Multiscale Modeling for Predicting of Radiation Effects on Nuclear Materials

Junhyun Kwon[a]*, Gyeong-Geun Lee[a], Chansun Shin[a]
[a]*Korea Atomic Energy Research Institute, 1045 Daedeok-daero, Yuseong, Daejeon 305-353, Korea*
*Corresponding Author: jhkwon@kaeri.re.kr

1. Introduction

Microstructural evolution due to irradiation results in changes in material properties. When a high-energy particle collides with lattice atoms in a solid, the displacement reactions produce point. Such defects, particularly point defects, diffuse over macroscopic length and develop into a mature microstructure by interacting with other defects. These defects alter the materials chemistry and microstructure. Radiation-induced microstructure changes property of materials, thereby degrading the integrity of structural components in a nuclear power plant. For example, the embrittle-ment of reactor pressure-vessel steels is an important issue that directly affects the safety and determines the lifetime of nuclear power plants.

Much effort has been made to develop improved methods for predicting embrittlement and solving related problems. Recent innovations in computational modeling, coupled with improved experimental tools, provide a basis for developing a multiscale model of pressure-vessel embrittlement. In this study, we briefly describe some of our ongoing work in this area, particularly with regard to multiscale modeling for evaluating microstructural evolution and mechanical property changes during irradiation. This modeling approach can be applied to nuclear power systems, including the currently operating light water reactors, GEN-IV nuclear power reactors, and further nuclear fusion systems.

2. Multiscale Modeling Methods

The modeling involves MD simulations, KMC methods, and DD simulations. Each model covers the relevant length and time scales to estimate the fate of defects and solutes, and to predict a microstructural evolution during irradiation. It is possible to predict the amount of radiation damage through the prediction of the material microstructure. Fig. 1 provides overview of a multiscale modeling approach [1]. The main objective of this approach is to keep track of point defects, impurities and solutes and to predict the microstructural evolution. MD simulations yield information about primary damage, particularly in terms of the cascade efficiency, the spatial distribution of point defects and the number density of defect clusters. All information is used as input in subsequent models such as KMC and DD simulations. Because the primary damage is totally dependent on the interatomic potential used, the use of suitable parameters in multiscale simulations is important. Multiscale modeling is not sufficient to predict the performance of commercial alloys composed of various elements. Hence, an experiment is required in conjunction with the modeling.

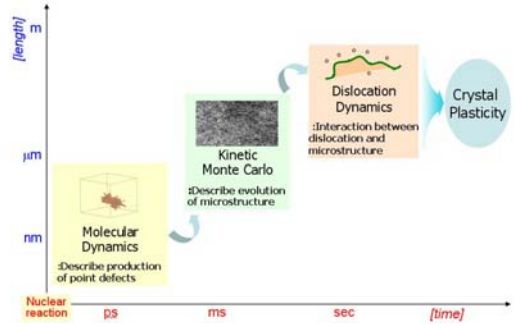

Fig. 1. Multiscale modeling for radiation damage simulation

2.1 Molecular Dynamics (MD) Simulations

The physics of primary damage production has been studied by means of MD simulations and theoretical work. Displacement cascades are caused by high-energy particles such as neutron, or heavy ions. In light water reactor environments, fast neutrons play a role in initiating displacement cascades. In this work, the formation of primary damage to reactor pressure vessel (RPV) steels is investigated under neutron irradiation.

Neutron damage to materials begins with the creation of primary knock-on atoms (PKA) from high-energy neutron-nuclear interactions. The PKA energy is determined by such factors as the incident neutron energy, the masses involved, and the angle between the incident neutron and the recoil direction. The MD method is a technique for simulating displacement cascades in ordered solids. The cascade simulations are carried by using the MD code, which produces the temporal behavior of point defects as a result of PKA injection. The MD simulation should be terminated when a slight change occurs in the number of point defects. The output of primary interest is the distribution of residual point defects after the in-cascade recombination. These residual defects are known to cause microstructural changes to irradiated material. Fig. 2 illustrates the evolution of the displacement reactions in the 5.3 keV PKA cascade; the figure shows each step from the beginning of a cascade to its relaxation in iron at 290^{o}C.

