THEORY AND MODELING OF RADIATION EFFECTS IN MATERIALS FOR FUSION ENERGY SYSTEMS- H. L. Heinisch (Pacific Northwest National Laboratory[1])

OBJECTIVE

The objective of this report is to present a brief summary of the recent US/Japan Workshop on Theory and Modeling of Radiation Effects in Materials for Fusion Energy Systems.

SUMMARY

The US/Japan Workshop on Theory and Modeling of Radiation Effects in Materials for Fusion Energy Systems, under Phase III of the DOE/Monbusho Collaboration, convened on July 17-18, 1995, at Lawrence Livermore National Laboratory. A brief summary of the workshop is followed by the workshop program.

PROGRESS AND STATUS

Several very positive trends in fusion materials research emerged from this workshop. Technically, the theory and modeling work is moving toward more technologically relevant problems. We have obtained a quantitative understanding of many of the "generic" fundamental issues of irradiation effects. In gaining that understanding, theories, models, and methodology were developed that can now be applied to more complicated problems. We are now focusing attention on the potential real materials of fusion energy. Atomic-scale modeling is presently under way on defect production in vanadium and silicon carbide. New methods for obtaining reasonable interatomic potentials for treating alloys and impurities look very promising. We can simulate the initial state of damage quite well now, and emphasis is moving toward understanding its influence on microstructure development. Massively parallel computers are available to handle much larger systems, and we are working to exploit this development.

Even as the number of neutron irradiation facilities available for testing and development of fusion materials is decreasing worldwide, the opportunities for advancement in theory and modeling are definitely improving. Using more computing power and better models, the new insights gained from theory and modeling activities can help us extrapolate our limited neutron irradiation information to more fusion-relevant environments.

Nineteen participants attended the workshop, eleven from Japan and eight from the US. An overview of the status of the collaboration and of the theory and modeling task was followed by technical presentations. The workshop concluded with group discussions on cascade simulations, microstructure evolution and mechanical properties, critical experiments and continuing specific collaborations. We were fortunate also to have a presentation on massively parallel computing by Dr. Alice Koniges from the National Energy Research Supercomputer Center at LLNL. A report containing extended abstracts of the presentations and summaries of the group discussions was distributed to participants and collaboration task leaders.

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[1]*Pacific Northwest National Laboratory is operated for the U.S. Department of Energy by Battelle Memorial Institute under Contract DE-AC06-76RLO 1830.*

PROGRAM

Introduction, H.L. Heinisch (PNL)

Overviews and Projections

Overview of JUPITER Collaboration, A. Kohyama (Kyoto U.)
Objectives for Theory and Modeling in the JUPITER Collaboration, N. Sekimura (U. Tokyo)
Historical Overview of Theory and Modeling of Irradiation Effects in Fusion Materials, S. Ishino (Tokai U.)

Computational Resources

MPP Computing Resources at NERSC, A. Koniges (NERSC, LLNL)
Japanese Computing Resources and Needs, Y. Katoh (NIFS)

MD Simulations of Defect Production

Interatomic Potentials, J.B. Adams (U. Illinois)
Critical Review of Molecular Dynamics Simulations of Cascades, T. Diaz de la Rubia (LLNL)
MD Cascades in BCC Metals, R.E. Stoller (ORNL)
Defect Production in SiC, N.M. Ghoniem (UCLA)
Molecular Dynamic Simulation of Si, M.J. Caturla (LLNL)
Critical Evaluation of Various Interatomic Potentials for Radiation Damage Studies of Vanadium, K. Morishita (U Tokyo)

Simulations of Defect Behavior

Defect Clusters in Irradiated Metals, Y. Shimomura (Hiroshima U.)
MD Simulations of Point Defect Behavior Near a Dislocation, H. Matsui (Tohoku U.)
Stochastic Annealing Simulation, H.L. Heinisch (PNL)
Defect Clusters in SiC, K. Fukumoto (Tohoku U.)

Microstructure Evolution and Mechanical Properties

Modeling Radiation-induced Segregation, S. Watanabe (Hokkaido U.)
Modeling of Radiation Embrittlement of Steels, R.E. Stoller (ORNL)
Development of an Integrated Code for Swelling Evaluation, Y. Katoh (NIFS)
Microstructure-Mechanical Properties Correlations, G.R. Odette (UCSB)
Numerical Analysis of Microstructural Evolution under Applied Stress in Irradiated Fe-Cr-Ni Alloys, H. Tanigawa (U. Tokyo/Kyoto U.)
Application of Various Irradiation Methods for Advanced Modeling of Microstructure Evolution, T. Iwai (U. Tokyo, Tokai-mura)

Group Discussion

Simulating Cascade Damage, Leader, T. Diaz de la Rubia (LLNL)
Microstructure Evolution, Mechanical Properties, Leader, G.R. Odette (UCSB)
Critical Experiments, Leader, N. Sekimura (U. Tokyo)
Specific Collaborations, Leader, A. Kohyama (Kyoto U.)

ACKNOWLEDGEMENTS

On behalf of all the participants, we would like to thank Dr.Tomas Diaz de la Rubia and Lawrence Livermore National Laboratory for providing the workshop facilities. We are indebted to Mrs. Margie Altenbach for artfully coordinating the local arrangements.