Advanced Energy Structural Materials Research Section

K. Morishita, Associate Professor
K. Yabuuchi, Assistant Professor
A. Kimura, Researcher

1. Introduction

In order to achieve the safety and efficient operations of advanced nuclear energy systems, the development and use of robust materials and the establishment of reliable system maintenance management are essential. This section addresses the mission of establishing the 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) Materials modeling and data-driven science & technology

Radiation damage processes in nuclear materials occur at a wide variety of time and length scales. To understand this process, so-called multiscale viewpoint and statistical arguments are required. In this section, efforts are made to model material behavior during irradiation complementarily using several computational techniques such as molecular dynamics, ab-initio quantum calculations, kinetic Monte-Carlo, rate-equation theory analysis, FEM and CFD. Recently, additional efforts have also been devoted to this research using machine learning, AI (artificial intelligence) and data-driven techniques.

(2) Plant integrity analysis

The structural integrity of the reactor pressure vessel (RPV) is critical to the reactor safety. Here, this is evaluated using three-dimensional computational fluid dynamics (3D-CFD) and the finite element method (FEM). Pressurized thermal shock (PTS) events during emergency water cooling, the most severe situation, are focused in this study. Through this evaluation, the risk of the RPV function loss is quantified and it is proposed as an indicator available for optimizing maintenance strategy.

(3) Effects of irradiation on the microstructure and mechanical property changes 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. 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. Statistical arguments on non-equilibrium point defect production in materials under irradiation

In fusion reactor structural materials, displacement cascade process is initiated by collisions of incident high energy neutrons with target atoms, resulting in the production of a large number of athermal point defects, which significantly affects the microscopic composition and microstructure of the materials and changes their mechanical properties; hence, it is of great importance to investigate this process in depth. However, since the displacement cascade process occurs on a time scale of several tens of picoseconds, it is very difficult to observe by experiments, and computer simulation techniques are needed instead. Molecular dynamics (MD) is one of the most powerful tools to investigate the defect production process in materials due to displacement cascades. In this study, molecular dynamics simulations are performed to investigate displacement cascades in Fe as a function of primary knock-on atom (PKA) energy. The statistics of defect production due to displacement cascades is focused, where 1000 cases are simulated for individual PKA energies. It is found in our simulations that the simulated probability density function of the number of athermal point defects produced by displacement cascade exhibits approximately a normal distribution as shown in Fig. 1. For PKA energies below

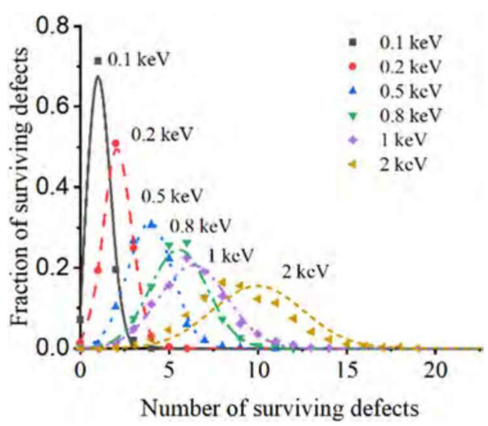

Fig. 1: PKA energy dependence of the number of point defects produced by displacement cascades.

100 eV, the average number of surviving point defects is in proportion to PKA energy with a constant standard deviation. For higher energies, on the other hand, the average and the standard deviation individually show power dependence on PKA energy. These PKA energy dependences of the average number of surviving point defects are consistent with those of the NRT and Bacon models for lower and higher PKA energies, respectively. Statistical characteristics of displacement cascades will help to describe the changes in the microstructure and mechanical properties of materials under irradiation.

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 current judgments in Japan are made by only deterministic, and the degree of satisfaction is beyond their scope. In the present study, to quantify the degree of satisfaction, uncertainties in the structural integrity are assessed. 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. This means that this indicator is more appropriate for representing aging risk than the conventional $\Delta DBTT$ (ductile-to-brittle transition temperature shift).

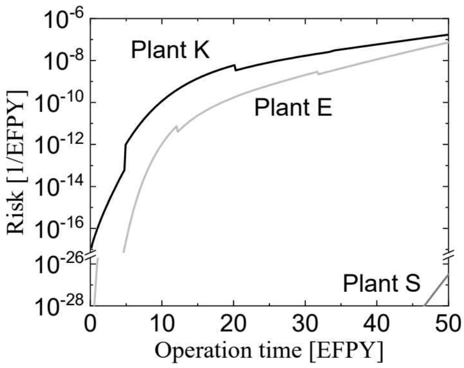

Fig. 2: The time evolutions of the predicted and corrected DBTT values and embrittlement risks for the three plants.

