Advanced Energy Structural Materials Research Section

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1. Introduction

For the safe and efficient operation of advanced nuclear energy systems, development of robust materials and establishment of reliable system management methods 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. Our research interests are as follows:

(1) Theory, modeling, numerical simulation and data-driven science & technology of irradiated materials

Radiation damage processes in materials during irradiation 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

Structural integrity of a reactor pressure vessel (RPV) during a pressurized thermal shock (PTS) events is of critical importance in the quantitative assessment of reactor safety. We evaluate this using three-dimensional computational fluid dynamics (3D-CFD) and the finite element method (FEM). 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. Mechanism of non-equilibrium point defect production in irradiated materials

In materials of fusion reactor components, high energy neutrons entering the material collide with many target atoms, initiating displacement cascade processes. This process produces locally dense athermal point defects within the material. This has a profound effect on the material's microscopic composition and structure thus altering its mechanical properties. Therefore, it is important to investigate the impact of these processes in the design and selection of component materials. However, the displacement cascade process occurs on an extremely short timescale of several tens of picoseconds, it is very difficult to observe it experimentally. As such, computer simulation techniques are often employed instead. Among them, molecular dynamics (MD) is one of the most powerful tools. In this study, the MD technique was used to simulate displacement cascades in Fe. Fig. 1 shows a simulated example of the time evolution of this process initiated from a 50 keV recoil atom.

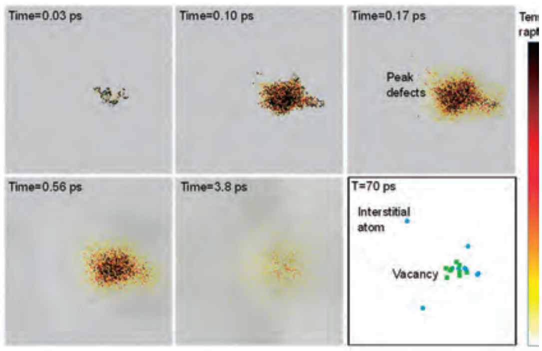

Fig. 1: Our molecular dynamics simulation shows the time evolution of athermal defect production process in Fe during irradaition.

As shown in the figure, at about sub-ps after the primary recoil atom starts to move, a large number of displaced atoms are formed with a very high density. In the central region, the kinetic energies and arrangement of the atoms exhibit a quasi-molten state. As time evolves, the cascade core cools down gradually, during which the displaced atoms in the molten zone return to their lattice point positions and annihilate. Almost all of the displaced atoms are annihilated (disappeared) during this cooling phase, but some still remain. These can be described as lattice defects (i.e., interstitial atoms) that are athermally introduced into the material by the effects of incident neutrons. Interestingly, some of these interstitial atoms are isolated at this time, while others are grouped together to form clusters. Such information is highly valuable, as whether the interstitial atoms thus produced are isolated or clustered can have a significant impact on subsequent defect reactions.

The mechanism of defect production demonstrated here is quite different from the conventional one employed by the NRT model for evaluating *dpa*. A more detailed model construction is underway.

3. Size and temperature dependence of point defect binding free energy to defect clusters in Fe

Size and temperature dependence of the point defect binding free energy has numerically evaluated for self-interstitial atom (SIA) clusters and vacancy clusters in bcc Fe by using continuum models based on thermodynamics and linear elasticity. The estimated binding free energy of SIAs to SIA-clusters is much higher than that of vacancies to vacancy clusters, indicating that SIA-clusters are more thermally stable than vacancy clusters. For relatively small clusters, the estimated binding free energy at 0 K is comparably consistent with atomistic calculation data; and then, the SIA biding free energy at 850 K is averagely about 35 % lower than that at 0 K, while the vacancy binding free energy is about 6 % lower; which may remarkably affect the formation kinetics of those defect clusters under irradiation. These kinds of information will be one of the basic parameters for a theoretical model of the microstructural evolution of Fe-based materials in the nuclear fusion DEMO environment.

This work was performed in the collaboration with Dr. Watanabe et al. at of National Institutes for Quantum Science and Technology (QST).

