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Sensitivity analysis and optimization of multi-scale models for microstructural evolution in metal materials under neutron irradiation

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Outline

1) Introduction

Irradiation damage in tungsten

Multi-scale modeling of irradiation effects

Uncertainty quantification & sensitivity analysis

2) Method

The OKMC model

Sensitivity analysis

Surrogate model

3) Sensitivity Analysis

Sensitivity at 733K and 0.02dpa

Factors affecting the sensitivity potentially

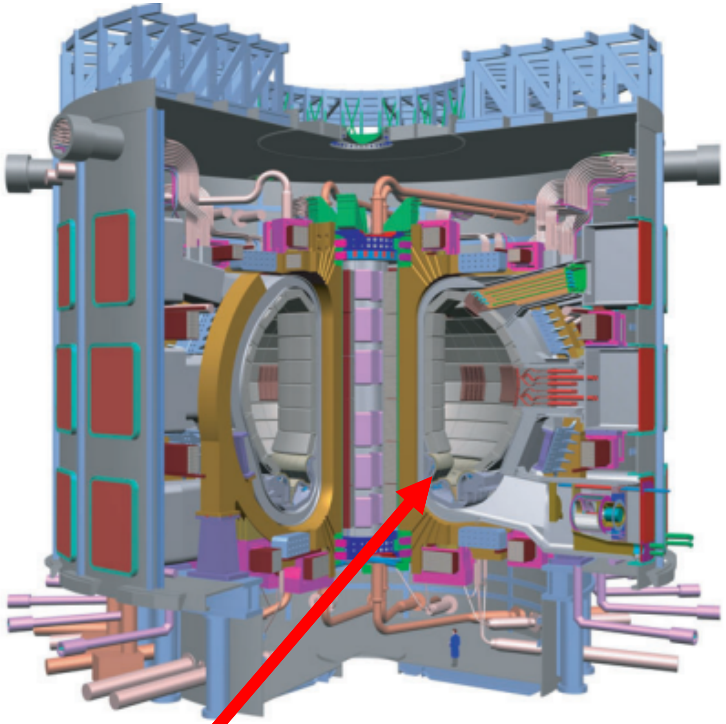
4) Surrogate Models

Polynomial Chaos Expansion

Artificial Neural Network

5) Conclusion & Fututure Work

Irradiation damage in tungsten



Plasma-Facing Components

Tungsten

- High flux of H and He ions
- Intense neutron irradiation

Research on Irradiation Damage in Tungsten

Experiments

Simulations

Efficient

Fusion neutron irradiation

Microscopic mechanisms

Lack of devices to generate fusion neutron of 14.1 MeV

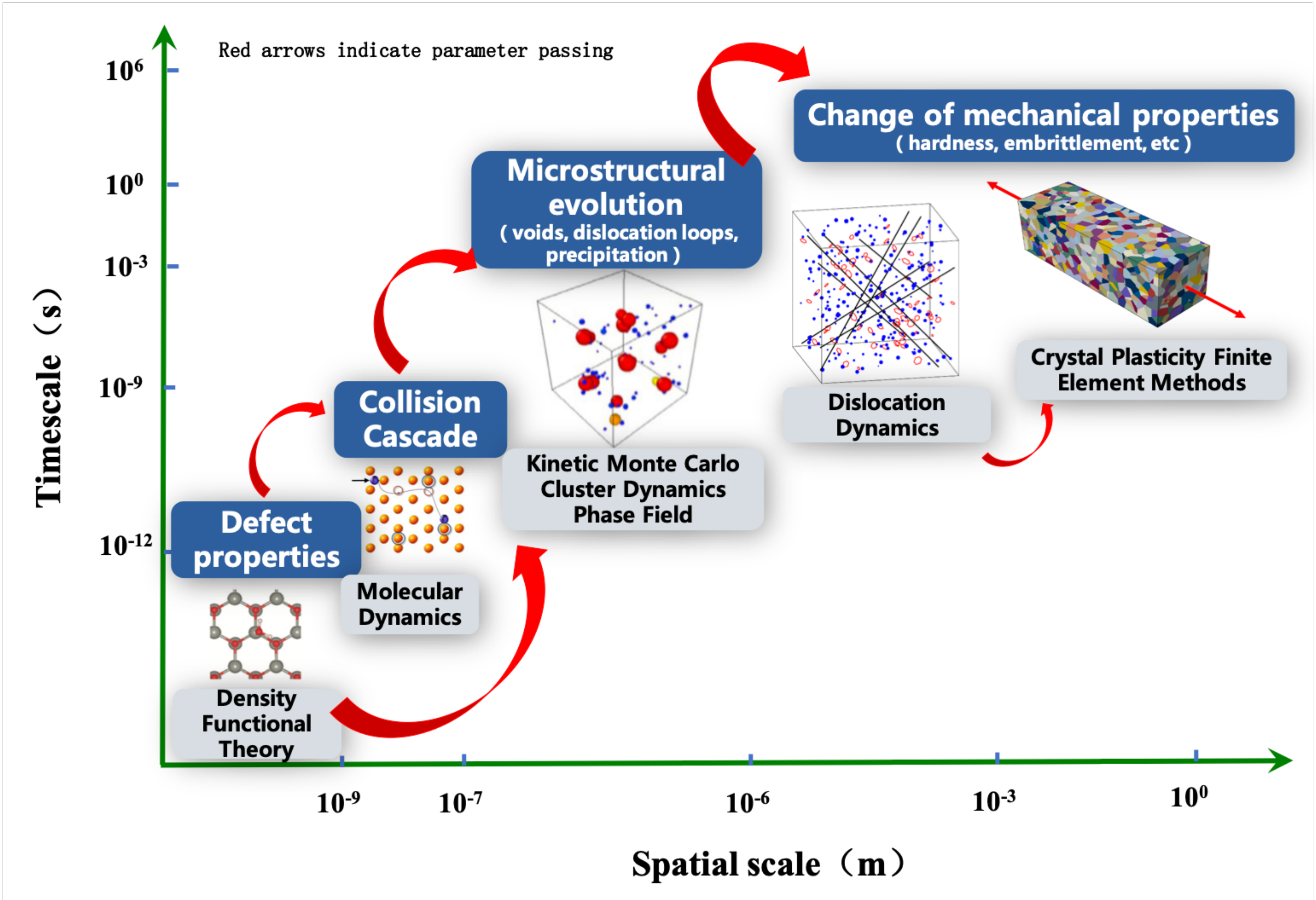
Emulated with

Extrapolated to the prediction

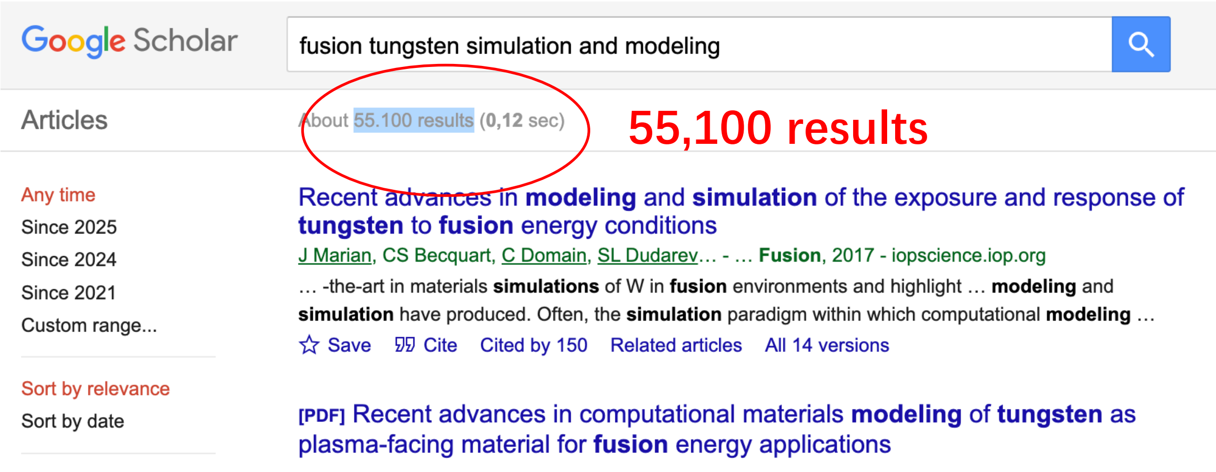
Fission neutron & Ion irradiation

Aymar, R., Barabaschi, P., & Shimomura, Y. (2002). The ITER design. Plasma physics and controlled fusion, 44(5), 519.

Multi-scale modeling of irradiation effects



Multi-scale modeling of irradiation effects



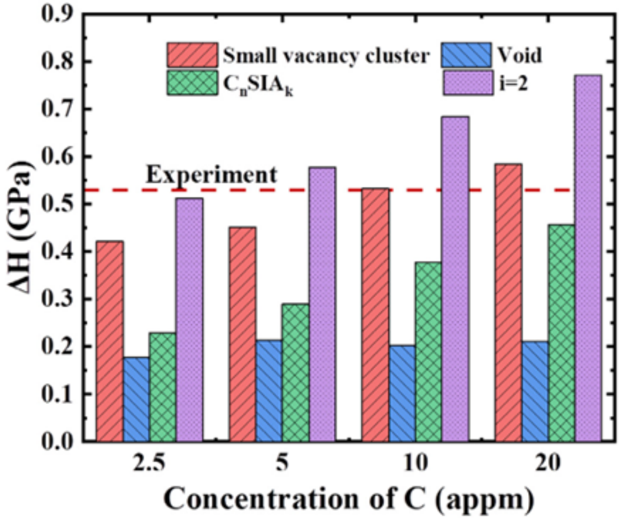
- Thousands of related research work (Google Scholar: 55100 results).
- Most of them use DFT or MD methods, forming a solid foundation for mesoscale methods such as Object kinetic Monte Carlo (OKMC) and Cluster Dynamics (CD).

OKMC

Simulate defect diffusion and microstructure evolution processes

Defect size, concentration | Microstructural morphology

Can be easily compared with experimental findings



Niu, Y. Z., et al. JNM (2023)

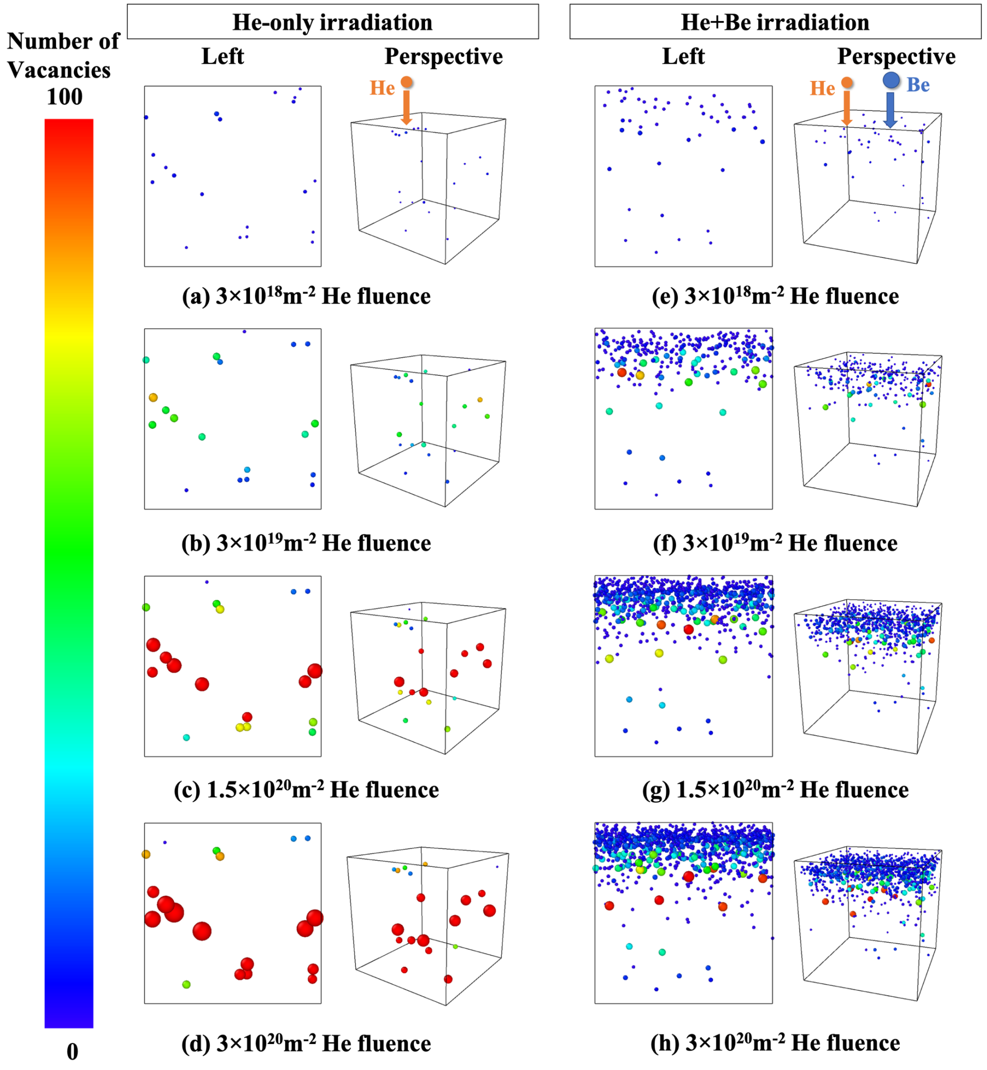
Information of microstructures can be fed to further predict the change of mechanical properties..

