Radiation Damage Effects in Beryllium for Next Generation Neutrino Beam Targetry

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THE UNIVERSITY of WISCONSIN MADISON

Computational Materials Group

Introduction to Radiation Damage Effects in Target and Window Be Material

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Simulation Tools for Modeling Radiation Damage in Materials

Summary and Future Work

Introduction to Radiation Damage Effects in Target and Window Be Material

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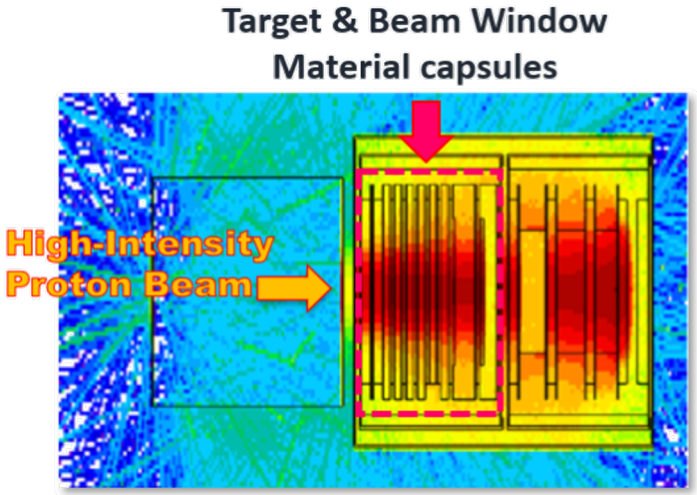
Simulation Tools for Modeling Radiation Damage in Materials

Summary and Future Work

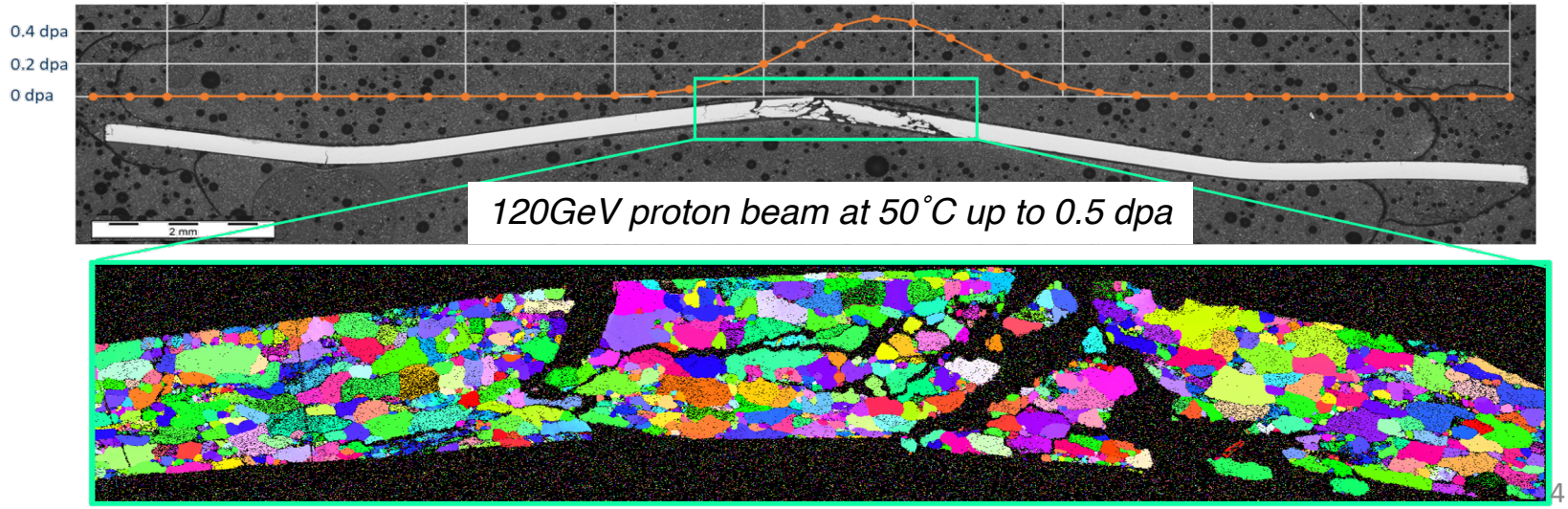
Background

Primary beam window of the NuMI neutrino source at Fermilab



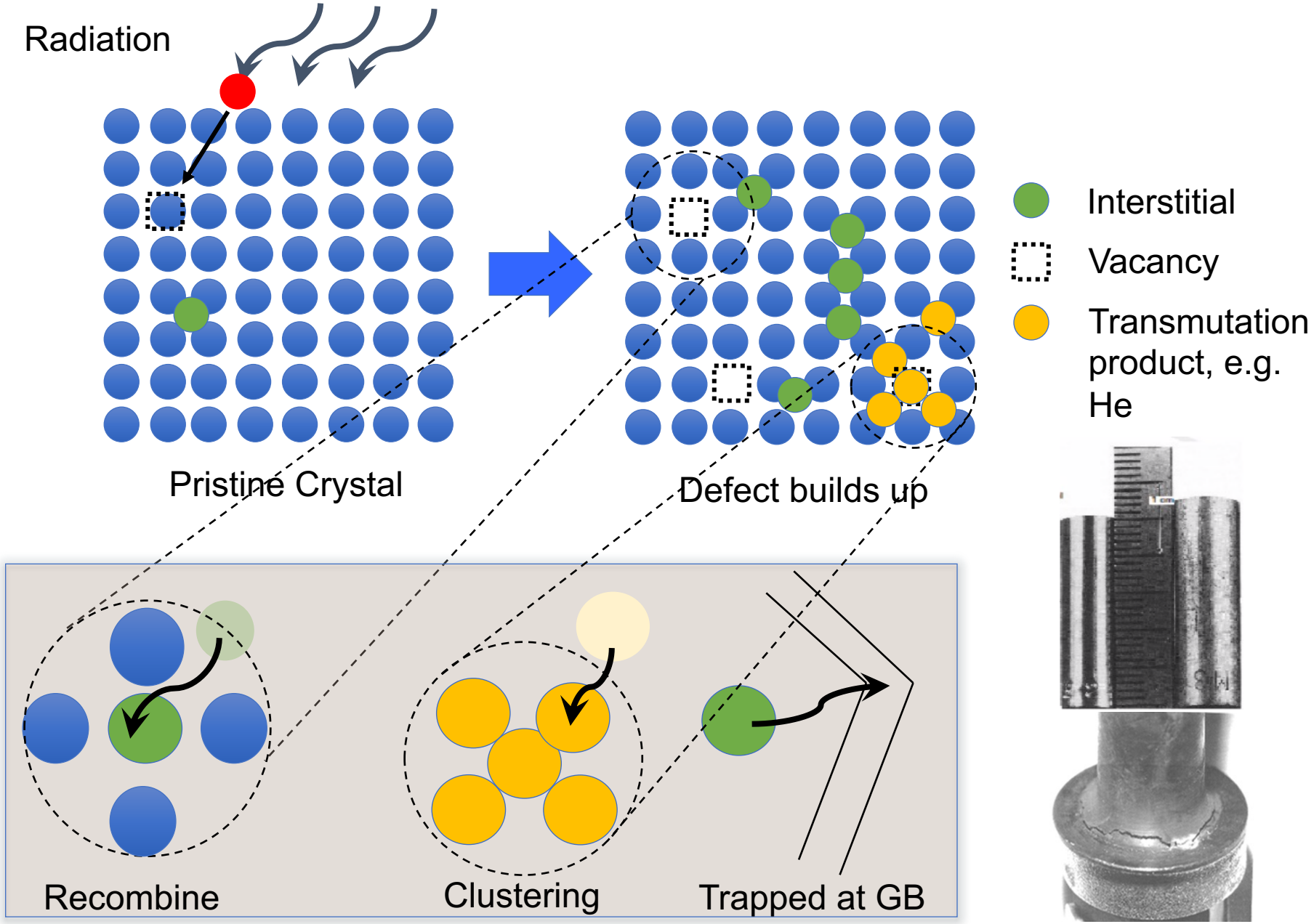
Operation conditions: *120 GeV proton* *beam at 1MW, ~40-100 ℃ for current accelerator; at 4MW, ~100-340 ℃ for future accelerator.*

