

Advanced Energy Structural Materials Research Section

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1. Introduction

The development of robust materials and the implementation of reliable system management are crucial for ensuring the safe and efficient operation of advanced nuclear energy systems. This section explores the mission of establishing maintenance management methodologies and advancing materials research and development for cutting-edge nuclear energy systems, including fusion and fission reactors. Our research interests include:

(1) Theory, modeling, numerical simulation, and data-driven science & technology: Radiation damage in materials during irradiation occurs across various time and length scales. To gain a comprehensive understanding of the processes, a multiscale perspective and statistical approaches are essential. This section focuses on modeling material behavior under irradiation through a combination of computational techniques, including molecular dynamics (MD), ab-initio calculations, kinetic Monte-Carlo, rate-equation analysis, finite element method (FEM), and computational fluid dynamics (CFD). Recently, additional efforts have also been dedicated to integrating machine learning and data-driven methodologies to enhance this research.

(2) Plant integrity analysis: Structural integrity of a reactor pressure vessel (RPV) during pressurized thermal shock (PTS) events is crucial for the quantitative assessment of reactor safety. To evaluate this, we employ 3D computational fluid dynamics (CFD) and finite element method (FEM) simulations. The risk of RPV function loss is then quantified for optimizing maintenance strategies.

(3) Effects of irradiation on microstructure and mechanical property changes: High-energy particle irradiation generates oversaturated interstitials and vacancies, whose behavior drives microstructural evolution and may lead to the degradation of material's mechanical properties. Understanding the behavior of these point defects is essential for elucidating the mechanisms behind such property changes. In our research, we investigated microstructure evolution under irradiation through both experiments and computational modeling.

2. Evaluation of the formation free energy of clusters in Fe

The safety of reactor pressure vessel (RPV) steel is a critical issue in the field of nuclear energy. In par-

ticular, atomic clusters in alloys influence the crystal-line properties of materials and accelerate the embrittlement of RPV steel. During the evolution of clusters, growth occurs primarily through atomic absorption and dissociation processes, and the associated kinetics are governed by variations in free energy.

Previous studies have generally evaluated cluster behavior using average free energy. However, due to differences in atomic configurations and local chemical environments, the free energy exhibits a discrete distribution even for clusters of the same size. Therefore, a systematic analysis of the influence of cluster configurations on the free energy distribution is of significant importance. In this study, the effect of cluster structure on the characteristics of free energy distributions is quantitatively investigated.

Fig.1 shows the variation of the free energy distributions of Cu, Mn, and Ni clusters as a function of cluster size at 900 K. The horizontal axis represents the cluster size, while the vertical axis denotes the free energy. The violin plot correspond to the probability distributions of cluster free energies arising from different configurations at the same cluster size, and the curves represent the average free energy as a function of cluster size. For Cu clusters, the free energy generally increases with increasing cluster size, while the distribution progressively concentrates in the low-free-energy region. For Mn and Ni clusters, similar trends in free energy variation with cluster size are observed, with the average free energy turning from an increasing to a decreasing trend at size = 4 for Mn and size = 2 for Ni, respectively, and approaching or falling below zero near size ≈ 6 , indicating a pronounced self-aggregation tendency.

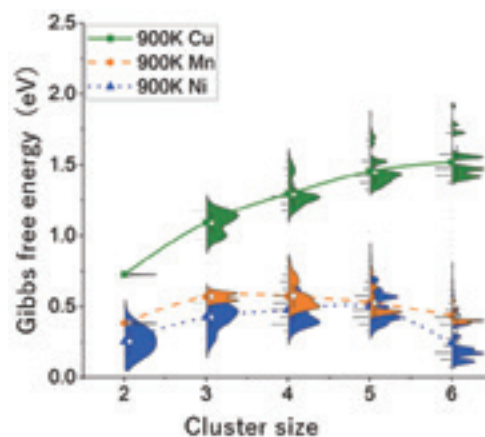


Fig. 1 Formation free energy distributions of Cu, Mn, and Ni clusters in Fe.

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 considering 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 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 (MD) and Kinetic Lattice Monte Carlo (KLMC) simulations. 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 show that in the early stage of irradiation, most of the defect clusters are generated by cascade clusters and their fluctuations are fluctuations in the cascade cluster generation rate. As the irradiation progresses, the fluctuations flow into the larger-sized clusters, and the fluctuations in the larger-sized clusters increase. The swelling fluctuation exceeds 20% for 10% of the defect generation.

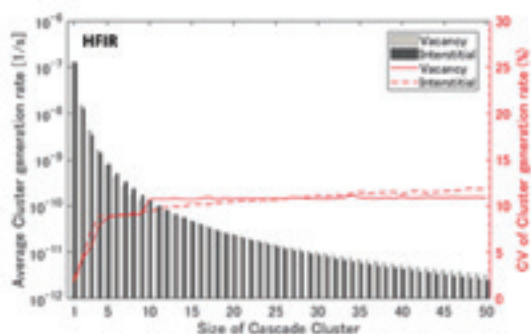


Fig. 2 Cascade clusters generation rate and fluctuations

4. Development of a First-Principles Database for Neural Network Potential of Fe-Mn-Ni-Si Alloys

Irradiation damage in nuclear materials under fusion and fission environments can significantly

affect microstructure and material properties. Molecular dynamics (MD) simulations are widely used to investigate irradiation damage behavior. However, the accuracy strongly depends on the quality and coverage of the interatomic potential. In recent years, machine learning based neural network potential has attracted increasing attention, making the construction of reliable first-principles databases a key prerequisite for their development. Following methodological studies using empirical potentials in the previous year, the present year focused on constructing a first-principles database for machine learning applications. The target system is the Fe-Mn-Ni-Si alloy, which is representative of reactor pressure vessel steels. First-principles calculations were performed using the VASP code. To efficiently sample diverse atomic environments, multiple data generation strategies were employed to include solid solution structures, defect-containing configurations, and thermally disordered structures. Atomic perturbations, random substitutions, and defect structures were intentionally introduced to avoid excessive clustering around ideal crystal configurations. Fingerprint checks and random seed control were applied to prevent duplication of similar structures. As a result, the constructed database contains approximately 20,000 structures, corresponding to about 3.24×10^7 distinct atomic environments. The distribution of atomic environment descriptors was analyzed to assess database quality and diversity.

As shown in Fig. 3, the density distribution exhibits a continuous and approximately Gaussian-like shape, with data points distributed across both central and outer regions of the descriptor space, reflecting well-balanced sampling behavior. This indicates broad configurational coverage without strong bias toward specific atomic configurations. This first-principles database provides a foundation for future neural network potential training and subsequent MD simulations of irradiation damage behavior in Fe-Mn-Ni-Si alloys.

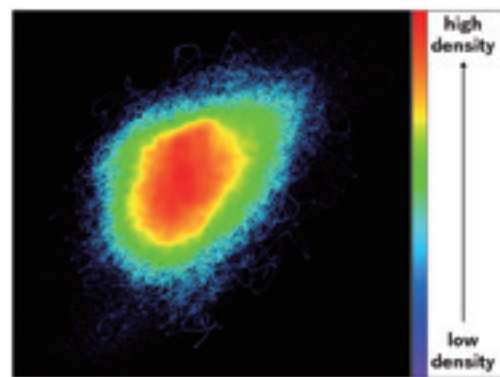


Fig. 3 Density distribution of atomic environment descriptors, illustrating the coverage and diversity of the constructed database.

Collaboration Works

(該当なし)

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