OKMC bridges the simulation of microscopic mechanisms with the macroscopic observations.

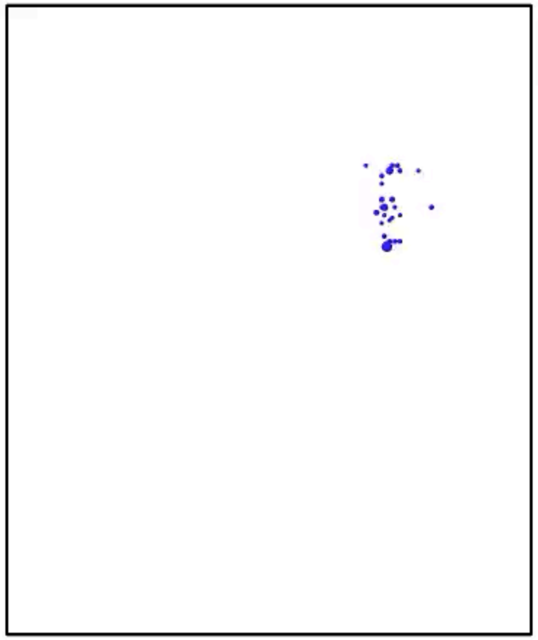
Niu, Y. Z., Li, Y. H., Ren, Q. Y., Li, Z. Z., Terentyev, D., Ma, H. Z., ... & Lu, G. H. (2023). Influence of carbon on the evolution of irradiation defects in tungsten. Journal of Nuclear Materials, 579, 154393.
Li, Y., & Ghoniem, N. (2020). Cluster dynamics modeling of irradiation growth in single crystal Zr. Journal of Nuclear Materials, 540, 152312.

The application of OKMC methods: examples

Suppression of He-induced damage by Beryllium

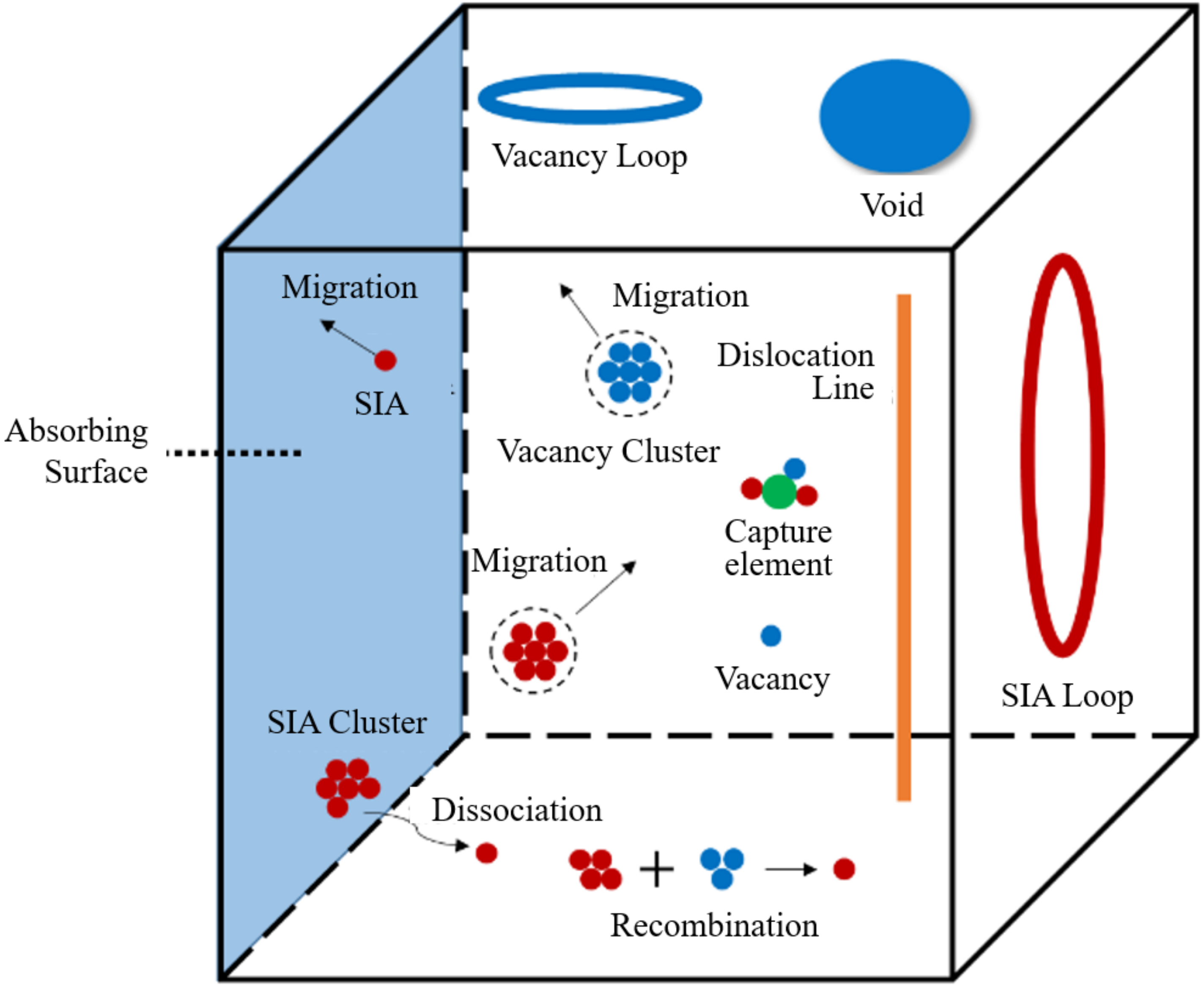


Void lattice formation



[1] Zhou et al., Nuclear Fusion. 64 (2024) 106021.
[2] Li et al., Acta Materialia. 219 (2021) 117239.

The OKMC model



Self-Interstitial Atom

- SIA
- Vacancy

Thermal-activated

Based on probability

Migration	Defects **move** to neighboring locations.
Rotation	Defects change the current migration **direction**.
Dissociation	Individual defects **emit** from clusters.

Non-thermal-activated

Based on capture radius

Aggregation	Defects or clusters **combine** to form larger clusters.
Recombination	Dissimilar defects or clusters combine and **heal**.
Capture	Defects are **absorbed** by capture elements.
Annihilation	Defects are **removed** when moving to absorbing surfaces.

Niu, Y. Z., Li, Y. H., Ren, Q. Y., Li, Z. Z., Terentyev, D., Ma, H. Z., ... & Lu, G. H. (2023). Influence of carbon on the evolution of irradiation defects in tungsten. Journal of Nuclear Materials, 579, 154393.

Uncertainty quantification & sensitivity analysis

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Uncertainty

E_a, ν_0

Migration energies

Binding energies

Rotation energies

e.g. **Monovacancy migration energy：** **1.68eV, 1.50eV, 1.97eV …**

Divacancy binding energy ： **-0.41eV, - 0.06eV, +0.42eV, +0.7 eV …**

Probability of dissociation： **1.44e-5, 2.17e-10 …**

Stochastic events

based on probabilities

Different outputs in several simulations **with same probabilities.**

Uncertainty Quantification —optimization→ **Parameter**

Uncertainty Quantification → **Mechanism**

- Parameter estimation
- Uncertainty propagation
- Surrogate models
- Sensitivity Analysis

Reduce calculational costs of parameter calibration

Sensitivity Analysis

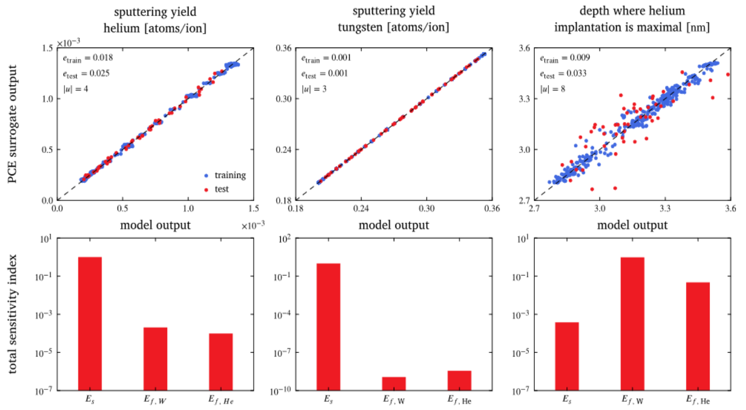
- Identify sensitive parameters
- Perform calibration

- The stochastic mechanism is crucial to the OKMC model.

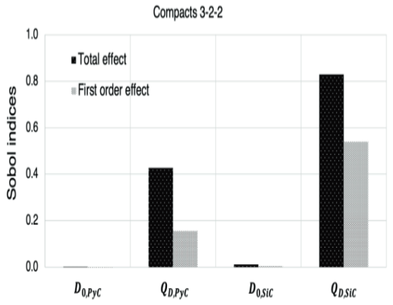
Uncertainty quantification & sensitivity analysis

PCE surrogate model + Sobol' indices

(PCE: Polynomial Chaos Expansion)



Pieterjan Robbe, et al. (2023)



Seok Bin Seo, et al. (2023)

There have been attempts in nuclear materials field to employ the approach.

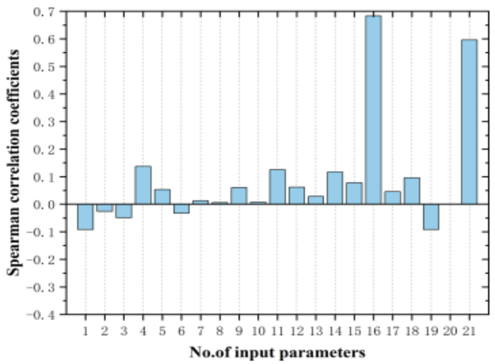
Characteristics

A large number of training samples

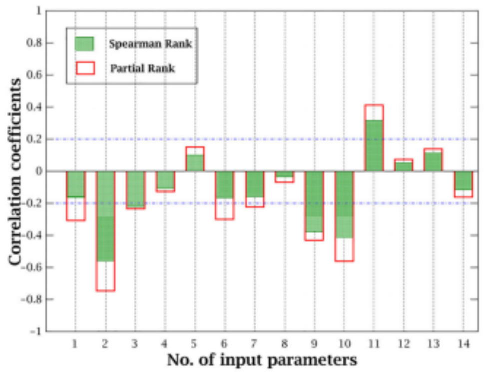
The increase of uncertainty

LHS + Spearman correlation coefficient

(LHS: Latin Hypercube Sampling)



C. Peng, et al. (2023)



Ye Yang, et al. (2021)

The method was applied in many studies on severe accidents and thermal-hydraulics in fission reactors.

Characteristics

More universal / Broad applicability

Relatively low computational cost

Robbe, P., Blondel, S., Casey, T. A., Lasa, A., Sargsyan, K., Wirth, B. D., & Najm, H. N. (2023). Global sensitivity analysis of a coupled multiphysics model to predict surface evolution in fusion plasma–surface interactions. Computational Materials Science, 226, 112229.

Seo, S. B., & Wirth, B. D. (2023). Sensitivity analysis of cesium and strontium release from TRISO particle under irradiation and high temperature conditions. Nuclear Engineering and Design, 408, 112333.