Fracture of the Be specimen



Courtesy of Dr. S. Kuksenko and Mr. P. Hurh

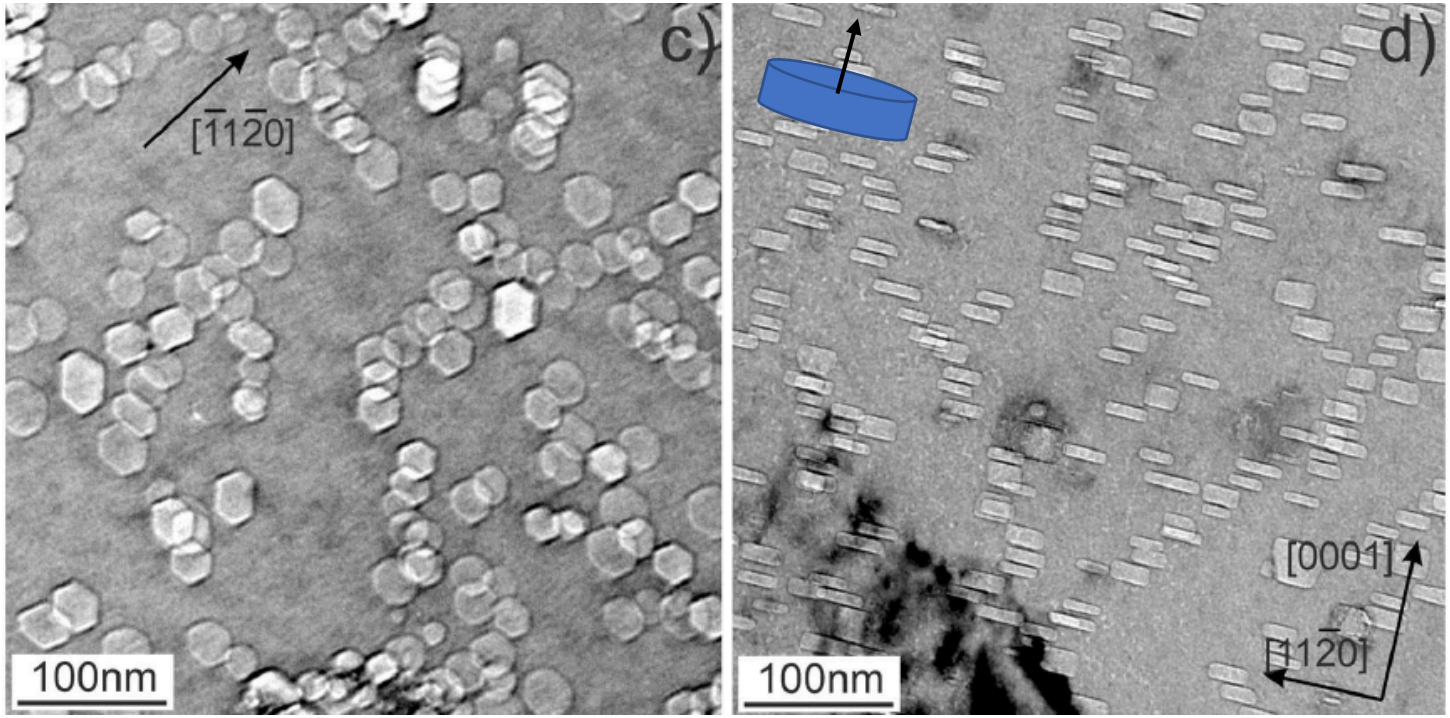
Radiation Damage in Materials



Radiation Damage in Beryllium

Radiation in Be induce the formation of He bubbles in fusion application

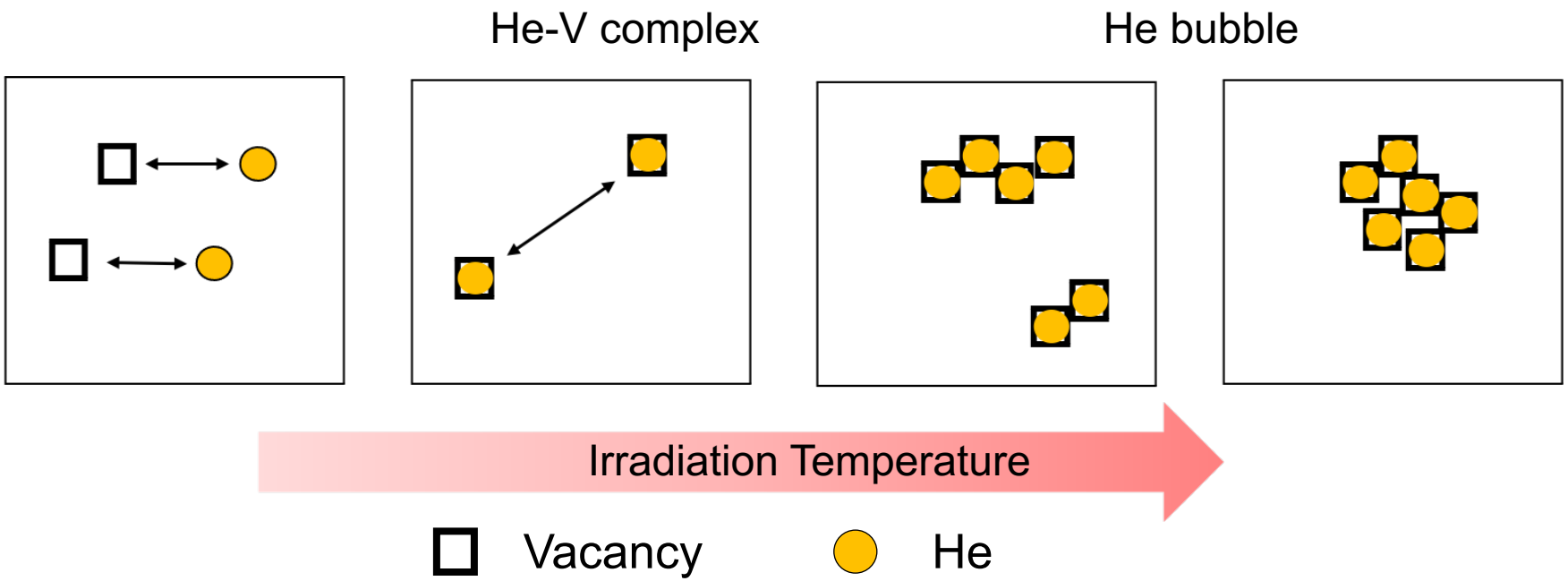
Neutron irradiation @ 713 K, >3000 appm He



M. Klimenkov, et al. *Sci. Rep. 10 (2020) 8042*

Radiation Damage in Beryllium

The temperature-dependent He bubble formation [1-4].



High energy proton irradiation of beryllium results in He production rates **1,000 times** higher than in the fusion environment (neutron irradiation).

[1] M. Klimenkov, et al. JNM, 443 (2013) 409; [2] K. Chakin, et al. JNM, 307 (2002) 657;
[3] W. V. Renterghem, et al, JNM, 374 (2008) 54; [4] P. Liu, et al. Fusion Eng. Des, 140 (2019) 62.

