron irradiation on defect accumulation in copper, J. Nucl. Mater. 283-287 (2000) 297.

H. L. Heinisch, B. N. Singh and S. I. Golubov, The effects of one-dimensional glide on the reaction kinetics of interstitial clusters, J. Nucl. Mater. 283-287 (2000) 737.

K. Morishita, T. Diaz de la Rubia, E. Alonso, N. Sekimura and N. Yoshida, A molecular dynamics simulation study of small cluster formation and migration in metals, 283-287 (2000) 753.

ANALYTICAL

E. Donahue, G. R. Odette and G. E. Lucas, On the mechanisms and mechanics of fracture toughness of V-4Cr-4Ti alloy, J. Nucl. Mater. 283-287 (2002) 518.

E. Donahue, G. R. Odette and G. E. Lucas, A physically based constitutive model for a V-4Cr-4Ti alloy, J. Nucl. Mater. 283-287 (2000) 637.

S. Sharafat and N. M. Ghoniem, Comparison of a microstructure evolution model with experiments on irradiated vanadium, J. Nucl. Mater. 283-287 (2000) 789.

N. M. Ghoniem, L. Sun, Fast sum method for the elastic field of 3-D dislocation ensembles, Phys. Rev. B, 60 (1999) 128 .

N. M. Ghoniem, B. N. Singh, L. Z. Sun and T. Diaz de la Rubia, Interaction and accumulation of glissile defect clusters near dislocations, J. Nucl. Mater. 276 (2000) 166.

Y.Katoh, R. E. Stoller, T.Muroga and A.Kohyama, Simulating the influence of radiation temperature variations on microstructural evolution, J. Nucl. Mater. 283-287 (2000) 313.

M. Ando, Y. Katoh, H. Tanigawa and A. Kohyama, The contribution of various defects to irradiation-induced hardening in austenitic model alloy, J. Nucl. Mater. 283-287 (2000) 423.

N. M. Ghoniem, L. Z. Sun, And B. N. Singh , 3-D dislocation dynamics study of plastic instability in irradiated copper," J. Nucl. Mater., 283-287 (2000) 741.

N. M. Ghoniem, S.- H. Tong, and L. Z. Sun, Parametric dislocation dynamics: a thermodynamics-based approach to investigations of mesoscopic plastic deformation, Phys. Rev. B, 61 (2000) 913.

N. M. Ghoniem, Computational methods for mesoscopic, inhomogeneous plastic deformation, Proc. First Latin American Symposium on Materials Instabilities, Valpareso, Chile, Kluwer Publication, 2000.

N. M. Ghoniem, S.- H. Tong, B. N. Singh, and L. Z. Sun, On dislocation interaction with radiation- induced defect clusters and plastic flow localization in FCC metals, Phil. Mag., submitted (2001).

J. M. Huang and N. M. Ghoniem, The dynamics of dislocation interaction with sessile self-interstitial atom (sia) defect cluster atmospheres, accepted for publication, J. Comp. Mat. Science, (2001).

L. Z. Sun, N. M. Ghoniem, Z. Q. Wang, Analytical and numerical determination of the elastic interaction energy between glissile dislocations and stacking fault tetrahedra in FCC metals, accepted for publication, J. Mat. Sci. & Engr., (2001).

EXPERIMENTAL

N. Nita, T. Iwai, K, Fukumoto and H. Matsui, Effects of temperature change on the mechanical properties and microstructural evolution of vanadium alloys under ion irradiation, J. Nucl. Mater. 283-287 (2000) 60

N. Sekimura, T. Iwai, Y. Arai, S. Yonamine, A. Naito, Y., Miwa, and S. Hamada, Synergistic effects of hydrogen and helium on microstructural evolution in vanadium alloys by triple ion beam irradiation, J. Nucl. Mater. 283-287 (2000) 224.

H. Watanabe, T, Arinaga, K. Ochiai, T. Muroga and N. Yoshida, Microstructure of vanadium alloys during ion irradiation with stepwise change of temperature, J. Nucl. Mater. 283-287 (2000) 286.

K.-i. Fukumoto, H. Matsui, H. Tsai and D. L. Smith, Mechanical behavior and microstructural evolution of vanadium alloys irradiated in ATR-A1, J. Nucl. Mater. 283-287 (2000) 492.

K.-i. Fukumoto, H. Matsui, Y. Candra, K. Takahashi, H. Sasanuma, S. Nagata, and K. Takahiro, Radiation induced precipitation in V-(Cr,Fe)-Ti alloys irradiated at low temperature with low dose during neutron or ion irradiation, J. Nucl. Mater. 283-287 (2000) 535

D. T. Hoelzer, M. K. West, S. J. Zinkle and A. F. Rowcliffe, Solute interactions in pure vanadium and V-4TCr-Ti alloy, J. Nucl. Mater. 283-287 (2000) 616.

T. Nagasaka , H. Takahashi , T. Muroga, T. Tanabe (c) and H. Matsui, Recovery and recrystallization behavior of vanadium at controlled various nitrogen and oxygen levels, J. Nucl. Mater. 283-287 (2000) 816.

T. Hayashi, K. Fukumoto and H. Matsui, Study of point defect behaviors in vanadium and its alloys by using HVEM, J. Nucl. Mater. 283-287 (2000) 868.

D. T. Hoelzer, S. J. Zinkle, and A. F. Rowcliffe, The defect microstructure of V-4Cr-4Ti alloy following neutron irradiation at 323°C, Symposium R on Microstructural Processes in Irradiated Materials, 2000 MRS Fall Meeting, Boston, Nov. 27 - Dec. 1, 2000.

M. Satou, Radiation hardening of vanadium alloys, Symposium R on Microstructural Processes in Irradiated Materials, 2000 MRS Fall Meeting, Boston, Nov. 27 - Dec. 1, 2000.

T.Okita, T. Kamada and N. Sekimura, Effects of dose rate on microstructural evolution and swelling under neutron irradiation, J. Nucl. Mater. 283-287 (2000) 220.

FUTURE WORK

With the completion of the JUPITER Collaboration March 31, 2001, IFFS-VI will be officially terminated, but the overall concept of the IFFS-VI approach and the progress and cooperative efforts in theory, modeling and fundamental experiments that resulted from it will be carried on within the next collaboration.