Development of a radiation damage structure classifier in bcc-W using molecular dynamics simulation and deep learning

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1. Introduction

Due to favorable properties in high heat-load environments such as high melting point, low coefficient of thermal expansion, and high thermal conductivity, tungsten (W) has been considered as a plasma-facing material for fusion reactors [1][2]. Materials used in nuclear fission/fusion reactors are subjected to neutron irradiation, and the radiation damages can affect the safety and performance of the nuclear power systems [3]. Therefore, it is important to understand how radiation damages are formed and how they evolve in materials.

In a material exposed to neutron irradiation, primary knock-on atoms (PKAs) are generated by receiving excess energy by collision with neutrons. If a PKA has a high kinetic energy, defects such as self-interstitial atoms (SIAs) and vacancies are generated due to energy transfer in a sequence of collisions [4]. To predict the radiation damage phenomena, molecular dynamics (MD) simulation, which is a computationally intensive method for simulating many-body collision [5], has been widely used. However, it is not easy to apply MD to simulations of high-energy and high-dose damages because of its high computational cost.

Recently, convolutional neural network (CNN), which is a kind of deep learning method, has shown high performance in image classification tasks [6]. Thus, in this research, to reduce the computational cost of radiation damage simulations significantly, we investigate whether radiation damage structures obtained by MD can be identified and imitated by CNN deep learning. If such a machine-learning classifier is successfully constructed, a radiation damage simulator for high-energy and high-dose damage, which is important in the development of fusion and fast reactors, can be developed in the future.

In this research, bcc-W was used as a test system. Radiation damage structures were generated by MD recoil simulations and were used as training and test data in developing the classifier using CNN. The classification performance was evaluated and effects of training conditions were analyzed.

2. Methods

In this section, we present processes to build the radiation damage structure classifier. First, defect structure data after collision cascades in W were generated by MD recoil simulations. Second, data preprocessing was conducted to convert MD simulation data into an appropriate data format for deep learning. Third, a CNN deep learning model for radiation damage classification was built and optimized. Lastly, the classifier was tested with non-trained dataset to evaluate the classification performance.

2.1 MD simulation

Radiation damage structures used as training and test datasets for the classifier were generated by MD recoil simulations using LAMMPS code [7]. To simulate the bulk structure of bcc-W, 110×100×90 (1980000 atoms) supercells were basically used, while 144×72×72 (1492992 atoms) supercells were used only for near <100> displacement simulations. The system was first equilibrated under the condition of 30 K and 1 bar with an NPT ensemble. Subsequently, we introduced excess kinetic energy to an atom that will become a recoil atom. The time evolution in a recoil simulation was simulated with an NVE ensemble using a variable timestep method. The recoil simulations were continued for around 6~15 ps until defect structures converged. The embedded-atom method (EAM) [8] potential parameterized by Derlet et al. [9] and modified by Bjorkas et al. [10] was used as the potential model for recoil simulations. Damage structures were obtained under total 90 settings (6 energies and 15 directions). To account for the stochastic nature of radiation damage, 100 time samples were collected for each setting.

2.2 Data preprocessing

The results of MD recoil simulations were given as 3-dimensional Cartesian coordinates of atoms. We converted atomic position data into defect structure data. In addition, we reduced the dimension of original defect structure data to 2 dimensions since CNN has showed good performance with 2-dimensional data.

These data preprocessing tasks were completed in four steps. First, vacancies and SIAs position data were extracted from atomic position data using Wigner-Seitz defect analysis method [11]. Second, since two supercell sizes were used in MD, they were adjusted to 125×125×125 supercell size. Third, the 3-dimetional data were projected onto the xy, yz, and xz planes. Therefore, one MD recoil simulation has a set of six data of 125×125 2-dimentional cells. Finally, six data were merged so that (125, 125, 6) array data is finally generated for training and test in CNN deep learning.

2.3 Deep learning model

CNN deep learning was adopted to build radiation damage structure classifier. The CNN training architecture used in this study is presented in Figure 1. As described in the previous section, each input has a (125, 125, 6) array format. The output is a classification result, classifying an input into radiation damage structure ("*Yes*") or not ("*No*").

The training and test datasets consist of YES data and NO data. YES data, which are defect structures that can be formed by radiation damage, were generated by MD recoil simulations and data preprocessing as described in Section 2.1 and 2.2. NO data, which are defect structures that cannot be formed by radiation, were prepared randomly. To be specific, vacancies and SIAs were randomly distributed in a 125×125×125 supercell, while limiting the number of defects to 4~80. In addition, to make NO data more similar to YES data, some NO data were prepared considering statistics of defect numbers and locations obtained by MD. In total, 8200 YES data and 5800 NO data were generated.

As shown in Figure 1, the CNN architecture has two convolutional layers with a Rectified Linear Unit (ReLU) activation function and max-pooling layers. Finally, the extracted features are flattened and classified with Softmax function. The learning architecture was optimized to maximize the prediction accuracy of the classifier.