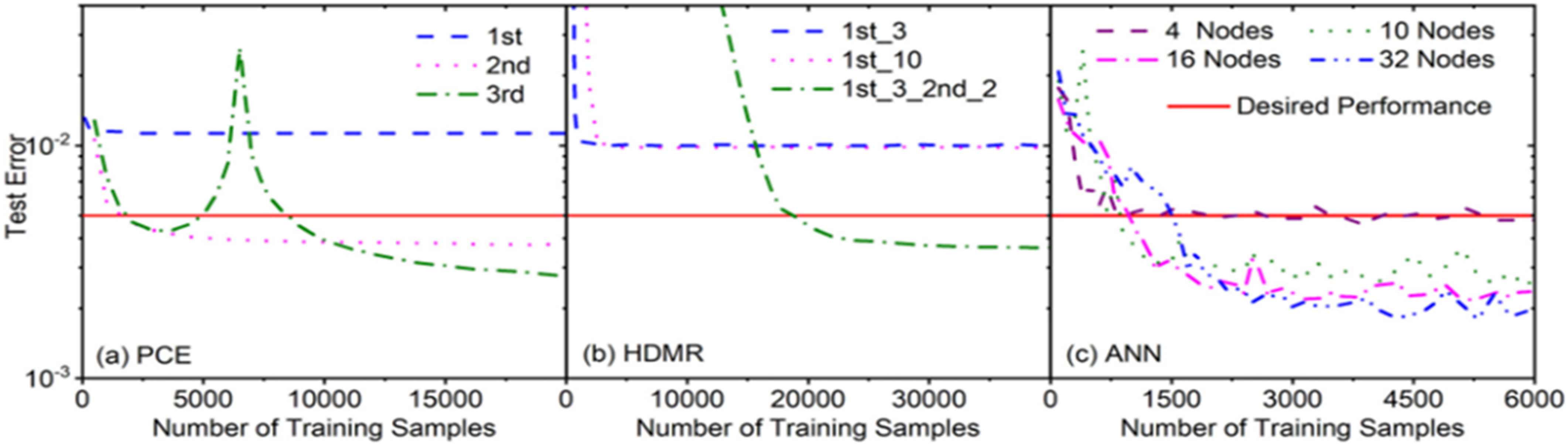
Peng, C., et al. (2023, May). Best Estimate Plus Uncertainty Analysis of a Pressurizer Surge Line Break LOCA on China's Advanced PWR. In Proceedings of the 23rd Pacific Basin Nuclear Conference, Volume 2: PBNC 2022, 1-4 November, Beijing & Chengdu, China (pp. 490-505). Singapore: Springer Nature Singapore.

Yang, Y., Deng, C., & Yang, J. (2021). Best estimate plus uncertainty analysis of a small-break LOCA on an advanced Generation-III pressurized water reactor. International Journal of Energy Research, 45(8), 11916-11929.

Uncertainty quantification: surrogate models

In an inverse UQ study of combustion kinetic models, the test errors of three typical surrogate models are compared.

Polynomial Chaos Expansion | **High Dimentional Model Representatiaon** | **Artificial Neural Network**



J. Wang, et al. (2020)

PCE & ANN	**High convergence speed** / **High accuracy**
HDMR	**Convergence speed and accuracy are mutually exclusive.**

Wang, J., Zhou, Z., Lin, K., Law, C. K., & Yang, B. (2020). Facilitating Bayesian analysis of combustion kinetic models with artificial neural network. Combustion and Flame, 213, 87-97.

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The OKMC model

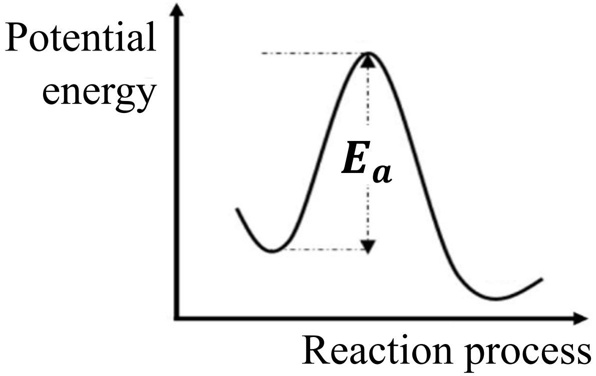
How to calculate the probabilities/rates ?

Arrhenius formula

$$R = \nu_0 \times \exp\left(-\frac{E_a}{k_B T}\right)$$

- R : rates of events
- ν_0: attempt frequency
- **E_a: activation energy**
- k_B: Boltzmann constant
- T: temperature

Transition-state theory



E_a ↑ , R ↓

T ↑ , R ↑

What outputs need attention ?

Defects mainly affecting the **mechanical properties** of tungsten → **Vacancy Clusters** / **SIA Clusters**

Characteristics →
- **Average Size**
- **Number Density**

Sensitivity analysis: flow chart

Identification & Characterization of Uncertainties

Migration energies
Binding energies
Rotation energies
Capture radiuses
etc.

Probability estimation → **Filter the parameters to be analyzed**

Generation of Samples

Latin Hypercube Sampling (LHS)

A method creating **more representative samples**

Simulation of OKMC

Facility of the experiments

High Flux Isotope Reactor (**HFIR**) at Oak Ridge National Laboratory (**ORNL**)

The thermal and cold neutrons produced by HFIR are used to study physics, chemistry, materials science, engineering, and biology.

The outputs of OKMC

- Average size of Vac clusters
- Number density of Vac clusters
- Average size of SIA clusters
- Number density of SIA clusters

Sensitivity Analysis

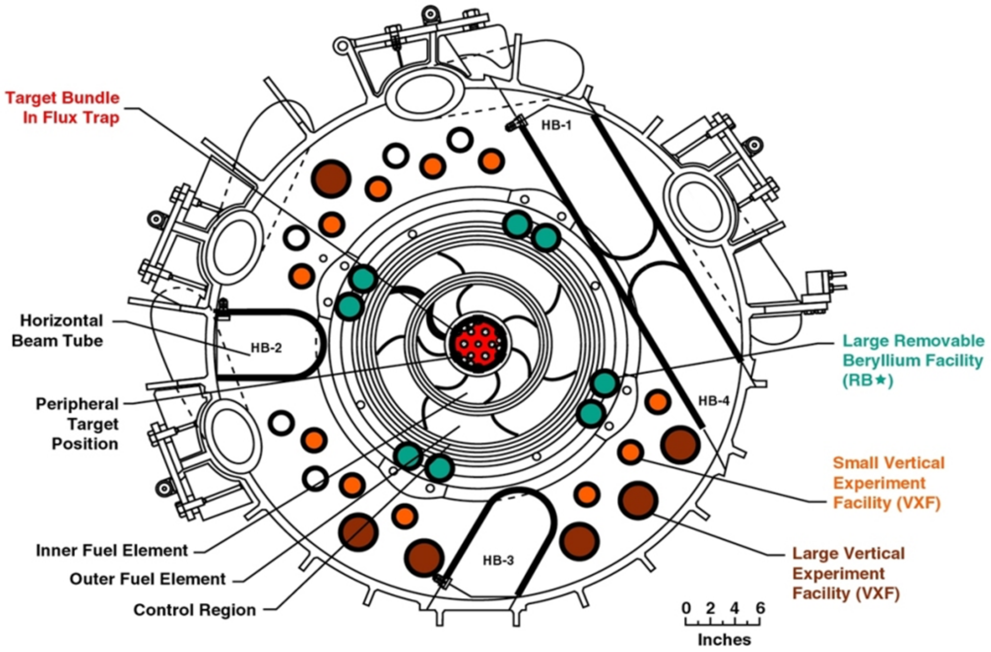
Spearman correlation coefficient

Potential factors

- Range of values
- Irradiation dose
- Multiparameter
- Temperature

Hu, X., & et al. (2016). Defect evolution in single crystalline tungsten following low temperature and low dose neutron irradiation. Journal of Nuclear Materials, 470, 278-289.

Experiments



High Flux Isotope Reactor (**HFIR**)

Irradiation test samples

733K, 0.02dpa

Fission reactor	Material Type	Irradiation temperature [°C]	Dose [dpa]
HFIR (mixed neutron spectrum) [21–23,37]	Single crystal	~90	0.02
		~90	0.39
		460	0.02
		797	0.092
		700	0.44
		770	1.80
		1100	0.47
	Polycrystalline	800	1.50
		700	2.80
JMTR (mixed neutron spectrum) [13,17]	Polycrystalline	600	0.15
		800	0.15
Joyo (Fast reactor) [8,11]	Polycrystalline	400	0.17
		531	0.44
		538	0.96
		583	0.47
		740	0.40
		750	1.54
		756	0.42
HFR (mixed neutron spectrum) [38]	Single crystal	900	1.67
	Polycrystalline		
BR2 (mixed neutron spectrum) [24,39,40]	Polycrystalline	800	1.25
	Single crystal	600	0.2
		800	
		1200	
	ITER grade	600	0.2
		800	
		1200	
		1200	0.18
	Cold rolled pure polycrystalline	600	0.2
		800	
		1200	

https://neutrons.ornl.gov/hfir

Hu, X. (2022). Recent progress in experimental investigation of neutron irradiation response of tungsten. Journal of Nuclear Materials, 568, 153856.

Sensitivity analysis: flow chart

ICARE
华中科技大学 Huazhong University of Science and Technology

Identification & Characterization of Uncertainties

Migration energies

Binding energies

Rotation energies

Capture radiuses

Probability estimation →

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- Range of values
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- Multiparameter
- Temperature

Hu, X., & et al. (2016). Defect evolution in single crystalline tungsten following low temperature and low dose neutron irradiation. Journal of Nuclear Materials, 470, 278-289.

Sensitivity analysis: sampling settings

Parameters to be analyzed

Physical Meaning	Symbol	Reference value	Range
Capture radius of vacancy	R_V	1	*(0.8~1.2)
Capture radius of SIA	R_W	1	*(0.8~1.2)
Migration energy of monovacancy	$E_{m,1V}$	1.68 eV	+(-0.1~0.1) eV
Migration energy of divacancy	$E_{m,2V}$	1.44 eV	+(-0.1~0.1) eV
Migration energy of tri-vacancy	$E_{m,3V}$	0.83 eV	+(-0.1~0.1) eV
Binding energy of divacancy	$E_{b,2V}$	-0.12 eV	+(-0.1~0.1) eV
Binding energy of tri-vacancy	$E_{b,3V}$	-0.0636 eV	+(-0.1~0.1) eV
Migration energy of SIA	$E_{m,W}$	0.023 eV	+(-0.01~0.01) eV
Rotation energy of SIA	$E_{r,W}$	0.38 eV	+(-0.1~0.1) eV

Settings

- **Number of samples**: 60;
- **Number of recalculations for one sample**: 15.

Surrogate model: PCE

Expansion

$$y = F(X) = \sum_{\alpha \in I^d} c_\alpha \Psi_\alpha(X)$$

- y: model outputs, QoI
- $F(X)$: Functional relationship
- I^d: d-dimentional parameter space
- c_α: PCE coefficient
- $\Psi_\alpha(X)$: orthogonal multivariate basis function

Truncation

$$P = \binom{d+p}{p} = \frac{(d+p)!}{d!\,p!}$$

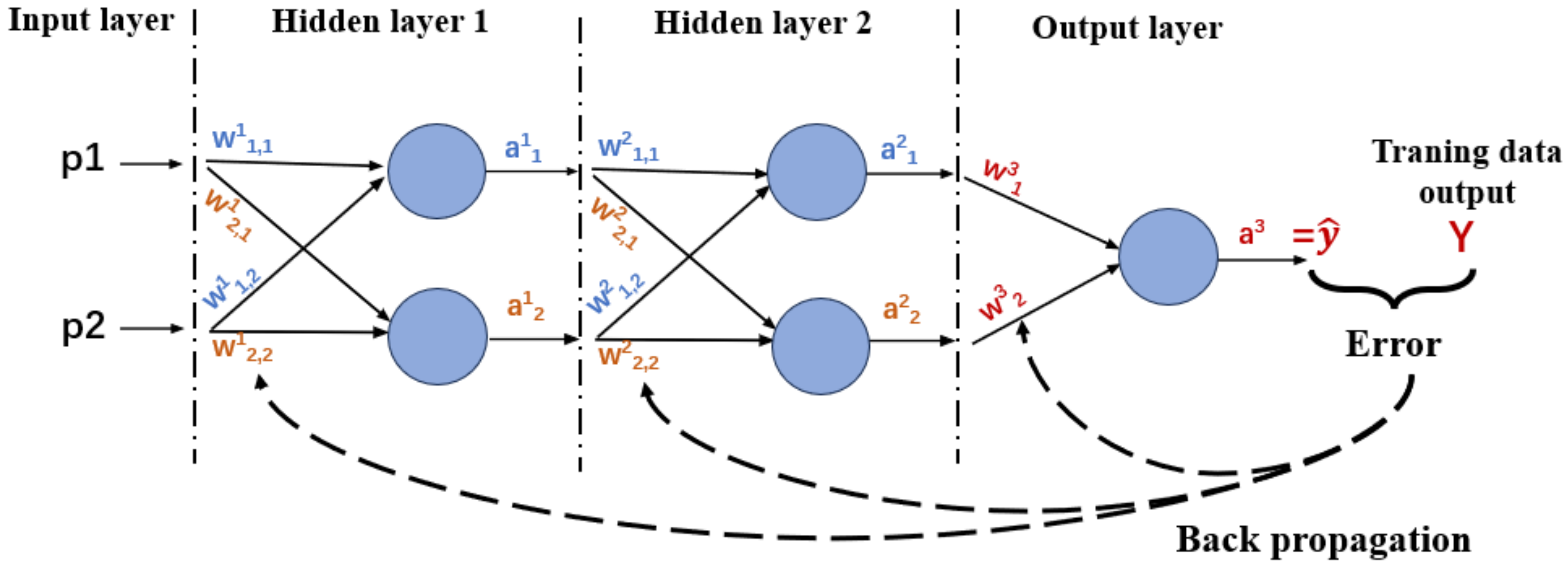
- P: number of polynomial terms
- p: highest order of polynomials

Calculation of PCE coefficients

Intrusive methods	Galerkin projection	• Requiring modifications of the numerical code ✗→ **OKMC**
Non-intrusive methods	Spectral projection	• Gaussian quadrature rules, Smolyak sparse grid
	Regression	• Least squares methods, compressed sensing methods

Surrogate model: ANN

Multilayer Perception trained with Backpropagation Algorithm



- (1) Randomly assign the weights and compute the network solution;
- (2) Compute the error between the outputs of network and training data, and back propagate the weights to each layer;
- (3) Re-assign the weights to avoid the same error, and so on do iterations;
- (4) Obtain the optimal weight matrix as the best approximation.

