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Nuclear Fuel and Materials

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

Jonghyeon Park and Takuji Oda*
Seoul National University

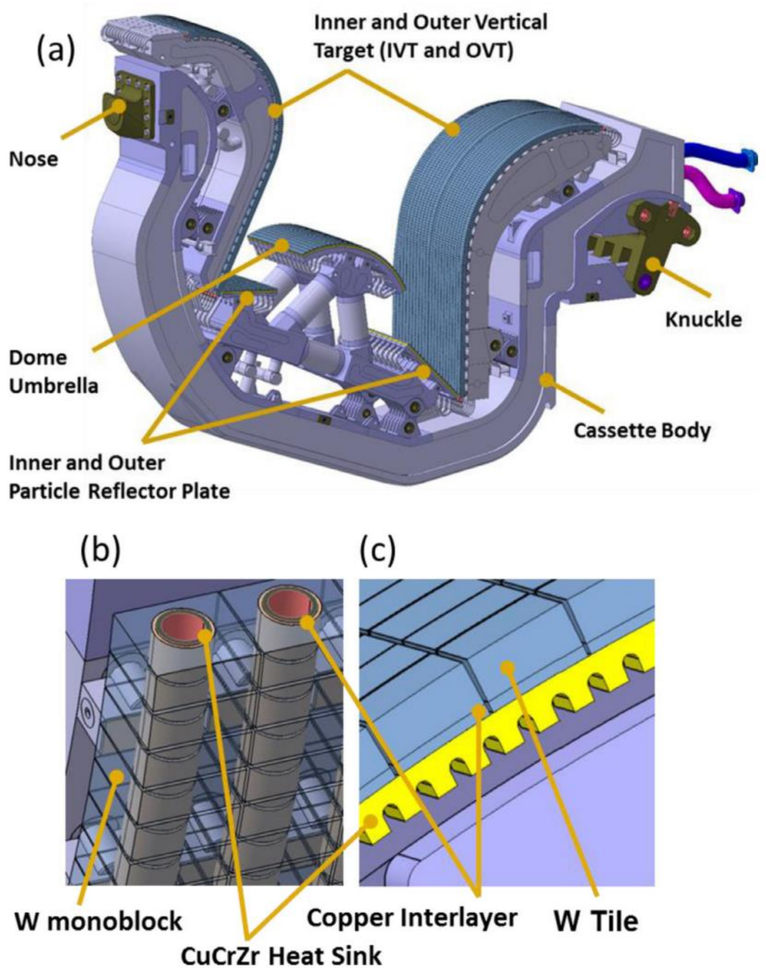
**** E-mail: oda@snu.ac.kr***

서울대학교
SEOUL NATIONAL UNIVERSITY
SNU · Nuclear Materials Modeling Lab.

Radiation damage in tungsten

❑ Tungsten (W)

- W is used as a plasma-facing material for nuclear fusion reactor due to its favorable properties, such as high melting point.
- The extreme environment of fusion reactors, characterized by intense energetic particle fluxes, causes adverse effects, such as increased tritium retention and degradation of mechanical properties.

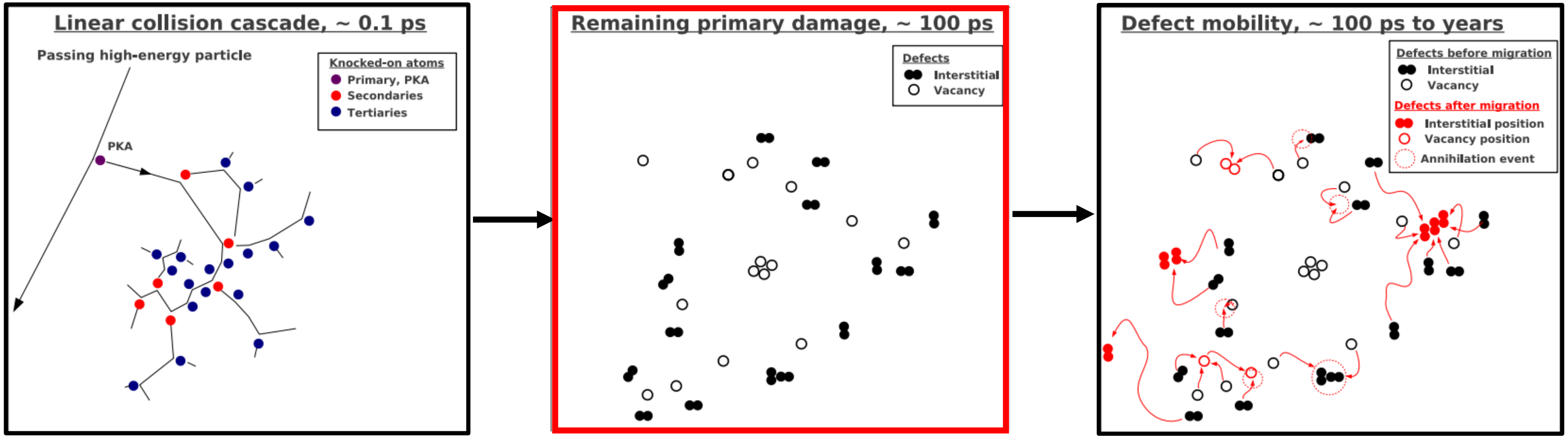


* T. Hirai, et al., Journal of Nuclear Materials and Energy, 2016, Vol. 9, 616-622

Radiation damage structure

❑ Primary damage and radiation damage structure

- The initial stage of the radiation damages starts with the generation of primary knock-on atoms (PKAs) which cause atomic displacement.
- After collision cascades, radiation damage structures are formed, which consists of defects such as vacancy and self-interstitial atom (SIA).