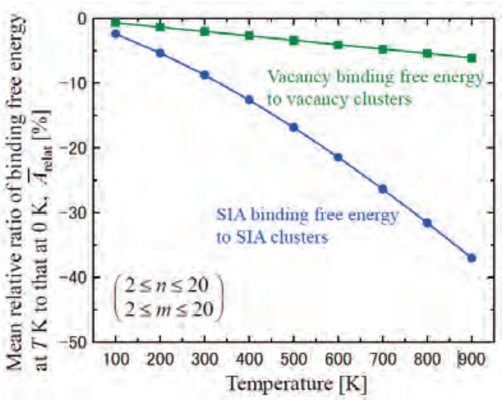

Fig. 2: Temperature dependence of the free energy of point defects to small defect clusters in Fe.

4. Development of new power device "DISTAR"

With the aim of developing new energy devices with higher functionality, we prototyped a small device (Distar) that combines a light-receiving element (LED) and a light-emitting element (solar panel), which is inspired by the operating principle of a conventional bipolar transistor. By applying positive feedback to the current flowing through the circuit, our prototype device showed a current amplification factor of about 1000. Then, this prototype circuit was modeled theoretically, and a simulation model was constructed so that the relationships between the current, voltage, resistance, etc. of the circuit could be understood. It was found from the model calculations that although the current amplification factor reaches 1000, the Joule heat in the resistor is very large, and the energy efficiency of the entire circuit is extremely low (90 percent of input energy is lost). Based on this fact, it is currently concluded that further efforts are necessary to improve energy efficiency. This research is a joint research with Professor Emeritus Kensho Okamoto of Kagawa University.

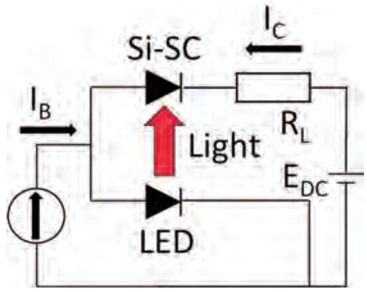

Fig. 3: DISTAR circuit

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 AI 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.

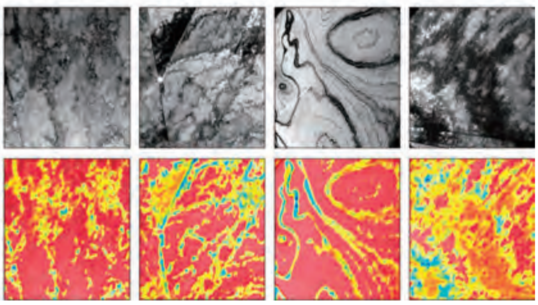

Fig. 4: Image analysis using AI

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2. Others

藪内聖皓，中部電力（株）原子力安全技術研究所，圧力容器非照射材の硬化部に関する研究

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 Si 影響の検討

藪内聖皓，東北大学，「プロセスインフォマティクスによる成膜技術の探索」（令和４年度エネルギー対策特別会計委託事業「フルセラミックス炉心を目指した耐環境性３次元被膜技術の開発」の一部）

Publications

K. Tougou, M. Fukui, K. Fukumoto, R. Igarashi, K. Yabuuchi, Dynamic interaction between the dislocations and cavities in tungsten during tensile test, Nuclear Materials and Energy, 30, 101130, 2022

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

K. Fukumoto, K. Umehara, K. Yabuuchi, Dynamic Interaction between Dislocation and Irradiation-Induced Defects in Stainless Steels during Tensile Deformation, Metals, 12, 762, 2022

S. NogamiI, Ozawa, D. Asami, N. Matsuta, S. Nakabayashi, S. Baumgärtner, P. Lied, K. Yabuuchi, T. Miyazawa, Y. Kikuchi, M. Wirtz, M. Rieth, A Hasegawa, Tungsten–tantalum alloys for fusion reactor applications, Journal of Nuclear Materials, 566, 153740, 2022

P. Song, K. Yabuuchi, P. Spatig, Insights into hardening, plastically deformed zone and geometrically necessary dislocations of two ion-irradiated FeCrAl(Zr)-ODS ferritic steels: A combined experimental and simulation study, Acta Materialia, 234, 117991, 2022

