Advanced Energy Structural Materials Research Section

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1. Introduction

The development of robust materials and the establishment of reliable system management are essential for the safe and efficient operation of advanced nuclear energy systems. This section addresses the mission of establishing maintenance management methodologies as well as materials R & D for advanced nuclear energy systems such as fusion and fission reactors. Our research interests include:

(1) Theory, modeling, numerical simulation, and data-driven science & technology of irradiated materials: Radiation damage processes of materials during irradiation occur at various time and length scales. To understand these processes, 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 MD, ab-initio calculations, kinetic Monte-Carlo, rate-equation analysis, FEM and CFD. Recently, additional efforts have also been devoted to this research using machine learning, AI, and data-driven techniques.

(2) Plant integrity analysis: Structural integrity of a reactor pressure vessel (RPV) during pressurized thermal shock (PTS) events is of critical importance in the quantitative assessment of reactor safety. We evaluate this using 3D CFD and FEM. The risk of the RPV function loss is quantified and then 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 those defects is responsible for the evolution of the microstructure, which may cause degradation 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. Size distribution of defect cluster 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, some of the point defects aggregate to form defect clusters. 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 factors influencing the generation of clusters were investigated through the MD simulation of the collision cascade in Fe.

Fig.1 shows a snapshot of the displacement cascade in Fe at 0.2 ps, which is initiated from a PKA with a kinetic energy of 50 keV. It can be seen from this figure that the nucleation of an SIA loop (marked by green line) is formed at a relatively early stages. The formation of such cascade clusters is thought to have a major impact on the subsequent microstructural developlement, making it difficult to develop fusion reactor materials with excellent radition resistance.

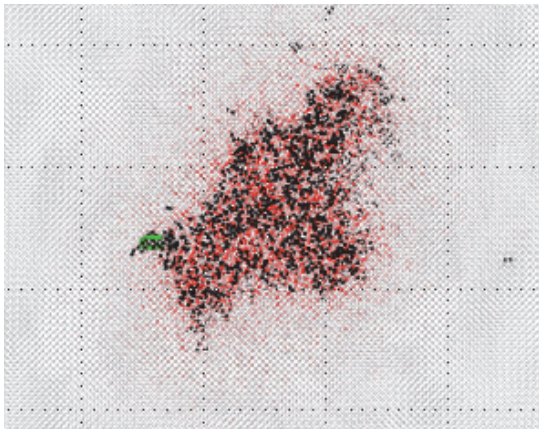

Fig. 1: Evolution of displacement cascades in Fe

3. Effect of irradiation environments on microstructural evolution in Fe during irradiation

Many studies have been done so far using numerical simulations to develop tools to predict material degradation under irradiation. However,

many conventional predictions mainly evaluate the "average" behavior of the changes due to irradiation without taking into account the effects of fluctuations. The fracture behavior of a material does not depend on the average behavior of the material, but rather is dominated by the material's property at its weakest point. Therefore, it is important to focus on fluctuations in defect microstructural evolutions.

In this study, the fluctuations in defect generation and associated microstructural changes caused by irradiation are focused. The probability distribution function (PDF) of the number of point defects and that of the number of cascade clusters are obtained as a function of recoil energy using our molecular dynamics simulations (MD). The recoil energy spectrum for a specific neutron irradiation facility, e.g., high flux isotope reactor (HFIR) in ORNL, is then obtained using the nuclear library JENDL constructed by JAEA. Using these data evaluated here, the average and fluctuations of point defect generation rate and those of cascade cluster generation rate are evaluated individually for the specific irradiation facility. These generation rates are furthermore employed as a source term in the rate theory equations to evaluate the microstructural changes of materials during irradiation. Our calculation results showed that the fluctuation in microstructural changes is highly dependent on irradiation conditions; for example, the coefficient of variation in concentrations of defect clusters accumulated varies by up to 40 % in HFIR.

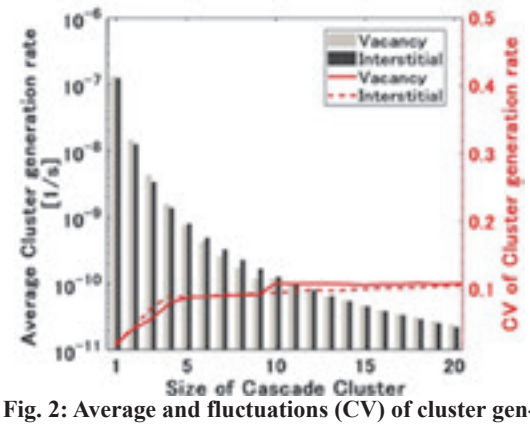

Fig. 2: Average and fluctuations (CV) of cluster generation rate

4. Modeling of SiC materials for application in nuclear energy system: first principles calculations

Since its excellent properties such as high strength and low induced radioactivity, SiC materials are being developed and validated as nuclear materials. However, before practical application in nuclear reactors, it is necessary to study the effects of high temperature and irradiation environment of nuclear systems on the properties of SiC materials.

To simulate the radiation damage behavior of materials using molecular dynamics methods, a reliable potential function is required. However, it is known that the Tersoff, MEAM, and GW potential functions widely used in molecular dynamics simulations of SiC materials are inconsistent with highly accurate first principles calculations. Therefore, it is necessary to develop new potential functions that can accurately describe the interactions between atoms.

On the other hand, with the development of artificial intelligence technology, neural networks have been proven to be able to construct high-precision potential functions and apply them to material modeling research. Therefore, in order to conduct reliable molecular dynamics simulations of irradiation behavior, this study used a high-precision first principles calculation method to calculate the total potential energy of SiC materials and provided teaching data for constructing neural network potential energy functions.

First principles calculation was carried out by supercomputer system using SIESTA code. We constructed 3C-SiC model with 216 atoms composed of $3 \times 3 \times 3$ supercells and approximated the exchange interaction of electrons using generalized gradient approximation. To obtain a good generalization ability for the neural network potential function to be developed, not only the calculation of the perfect crystal SiC but also the cases for different lattice constants, vacancies and interstitial atoms were calculated. A total of 149 calculations were conducted. As input parameters for the neural network potential function, atomic coordinates, energy and force have been calculated and extracted.

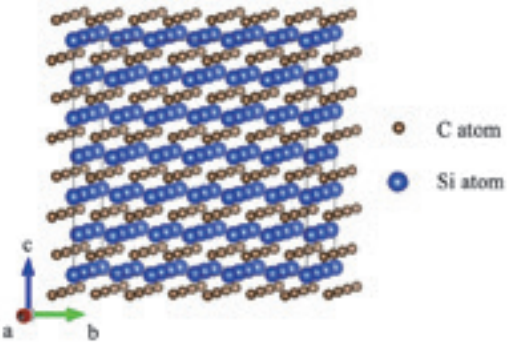

Fig. 3: 3C-SiC perfect crystals.

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.

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