

Advanced Energy Structural Materials Research Section

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1. Introduction

Materials development and maintenance management is essential for establishment of the safety and efficient operation of advanced nuclear energy systems. This section addresses the mission of establishing a maintenance management methodology as well as material R & D for advanced nuclear energy systems such as fusion and fission reactors. Current main researches are as follows:

(1) Plant integrity analysis: The structural integrity of a reactor pressure vessel (RPV) is important for reactor safety and was investigated using three-dimensional computational fluid dynamics (3D-CFD) and the finite element method (FEM). Pressurized thermal shock (PTS) during emergency water cooling, the most severe situation, was focused in the present study. Through this investigation, the magnitude of the risk of the RPV function loss was evaluated and proposed as an indicator available for optimizing the maintenance strategy.

(2) Materials multiscale modeling and data science: Radiation damage processes in nuclear materials take place at a wide variety of time and length scales. So-called the multiscale viewpoint and statistical arguments are required to understand the processes. To do this, modeling effort has been made using several computational techniques complementarily such as molecular dynamics, ab-initio quantum calculations, kinetic Monte-Carlo, rate-equation theory analysis, FEM and CFD.

(3) Irradiation effects on microstructure evolution and properties of materials: High energy particle irradiation leads to the formation of oversaturated interstitials and vacancies. The behavior of point defects is responsible for the evolution of the microstructure, which may cause degradation, (or development), of the mechanical properties of the material. Hence, the elucidation of the behavior of point defects is essential for understanding the mechanisms responsible for the changes in mechanical properties. In our study, the microstructure evolution under high energy particle irradiation has been investigated experimentally and computationally.

2. PKA energy dependence of defect production in collision cascades

Since there are no fusion reactors at present, it is necessary to understand material behavior in a fusion reactor for a realistic design of fusion DEMO reactor. The production of primary defects in collision cascades in a material is a phenomenon that occurs in a very short time; therefore, it should be analyzed by computational simulation technique based on molecular dynamics (MD) method. In the MD simulation, behavior of collision cascades can much depend on some variable parameters such as PKA energy and the incident direction of a PKA (primary knock-on atom). The objective of this study is to systematically investigate the parameter dependence of the collision cascade behavior with a statistical analysis.

In this study, by means of MD method, we examined the relationship between the PKA energy and the number of non-equilibrium produced defects, in which Mendelev potential was applied to evaluate the cascade damage process in α -Fe. In the MD simulations, the number of produced defects was evaluated as a function of PKA energies ranging from 0.02 to 10 keV, with 1000 case calculations for each of the PKA energies. In this analysis, when PKA energy is lower than 0.1 keV, the number of surviving defects increases in proportion to PKA energy, leading to a good agreement with the NRT model. In contrast, when PKA energy is higher than 0.1 keV, the number of surviving defects nonlinearly increases with PKA energy,

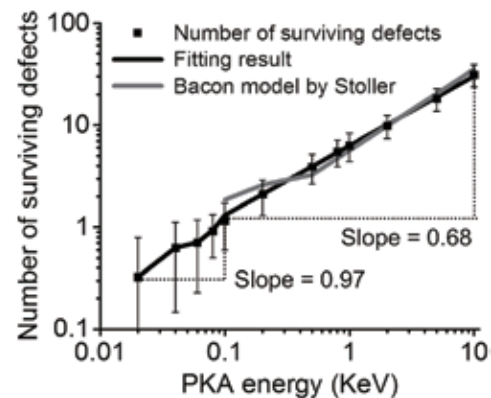


Fig. 1: PKA energy dependence of the number of point defects produced by displacement cascades.

resulting in a similar trend to Bacon' model.

3. Structural integrity assessment of reactor pressure vessels: A probabilistic risk evaluation

Reactor pressure vessels (RPVs) are an important component in nuclear power plants and function to keep nuclear fuel and radioactive materials confined. The structural integrity of RPVs has been verified by regulation through periodic and special inspections, where judgments are made as to whether regulations are satisfied. Unfortunately, however, the judgments are only deterministic, and the degree of satisfaction is beyond their scope. In the present study, to clarify the degree of satisfaction, uncertainties in the structural integrity are quantified. Using the probability density distribution function of the stress intensity factor and that of the fracture toughness, the probability of the occurrence of the irradiation-induced brittle fracture of RPVs during pressurized thermal shock (PTS) events is evaluated and defined as an indicator representing fracture risks. The characteristics of the indicator are found to show that it increases significantly with the reactor operating time and therefore indicates a more appropriate quantified parameter of aging phenomena than the conventional $\Delta DBTT$ (ductile-to-brittle transition temperature shift). The indicator is finally proposed to be employed for the optimization of the inspection and maintenance of RPVs.