Settings

- **Activation function**: the hyperbolic tangent, a = tanh(n)
- **Training method**: Levenberg-Marquardt algorithm, a second-order Quasi-Newton optimization method

D. Atabay. Pyrenn: a recurrent neural network toolbox for python and matlab. Available at: http://pyrenn.readthedocs.io/en/latest/, 2018

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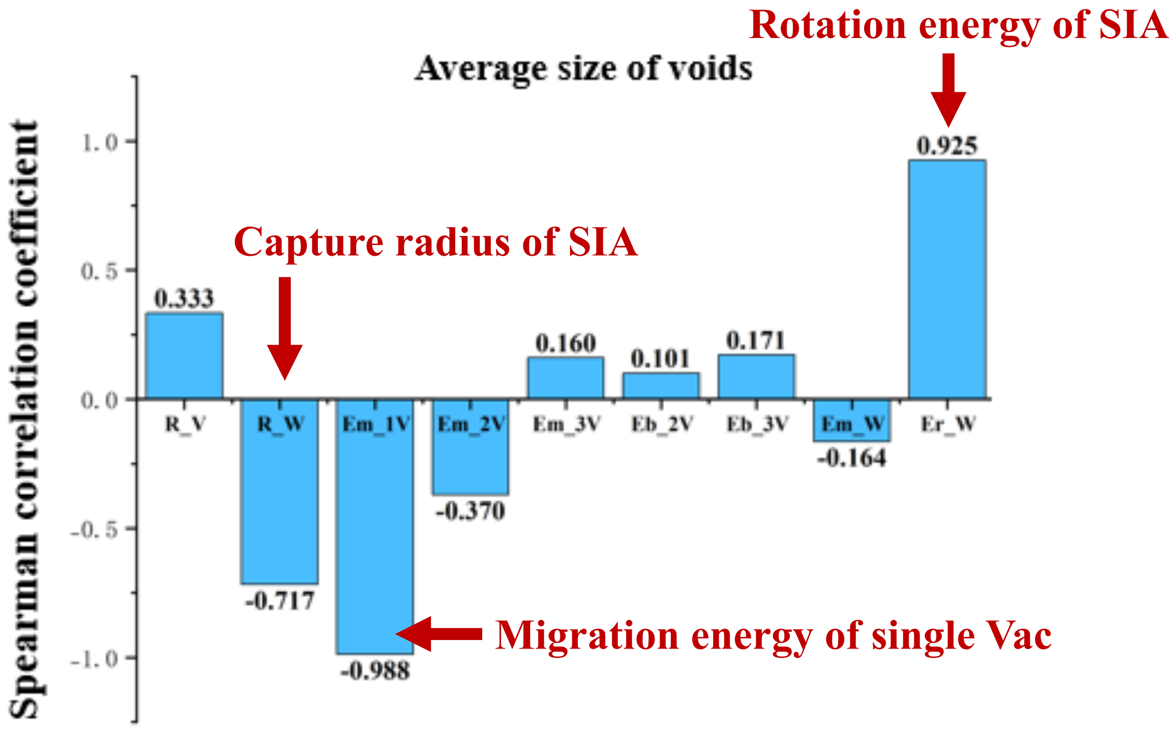
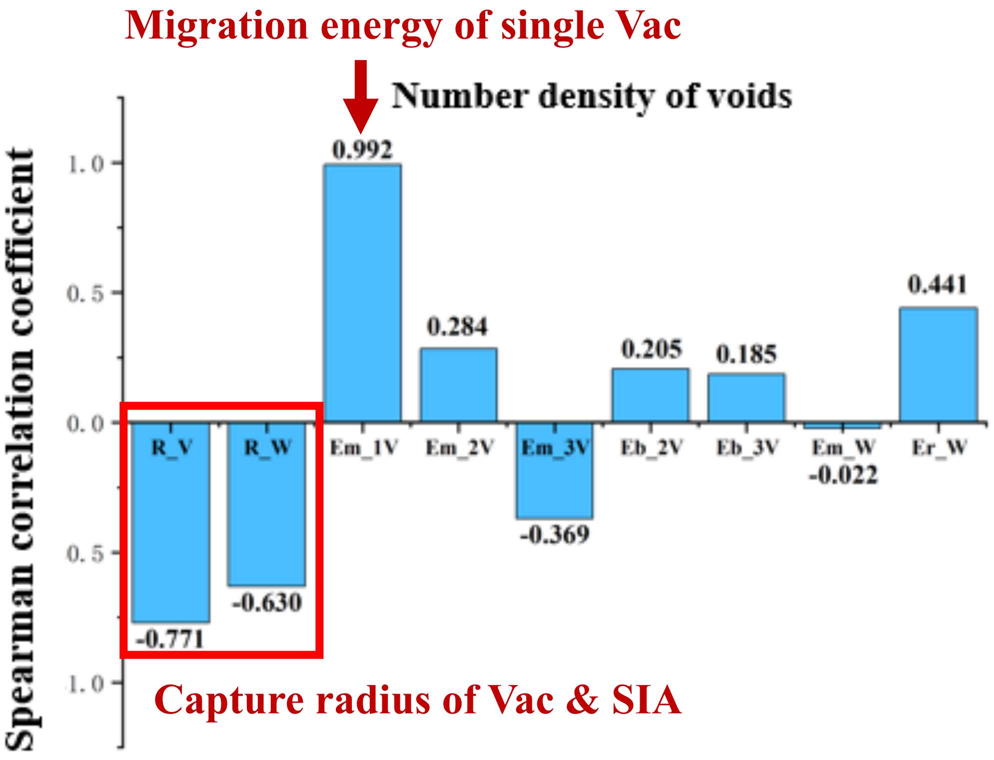
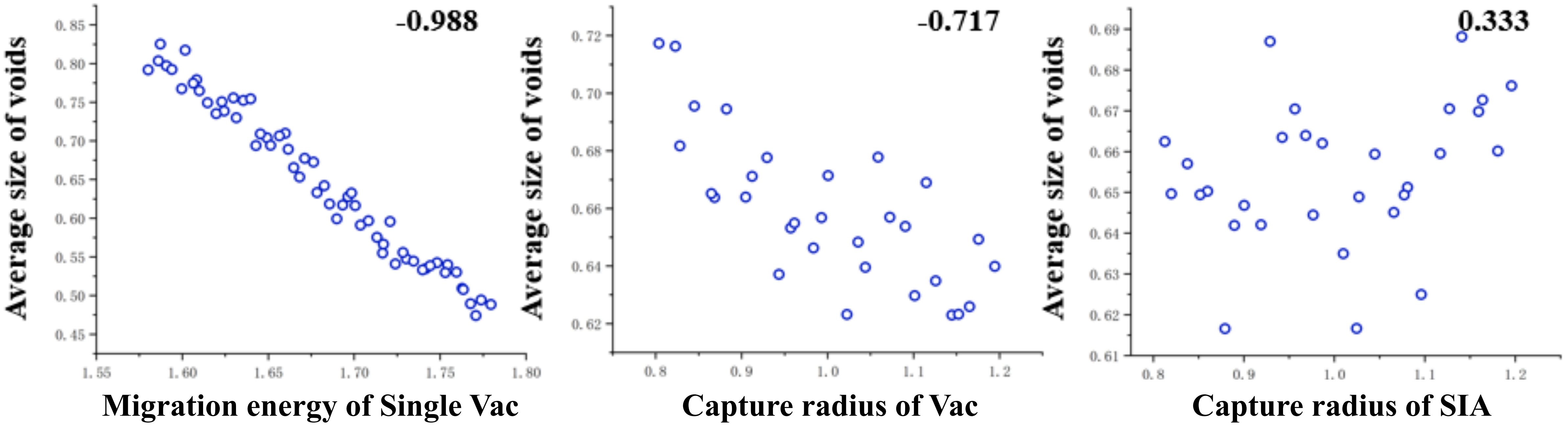