4. Effects of irradiation on microstructural evolution in materials and corresponding mechanical properties

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 has investigatd the irradiaton effect of tungsten (W), which is a candidate material for fusion divertar, using an ion accerelator (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} surafcace 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 diverter 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.

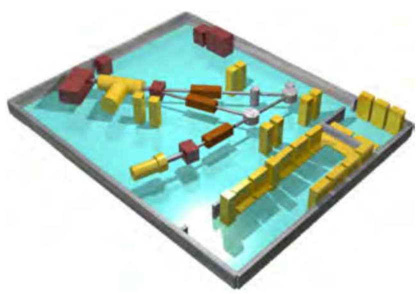

Fig. 3: Ion-accelerator (DuET)

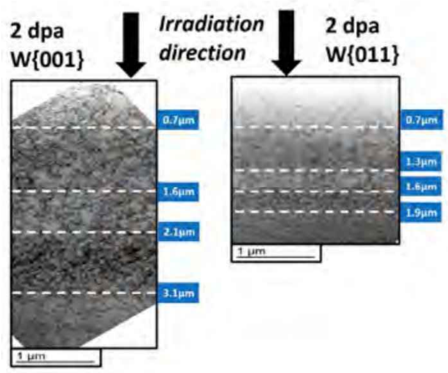

Fig. 4: TEM micrographs of W single crystals after irradiation

5. Application of AI technology to the image analysis for nuclear materials development

TEM image analysis of post-irradiation metals has often been conducted in the field of nuclear material development research, where an interpretation of imges is different unfortunately from person to person. To avoid this gap, a new attempt is being made to apply the state-of-the art AL technology to the image analysis. If this attempt progresses successfully, it should be possible to bridge the gap between the skill levels of skilled and novice users.

Financial Support

1. Grant-in-Aid for Scientific Research

森下和功，基盤研究(C)，ミクロからマクロまで総動員して老朽化設備の破損リスクを管理する方法

藪内聖皓，基盤研究(B)，超微小試験技術による照射脆化のミッシングリンク解明（分担金）

木村晃彦，基盤研究(B)，低放射化 ODS 鋼における耐照射脆性のナノ・メゾ組織定量化モデルの構築（繰越し）

2. Others

森下和功，量子科学技術研究開発機構，核融合中性子照射場の理論的定量化に関する研究

藪内聖皓，長瀬産業（株），インフラ鋼構造物に生成するさびの構造解明

藪内聖皓，（株）原子力安全システム研究所，原子炉容器鋼の照射ミクロ組織変化へのＮｉ影響の検討

Publications

H. Yuya, R. Kobayashi, K. Otomo, K. Yabuuchi, A. Kimura, Microstructure and mechanical properties of HAZ of RPVS clad with duplex stainless steel, Journal of Nuclear Materials, 545, 152756, 2021

X. Yi, Y. Du, D. Geng, Z. Li, W. Han, P. Liu, J. Chen, K. Yabuuchi, K. Yoshida, S. Ohnuki, Q. Zhan, F. Wan, Y. Nagai, Heavy-ion irradiation and post-irradiation annealing effects in explosion-welded CuCrZr/316LN joints for ITER application, Materials Characterization, 178, 111252, 2021

K. Fukumoto, T. Mabuchi, K. Yabuuchi, K. Fukui, Irradiation hardening of stainless steel model alloy after Fe-ion irradiation and post-irradiation annealing treatment, Journal of Nuclear Materials, 557, 153296, 2021

H. Yuya, K. Yabuuchi, A. Kimura, Radiation embrittlement of clad-HAZ of RPV of a decommissioned BWR plant, Journal of Nuclear Materials, 557, 153300, 2021

L. Zhang, Y.F. Du, W.T. Han, P.P. Liu, X.O. Yi, K. Yabuuchi, S. Ohnuki, F.R. Wan, An approximate in-situ method for investigating irradiation damage of grain boundary, Nuclear Materials and Energy, 29, 101056, 2021

K. Yabuuchi, S. Kondo, T. Hinoki, R. Kasada, 複合ビーム材料照射装置 DuET を用いた核融合炉材料研究と関連材料研究の展開, Journal of Plasma and Fusion Research, 97, 7, 403, 418, 2021

