PROGESS ON THE 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) is 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 is 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 at 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 recent progress and future plans are discussed.

PROGRESS AND STATUS

Introduction

IFFS-VI is 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 program was devised and embraced by both sides of the JUPITER collaboration as a means of focusing our individual and joint efforts. The problem chosen aims our theory and modeling programs at the prime candidate material that has received the least attention in that regard so far, but it does not preclude advancements in the general fundamental understanding of irradiation effects. The primary temperature variation experiments, already planned before IFFS-VI was started, are currently underway as a major JUPITER irradiation in HFIR. They will provide experimental information on defect accumulation and property changes under well-controlled and monitored conditions. The temperature variation experiments will provide 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 are among the materials included in the experiments. Separate low-dose irradiations will be performed in the JMTR reactor and with heavy ions in Japan.

IFFS-VI is 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.

IFFS-VI Tasks

The experimental tasks associated with the neutron irradiations in HFIR and JMTR are underway or in the development stage, and their performance will not be directly affected by IFFS-VI. At present, the theory and modeling tasks fall into the broad categories of

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Interatomic Potentials, Defect Properties, Cascade Generation, Annealing Simulation and Comparison with Experiments. A more detailed breakdown of the tasks is indicated below. It is not anticipated that sufficient resources will exist for the completion of all the tasks within the remainder of the JUPITER collaboration. However, the task lists serves as an important instrument for focussing and integrating the activities of both sides.

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 Proposed Schedule

IFFS-VI was initiated as a two-year program, with a goal of predicting the outcome of the HFIR experiments, from which experimental data should be available starting in late 1999 or early 2000. Good progress toward this goal is expected to be made by building on existing models and using the experimental data that already exist for vanadium. Although there is a logical sequence of activities toward meeting the goal, many of the IFFS-VI tasks can be worked on simultaneously and at various levels of physical realism until all the pieces fit together with the requisite level of physical reality.

It is expected that many of the ongoing developments in theory and modeling of irradiation effects are directly relevant to IFFS-VI without being developed specifically for V-4Cr-4Ti or pure V or even bcc metals and alloys, especially developments of models dealing with defect accumulation and microstructure evolution. These models can be developed in a general way and made specific to V-4Cr-4Ti when cascade and defect property information for that material is available from MD simulations and first principles calculations.

Basic information that must be established early on includes interatomic potentials for pure V (some cascade simulations have been done using an embedded atom potential, see below) and for the V-impurity and V-4Cr-4Ti alloy element interactions. These potentials should be developed and tested before further atomistic calculations are performed.

Progress is to be shared informally through email, conference presentations, and postings on a potential Internet web site. Progress will be formally reviewed at a JUPITER collaboration workshop on theory and modeling, now scheduled to be held in conjunction with the ICFRM-9, October 10-15, in Colorado Springs.

IFFS-VI Progress in Theory, Modeling and Experiments

The following is a list of papers, presentations and work in progress on fundamental studies of radiation damage relevant to IFFS-VI objectives involving US and Japanese JUPITER participants:

The following papers, specifically on vanadium, are in the Proceedings of ICFRM-8, October 26-31, 1997, Sendai, Japan, Part C, J. Nucl. Mater., in press.

"Defect Cluster Formation in Vanadium Irradiated with Heavy Ions," N. Sekimura, Y. Shirao, H. Yamaguchi, S. Yonamine and Y. Arai.

"A Molecular Dynamics Simulation Study of Displacement Cascades in Vanadium," K. Morishita and T. Diaz de la Rubia.

The following papers, on vanadium and fundamental aspects of radiation damage in BCC metals, were presented at the International Workshop on Basic Aspects of Differences in Irradiation Effects between FCC, BCC and HCP Metals and Alloys, October 15-20, 1998, Cangas de Onis, Spain. The proceedings will be published in J. Nucl. Mater.

"Damage Evolution and Accumulation in Pure Vanadium," E. Alonso, T. Diaz de la Rubia and J.M. Perlado.

"Cascade Damage in FCC and BCC Metals, N. Sekimura.

"Modeling of Irradiation Damage Evolution in FCC and BCC Metals," T. Diaz de la Rubia and N. Soneda.

"Primary Defect Formation in BCC Iron: The Role of Cascade Energy and Temperature and Pre-existing Defects," R. Stoller.

"Atomistic Simulation of Self-interstitial Dislocation Loop Structure and Mobility in BCC Iron," B.D. Wirth, G.R. Odette and G.E. Lucas.

"Kinetic Monte Carlo Studies of the Effects of One-dimensional Glide on the Reaction Kinetics of Interstitial Clusters," H.L. Heinisch, B.N. Singh and S.I. Golubov.

"New Aspects of Void Formation in Neutron-irradiated Copper and Nickel at High Temperature," Y. Shimomura and I. Mukouda.

"Deformation and Fracture Mechanisms in Irradiated FCC and BCC Metals," S.J. Zinkle and G.E. Lucas.

"Computer Simulation of Fundamental Behaviors of Interstitial Clusters in Fe and Ni," E. Kuramoto.

"Three-dimensional Dislocation Dynamics for Computer Simulation of Localized Plastic Deformation," N.M. Ghoniem.

The following papers on vanadium were presented at Symposium N on Microstructural Processes in Irradiated Materials, at the Materials Research Society 1998 Fall Meeting, November 30-December 3, 1998, Boston, MA, USA. Papers will be published in the MRS Proceedings for this symposium.

"Dislocation Loops Interaction With Dislocations in Vanadium: An Atomistic Study with Flexible Boundary Conditions," E. Alonso, T Diaz de la Rubia and J.M. Perlado.

"Effects of Neutron Irradiation on Tensile Properties of V-Ti-Cr-Si Type Alloys with Helium Pre-existence," M. Satou and K. Abe.

A direct collaboration under JUPITER was established between Q. Xu and H.L. Heinisch during Dr. Xu's assignment at PNNL. Progress on their study of "The Effects of Temperature Variation on Defect Accumulation During Irradiation" using KMC simulations will be reported at ICFMR-9, October 10-15, 1999, Colorado Springs, CO, USA.

FUTURE WORK

Progress by the participants in IFFS-VI will be reviewed at the US/Japan JUPITER Workshop on Theory and Modeling to be held in conjunction with ICFRM-9.