Introduction to Radiation Damage Effects in Target and Window Be Material

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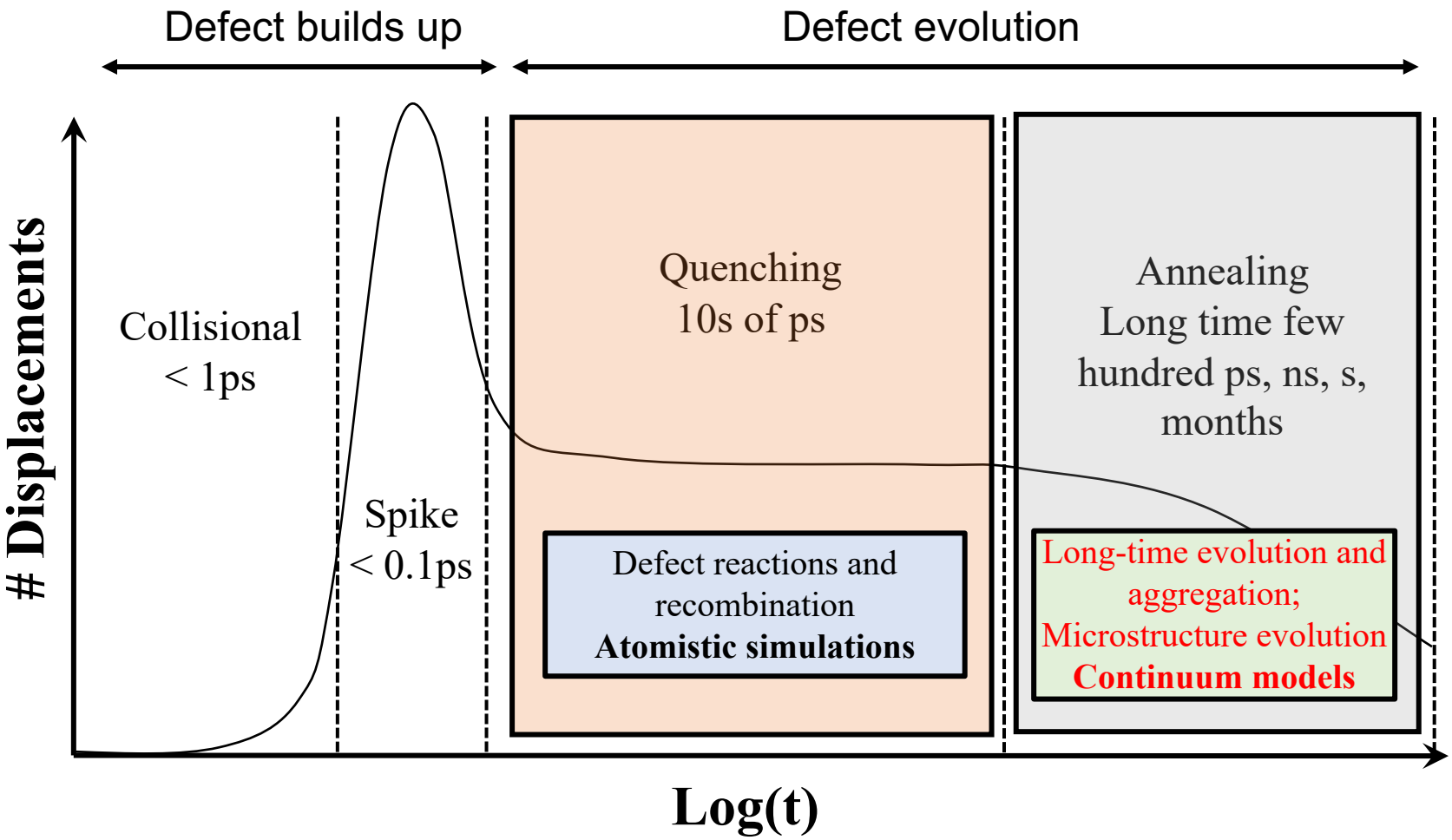
Simulation Tools for Modeling Radiation Damage in Materials

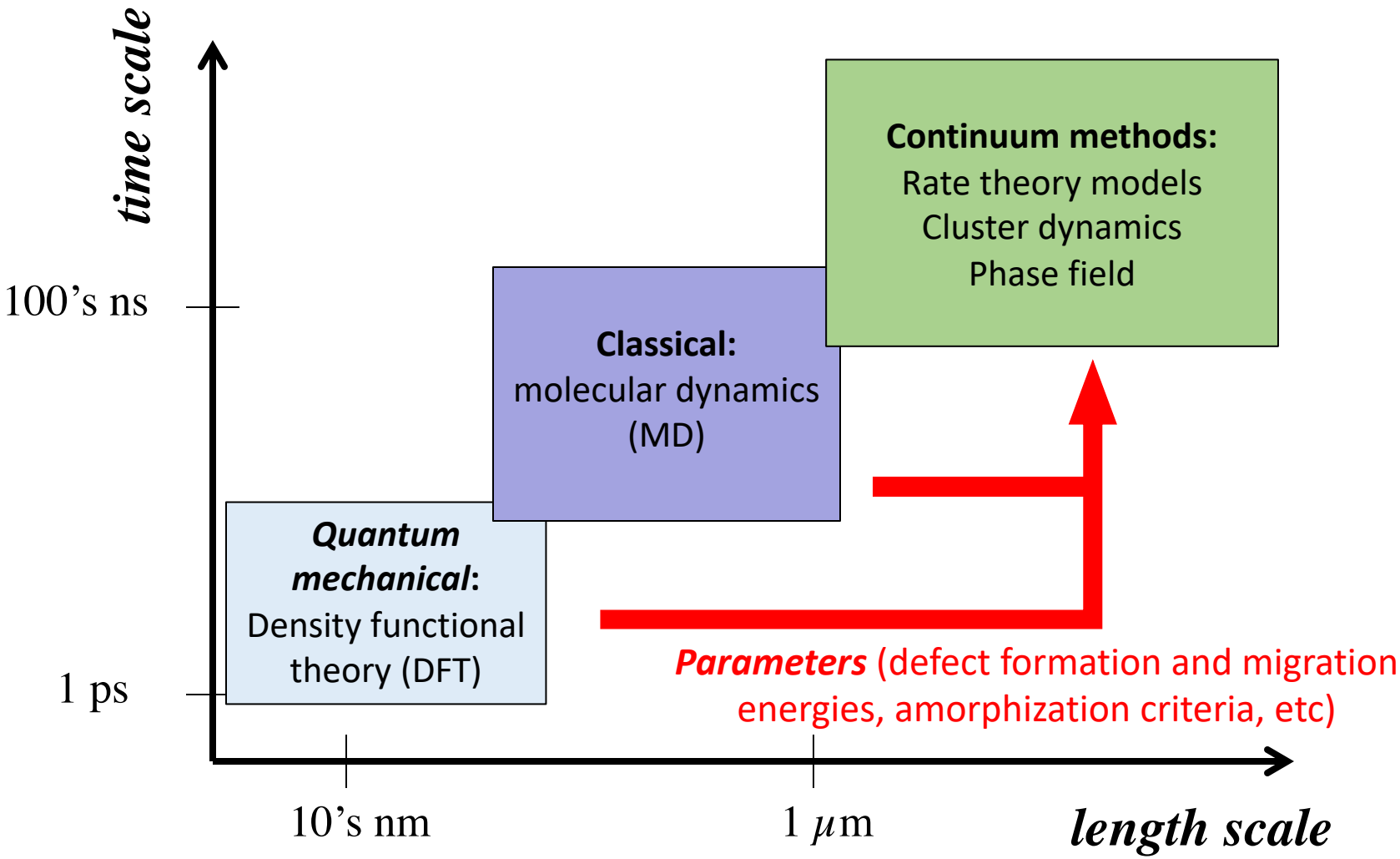
Summary and Future Work

Time Scales in Radiation Effects



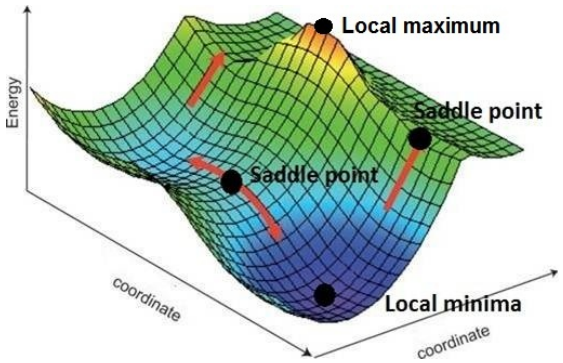
Adapted from Gary S. Was, *Fundamentals of radiation material science*, Springer, 2007