Y. Chen, K. Morishita, Molecular dynamics simulation of defect production in Fe due to irradiation, Nuclear Materials and Energy, 30, 101150, 2022

Presentations

森下和功, 福島第一原発事故で顕在化した課題, 日本保全学会第 17 回学術講演会, オンライン開催, 2021.7.6-8

阮小勇，森下和功, RPV 保全最適化のための３D-CFD＆FEM による PTS 時の構造健全性評価：非対称原子炉冷却の効果, 日本保全学会第 17 回学術講演会, オンライン開催, 2021.7.6-8

陳昱婷，豊田達也，祝梁帆，森下和功，渡辺淑之，野澤貴史, 核融合中性子照射場の理論的定量化に関する研究, 量子科学研究開発機構六ケ所研究所 BA 共同研究令和 3 年度キックオフ会合, オンライン開催, 2021.7.30

阮小勇，渡辺淑之，安堂正巳，野澤貴史，森下和功, 核融合中性子照射場の理論的定量化に関する研究, 量子科学研究開発機構六ケ所研究所 BA 共同研究令和 3 年度キックオフ会合, オンライン開催, 2021.7.30

陳昱婷，豊田達也，祝梁帆，森下和功，渡辺淑之，野澤貴史, PKA energy dependence of defect production in collision cascades, Institute of Advanced Energy, Kyoto University, 12th International Symposium of Advanced Energy Science, オンライン開催, 2021.9.7

祝梁帆，森下和功，渡辺淑之，藪内聖皓, 中性子照射下における材料損傷過程の反応速度論解析, 日本原子力学会 2021 年秋の大会, オンライン開催, 2021.9.10

豊田達也，森下和功，藪内聖皓, 破壊き裂進展における照射効果の分子動力学評価, 日本原子力学会 2021 年秋の大会, オンライン開催, 2021.9.10

國分悠輔，藪内聖皓，森下和功, Deep Learning を用いた透過型電子顕微鏡画像解析技術の開発, 日本原子力学会 2021 年秋の大会, オンライン開催, 2021.9.14

Y. Chen, K. Morishita, Y. Watanabe, T. Nozawa, Molecular Dynamics Simulation of Defect Production in Fe due to Irradiation, ICFRM-20 組織委員会 20th International Conference on Fusion Reactor Materials (ICFRM-20), オンライン開催, 2021.10.24-29

X. Ruan, Y. Watanabe, K. Morishita, M. Ando, T. Nozawa, Relaxation volume of irradiation-induced defects in pure iron: Molecular-statics calculation with linear elasticity theory, ICFRM-20 組織委員会 20th International Conference on Fusion Reactor Materials (ICFRM-20), オンライン開催, 2021.10.24-29

岡本研正，岡本賢一郎，森下和功, 光電変換型トランジスタ「ダイスター」を用いた電力制御, 電気学会半導体電力変換／モータドライブ合同研究会, 立命館大学びわこ・くさつキャンパス＆WEB（ハイブリッド）, 2022.1.27

Yuting Chen，豊田達也，祝梁帆，森下和功, 核融合中性子照射場の理論的定量化に関する研究, 量子科学研究開発機構六ケ所研究所令和３年度原型炉研究開発共同研究成果報告会，オンライン開催, 2022.2.7

祝梁帆，森下和功，渡辺淑之，藪内聖皓, 軽水炉圧力容器鋼における溶質原子クラスター形成のシミュレーション（ポスター），日本原子力学会春の年会，オンライン開催, 2022.3.16

祝梁帆，森下和功，渡辺淑之，藪内聖皓, 軽水炉圧力容器鋼における溶質原子クラスター形成のシミュレーション（口頭），日本原子力学会春の年会，オンライン開催, 2022.3.17

Yuting Chen，森下和功, 照射カスケード損傷による鉄の欠陥クラスター生成に関する統計的な研究 分子動力学シミュレーション，日本原子力学会春の年会，オンライン開催, 2022.3.17

岡本賢一郎，岡本研正，森下和功, バイポーラトランジスタの動作に関する新仮説－トランジスタ光動説－, 応用物理学会春季学術講演会，青山学院大学相模原キャンパス, 2022.3.22-26

岡本賢一郎，岡本研正，森下和功, パワーダイスター―を用いたEV制御とDC/AC変換, 電気学会全国大会，オンライン開催, 2022.3.23