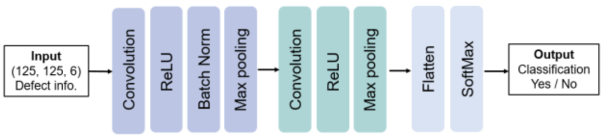

Fig. 1. Convolutional neural network (CNN) architecture used to build the radiation damage structure classifier.

3. Results and Discussion

3.1 Classification performance test

In the process of training, we used 7200 YES data and 4800 NO data for 6 recoil energies (1, 2, 4, 8, 16, 32 keV) and 15 recoil directions. Subsequently, the classification performance was evaluated with 1990 test data composed of 1000 YES data and 990 NO data. The information of recoil energies and directions used in the training and test is summarized in Table 1 together with obtained classification accuracy.

The classification results showed 95.3% accuracy, with 95.6% accuracy for YES data and 95.1% for NO data. Figure 2 shows the error rate of classifying YES and NO data as a function of recoil energy. When the test recoil energy was lower, the error rate became higher. Although the total error rate was below 5%, NO data error rate reached 15~30% when the recoil energy was below 6 keV.

Table I: Summary of training and test data information and classification performance.

Training dataset (recoil energy [KeV])		
1, 2, 4, 8, 16, 32		
Training data amount		
YES data	No data	Total
7200	4800	12000
Test data amount		
YES data	No data	Total
1000	990	1990
Classification accuracy [%]		
YES data	No data	Total
95.6	95.1	95.3

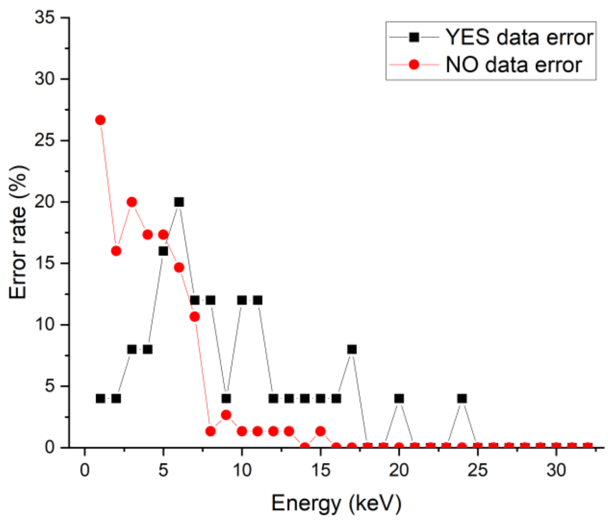

Fig. 2. Classification error rates of the radiation damage structure classifier as a function of recoil energy.

3.2. Analysis of classification results

To evaluate the performance of the classifier in detail, we analyzed the classification results. Figure 3 shows six typical cases as follows:

- ✓ First, most damage structures obtained by MD simulations were correctly distinguished as YES data. Figure 3 (a) shows one of YES data that was correctly classified as *Yes*.
- ✓ However, as in Figure 3 (b) and (c), some YES data were wrongly classified as *No*. These two structures show typical error cases: in (b), the radiation damage is composed of very few defects (less than 4); in (c), defects are widely separated and not clustered.
- ✓ In the case of NO data, as in Figure 3 (d), when the defects were widely spread so that it is obviously not radiation damage structure, the classifier perfectly classified as *No*.
- ✓ Even when NO data accidentally included clustered defects so that the damage structure became similar

to the structure that can be generated by MD simulations as in Figure 3 (e), our classifier correctly classified them as *No* in most cases. However, some of these structures were incorrectly classified as *Y*es, as in Figure 3 (f).