Multiscale Simulation Tools



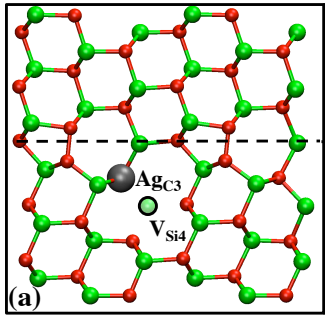
Quantum Mechanical Approach

Composition and structure
Atom positions, types



Thermodynamics and Kinetics information

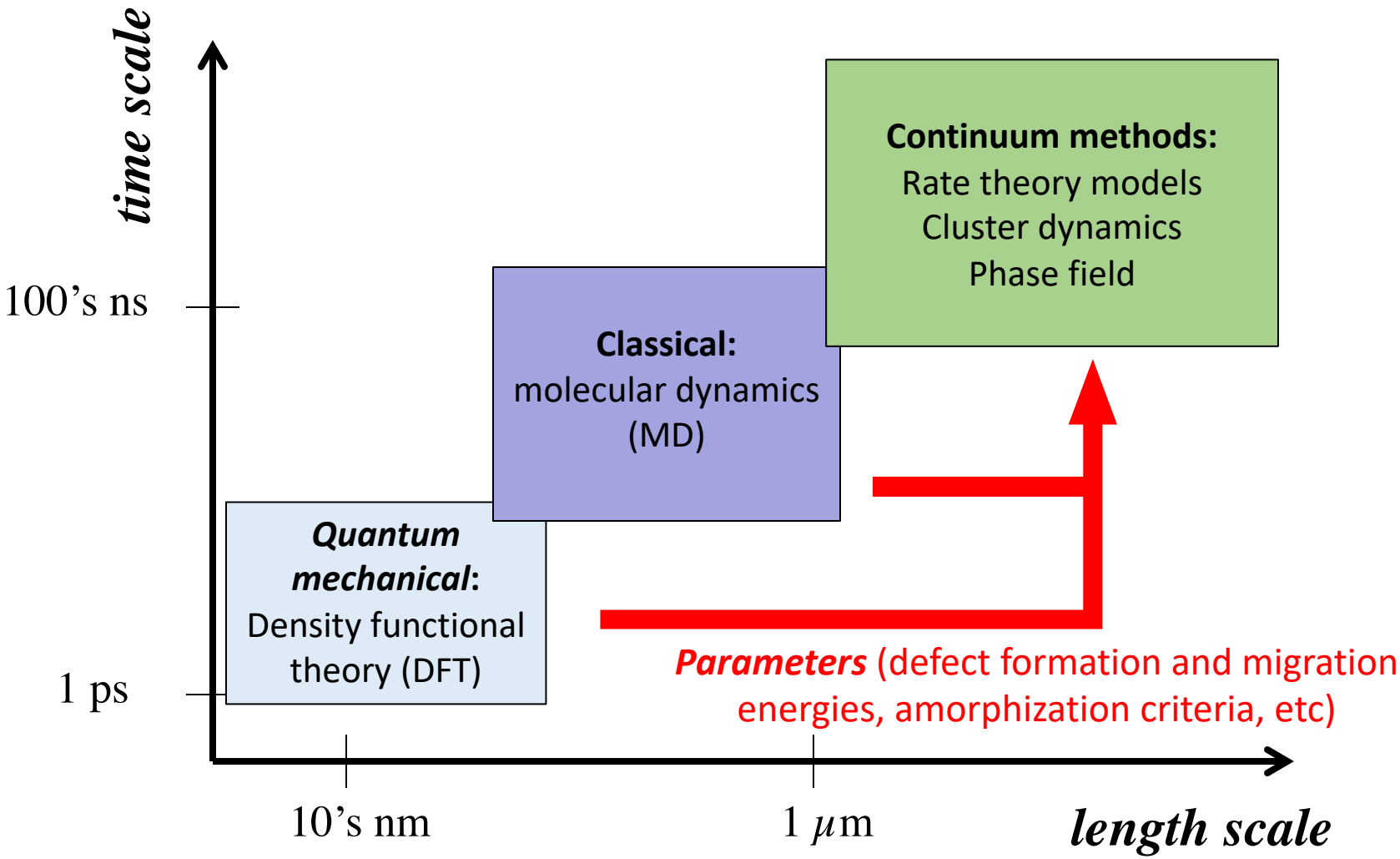
Solve Schrödinger equation
HF=eF



Segregation and diffusion of fission products to GBs in SiC

Electronic Structure
Defect Energies
Chemical Reaction Rates

Multiscale Simulation Tools



Classical Molecular Dynamics (MD)

Molecular dynamics technique

Atoms evolve according to Newton's equations of motion:

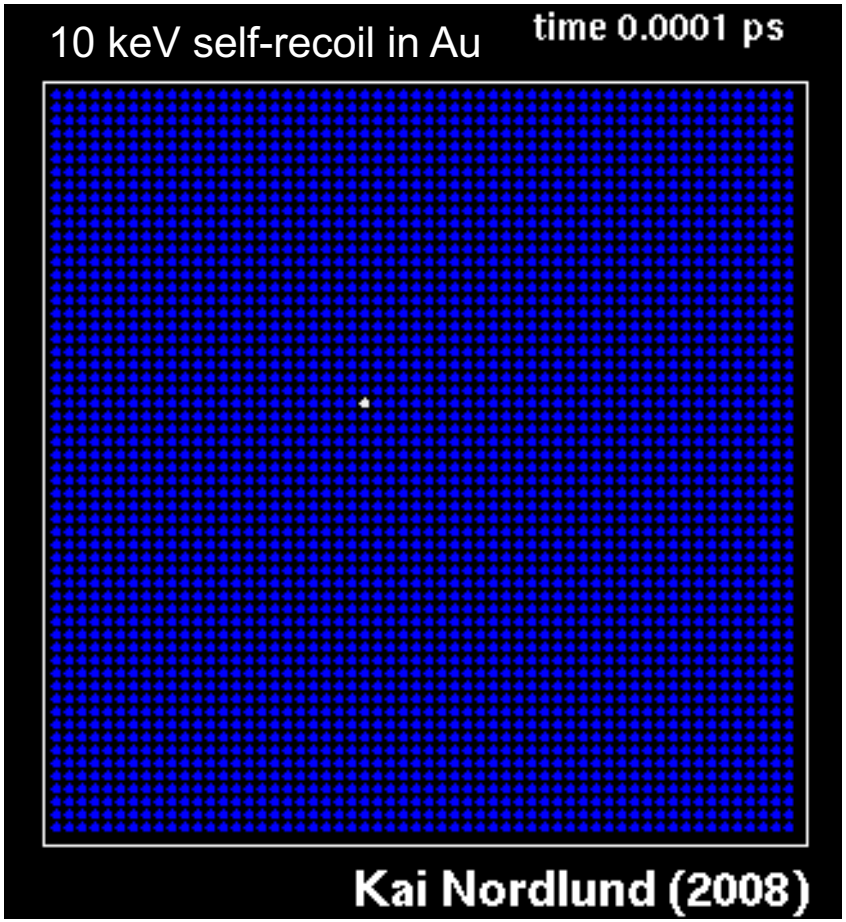
$$m_i \frac{\partial^2 \mathbf{r}_i}{\partial t^2} = -\frac{\partial V}{\partial \mathbf{r}_i}$$

Energy V can be calculated from empirical/machine learning **interatomic potentials**