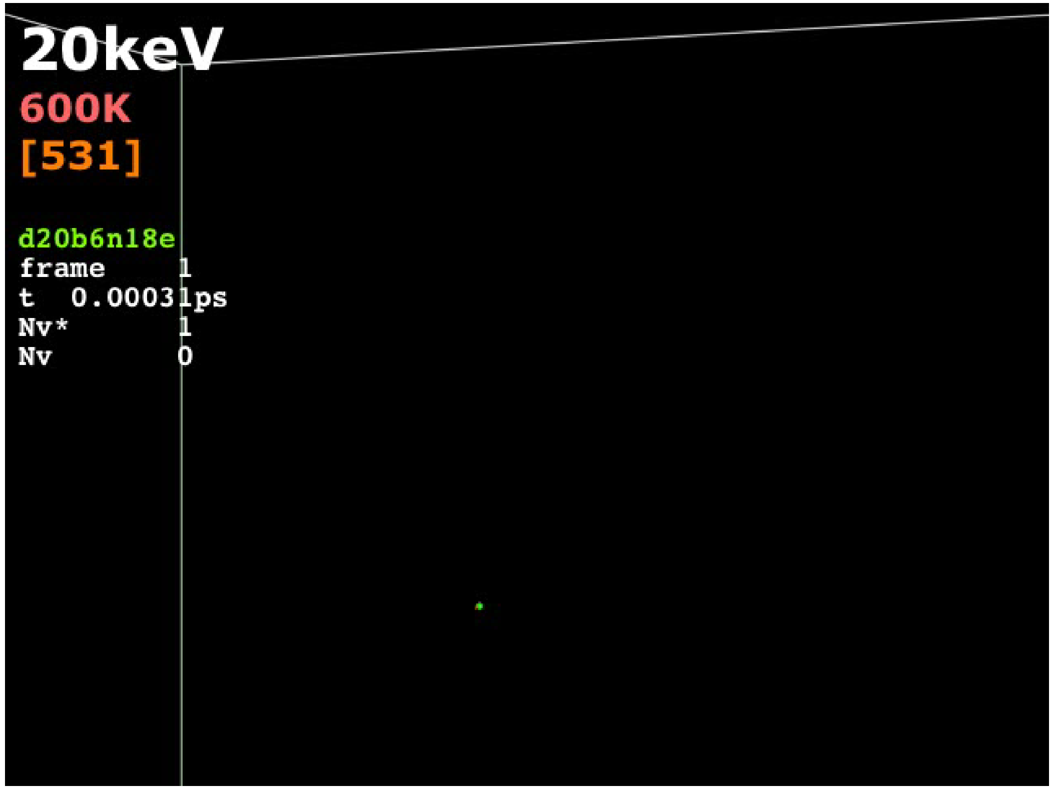


* Kai Nordlund, et al., Journal of Nuclear Materials, 2018, Vol. 512, 450-479

Radiation damage structure

❑ Molecular dynamics (MD)

- MD simulations is a suitable computational method to simulate atomic displacement by collisions.
- However, it is not easy to apply MD to simulate a high-dose environment due to its high computational cost.

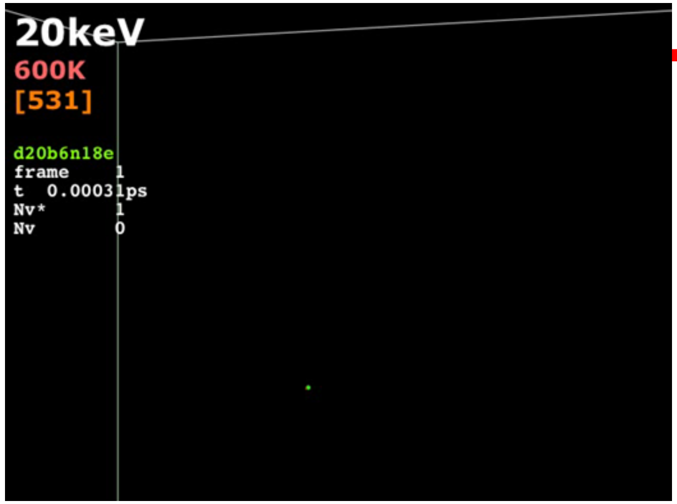


* http://www.youtube.com/watch?v=0btHd_8JFV4

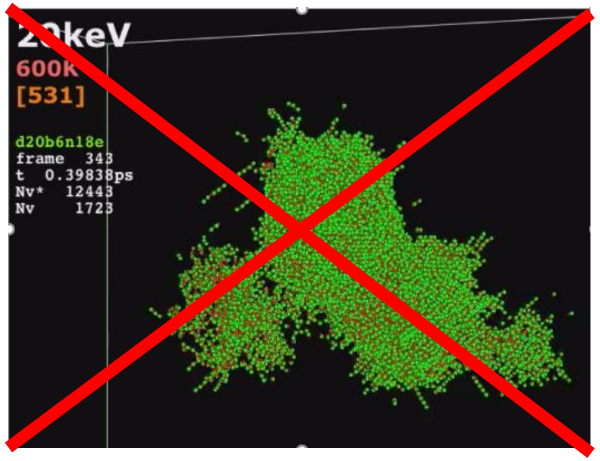
Radiation damage in tungsten

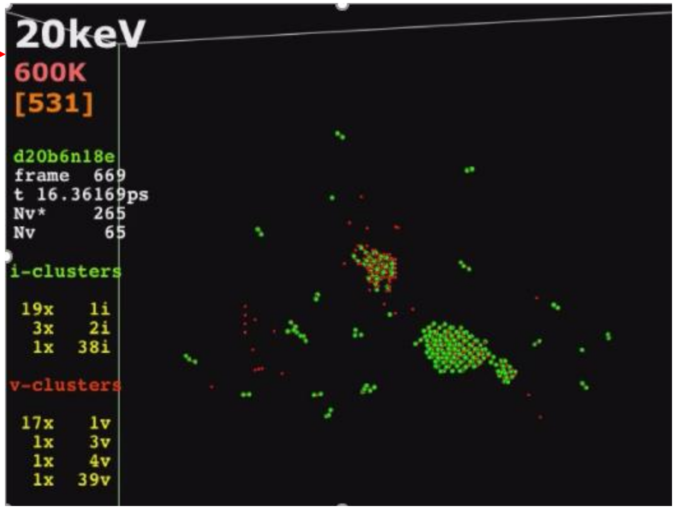
❑ Convolutional neural network (CNN)

- CNN is a kind of deep learning method, which has shown high performance in image classification tasks.
- If deep learning can be used to classify radiation damage structures, we can obtain radiation damage structures at low cost without simulations of collision processes



Skip collision cascades and replace it with CNN





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Research goals

<Objective>

Developing the classifier which is able to recognize and distinguish the radiation damage structures caused by PKAs in bcc-W

