Advanced Energy Structural Materials Research Section

K. Morishita, Associate Professor
K. Yabuuchi, Assistant Professor
A. Kimura, Researcher
J. Gao, Researcher
P. Song, Researcher
Y. Huang, Researcher

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,

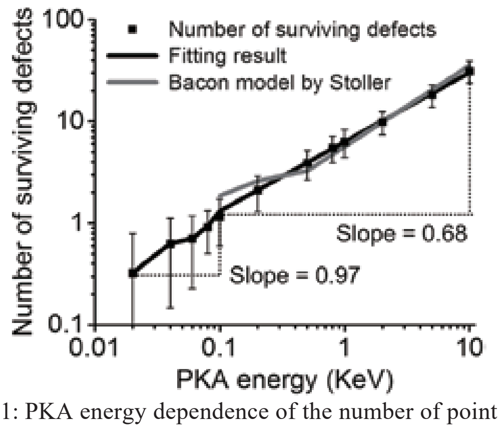

Fig. 1: PKA energy dependence of the number of point defects produced by displacement cascades.

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.

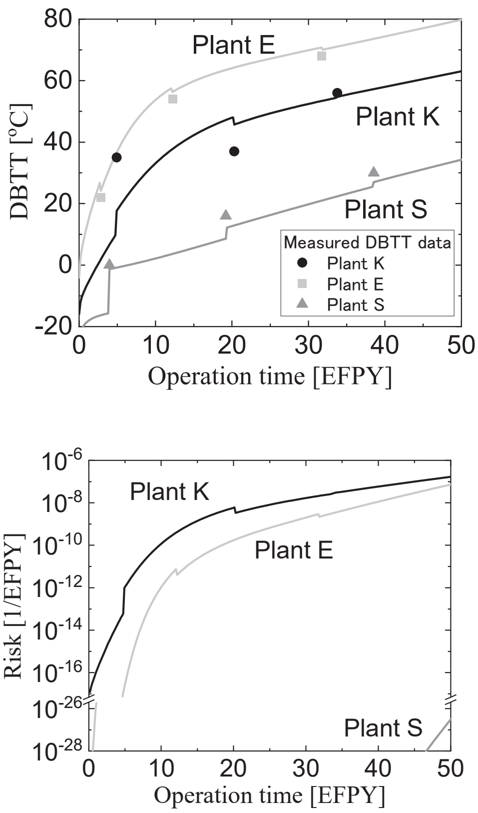

Fig. 2: The time evolutions of the predicted and corrected DBTT values and embrittlement risks for the three plants.

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 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 evolusion 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.

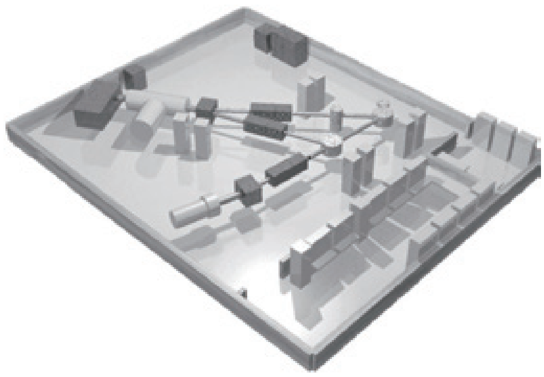

Fig. 3: Ion-accelerator (DuET)

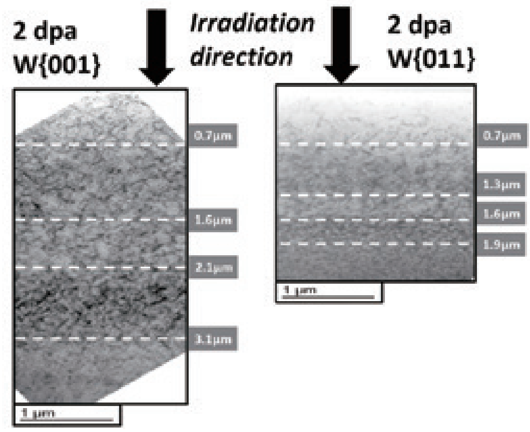

Fig. 4: TEM micrographs of W single crystals after 6.4 MeV Fe^{3+} ions.

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）

藪内聖皓，若手研究，格子欠陥の熱拡散に及ぼす磁壁の影響

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

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，中部電力（株）原子力安全技術研究所，圧力容器監視試験片のサイズ効果に関する研究

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，核融合科学研究所，耐照射性および再結晶遅延性能の向上のためのタングステン合金の開発

藪内聖皓，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

藪内聖皓，中部電力（株）原子力安全技術研究所，（研究題目非開示）

Publications

P. Dou, S. Jiang, L. Qiu, A. Kimura, Effects of contents of Al, Zr and Ti on oxide particles in Fe–15Cr–2W–0.35Y2O3 ODS steels, Journal of Nuclear Materials, 531, 152025, 2020

Y. Chen, C. Zhang, Z. Ding, X.L. Zhang, Y. Yang, Y. Song, A. Kimura, Annealing behavior of hardening and ductility loss of a 16Cr–4Al ODS ferritic steel irradiated with high energy Ne ions, Journal of Nuclear Materials, 531, 152030, 2020