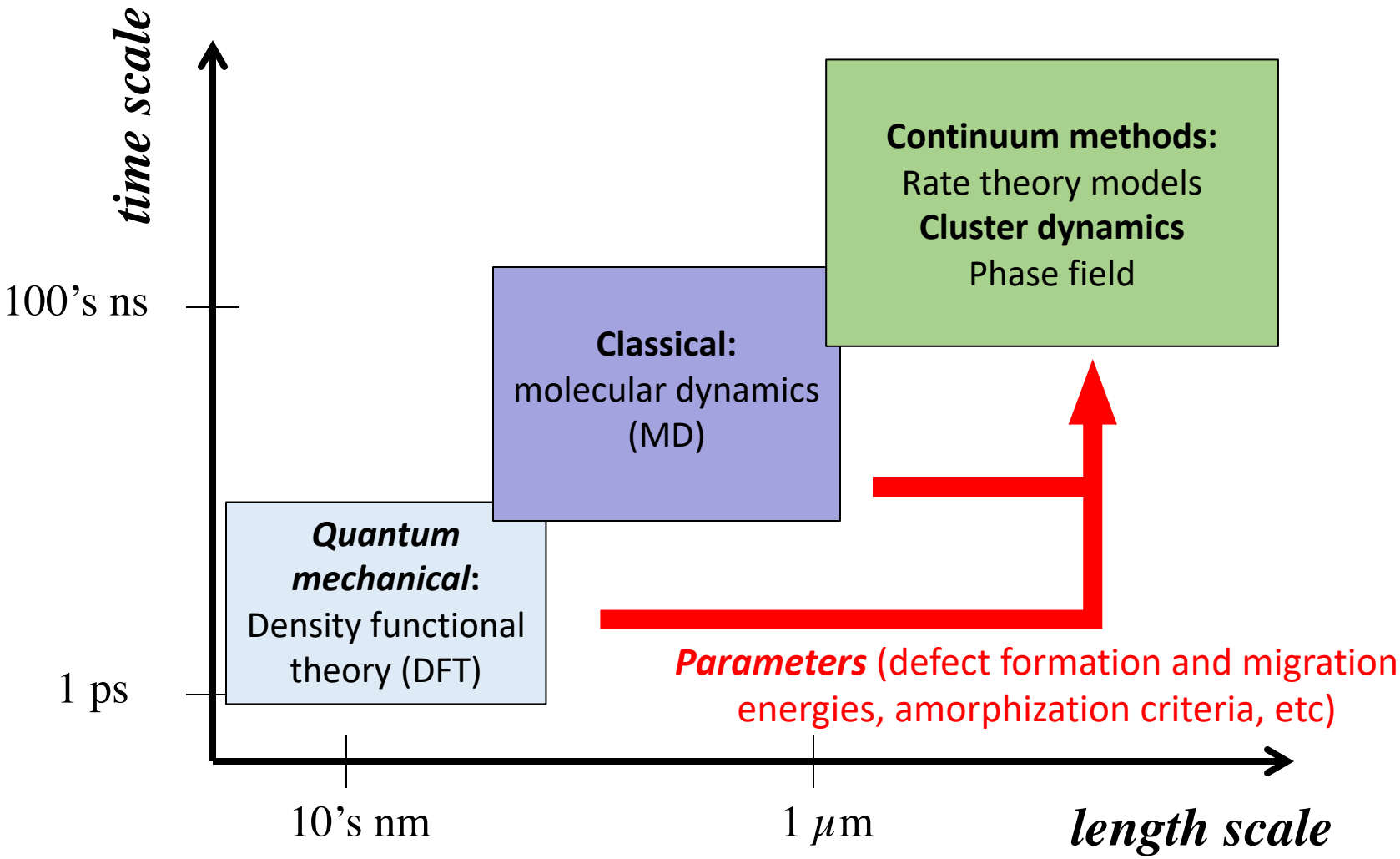
$$V = \sum_j V_2(\vec{r}_{ij}) + \sum_{jk} V_3(\vec{r}_{ij}, \vec{r}_{ik})$$

What can we learn from MD?

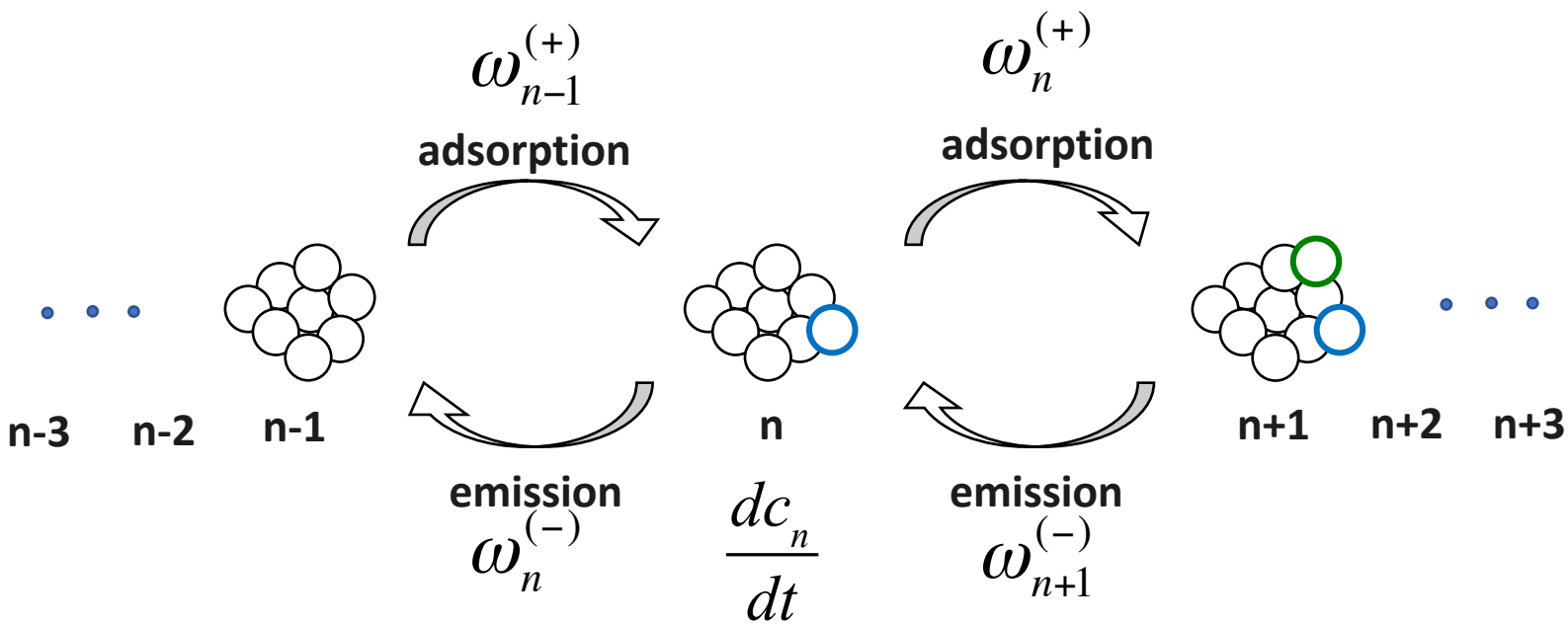
- Model radiation-induced collisions, defect formation, diffusion, clustering etc over relatively short time scales (< 1μs)
- Structural properties (dislocations, phase transformations)
- …



Multiscale Simulation Tools



What is Cluster Dynamics?



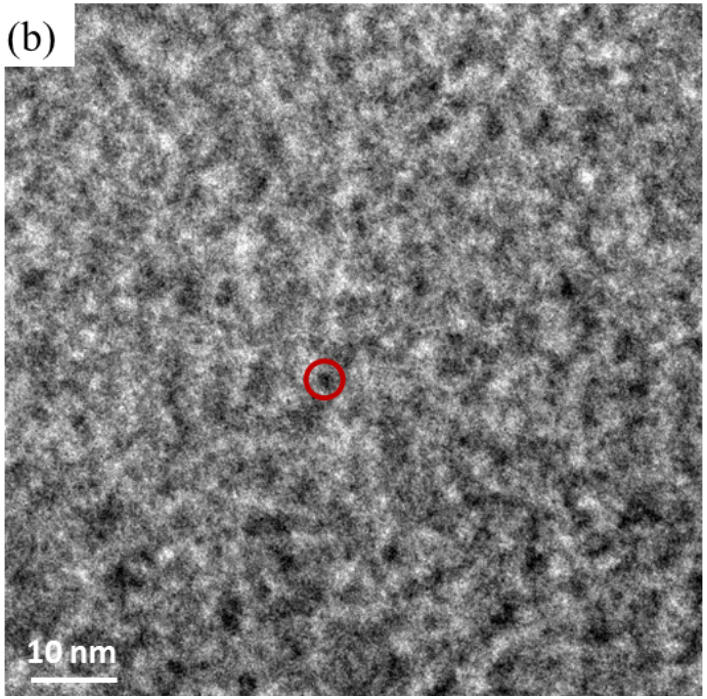
$$\frac{dc_n}{dt} = \underbrace{r_n}_{\text{Direct production}} + \underbrace{\omega_{n-1}^{(+)} c_{n-1} + \omega_{n-1}^{(-)} c_{n+1}}_{\text{Increase in } c_n} - \underbrace{\omega_{n}^{(+)} c_n - \omega_{n}^{(-)} c_n}_{\text{Decrease in } c_n}$$