❑ Contents

I. Method

(1) MD simulation

(2) Data pre-processing

(3) CNN deep leaning

II. Results and discussions

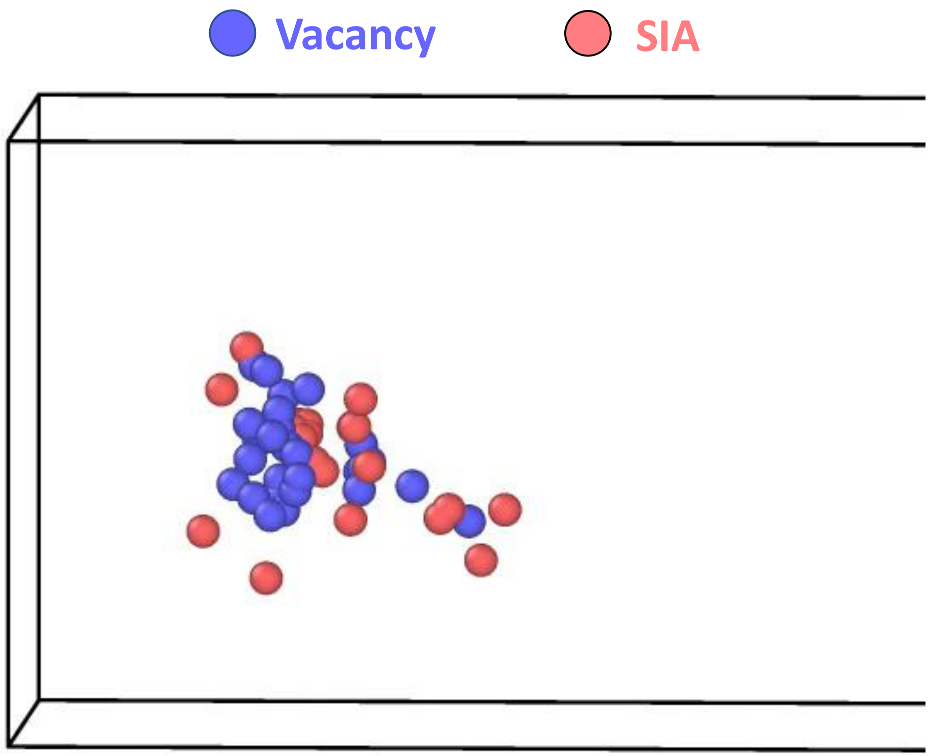
(1) Classification performance

(2) Classification results analysis

(3) Application

MD simulation

- Obtaining radiation damage structures
  - MD recoil simulation with LAMMPS code was conducted to obtain radiation damage structures.
  - Obtaining radiation damage structures with various conditions.
    - 135 recoil conditions (1~32 keV energies; 15 directions)
    - 100 samples for each conditions
  - These structures were used for training and test data in our classifier.



Data pre-processing

❑ Reducing dimension of radiation damage structures.

- To use our MD recoil simulation data as training and test data for CNN deep learning, we converted 3-dimensional into 2-dimensional data.
  (1) Radiation damage structures were obtained from MD recoil simulation
  (2) Vacancies and SIAs position data were extract by Wigner-Seitz analysis method
  (3) Supercell size was adjusted into $125 \times 125 \times 125$.
  (4) 3-dimentional defect structure was projected onto the xy, yz, zx planes.
  (5) Six data were merged so that $(125, 125, 6)$ array data is obtained.

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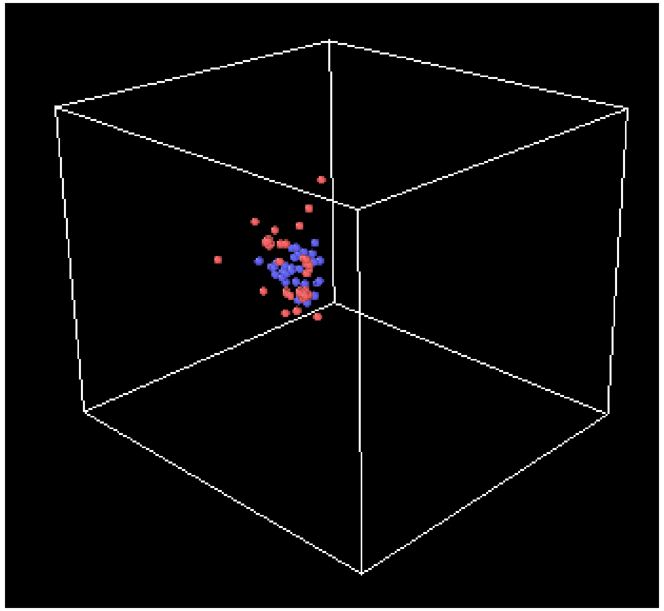

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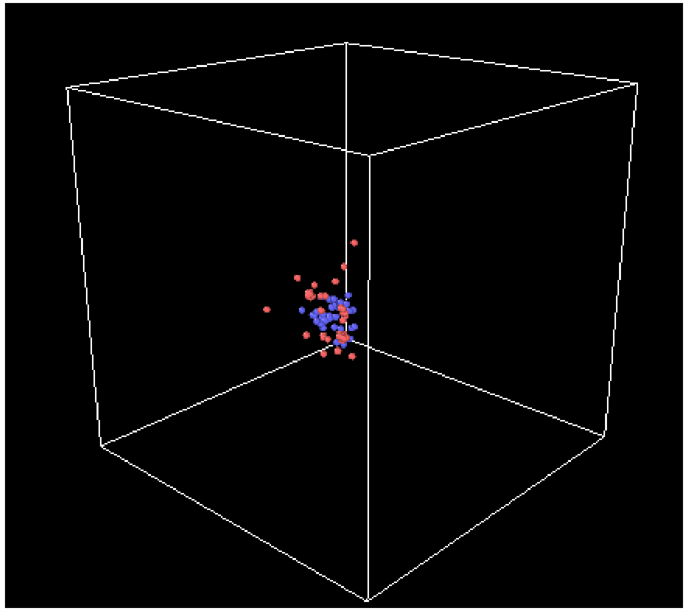

