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Multiscale modeling of radiation effects in nuclear reactor structural materials

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1. Introduction

The effect of radiation on materials is a multiscale phenomenon that involves various processes spanning a wide range of time and dimension. When a high-energy particle collides with lattice atoms in a solid, the displacement reactions produce non-equilibrium point defects within a nanometer range for several picoseconds. Such defects diffuse over macroscopic length and time scales and develop into a full-fledged microstructure by interacting with other extended defects. The pertinent processes include dimensions from an atomic size to a structural component that cover more than 15 orders of magnitude. The time scale also extends over a wide range, from femtoseconds (10^{-15} s) to the operation lifetime of a nuclear reactor [1]. Irradiation changes the microstructure and property of materials, thereby degrading the integrity of structural components and finally causing safety problems in nuclear power plants. Changes in the microstructure of materials are responsible for dimensional instabilities, such as swelling and irradiation creep, and mechanical property changes and degradation, including irradiation hardening and embrittlement. Most problems in irradiated materials originate from the atomic collision of high-energy particles and lattice atoms. This collision leads to displacement cascades through the energy transfer reaction and causes various types of defects such as vacancies, interstitials, and clusters. The behavior of the point defects created in the displacement cascades is important because these defects play a major role in a microstructural evolution and further affect the changes in material properties [2].

Rapid advances have been made in the computational capabilities for a realistic simulation of complex physical phenomena, such as irradiation and aging effects. At the same time, progress has been made in understanding the effect of radiation in metals, especially iron-based alloys. In this work, we present some of our ongoing work in this area, which illustrates a multiscale modeling for evaluating a microstructural evolution and mechanical property changes during irradiation. A short review of the multiscale modeling approach is given along with a summary of the main microstructural features observed in irradiated steels. Emphasis is placed on the problem of reactor pressure vessel (RPV) steel embrittlement [3]. We believe that the computational modeling approach is a valuable tool that can be applied to the evaluation of nuclear power structural materials.

2. Multiscale Modeling Approach

In this section, we illustrate the multiscale nature of radiation effects. Then, the multiscale modeling approach is described in simulating radiation effects on materials.

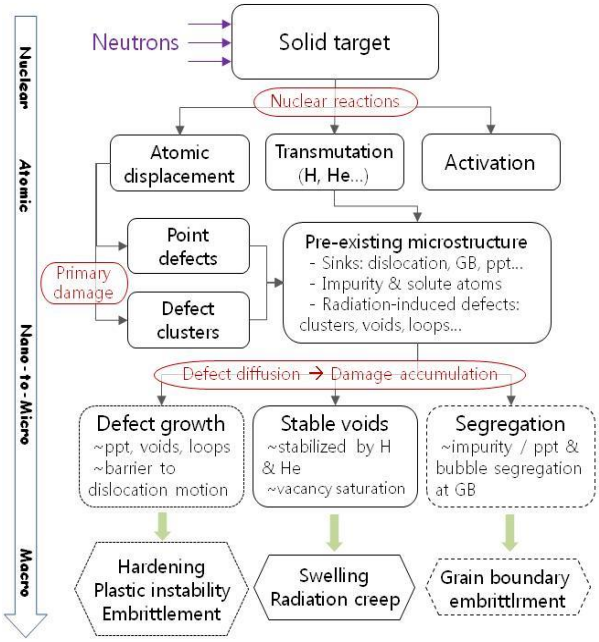

Fig. 1. Diagram describing radiation effects as multiscale phenomena. (GB = grain boundary, ppt =precipitate)

2.1 Radiation Effects

Radiation effects originate in the interaction of energetic neutrons entering the material and then striking the lattice atoms. The interaction is intrinsically nuclear, which takes only a fraction of femtosecond and leads to three main phenomena including transmutation, activation and atomic displacement. Besides activation, two other phenomena affect the materials behavior under irradiation. Transmutation is the production of chemical elements as a result of absorption of neutrons, which finally emits a hydrogen atom or an α-particle becoming a helium atom. Atomic displacements occur when the neutron bounce off the target nucleus by transferring a certain amount of kinetic energy. In case the given energy is high enough, the recoil atom may be ejected from its initial position. Recoil atoms lose their energy by inducing electronic excitation and/or causing atomic displacement. If the energy transferred to the

recoil atom is high enough, other displacement reactions can take place. When there are many secondary displaced atoms, a branching atomic displacement sequence is produced, which is called a displacement cascade. The overall lifetime of a displacement cascade is only a few picoseconds and the affected region has a characteristic length of a few nanometers. At the end of displacement cascade process, a number of point defects are created in the affected region, which are in the form of isolated interstitials and vacancies, and their clusters. The distribution of point defects at this point is defined as the primary damage state.

The primary defects are involved in the evolution of new microstructure by the interaction with pre-existent microstructure. They include grain boundary, precipitate, dislocation, *etc*. which are called a sink. A sink is any microstructural feature capable of absorbing point defects. A point defect cluster is a sink to single point defect upon absorption, which becomes a three-dimensional cavity (void) or a platelet (dislocation loop). While point defects migrate to sinks, defects can cause a redistribution of chemical elements by diffusion. As a result of interactions between primary defect and sink, new types of microstructure are created, which finally affect the properties of materials. The macroscopic effects, originating from the initial production of defects in nanometric displacement cascades over tens of years, manifest various consequences, including hardening, embrittlement, irradiation creep, swelling and plastic instability. The radiation effects described here are illustrated in Fig. 1.