V. Slezov, Kinetics of First-Order Phase Transitions, 1st ed., Wiley-VCH, 2009.

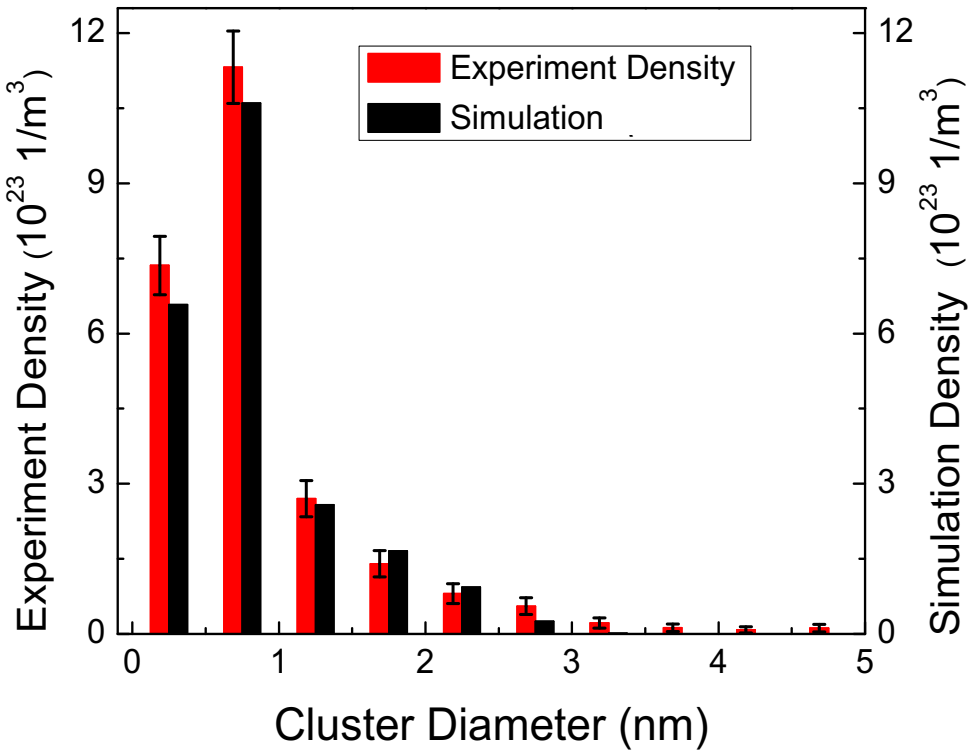
What Does Cluster Dynamics Output?

- Reveal mechanisms for defect evolution that cannot be observed in experiments

1 MeV Kr ions irradiate 3C-SiC for 120 s at 800 ˚C



TEM bright field image of SiC. Small clusters are indicated by red circles.



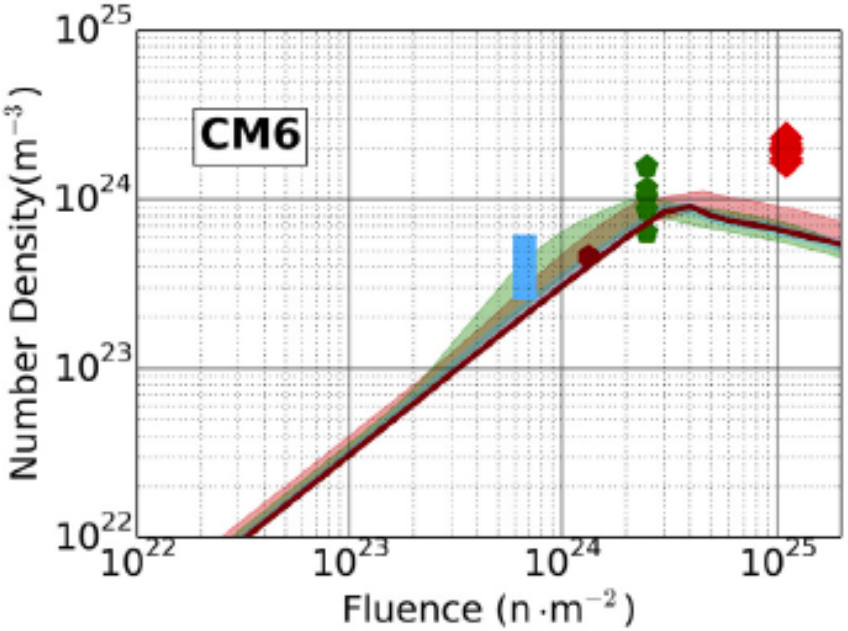
Cluster size distribution from CD based on potential physics

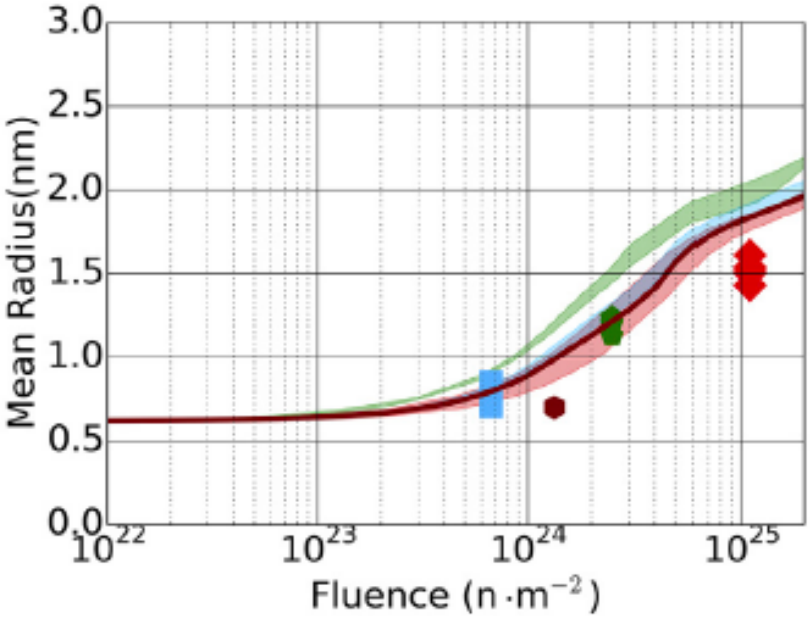
C. Liu, L. He, Y. Zhai, B. T. Puschel, P. M. Voyles, K. Sridharan, **D. Morgan, I. Szlufarska**., *Acta Materialia,* 125 (2017) 377-389

What Does Cluster Dynamics Output?

- Predict radiation damage at the conditions beyond the experimental observations