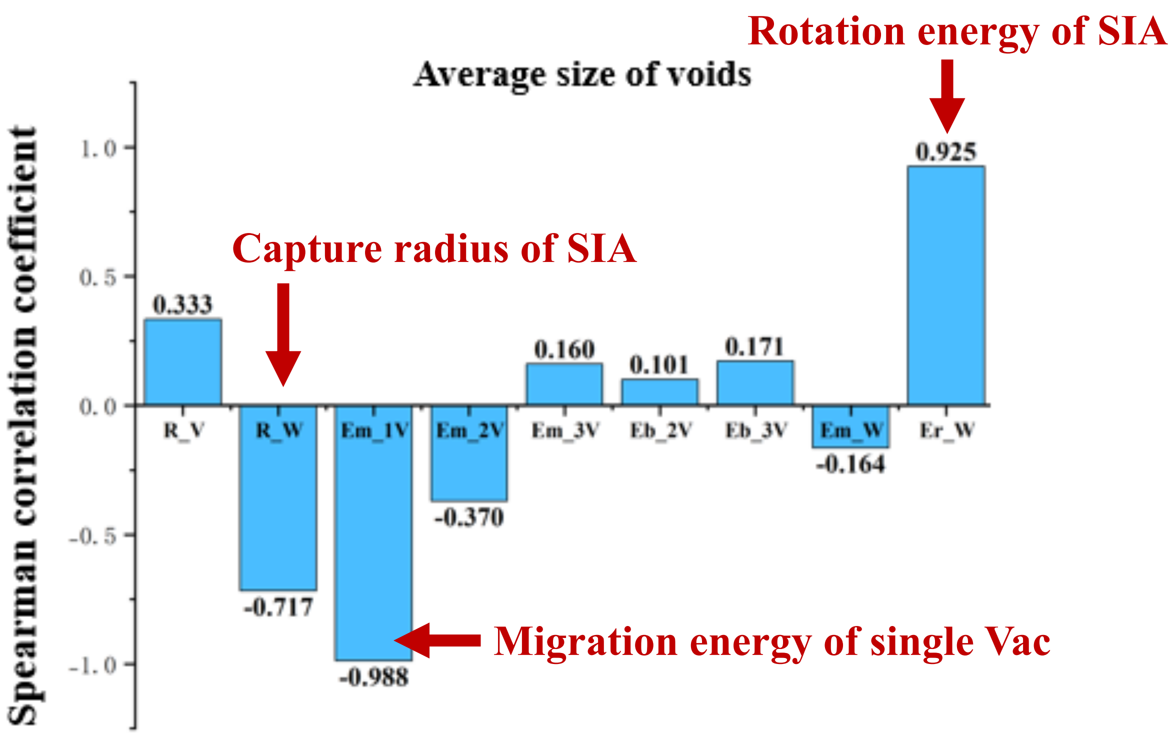
Sensitivity at 733K and 0.02dpa

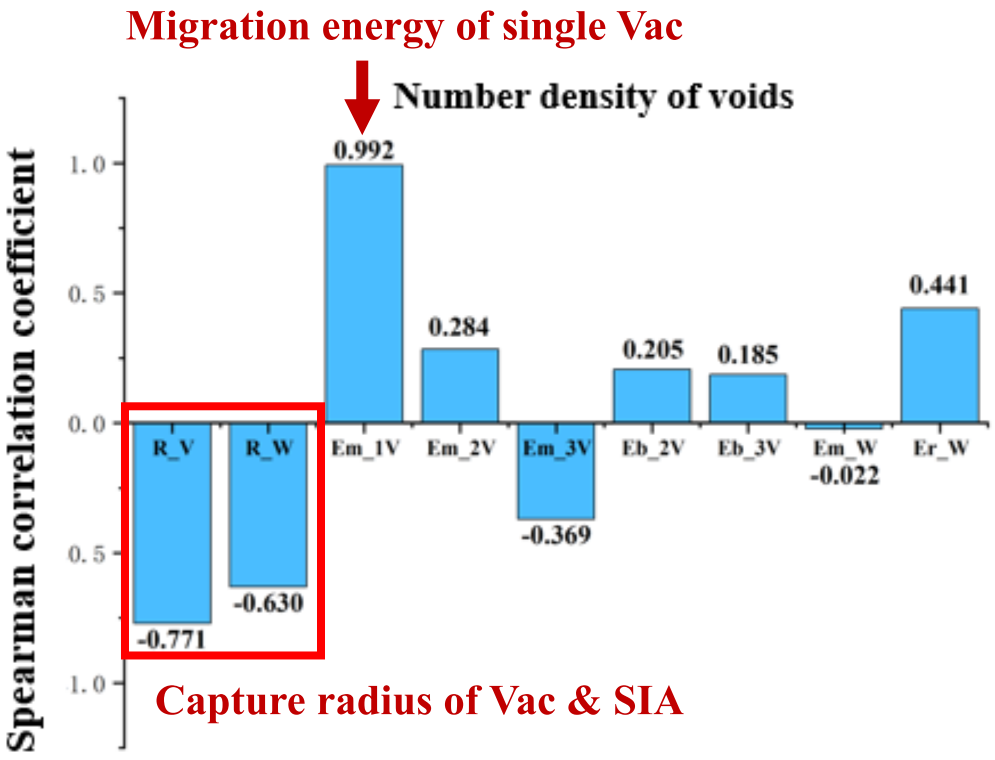


A distinct monotonic trend

Dispersed points

Sensitivity at 733K and 0.02dpa

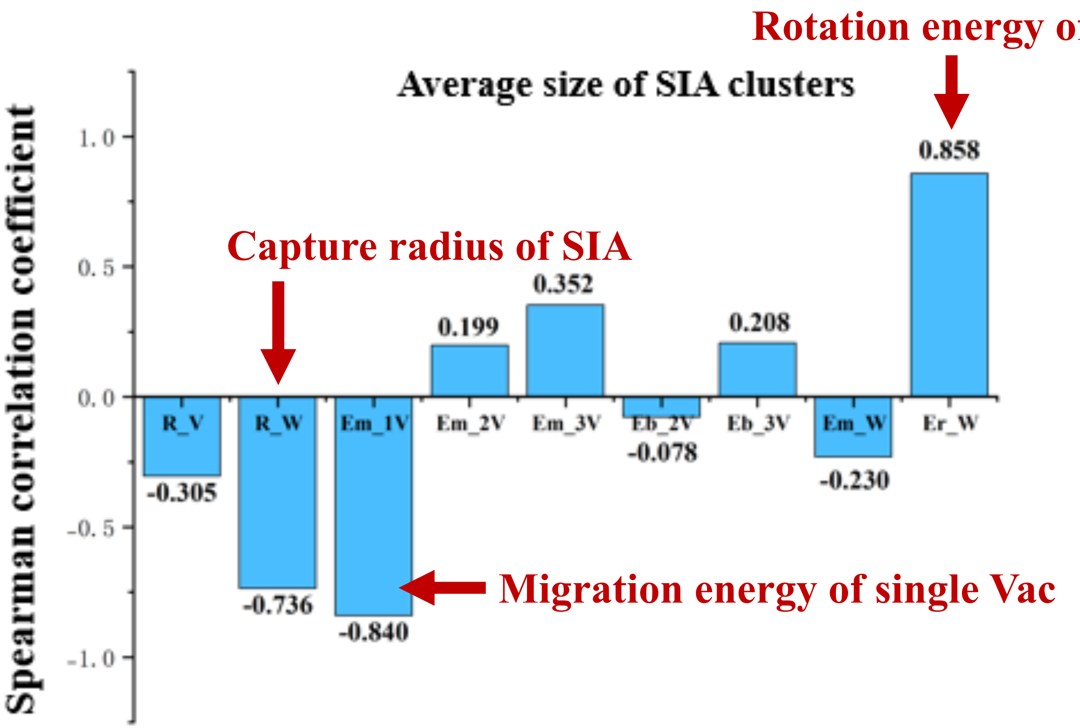


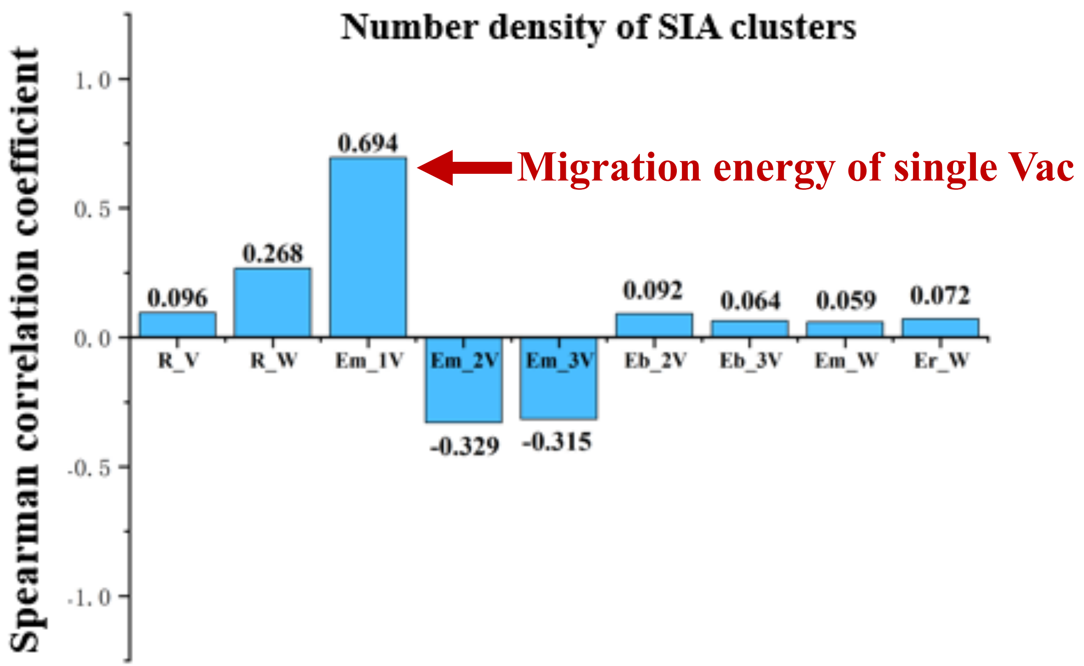


$$R = \nu_0 \times \exp\left(-\frac{E_a}{k_B T}\right)$$

- Single Vac migration ↓ → Large Vac clusters ↓ ; Small Vac clusters ↑
- SIA rotation ↓ → One-dimensional movements ↑ → Recombination ↓
- Capture radius ↑ → Aggregation & recombination ↑

Sensitivity at 733K and 0.02dpa





Four sensitive parameters

Migration energy of single Vac	Rotation energy of SIA
Capture radius of Vac	Capture radius of SIA

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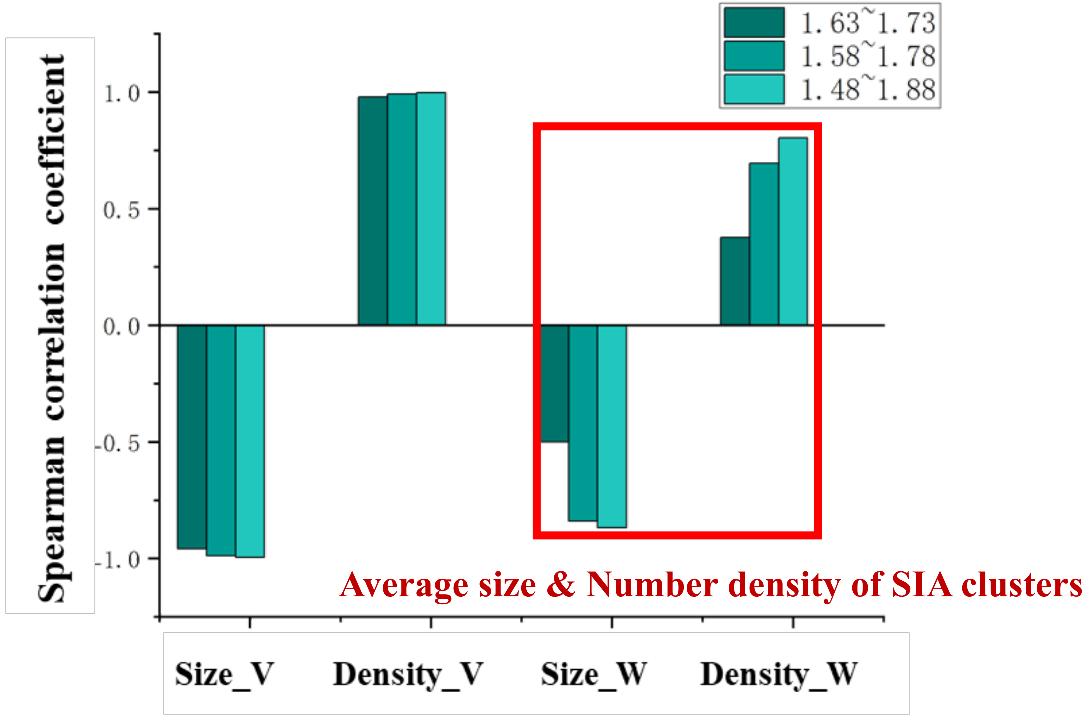
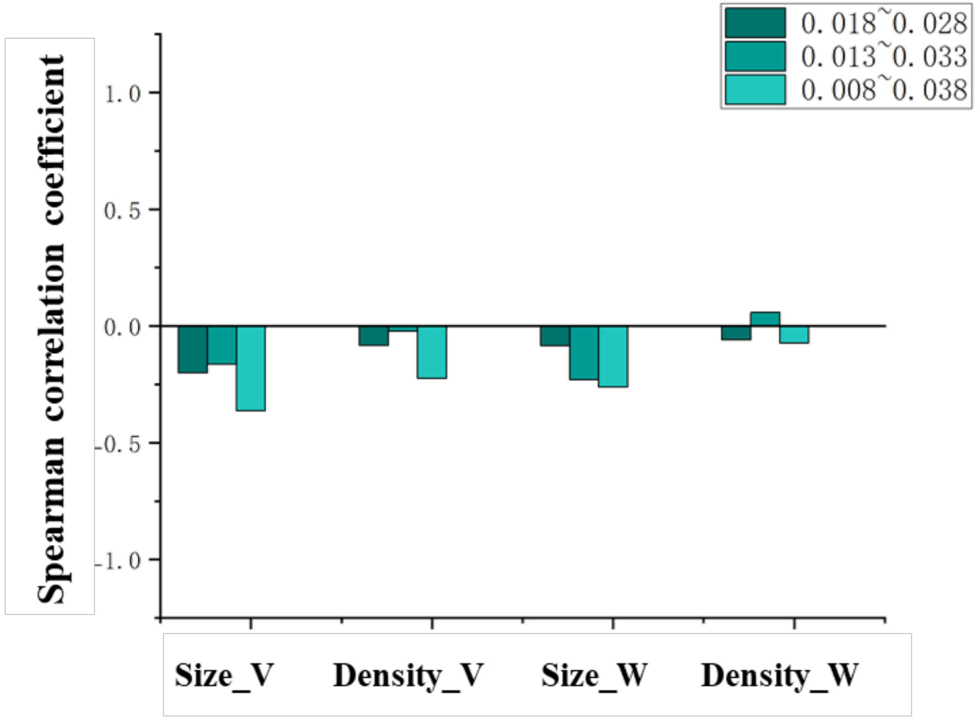
Potential factor: different ranges of values

We selected one high-sensitivity parameter (**Migration energy of single Vac,** <left>) and one low-sensitivity parameter (**Migration energy of SIA,** <right>) from the previous analysis results for further study.