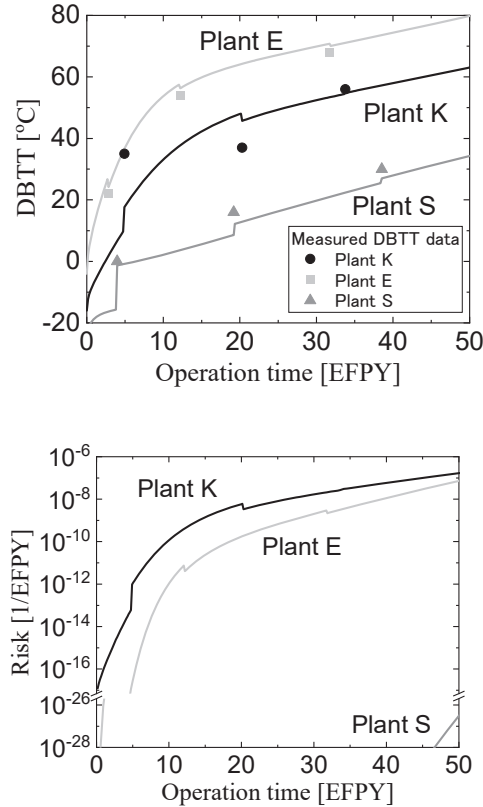


Fig. 2: The time evolutions of the predicted and corrected DBTT values and embrittlement risks for the three plants.

4. Irradiation effects on microstructure evolution and properties of materials

Tungsten (W) is considered to be the primary choice for the plasma facing materials (PFM) in fusion reactors due to its attractive combination of properties such as high melting point, good thermal conductivity, high creep resistance, good high-temperature strength and low vapor pressure. We have investigated the irradiation effect of tungsten (W), which is a candidate material for fusion divertor, using an ion accelerator (DuET: Fig. 3). We found that the microstructure evolution under ion irradiation depends on the crystal orientation using W single crystals with $\{001\}$ and $\{011\}$ surface orientation for ion-irradiation (Fig. 4). Defect zone depth is deeper in $\{001\}$ crystal than in $\{011\}$ crystal. The mechanism has been discussed with DFT, MD, and so on. The knowledge obtained in this study is fruitful for fusion divertor design and integrity. Moreover, we performed a systematic theoretical study of the interactions between transition metals (TM) elements and point defects in bcc W using density functional theory (DFT) calculations. The effects of transition metals elements on the microstructure evolution was discussed.

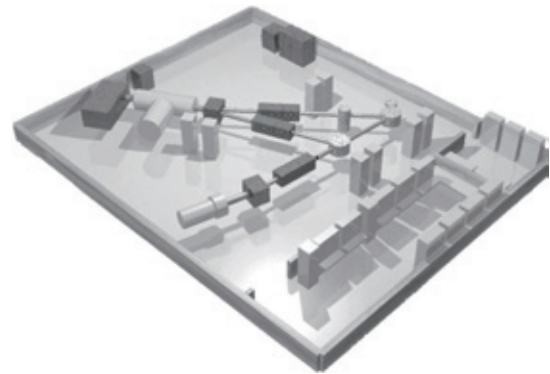


Fig. 3: Ion-accelerator (DuET)

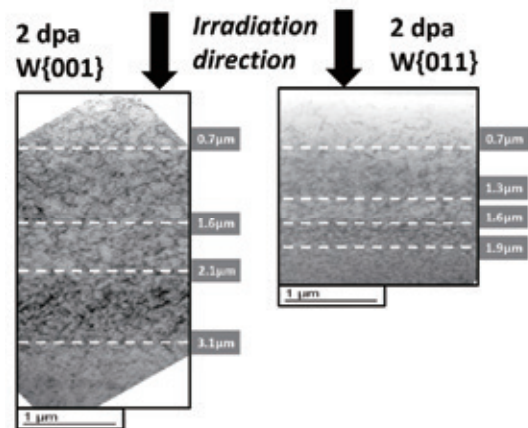


Fig. 4: TEM micrographs of W single crystals after 6.4 MeV Fe³⁺ ions.

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2. Others

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