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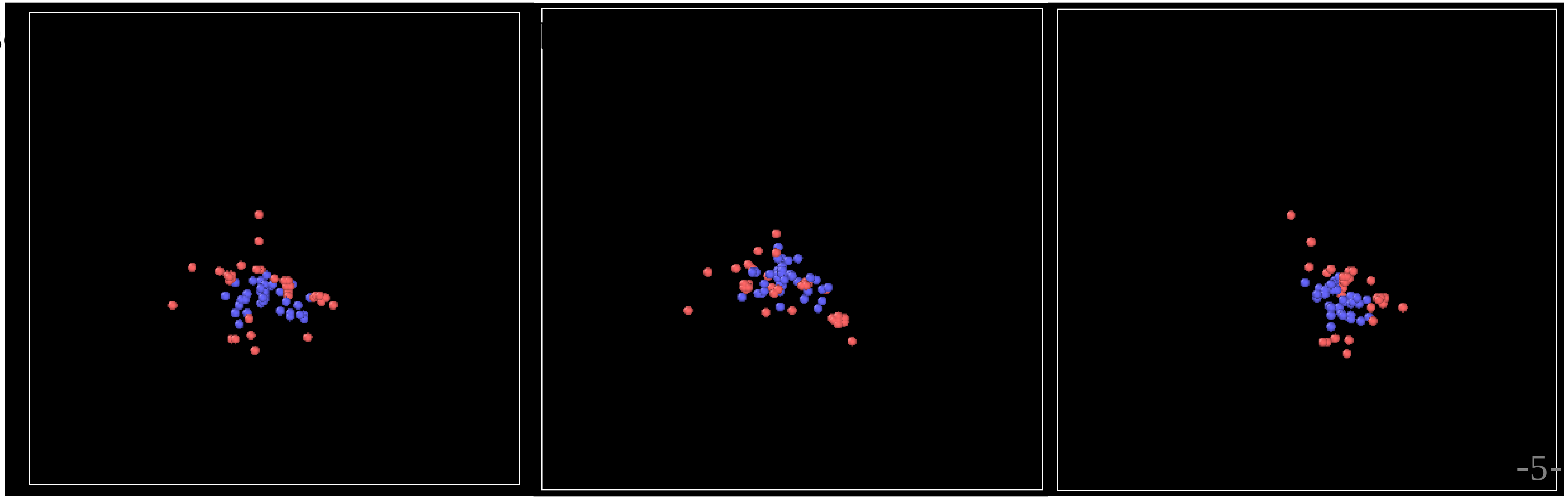

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Random defect structures

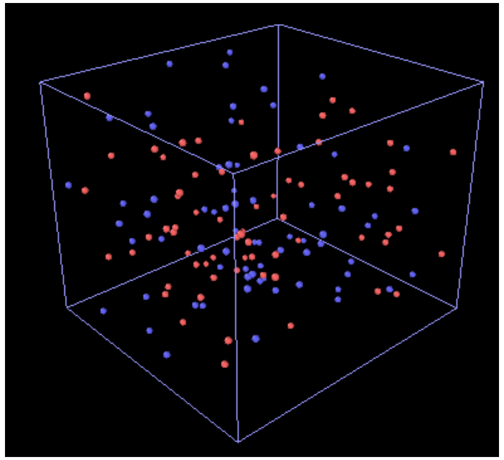
❑ Simple random and quasi random structures.

- To build high performance classifier, we should prepare not only correct radiation damage structure but also non-realistic defect structures for deep learning. We prepare two types:

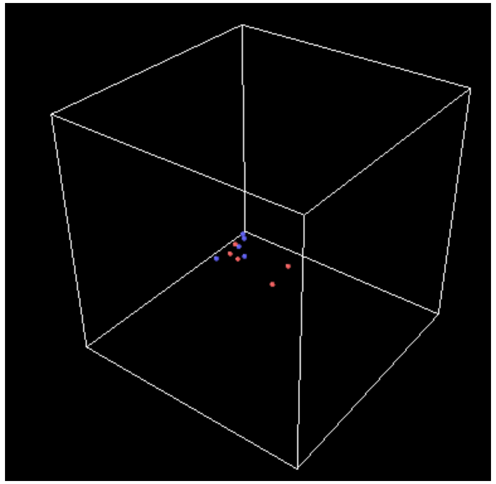
  (1) simple random, totally random.

  (2) quasi random which satisfies the defect number and position statistics derived from MD results.

<Simple random structures>



<Quasi random structure>



Deep learning model

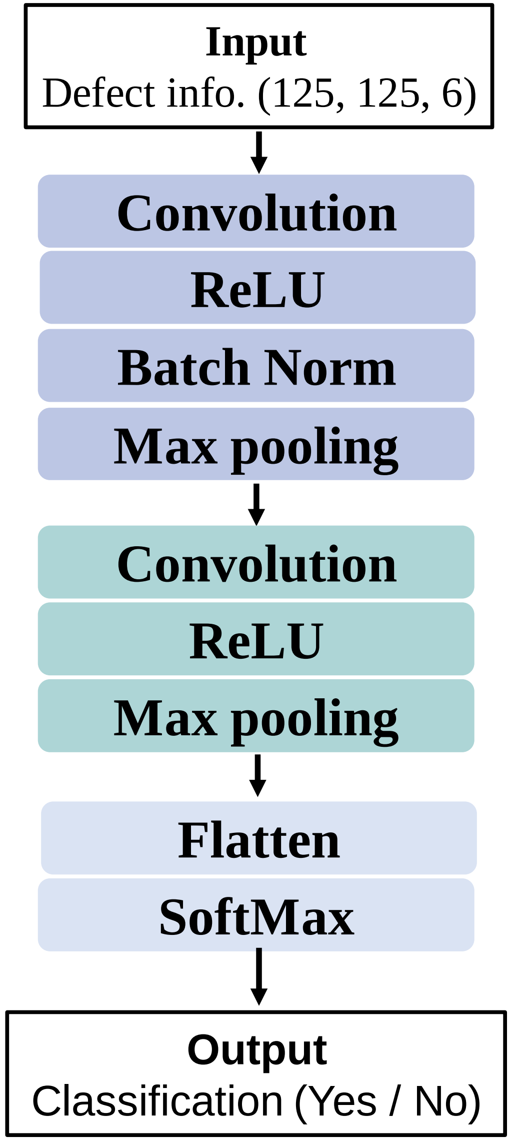
❑ CNN deep learning

- We defined YES data and NO data

  - YES data are defect structures that can be formed by radiation damage: MD simulation data (Total 8200)

  - NO data are defect structures that rarely formed by radiation damage: Simple random structure, quasi random structure (Total 5800)