P. Dou, Q. Ye, A. Kimura, Crystal and metal/oxide interface structures of nanoparticles in 15Cr–2W–0.1Ti–4Al–0.6Hf–0.35Y2O3 ODS steel, Journal of Nuclear Materials, 533, 152029, 2020

Y. Liu, S. Kondo, H. Yu, K. Yabuuchi, R. Kasada, Statistical Approach for Understanding the Effect of Specimen Size on the Yield Stress and Its Scattering in Mechanically-Alloyed Cu and ODS-Cu Obtained by Micro-Pillar Compression Test, Materials Transactions, 61, 5, 955-962, 2020

W. Sang, P. Dou, A. Kimura, Early-stage thermal ageing behavior of 12Cr, 12Cr–7Al and 18Cr–9Al ODS steels, Journal of Nuclear Materials, 535, 152164, 2020

K. Nakamura, Hi. Fujita, J. Engels, M. Tokitani, Y. Hishinuma, K. Yabuuchi, S. Kano, T. Terai, W. Inami, Y. Kawata,T. Chikada, Effects of helium implantation with heavy ion irradiation on deuterium permeation in yttrium oxide coating, Journal of Nuclear Materials, 537, 152244, 2020

P. Dou, W. Sang, A. Kimura, Effects of the contents of Al, Ti, W and Y2O3 on long-term thermal ageing behavior of 15Cr ODS ferritic steels, Journal of Nuclear Materials, 534, 152129, 2020

G. Yelia, D. Chenb, K. Yabuuchi, A. Kimura, S. Liu, W. Lin, Y. Zhao, S. Zhao, J.J. Kai, The stability ofg0precipitates in a multi-component FeCoNiCr-Ti0.2alloy under elevated-temperature irradiation, Journal of Nuclear Materials, 540, 152364, 2020

P. Dou, Z.-X. Xin. W. Sang, A. Kimura, Age-hardening mechanisms of 15Cr ODS ferritic steels with 5, 7 and 9 wt.% Al at 475 °C for 9000 h, Journal of Nuclear Materials, 540, 152368, 2020

X. Ruan, K. Morishita, Pressurized thermal shock analysis of a reactor pressure vessel for optimizing the maintenance strategy: Effect of asymmetric reactor cooling(, Nuclear Engineering and Design, 373, 111021, 2021

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, 152745, 2021

Y. Liu, S. Kondo, H. Yua, K. Yabuuchi, R. Kasada, Evaluation of irradiation hardening in ODS-Cu and non ODS-Cu by nanoindentation hardness test and micro-pillar compression test after self-ion irradiation, Nuclear Materials and Energy, 26, 100903, 2021

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

N. Almirall, P.B. Wells, T. Yamamoto, K. Yabuuchi, A. Kimura, G.R. Odette, On the use of charged particles to characterize precipitation in irradiated reactor pressure vessel steels with a wide range of compositions, Journal of Nuclear Materials, 536, 152173, 2020

Presentations

H. Iwakiri, S. Fujita, K. Morishita, Y. Watanabe, Behavior of hydrogen on the surface of fusion reactor materials by computer simulation, 11th International Symposium of Advanced Energy Science, Online, 2020.9.15

Y. Watanabe, K. Morishita, Y. Chen, Irradiation impact on the microstructural evolution in ferritic alloy, 11th International Symposium of Advanced Energy Science, Online, 2020.9.15

角田陽太郎，藪内聖皓，森下和功，FeCrNi 合金中に形成する積層欠陥四面体と空孔集合体のエネルギーハイラキーについての検討，2020 年秋季第 167 回講演大会，オンライン開催，2020.9.18

水田航平，中筋俊樹，藪内聖皓，森下和功，青木孝行，リスクに基づく事故炉廃止措置の最適化，2020 年秋の大会，オンライン開催，2020.9.17

森下和功，京大エネ理工研 Ze 研究会・シンビオ社会研究会・核融合エネルギーフォーラム炉工学・炉材料モデリングサブクラスター会合『先端 ICT 適用による原子力安全の高度化』趣旨説明，先端 ICT 適用による原子力安全の高度化，宇治おうばくプラザ/オンライン開催，2020.12.15

陳昱婷，水田航平，豊田達也，祝梁帆，森下和功，阮小勇，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，令和２年度共同研究成果報告会（BA 報告会），オンライン開催，2021.3.1

水田航平，中筋俊樹，藪内聖皓，森下和功，青木孝行，事故炉廃止措置最適化のための評価手法の検討，第 6 回次世代イニシアティブ廃炉技術カンファレンス（NDEC-6），オンライン開催，2021.3.3

岩切宏友，藤田旺生，森下和功，渡辺淑之，加藤太治，核融合炉材料表面における水素の基本的な挙動についてのコンピュータシミュレーション，ゼロエミッションエネルギー研究拠点 2020 年度共同利用・共同研究成果報告会，オンライン開催，2021.3.9

藪内聖皓，角田陽太郎，FeCrNi 合金中の積層欠陥四面体と空孔集合体の形成挙動，2020 年秋季講演大会，オンライン開催，2020.9.17