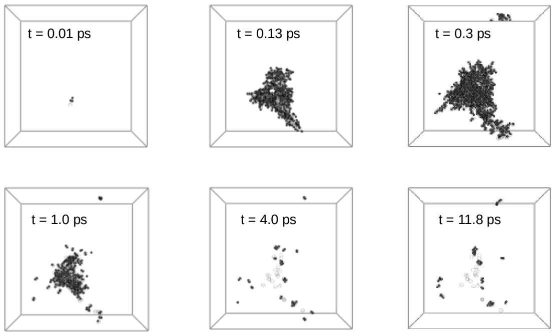

Fig. 2. Evolution of displacement cascade from a 5.3 keV MD simulation in α-iron at 290^{o}C as a function of time. The dots represent interstitials: the empty dots represent vacancies.

In the MD simulations, we obtained the cascade efficiency and the point defect clustering fractions, as well as the atomic distribution of residual defects. Those results are used as inputs to the subsequent model calculations, kMC and DD simulations.

2.2 Kinetic Monte Carlo (KMC) Simulations

After the production of primary damage, the processes of interest occur in much longer time scales. These processes include reactions between atoms, adsorption-desorption on the surface, occasional transitions from one state to another, and especially diffusion and annihilation of defects. Such events take much longer than general events such as an atomistic thermal vibration. This problem is called a time-scale problem and these types of processes are called rare events. KMC simulations attempt to overcome this limitation by exploiting the fact that the long-term dynamics of this kind of system typically consist of jumps from state to state. A KMC simulation can reach longer time scales, typically in the region of seconds and often much longer. The KMC calculation needs parameters about the rates of events: diffusion, formation of defects, dissociation of particles, and so on. Fig. 3 shows the various events treated by the KMC simulations.

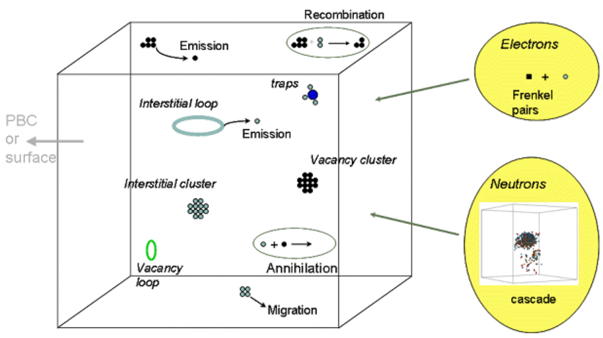

Fig. 3. The various events in a KMC simulations

2.3 Dislocation Dynamics (DD) Simulations

Deformation of metals can be, in theory, described as a collective motion of dislocations. The purpose of this simulation is to describe a general scheme for predicting radiation-induced property changes by simulating the behavior of dislocations under irradiation. DD solves the equation of motion of dislocation lines. The collective evolution of a large number of interacting dislocations is simulated under an external loading in DD simulations. An individual dislocation glide causes a plastic strain in the simulation volume; hence, the stress-strain behavior is an output of the DD simulations.

Radiation defects interact with moving dislocations and hinder the motion of dislocations. The interactions between dislocations and radiation defects are the origin of the changes in mechanical properties as well as the change in microstructure after deformation of nuclear materials. When radiation hardening is simulated in DD simulations, two types of information need to be passed from other simulations: firstly, the density and the size distribution of radiation-induced defects and, secondly, the defect strength, i.e. the barrier strength to the dislocation motion. Fig. 4 shows the interactions of the Frank loop with glide dislocations. The interactions between dislocations and defects play a role of irradiation hardening.

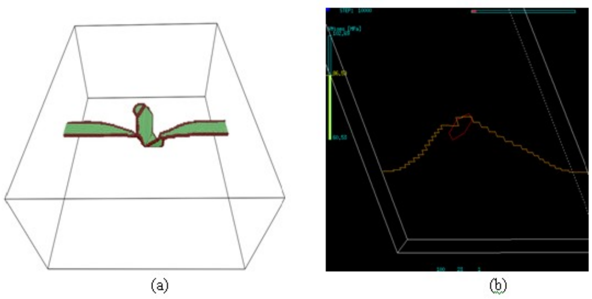

Fig. 4. Simulation of interaction between a Frank loop and a glide dislocation by (a) MD and (b) DD.

3. Discussion

This paper outlines the overview of multiscale modeling for radiation effects on nuclear materials. The hierarchical approach, with the combination of three models, can improve the prediction capability of material property changes due to irradiation. Worldwide effort to improve this technology is being made in corporation with IAEA and OECD NEA. Future work will focus on the multiscale code development and their application to nuclear field.

REFERENCES

[1] J. Kwon, G. Lee, and C. Shin, Multiscale Modeling of Radiation Effects on Materials: Pressure Vessel Embrittlement, Nuclear Engineering and Technology, Vol. 41, No. 1, p.11, 2009.