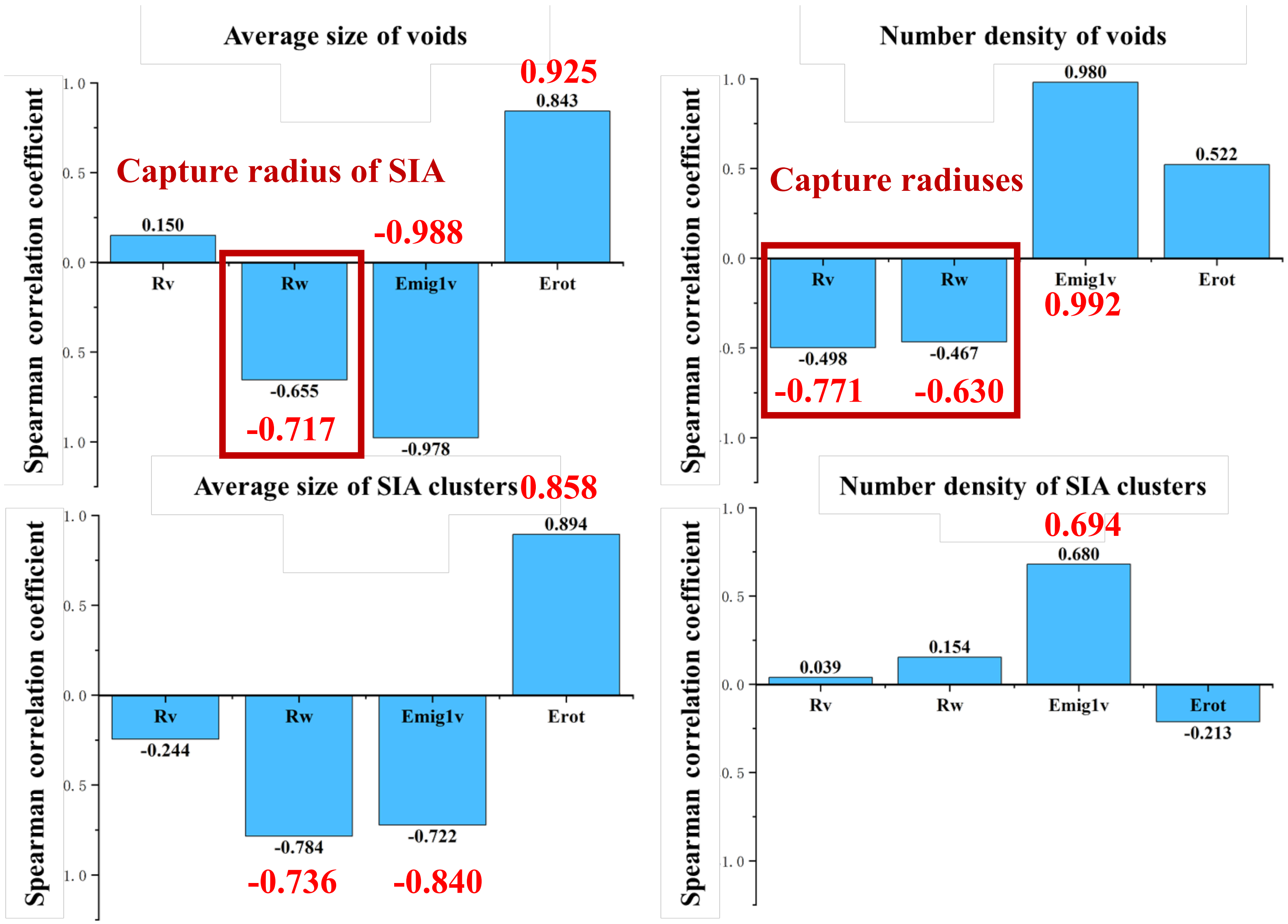




Samples concentrating within a smaller range may affect the accuracy of the analysis results.

No clear trends or patterns.

Potential factor: multiparameter analysis



We selected **the four sensitive parameters** as the target parameters for multi-parameter analysis.

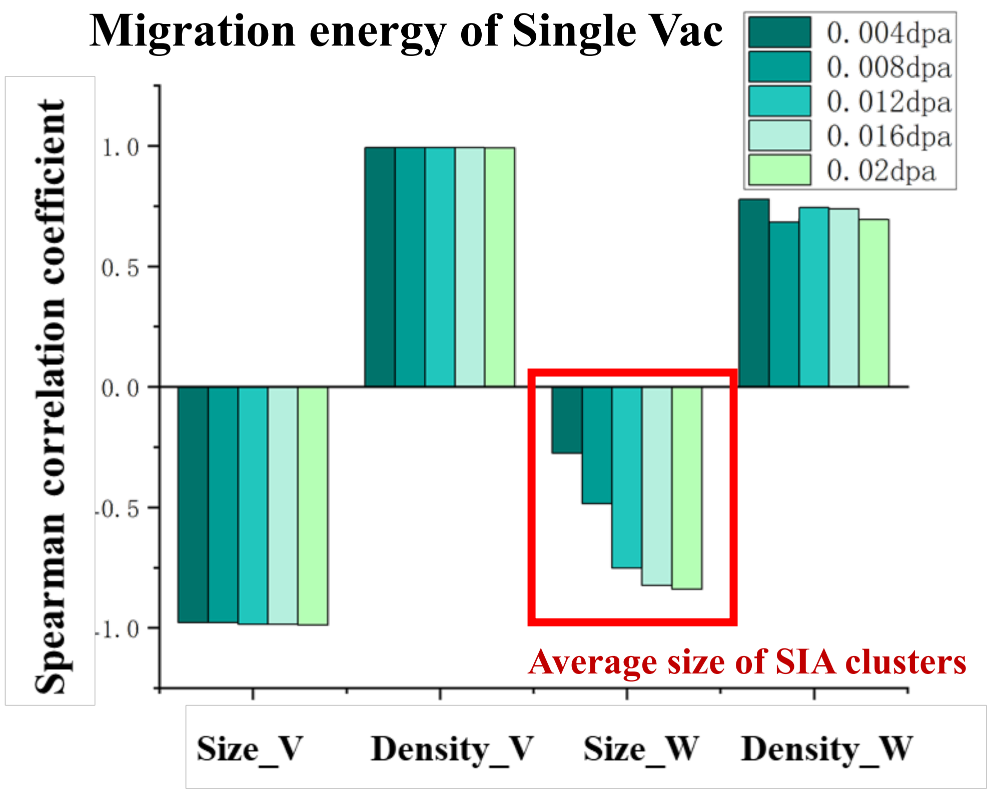
The sample size is 300.

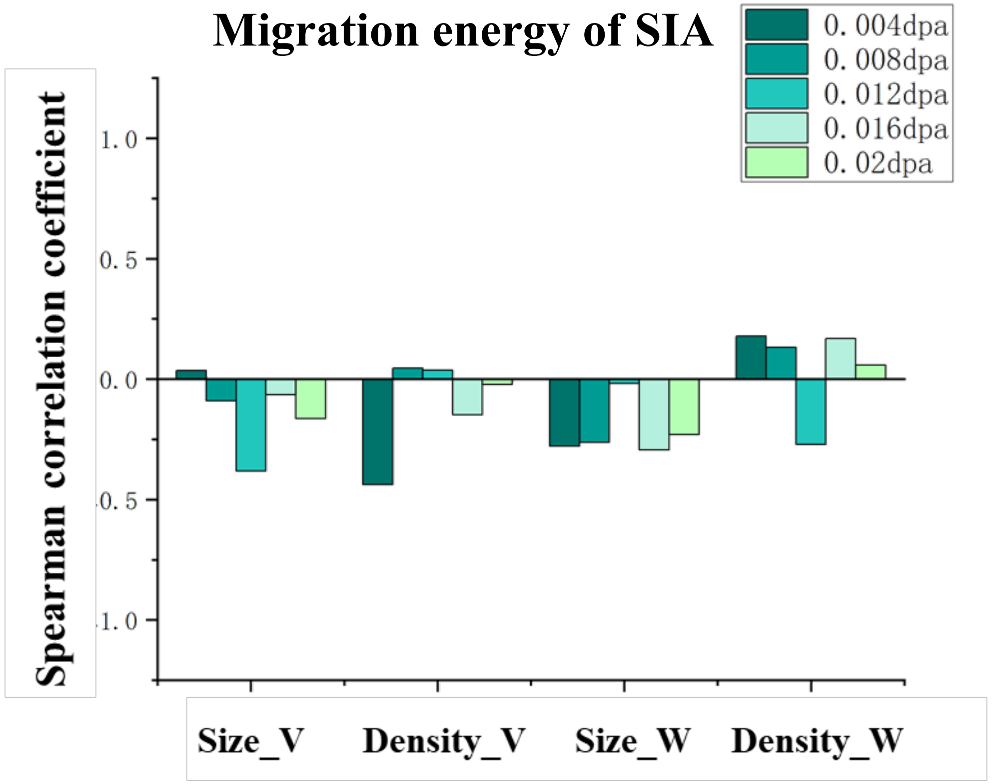
The numbers in red are the sensitivity for single-parameter analysis.

Sensitivity of **capture radiuses is reduced.**

No other substantial impact identified for now.

Potential factor: different irradiation doses

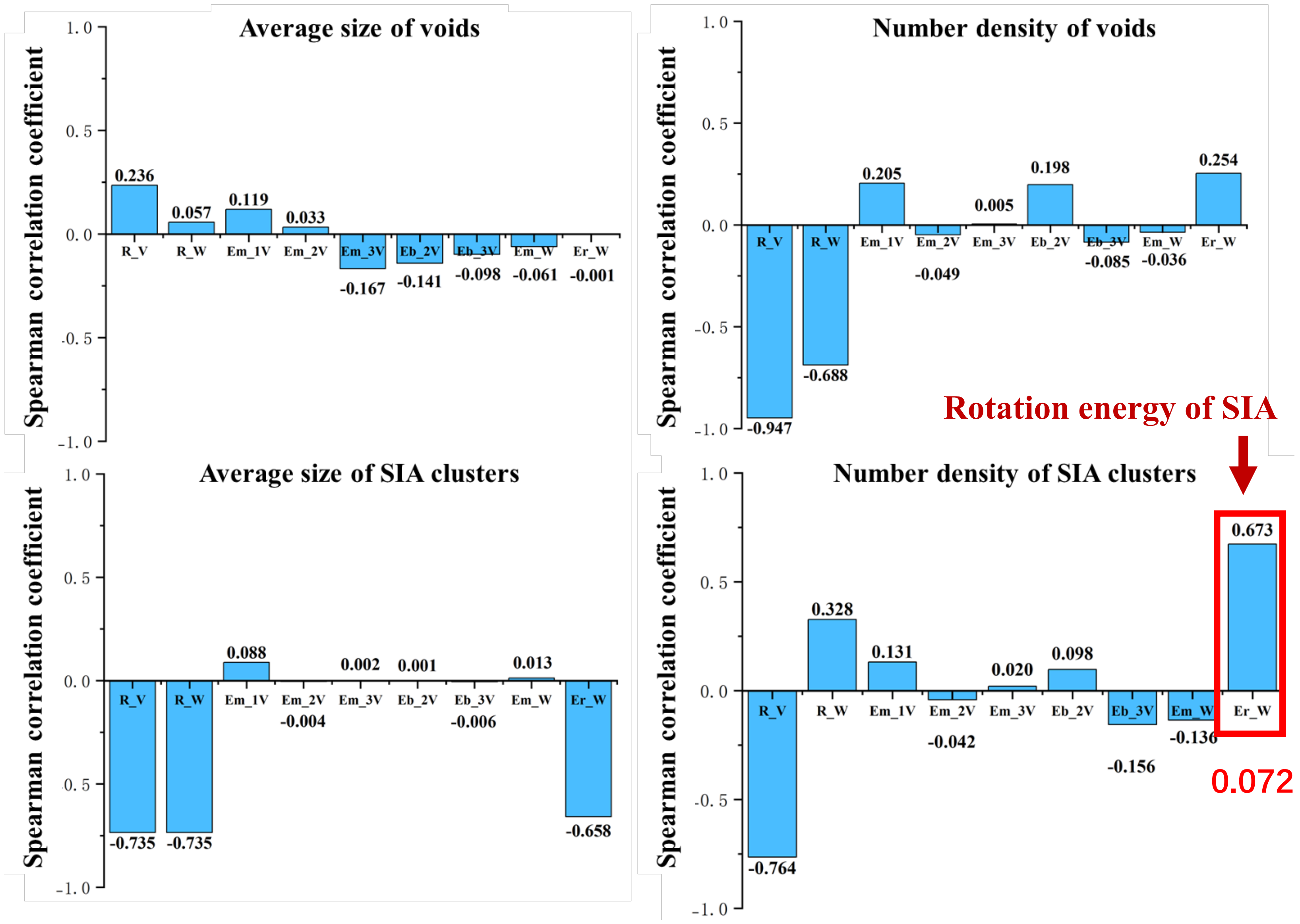




At low irradiation doses, recombination may be insufficient and the aggregation of SIAs dominates.

No clear trends or patterns.

Potential factor: different temperatures



363K, 0.004dpa

Vacancy migration events are almost nonexistent.