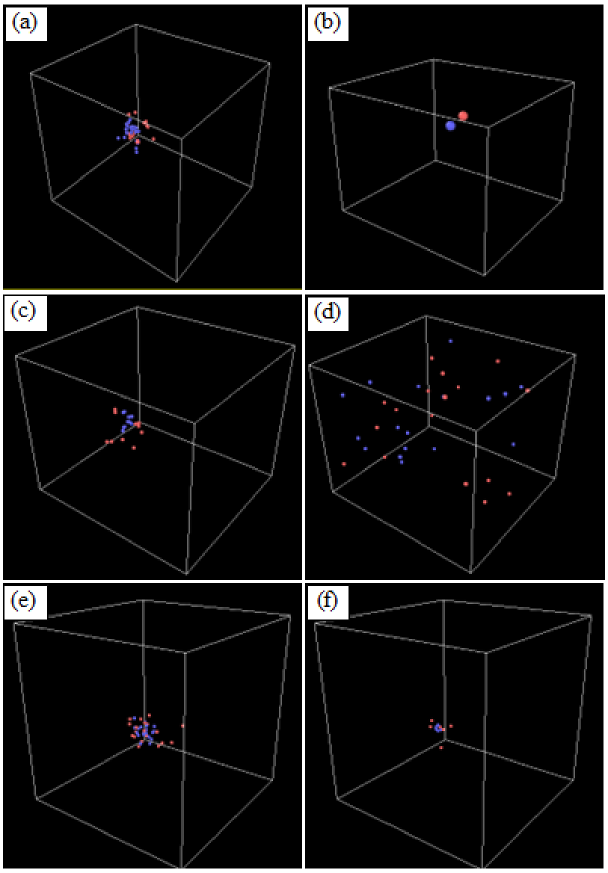

Fig. 3. Typical defect structures that correctly or wrongly identified by the classifier. The figures were drawn with OVITO software [12]. These 6 cases correspond to (a) YES data correctly classified as *Yes*, (b)(c) YES data wrongly classified as *No*, (d)(e) NO data correctly classified as *No*, and (f) NO data wrongly classified as *Yes*. Blue and red points indicate the positions of vacancies and SIAs, respectively.

In short, three types of structures often caused errors: (1) random structures that are coincidentally similar with MD recoil simulation results, (2) radiation damage structures composed of a small number of defects, and (3) radiation damage structures where defects are not so clustered.

The error type (1) is an intrinsic error of random structure generation and mostly happened with high recoil energy. On the other hands, the error types (2) and (3) occurred with low recoil energy, and causes the high error rate. This is because YES data, produced by MD recoil simulations, are no more special compared to randomly distributed defect data at low recoil energy. Accordingly, it is reasonable to consider that the relatively low classification performance at low recoil energy does not indicate the low performance of the classifier but merely reflects the nature of defect structures.

3.3 Classification performance improvement

Since the error rate due to (1) is below 0.5%, we focused on reducing error rate due to (2) and (3). To reduce the error rate by (2) and (3), the ratio of YES and NO data size in training dataset was changed and the error rates were analyzed. The performance was compared between four classifiers constructed with different data ratios (1:1.5, 2:1, 4:1, and 8:1). The total training size was fixed. The results are shown in Figure 4. Since the error types of (2) and (3) occurred mostly at low recoil energy, only error rates at low recoil energy are presented in Figure 4.

From the training data ratio test, a trade-off between YES data classification accuracy and NO data classification accuracy is observed at low energy. Since a defect structure that can be formed either by MD recoil simulation or by random generation should be classified as *Yes*, it is necessary to decrease the YES data error rate by allowing some increase in the NO data error rate. Thus, in the final version of the classifier whose classification performance is shown in Figure 2, we applied 4:1 data ratio so that the YES data error rate is reduced below approximately 10%, and the increase of the NO data error is suppressed as much as possible.

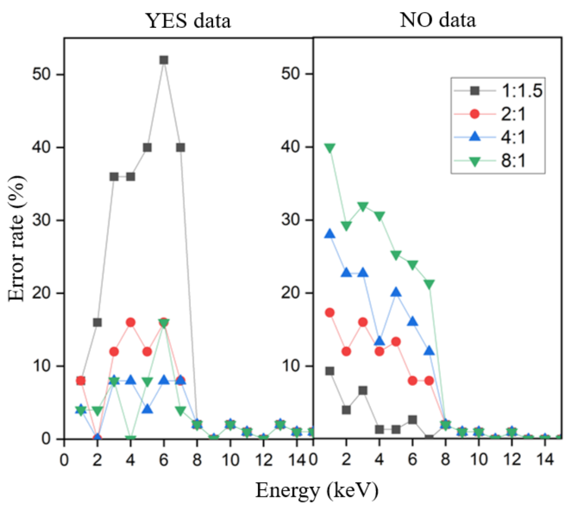

Fig. 4. Classification performance at low energy with different training data ratios. The tested ratios (YES data : NO data) are 1:1.5 (black), 2:1 (red), 4:1 (black), and 8:1(green). The left figure shows the YES data error rates, and the right figure shows the NO data error rates.

4. Conclusions

In this research, we proposed a radiation damage structure classifier with various recoil energy and directions in bcc-W using MD recoil simulations and CNN deep learning. The classification performance of classifier achieved 95.3% accuracy. However, the NO data error rate increased over 15% when the recoil energy was low, e.g., below 6~8 keV.

By analyzing the classification results, it was confirmed that most of errors were caused with low energy recoil when a small number of defects were formed and when the formed defects were not significantly clustered. To improve the classification performance of the classifier at low recoil energy, the training data ratio test was additionally conducted, and we concluded that including YES data and No data with 4:1 ratio can suppress the YES data error rate below 10% while the NO data error does not soar.

Through this study, we confirmed that radiation damage structures can be learned by CNN deep learning. Using the constructed classifier, we plan to develop a radiation damage simulator for high-energy and high-dose damage in future studies.

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