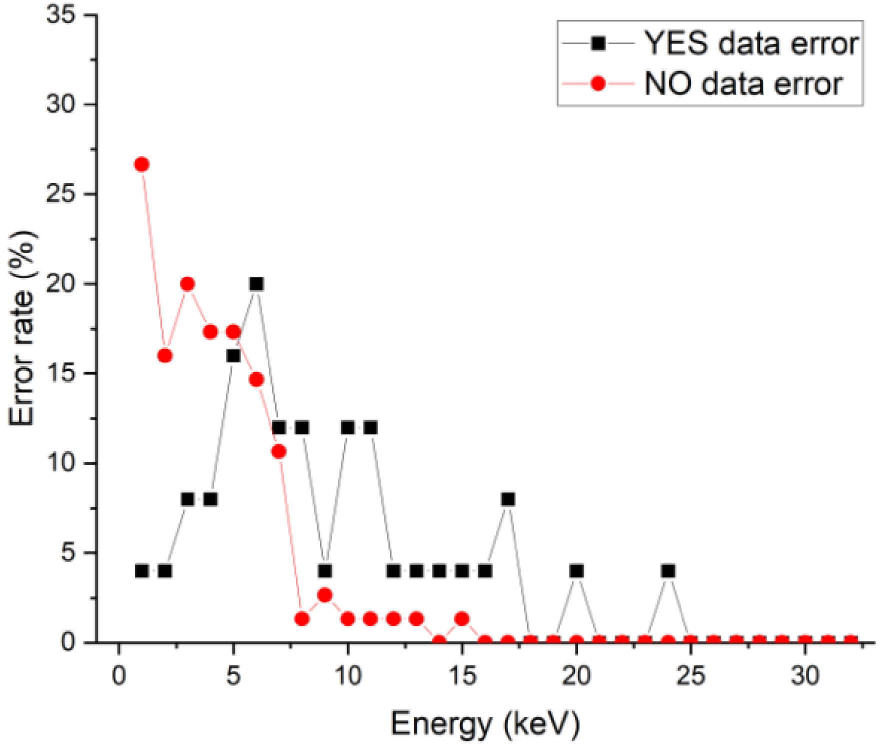
- Training with Keras library.



Classification performance test

❑ Performance results

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



Analysis of classification results

❑ Classification table

- To analyze how the classifier distinguish the defect structures and to confirm what make an error, we looked at classification case 1 ~ 4 results one by one.

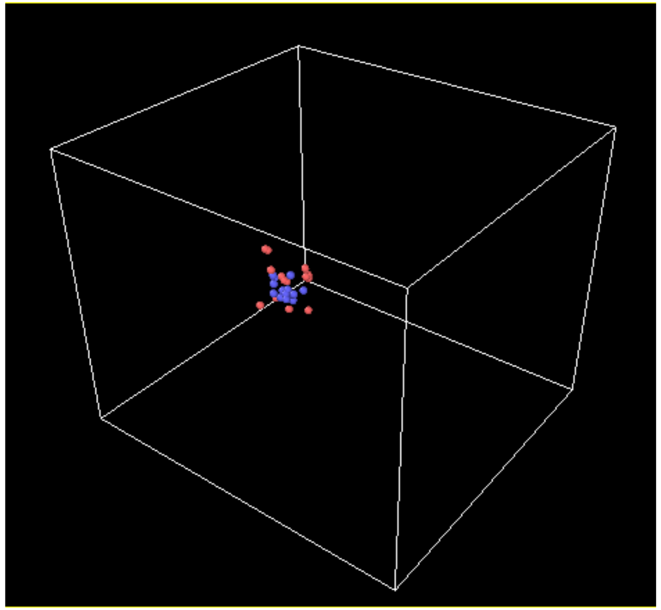
# of data		Real data	
		YES data	NO data
Prediction by classifier	*YES*	(Case 1) 956	(Case 4) 48
	NO	(Case 3) 44	(Case 2) 942

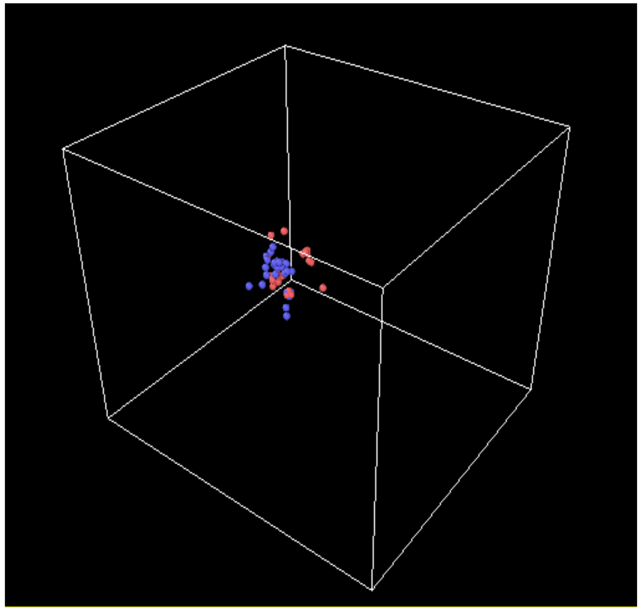
Analysis of classification results

❑ Case 1.YES data, correctly classified as *"YES"*

- Most damage structures obtained by MD simulations were correctly distinguished as YES data
- Especially the PKA energy has over 8keV, defects are mostly formed cluster.
- Below figures show examples of correctly classified YES data.

Real: YES data & Classification results: *YES*





Analysis of classification results

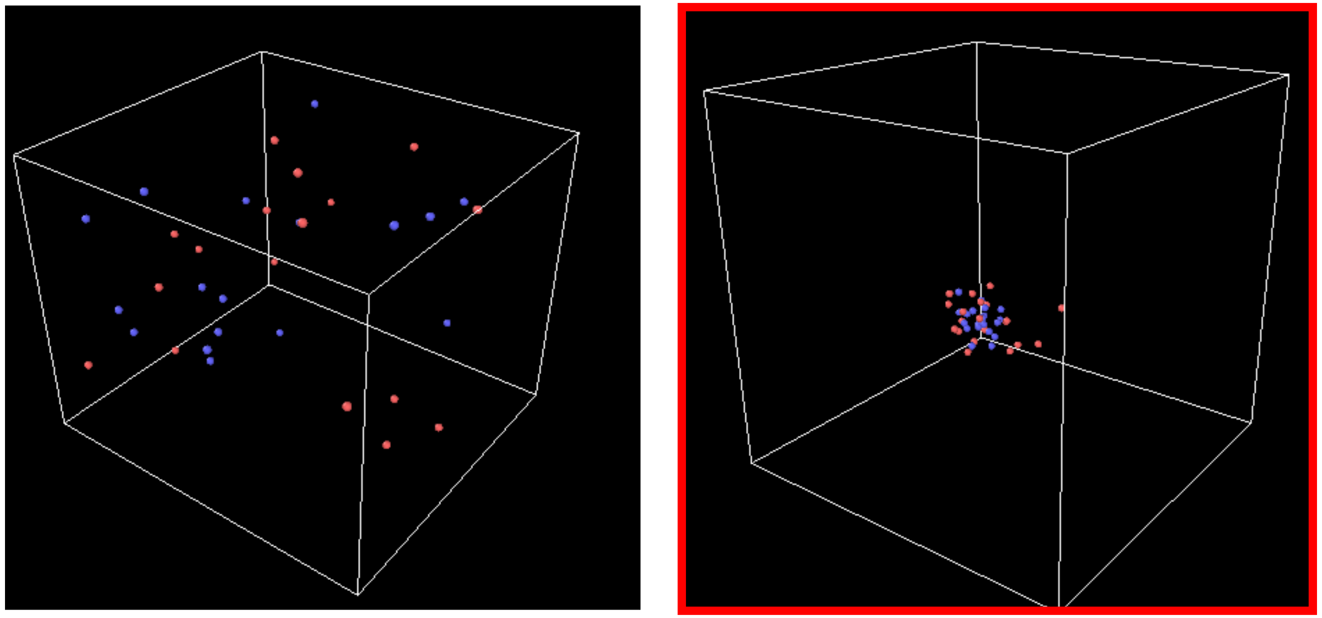
❑ Case 2.NO data, correctly classified as *"NO"*