Y. Watanabe, K. Morishita, T. Nozawa, H. Tanigawa, Size and Temperature Dependence of the Point Defect Binding Free Energy to Defect Clusters in bcc Fe, Plasma and Fusion Research, 17, 1205105, 2022

T. Yamamoto, Y. Wu, K. Yabuuchi, J. Haley, K. Yoshida, A. Kimura, G.R. Odette, Cavity Evolution and Void Swelling in Dual Ion Irradiated Tempered Martensitic Steels, Journal of Nuclear Materials, 154201, 2022

K. Yabuuchi, T. Suzudo, Interaction between an edge dislocation and faceted voids in body-centered cubic Fe, Journal of Nuclear Materials, 574, 154161, 2023

T. Miyazawa, Y. Kikuchi, M. Ando, J.H. Yu, K. Yabuuchi, T. Nozawa, H. Tanigawa, S. Nogami, A. Hasegawa, Microstructural evolution in tungsten binary alloys under proton and self-ion irradiations at 800 °C, Journal of Nuclear Materials, 575, 154239, 2023

A. Kimura, W. Sang, W.T. Han, K. Yabuuchi, Z.X. Xin, J.H. Luan, P. Dou, Twofold age-hardening mechanism of Al-added high-Cr ODS ferritic steels, Journal of Nuclear Materials, 575, 154223, 2023

K. Okamoto, K. Okamoto, K. Morishita, A. Okuno, Development of Photoelectric Conversion Transistor Consisting of High-power LED and Si Solar Cell, ICEP 2022 Proceedings, WC1-2, 2022

森下和功，特集連載　大学紹介(36)京都大学エネルギー理工学研究所における原子力/核融合材料・システム保全の研究，保全学, 21, 3, 53, 38, 2022

Presentations

K. Okamoto, K. Okamoto, K. Morishita, A. Okuno, Development of Photoelectric Conversion Transistor Consisting of High-power LED and Si Solar Cell, 2022 International Conference on Electronics Packaging (ICEP2022), Sapporo & Online Hybrid Conference, 2022.5.11-14

陳昱婷，森下和功，渡辺淑之，照射下材料中の非平衡欠陥生成に関する統計評価，第 14 回核融合エネルギー連合講演会, Online, 2022.7.7-8

阮小勇，渡辺淑之，森下和功，野澤貴史，分子静力学法と線形弾性論に基づく BCC 鉄中の照射欠陥の緩和体積の評価，第 14 回核融合エネルギー連合講演会, Online, 2022.7.7-8

祝梁帆，森下和功，中筋俊樹，藪内聖皓，渡辺淑之，軽水炉圧力容器鋼における溶質原子クラスター形成に関するモデリング研究，日本保全学会第 18 回学術講演会，京都大学＆Online, 2022.7.14

祝梁帆，森下和功，中筋俊樹，藪内聖皓，渡辺淑之，軽水炉圧力容器鋼の照射脆化に関するモデリング研究，日本保全学会第 18 回学術講演会，京都大学

＆Online, 2022.7.14

陳昱婷, 森下和功, 照射下 Fe 内の非平衡欠陥生成に関する分子動力学シミュレーション, 日本保全学会第 18 回学術講演会, 京都大学＆Online, 2022.7.14

濵﨑悠貴, 西川さくら, 岡本賢一郎, 森下和功, 岡本研正, 発光ダイオードと受光素子からなる新型増幅デバイス「ダイスター」に関する研究, 日本保全学会第 18 回学術講演会, 京都大学＆Online, 2022.7.14

堀池寛, 井出俊之, 蛯沢勝三, 鈴木孝寛, 高田毅士, 田中治邦, 宮野廣, 村田貴司, 森下和功, 基調講演「原発裁判から見る原子力発電の課題」, 日本保全学会第 18 回学術講演会, 京都大学＆Online, 2022.7.14