Recombination between SIA and Vac ↓

Aggregation of SIA ↑

↓

Number of SIA clusters ↑

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Polynomial Chaos Expansion

Input variables

- Migration energy of single Vac
- Rotation energy of SIA
- Capture radius of Vac
- Capture radius of SIA

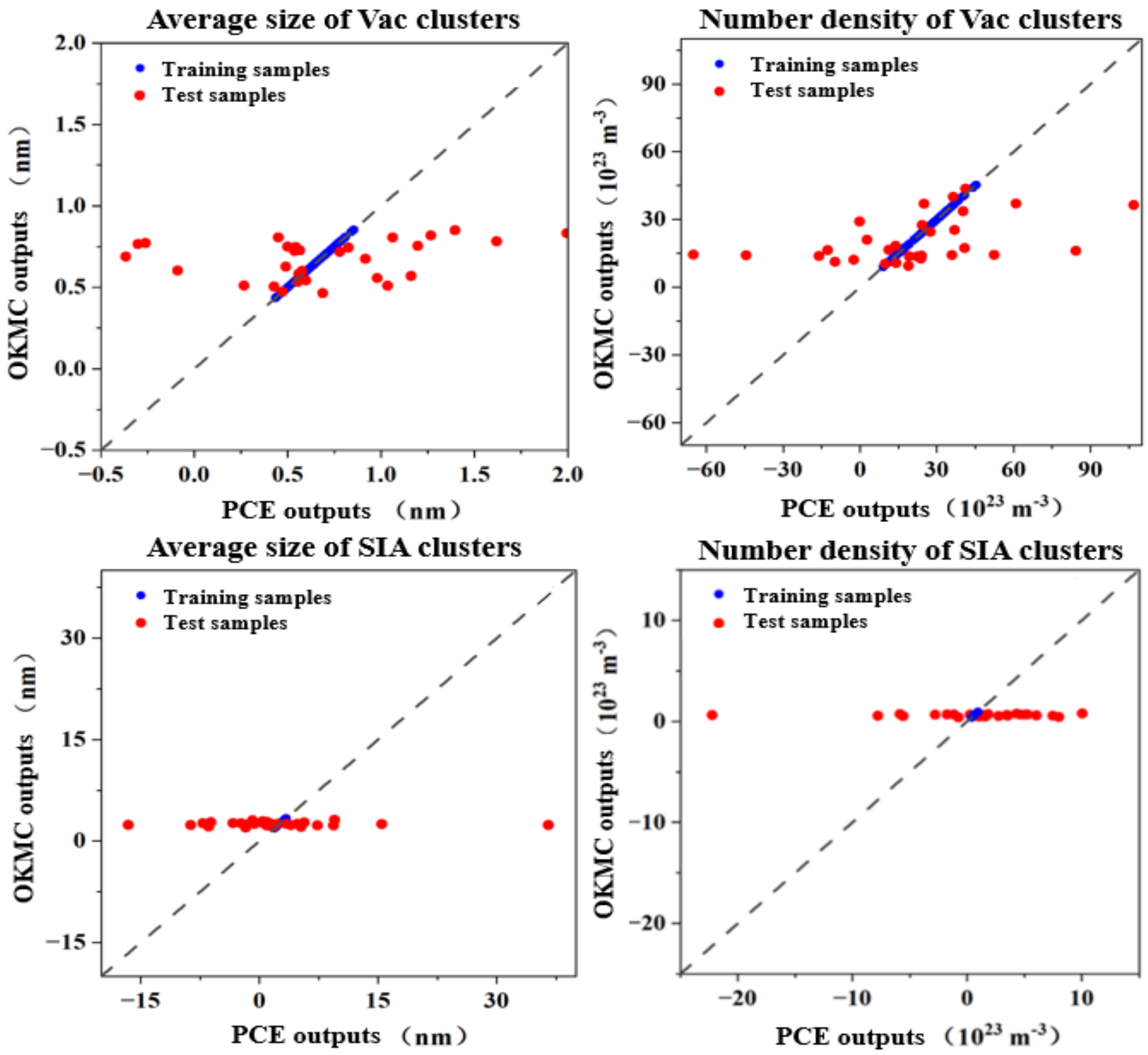
Settings of PCE surrogate models

Method	Order/ level	Number of training samples	Number of test samples
Linear regression	5	126	
Gaussian quadrature	4	256	30
Sparse grid	4	705	

- Minimization with least squares
- Limited training samples
- Multicollinearity of basis functions

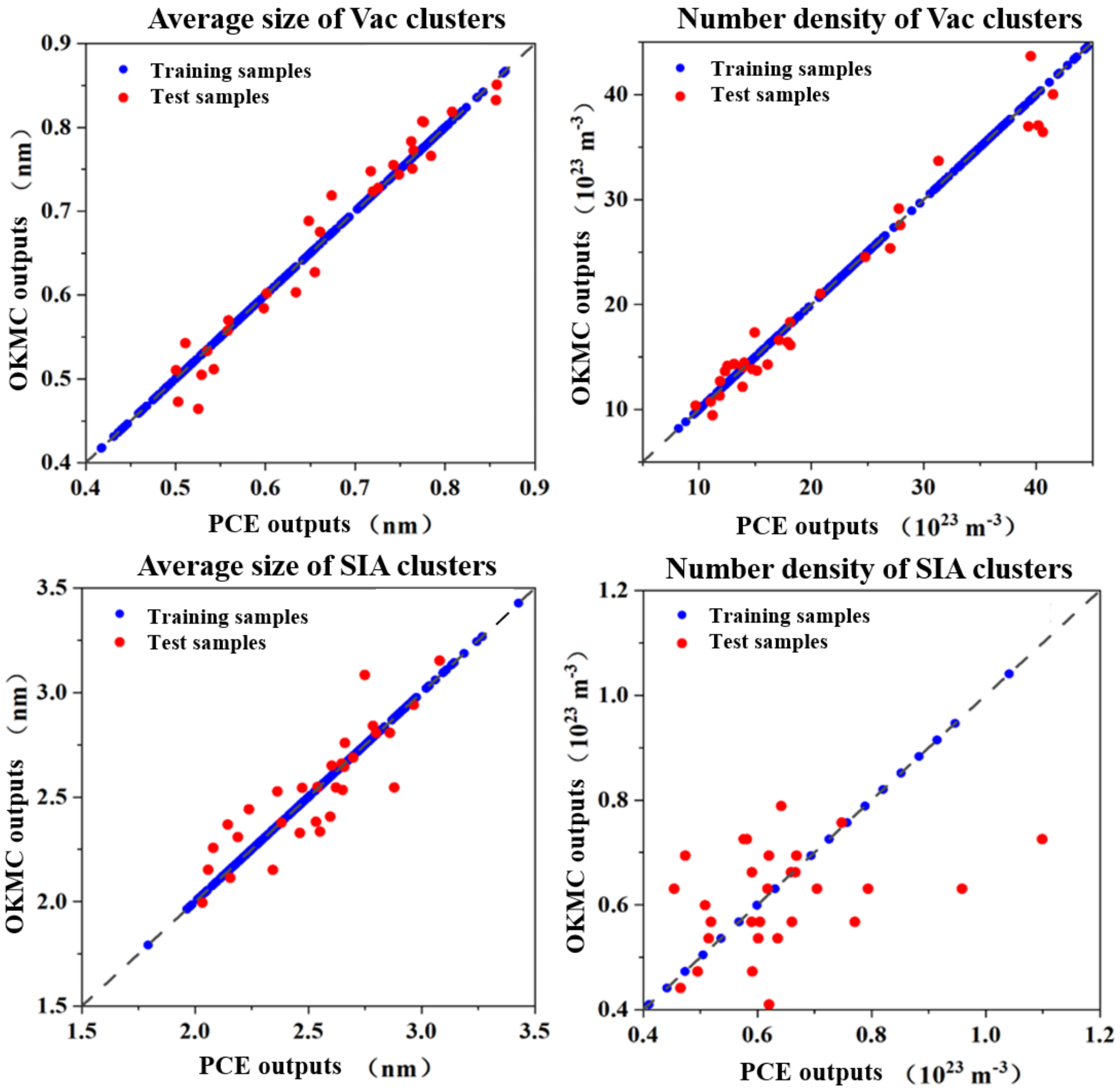
→ Noise-induced overfitting

Linear regression



Polynomial Chaos Expansion

Gaussian quadrature



Gaussian-quadrature PCE results match OKMC outputs better.

Smoothing and global averaging in the process of integral computation

Training samples that are **more uniformly distributed** in the parameter space

↓

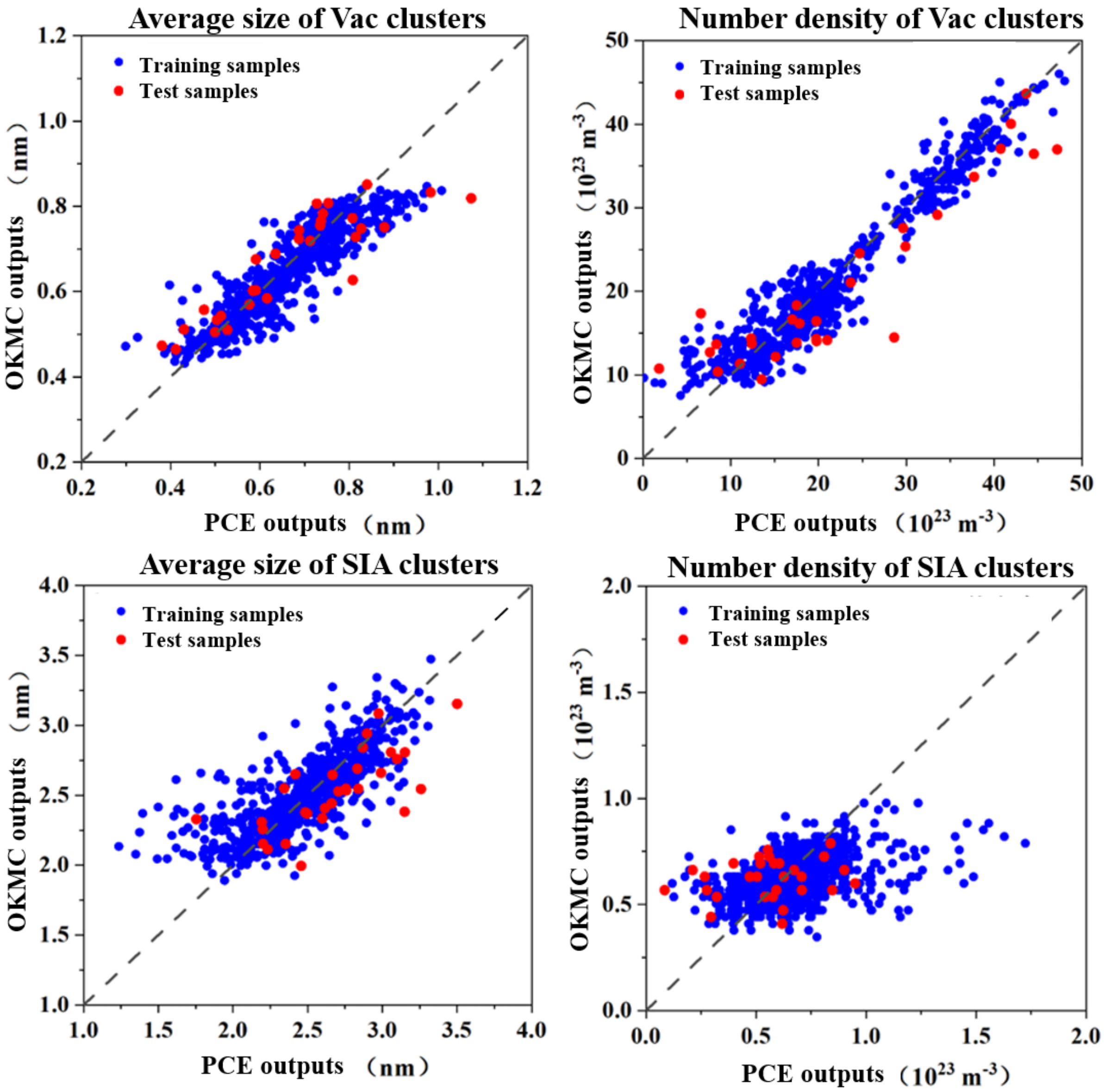
Reducing interference from data noise

Limitation:

Due to the **sample size**, it is difficult to build surrogate models that include more input parameters.

Polynomial Chaos Expansion

Sparse grid



Sparse-grid PCE results basically match the OKMC outputs, but some of the data are biased.