- Below figures show correctly classified NO data

  - Obviously not radiation damage structure (left)

  - NO data accidentally became similar to the structure generated by MD (right), but our classifier correctly classified.

Real: NO data & Classification results: *NO*

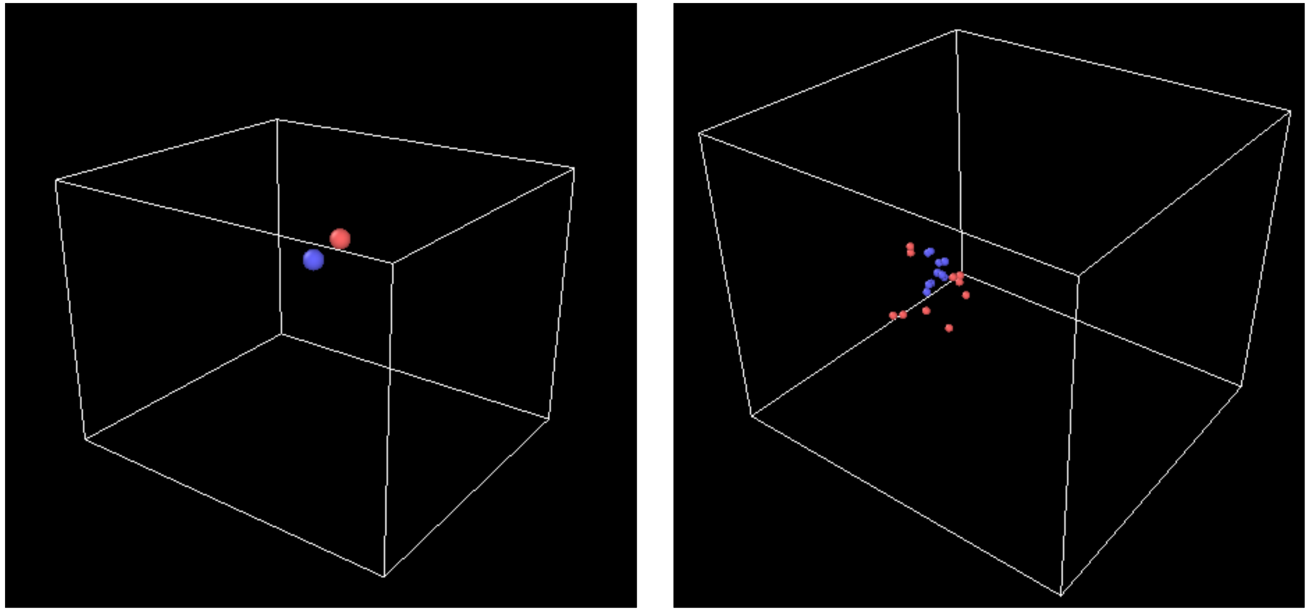


Analysis of classification results

❑ Case 3.YES data, wrongly classified as *"NO"*

- Below figures show typical error cases:
  - The radiation damage is composed of very few defects (left)
  - Defects are widely separated and not clustered (right)

Real: YES data & Classification results: *NO*

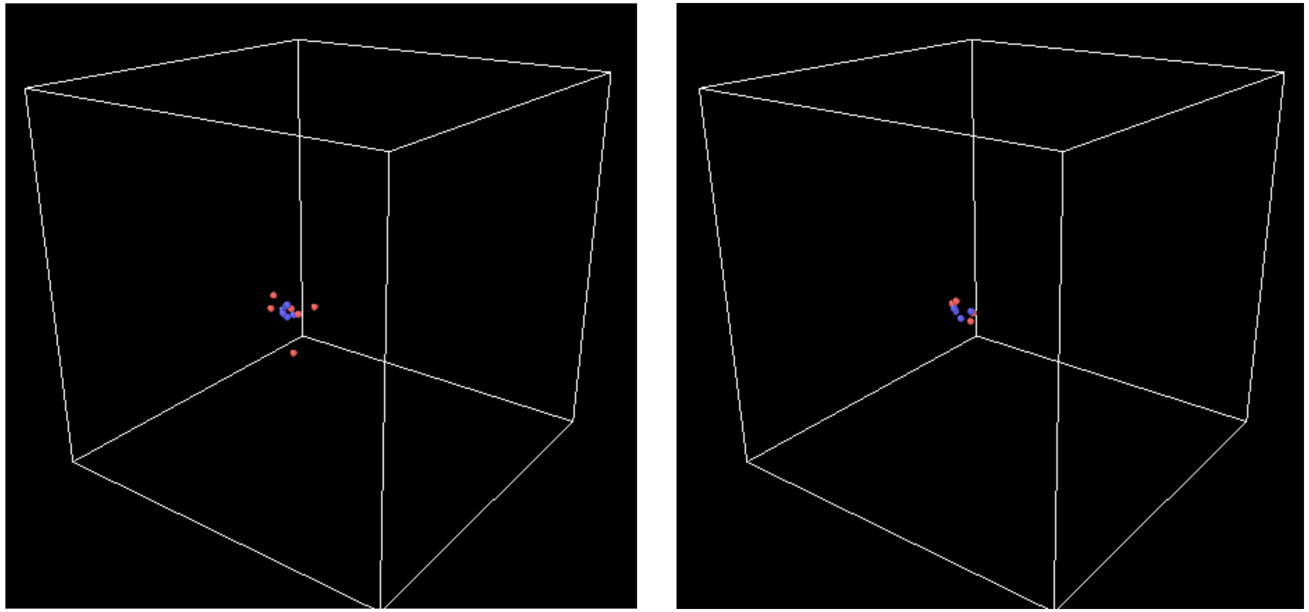


Analysis of classification results

❑ Case 4.NO data, wrongly classified as *"YES"*

- Below figures show typical error cases:
  - The random structure is composed of very few defects and accidentally closely located.