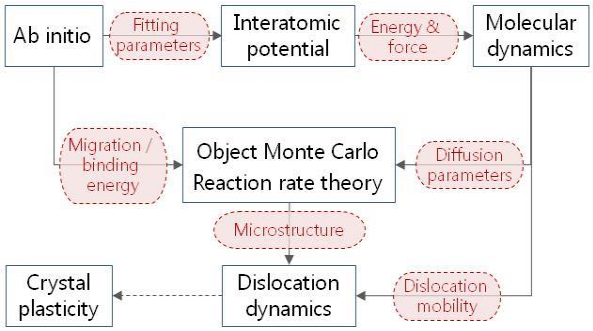

Fig. 2. Flowchart of the multiscale modeling frame applied to radiation effects in materials.

2.2 Multiscale Modeling

Different theoretical bases and computer simulation tools are existent, which can describe the physical mechanisms and simulate the production and evolution of radiation-induced microstructures from the atomic to the microscopic scale. Fig. 2. shows the flowchart of multiscale modeling approach applied to radiation effects in materials. The important function of each model is briefly described below.

In multiscale modeling approaches to radiation effects in alloys, *ab initio* data are transferred into interatomic potentials for large-scale molecular dynamics (MD) and Monte Carlo simulations of radiation damage production and short-term defect evolution. The goal of *ab initio* calculations is to obtain the value of a physical quantity by solving fundamental equations of physics where no empirical fitting parameters are involved. The effective technique, used for *ab initio* calculations in material science, is the application of density functional theory (DFT). DFT is an exact one-body reformulation of the many-body quantum mechanical problem governed by the Schrodinger equation. From the DFT calculations, we can extract the information on defects in pure elements or their interactions with impurities and solute atoms, including formation energy, binding energy and migration energy. Another important use for the DFT calculations is to fit potentials. Potentials are mathematical functions of the relative positions of atoms. The use of potentials is the only way to simulate the dynamic behavior and evolution of systems containing a large number of atoms up to several millions. The limitation of interatomic potential is that reliable potentials are difficult to produce for real alloys such as multi-element ones. Potentials are not only directly applied to molecular dynamics calculation but also used to produce important parameters for Monte Carlo simulation. The MD method is a suitable technique for simulating displacement cascades in ordered materials. It is relevant because the time and physical-length scales for displacement reactions are so small that the use of an experimental technique is difficult. With the rapid growth in computer modeling, we can simulate an atomic behavior to a degree of tens of picoseconds. The MD simulation is particularly useful for quantitatively defining the state of primary damage in a restricted space, which includes the size and density distribution of point defects and their clusters.

The MD simulation can describe the atomistic behavior exactly, but its total simulation time is typically limited to less than one microsecond. The processes we wish to study and observe often take place for much longer time scales, which include a reaction between atoms, adsorption-desorption on the surface, occasional transitions from one state to another, and especially diffusion and annihilation of defects after a cascade event in an irradiation experiment. These events need much more time to take place than general events like an atomistic thermal vibration. This is the "time-scale problem" and the processes are so-called "rare events." Kinetic Monte Carlo (kMC) attempts to overcome this limitation by exploiting the fact that the long-time dynamics of this kind of system typically consists of diffusive jumps from state to state [4]. The result is that kMC can reach vastly longer time scales, typically seconds and often well beyond. The kMC calculation needs parameters about the rates of events: diffusion, formation of defects, and dissociation of

particles, etc. However, the kMC method itself cannot predict them; these rates can be acquired by *Ab initio* calculation or MD simulation.

Radiation-induced defects affect the motion of dislocations which are microscopic carriers of the metallic plasticity. The changes in the behavior of dislocations due to such defects are the main source of the mechanical degradation of irradiated materials. It is thus desirable to simulate dislocations interacting with the defects in order to evaluate and predict the changes in the mechanical properties. Dislocation Dynamics (DD) is a method to simulate a collective motion of dislocations. The DD method represents a curved dislocation line as a connected set of discrete dislocation segments of edge and screw type [5]. We compute the stresses of each segment which includes the following: (i) the internal stress field produced by all the other dislocation segments present in the simulation box, (ii) the applied stress field which compensates for the proper boundary conditions on the surface of the finite volume, (iii) the Peierls stress which represents the lattice friction on the dislocation motion, (iv) the line tension of dislocation lines reflecting their self energy. The effective resolved shear stress acting on each dislocation segment is then computed by using the Peach–Koehler equation. Each dislocation segment moves according to a certain mobility law, which relates to the resolved shear stress and the velocity of a segment. The interactions of the dislocation segments, such as a junction formation, annihilation and cross-slip are implemented as local rules. From the DD simulation, we can compute the increase in the yield stress.

3. Conclusions

Multiscale modeling approaches are briefly presented here in the following order: nuclear interaction, atomic-level interaction, atomistic modeling, microstructural evolution modeling and mechanical property modeling. This is one of many possible methods for classifying techniques. The effort in developing physical multiscale models applied to radiation damage has been focused on a single crystal or single-grain materials. Fully integrating physical information on radiation damage from the lower scale models to the constitutive equations in the crystal plasticity model is not established yet. Although the overview of this work is not exhaustive, it would be a future goal to establish an efficient multiscale modeling methods for radiation damage study in the nuclear material fields.

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