Lower uniformity of training sample distribution

Larger training sample **size**

→ Increased noise interference

Lack of knowledge of the overall characteristics of training samples

→ Partial data bias

Limitation:

Less effectiveness in dealing with data noise

Outline

1) Introduction

Nuclear fusion in renewables-based system

Irradiation damage in tungsten

Multi-scale modeling of irradiation effects

Uncertainty quantification & sensitivity analysis

2) Method

The OKMC model

Sensitivity analysis

Surrogate model

3) Sensitivity Analysis

Sensitivity at 733K and 0.02dpa

Factors affecting the sensitivity potentially

4) Surrogate Models

Polynomial Chaos Expansion

Artificial Neural Network

5) Conclusion & Fututure Work

Artificial Neural Network

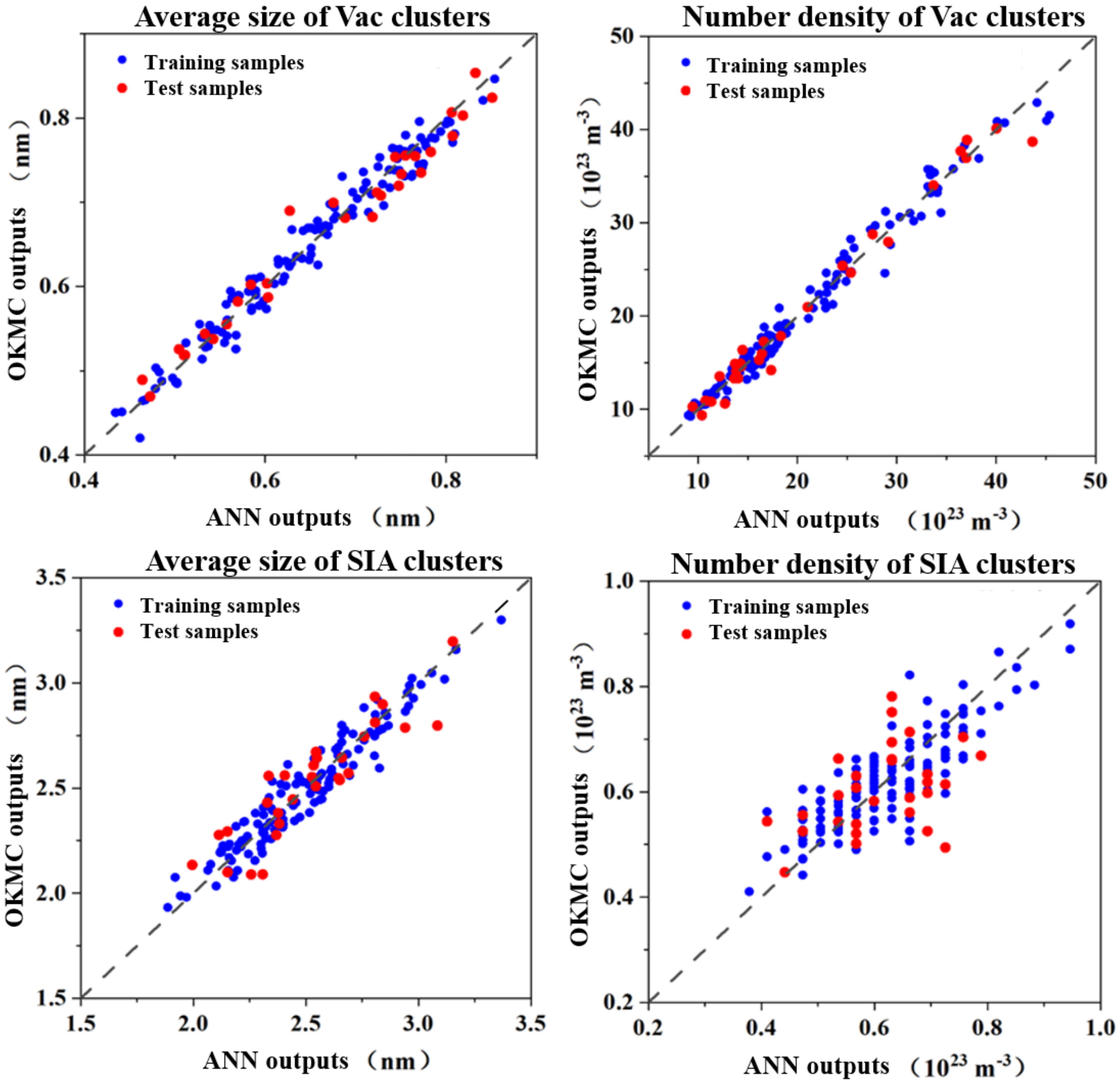
Settings of ANN surrogate models with 4 inputs and 4 outputs

Number of hidden layers	1	2	3
Number of nodes in each layer	10	8,8	6,6,6
	16	12,12	8,8,8

Six different surrogate models were built for each of the three sets of training samples in PCE part.

- ANN outperforms PCE in overall surrogate performance.
- MLP [4, 10, 4] and [4, 6, 6, 6, 4] have better performance in ANN surrogate models.
- **MLP [4, 10, 4]** is more computationally efficient than MLP [4, 6, 6, 6, 4].

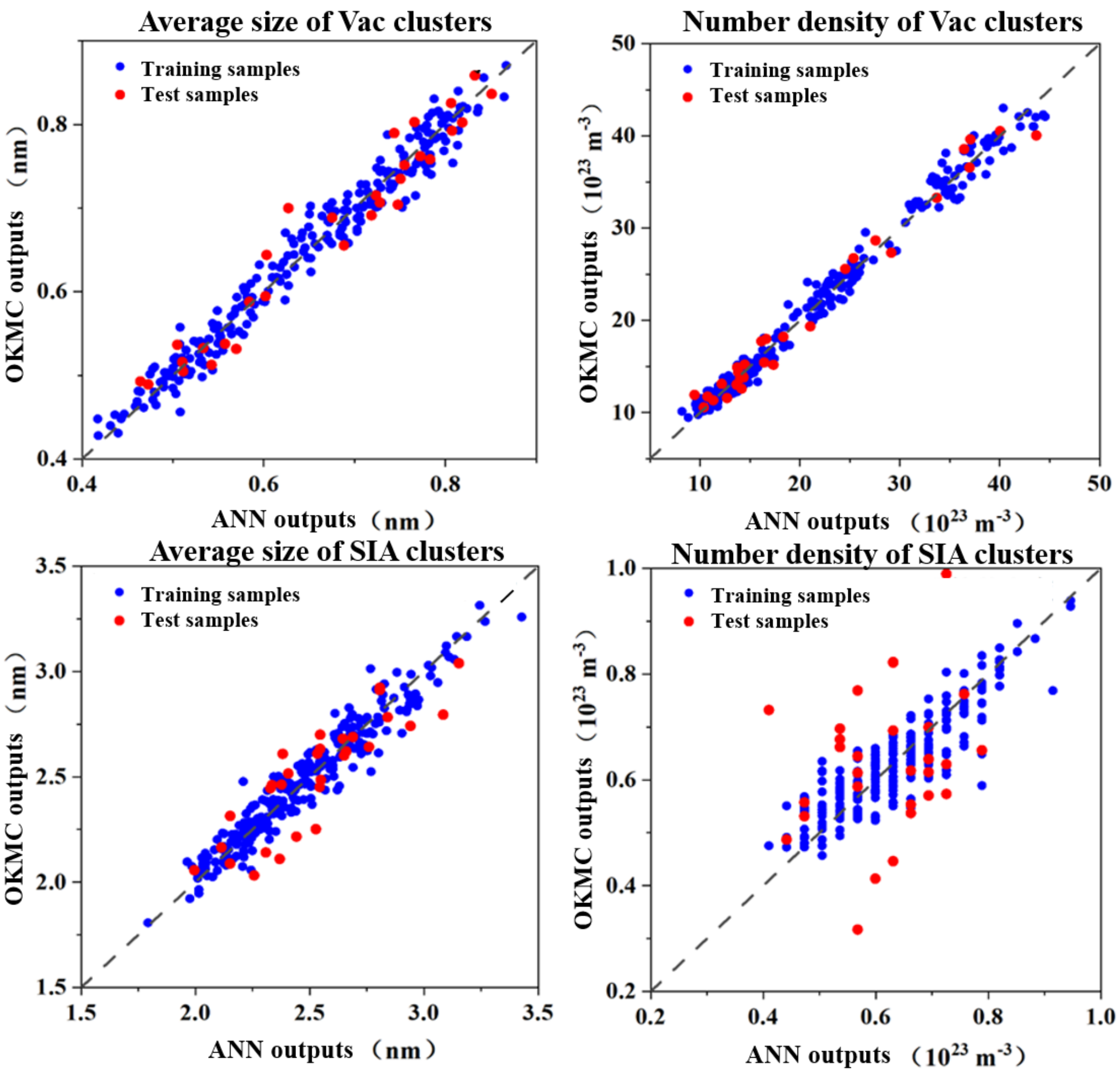
MLP [4, 10, 4] with 126 samples



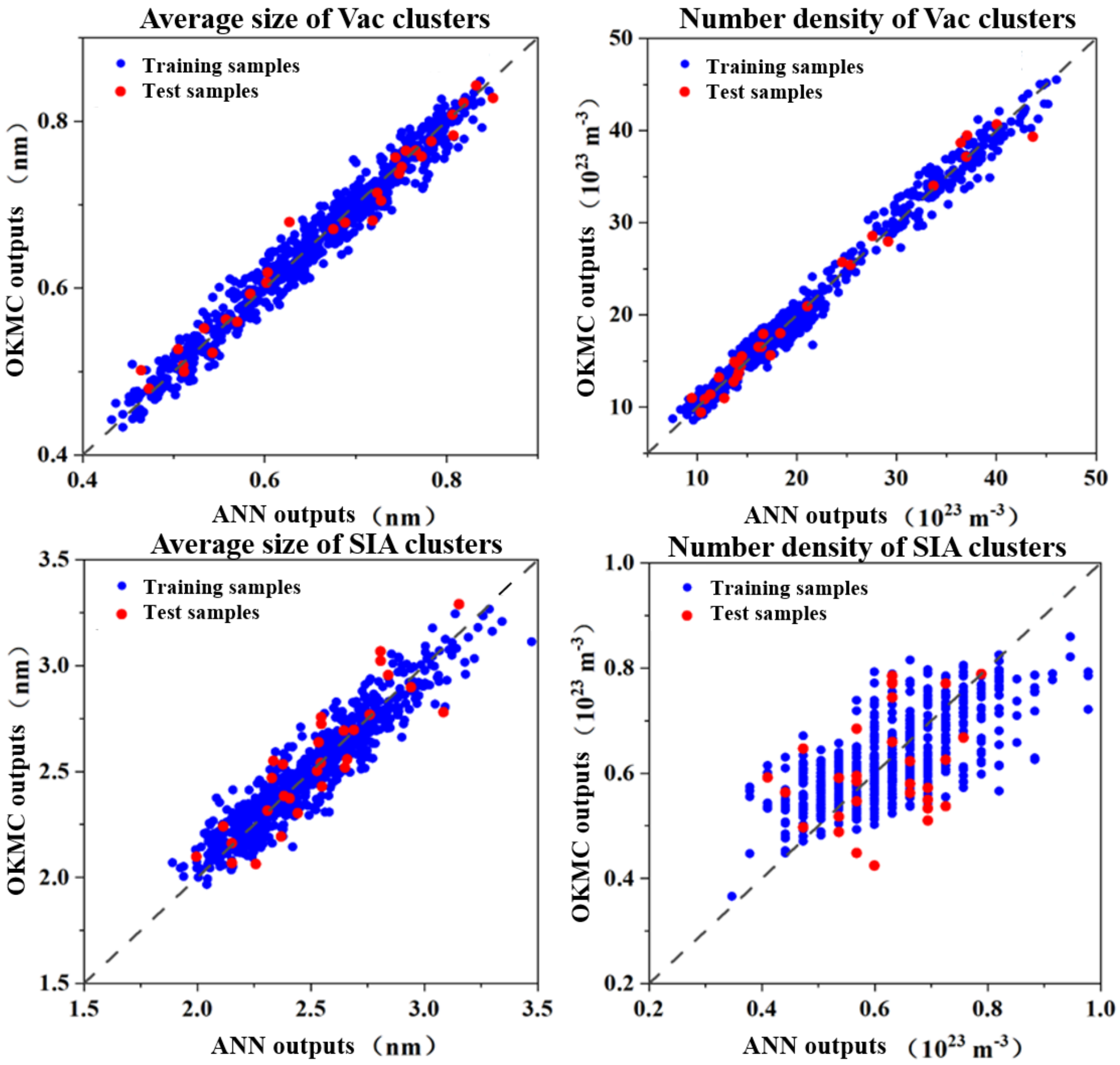
Artificial Neural Network

Huazhong University of Science and Technology

MLP [4, 6, 6, 6, 4] with 256 samples



MLP [4, 10, 4] with 705 samples



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Conclusion

To **better characterize the parameters** of OKMC and **optimize the model prediction**, we performed a **sensitivity analysis** of OKMC and assessed 4 **potential factors** that may affect the results of sensitivity.

- **Four sensitive parameters** with significant impacts on the OKMC simulation results were identified:

Migration energy of single Vac	**Rotation energy of SIA**
Capture radius of Vac	**Capture radius of SIA**

- ***Four potential factors***

Range of value	→	**Reasonable**
Multiparameter	→	**If computing resources are limited**
Irradiation dose	→	**Not too low**
Temperature	→	**Activation of specific processes**

Conclusion&Future Work

To **reduce the computational costs** of inverse uncertainty quantification, two types of **surrogate models** constructed for OKMC are analyzed and assessed in terms of method setup, surrogate performance, and error calculation.

- **Simple structure** ANN models **with fewer hidden layers** are preferred for building OKMC surrogate models.

Capable of reducing the interference of data noise | **Have stable performance**

- It is difficult for PCE models to fundamentally solve the **overfitting problem**. The Gaussian PCE model has a good surrogate performance. However, its obvious defects in high-dimensional problems cannot be ignored.

Future Work

▶ To reduce uncertainty, we need to **characterize** the sensitive parameters **more precisely**.

Inverse Uncertainty Quantification —(Experimental data / Surrogate model)→ **Parameter calibration**

Bayesian approach + MCMC method

Thank you for your attention!