Real: NO data & Classification results: *YES*



Analysis of classification results

❑ Three types of errors

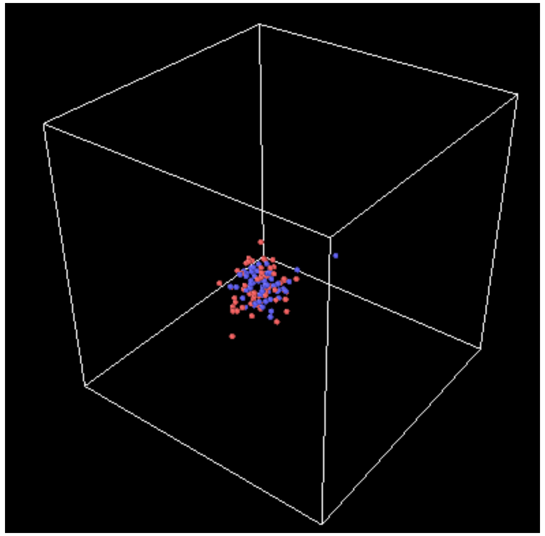
(1) (high energy) Random structures that are coincidentally similar to MD recoil simulation results.

- Intrinsic error of random structure generation and rarely affects final performance.

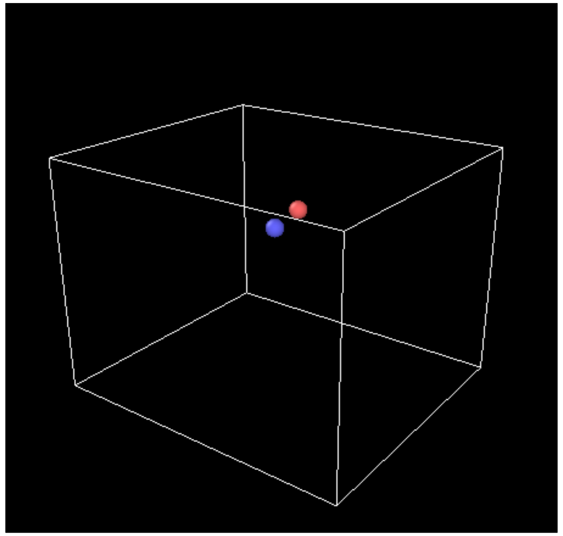
(2) (low energy) Damage structures composed of 4 or fewer defects each.

(3) (low energy) Defect number is small and the defects are not so clustered.

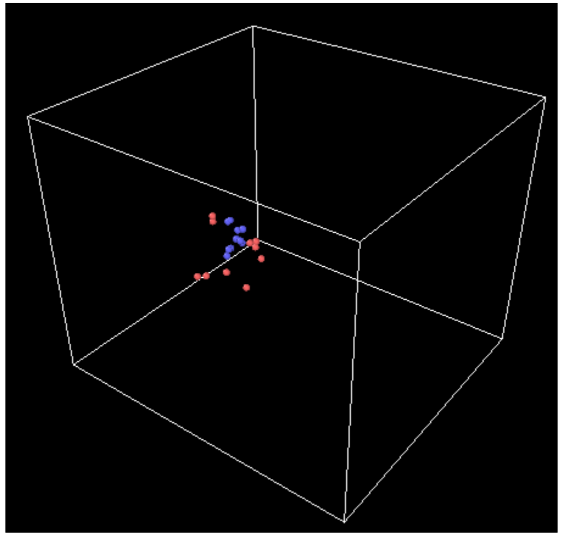
Error Type (1)



Error Type (2)



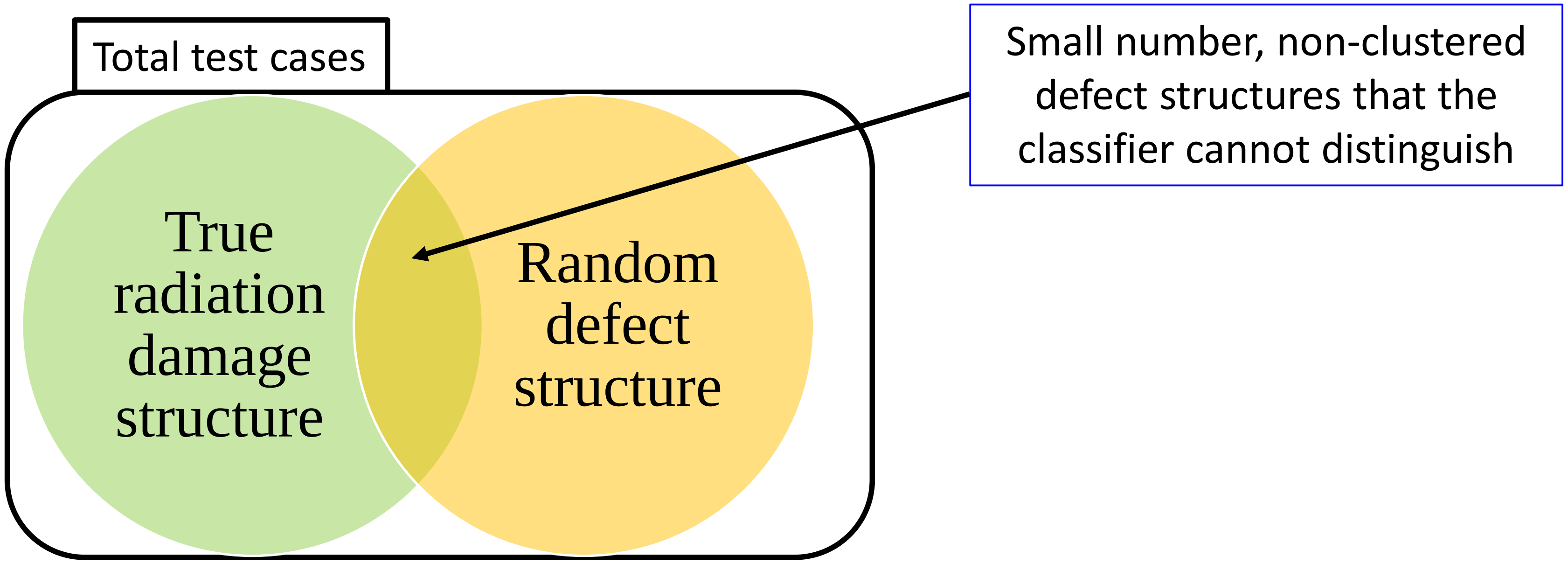
Error Type (3)



Analysis of classification results

- ❑ Errors at high energy (Over 7keV PKA)
  - ✓ No matter defects are clustered or not, our classifier can distinguish YES/NO data with 99% accuracy.