吉川榮和, 森下和功, 日本のエネルギーの未来を支える原子力発電を構想する, 日本保全学会第 18 回学術講演会, 京都大学＆Online, 2022.7.14

L. Zhu, K. Morishita, Monte-Carlo Simulation of Formation Process of copper-vacancy clusters in α-Fe during Irradiation, 13th International Symposium of Advanced Energy Science, Online, 2022.9.5-6

Y. Chen, K. Morishita, Statistical evaluation of non-equilibrium defect formation in materials during irradiation, 13th International Symposium of Advanced Energy Science, Institute of Advanced Energy, Kyoto University, Uji, Kyoto, Online, 2022.9.5-6

H. Yoshikawa, K. Morishita, K. Yabuuchi, Y. Tsujikura, A. Gofuku, T. Matsuoka, M. Abe, J. Nitta, Study on advanced ICT-based maintenance technology for zero-emission energy infrastructure, 13th International Symposium of Advanced Energy Science, Institute of Advanced Energy, Kyoto University, Uji, Kyoto, Online, 2022.9.5-6

K. Okamoto, K. Okamoto, Y. Hamasaki, K. Morishita, Development of New Semiconductor Power Control Devices Aiming for Carbon Neutrality, 13th International Symposium of Advanced Energy Science, Institute of Advanced Energy, Kyoto University, Uji, Kyoto, 2022.9.5-6

Y. Watanabe, K. Morishita, Y. Chen, L. Zhu, T. Nozawa, Effects of incascade defect clustering and defect cluster migration on microstructural evolution in F82H steel under irradiation: Mean field cluster dynamics simulation, 32nd Symposium on Fusion Technology (SOFT2022), Dubrovnik, Croatia and online Hybrid, 2022.9.18-23

陳昱婷, 森下和功, 衝突カスケードにおける点欠陥クラスター及び転位ループへの生成メカニズムの解明：大規模分子動力学 シミュレーション, 京都大学エネルギー理工学研究所第２回学生研究発表会, Online, 2022.12.16

濵﨑悠貴, 西川さくら, 岡本賢一郎, 森下和功, 岡本研正, 新型パワーデバイス「ダイスター」に関する研究, 京都大学エネルギー理工学研究所第２回学生研究発表会, Online, 2022.12.16

安部純弥, 藪内聖皓, 森下和功, Deep Learning による格子欠陥分類, 京都大学エネルギー理工学研究所第２回学生研究発表会, Online, 2022.12.16

石璵, 森下和功, ナノスケールき裂進展の分子動力学評価, 京都大学エネルギー理工学研究所第２回学生研究発表会, Online, 2022.12.16

祝梁帆, 森下和功, 原子力材料の照射脆化予測高度化のためのモデリング研究, 京都大学エネルギー理工学研究所第２回学生研究発表会, Online, 2022.12.16

岡本賢一郎, 濵﨑悠貴, 岡本研正, 森下和功, 池上和志, 宮坂力, ペロブスカイト太陽電池使用光電変換トランジスタを用いたモータ制御, 2023 年電子情報通信学会電子通信エネルギー技術研究会, Online, 2023.3.6

岡本賢一郎, 岡本研正, 森下和功, 池上和志, 宮坂力, ペロブスカイト太陽電池と LED からなる光電パワートランジスタ, 2023 年応用物理学会春季学術講演会, 上智大学＆オンライン, 2023.3.15

陳昱婷, 森下和功, 衝突カスケードにおける点欠陥クラスターの生成メカニズム : 大規模分子動力学シミュレーション, 日本原子力学会 2023 年春の年会, 東京大学, 2023.3.14

祝梁帆, 陳昱婷, 森下和功, 中性子照射下における Fe 内の非平衡欠陥生成に関する統計的評価, 日本原子力学会 2023 年春の年会, 東京大学, 2023.3.14

陳昱婷, 森下和功, 衝突カスケードにおける点欠陥クラスターの生成メカニズム : 大規模分子動力学シミュレーション, 日本原子力学会 2023 年春の年会, 東京大学, 2023.3.15

祝梁帆, 陳昱婷, 森下和功, 中性子照射下における Fe 内の非平衡欠陥生成に関する統計的評価, 日本原子力学会 2023 年春の年会, 東京大学, 2023.3.15