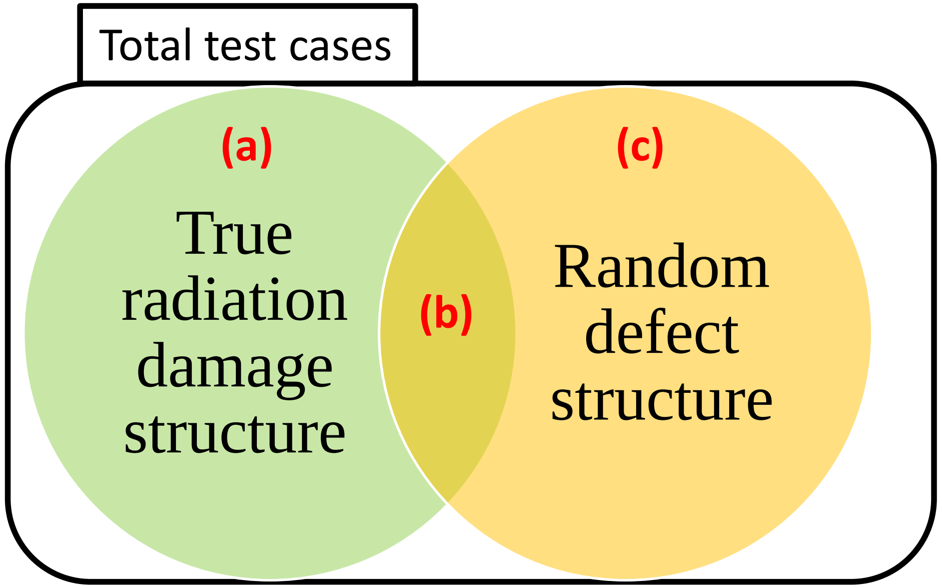
- ❑ Errors at low energy (Under 7keV PKA)
  - ✓ When defects form clusters, our classifier can recognize YES/NO data very well.
  - ✓ But for error type (2) and (3), it seems hard for the present CNN to distinguish YES/NO



Classification performance improvement

❑ Training data ratio test

- The classification results of indistinguishable defect structures are often affected by YES/NO data ratio in the training set



◆ When YES data has been trained more than NO data.

- (a): YES
- (b): more likely to predict YES
- (c): NO

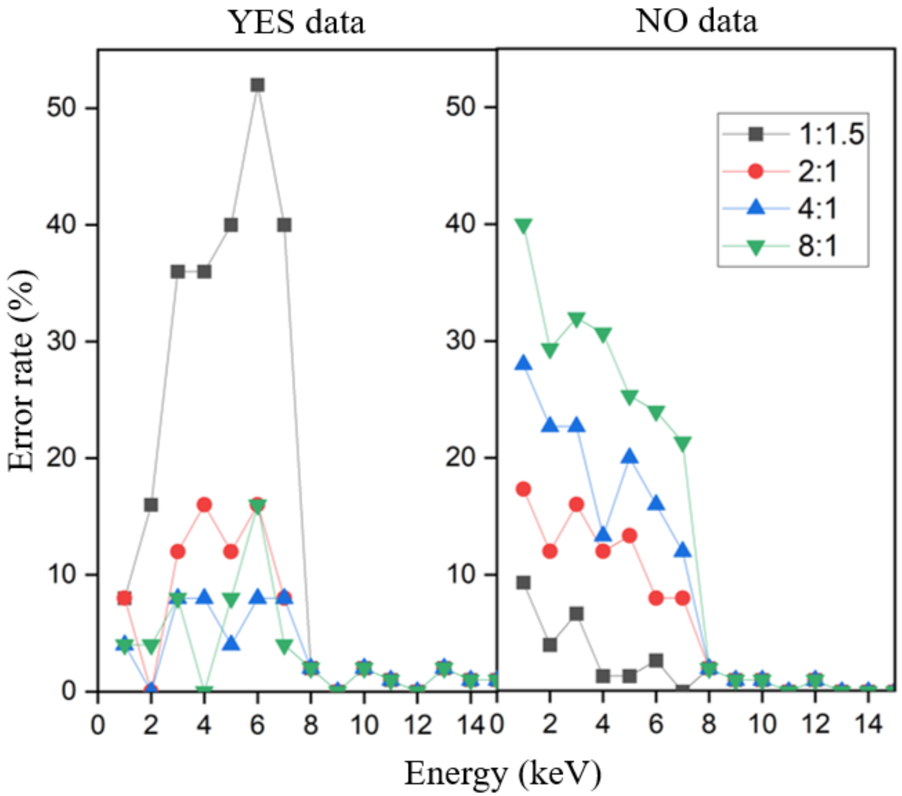
◆ When NO data has been trained more than YES data.

- (a): YES
- (b): more likely to predict NO
- (c): NO

Classification performance improvement

❑ Training data ratio changing test

- The ratio of YES and NO data size in training dataset was changed with the same CNN architecture and total data amount.
- There is a trade-off between YES&NO data classification error rate at low energy.
- We can select the data proportion based on the purpose of classifier.



Application of this method

❑ Radiation damage structure generator

- Since our classifier can distinguish radiation damage structure, we can produce radiation damage structure with a random structure generator.
- We can obtain radiation damage structure without high-cost MD calculation, the only needs are PKA energy and directions.

<Input>
PKA $E, \vec{d}$

Random generator
Random defect structures are generated

Classifier
Classify whether it is radiation damage structure or not

Valid

<Output>
radiation defect structure

repeat until valid

Conclusion

❑ Summary

- We obtained radiation damage structure in bcc-W by MD recoil simulation. And it was trained by CNN deep learning method.
- As a result, we developed the classifier that can distinguish whether an arbitrary defect structure is a radiation damage structure. And its classification performance showed 95.3% accuracy.
- There are indistinguishable defect structures at very low energy. The errors caused by these structures can be managed by training data ratio based on a purpose of the classifier.
- This classifier can be used in radiation damage research. Especially, we are building 'radiation damage structure generator' to reduce a computational cost of MD simulations.