Cu+Mn-Ni-Si precipitates form under irradiation in steels

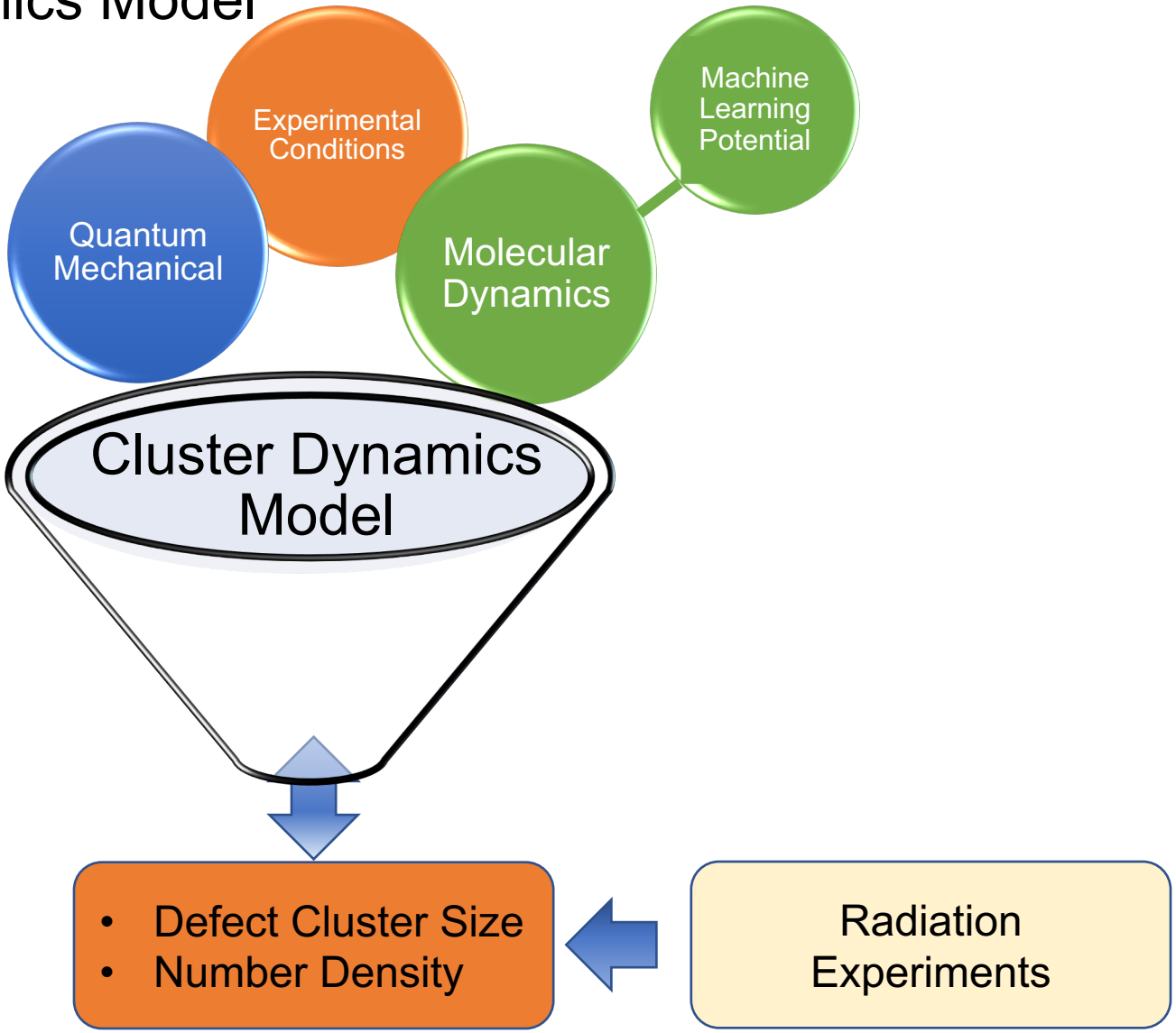




H. Ke, P. Wells, P. D. Edmondson, N. Almirall, L. Barnard, G. R. Odette, **D. Morgan**, *Acta Materialia* 138 (2017) 10-26.

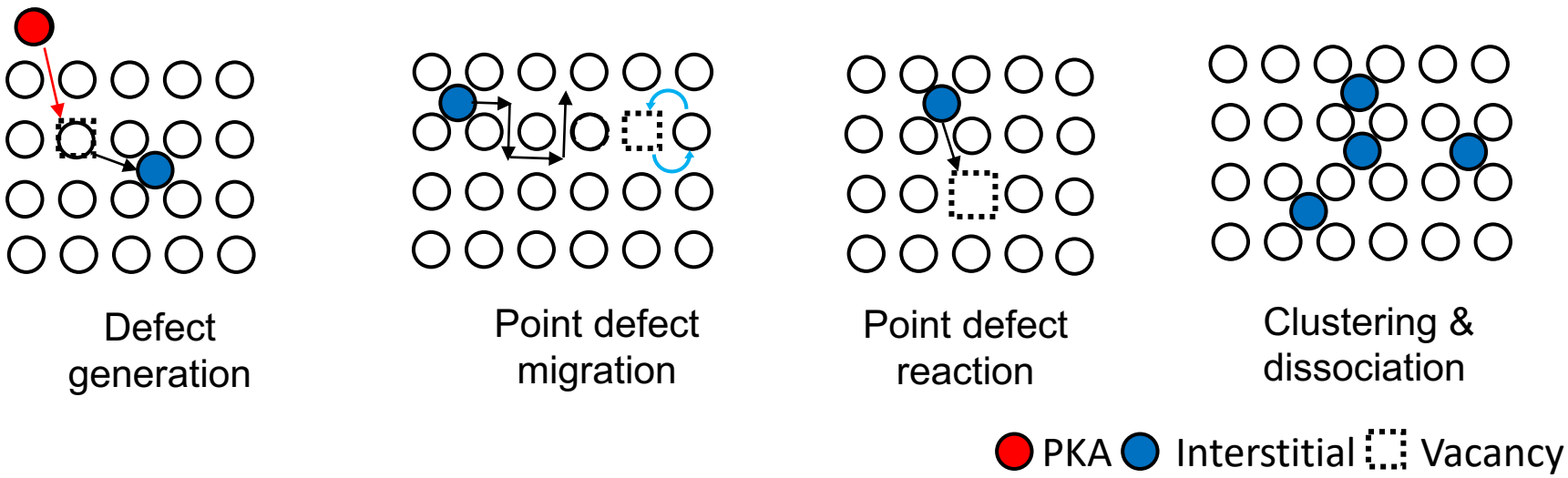
Our Strategy for Modeling Radiation in Be

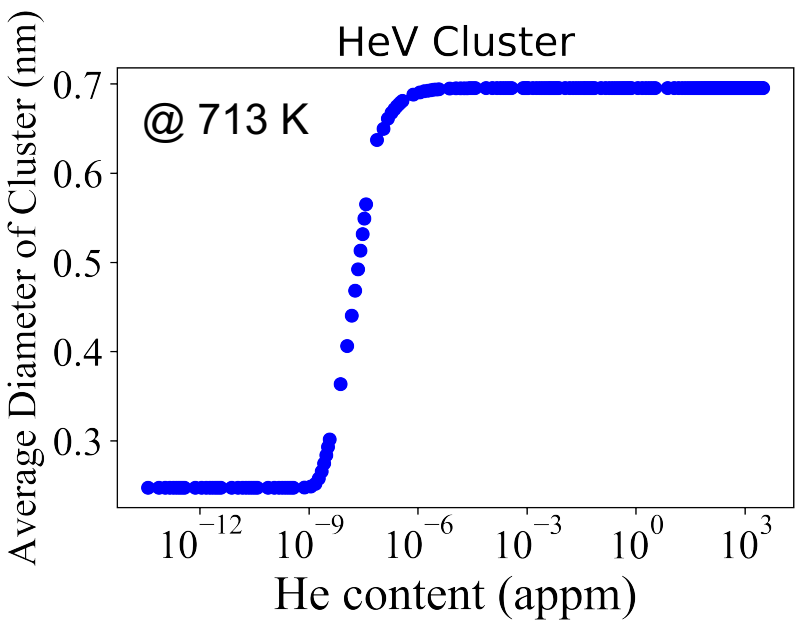
Atomistic Simulation based & Experimentally Validated Cluster Dynamics Model

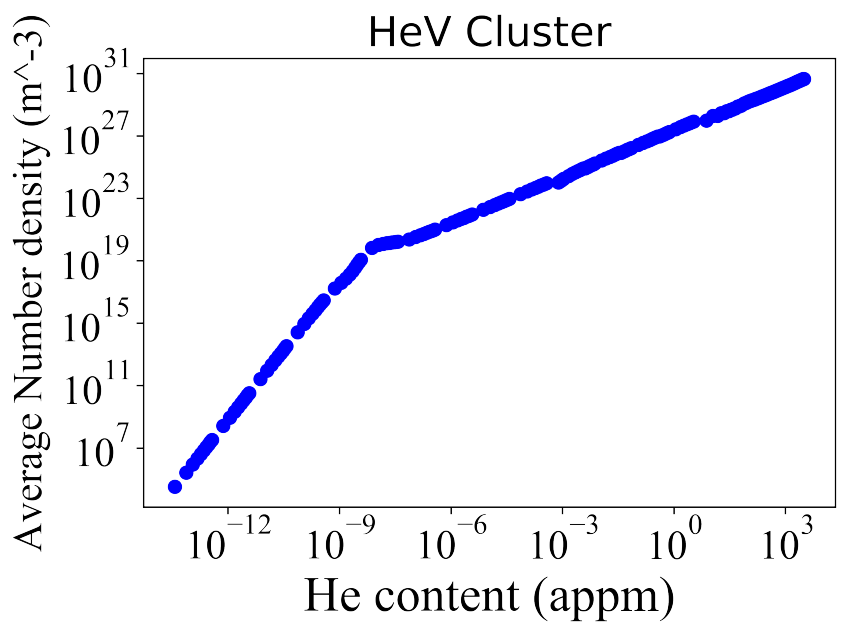


Current Status of the CD Model

- Physical processes have been involved:

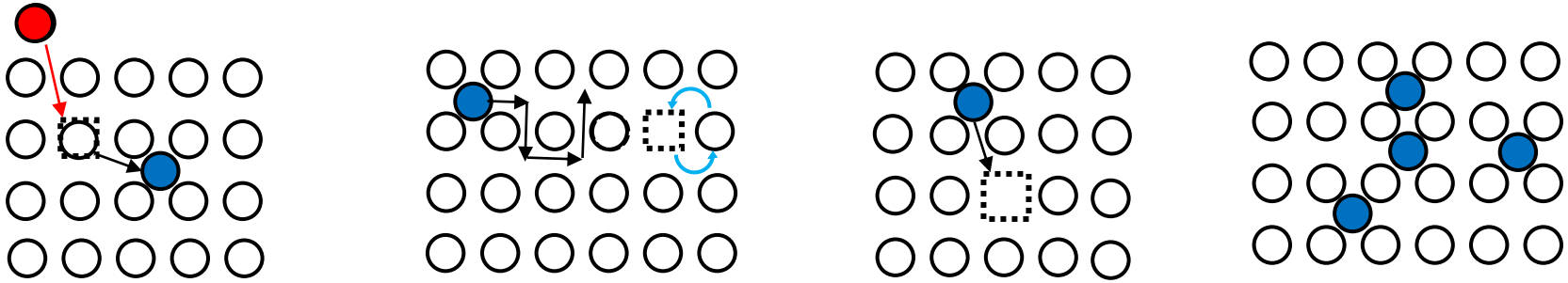






Next Plan of the CD Model

- Physical processes have been involved:

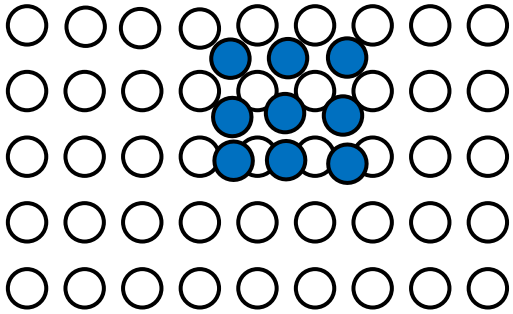


Defect generation | Point defect migration | Point defect reaction | Clustering & dissociation

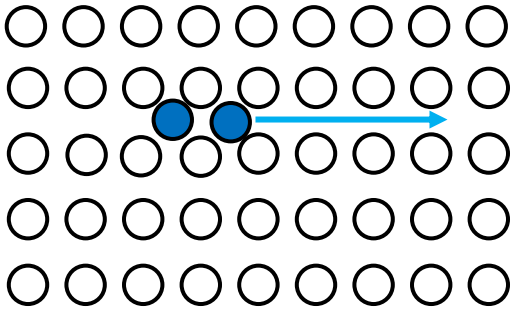
PKA Interstitial Vacancy

- Physical processes will be involved:

Large size cluster (N>10000)



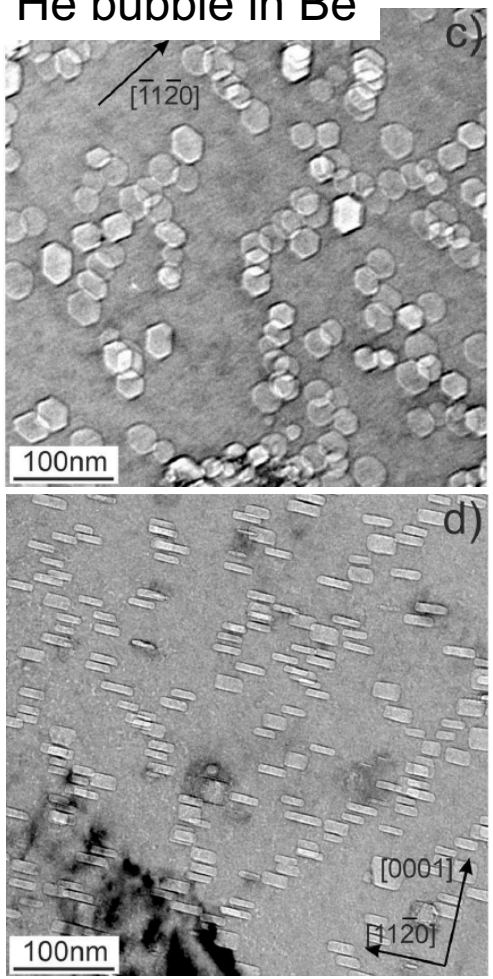
Cluster diffusion



Cluster

Experiments: Neutron vs Proton Irradiation

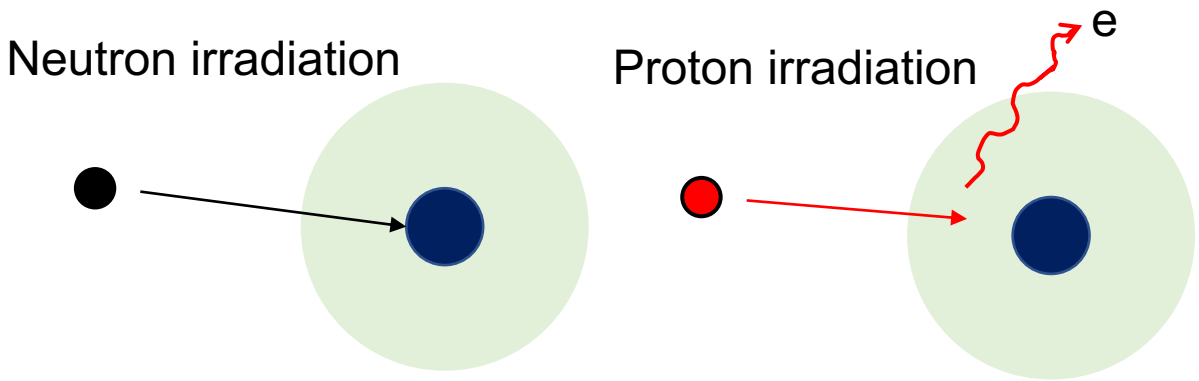
He bubble in Be



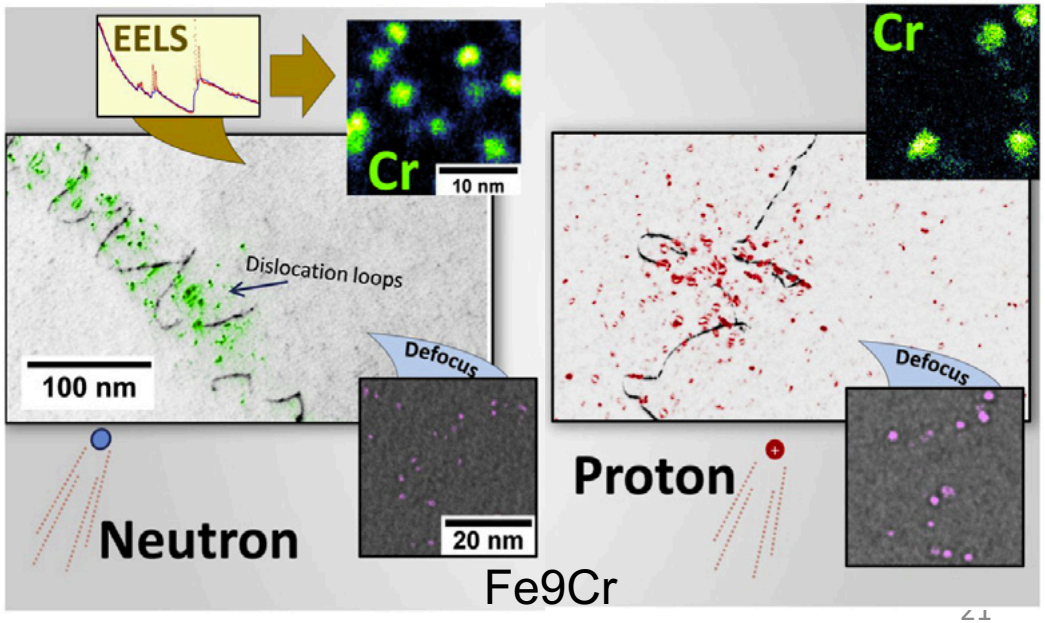
Neutron irradiation @ 713 K, >3000 appm He

M. Klimenkov, et al. *Sci. Rep. 10 (2020) 8042*

- *Stopping power difference:*



- *Radiation damage profile difference:*



J. C. Haley et al. JNM, 533 (2020) 152130.

Experimental Plan

Combine low-energy proton irradiation of Be with or without dual He ion implantation (Proton + He) and advanced materials characterization in order to include multiple DPAs and temperatures of interest

Beryllium dedicated glove box

Characterization Lab for Irradiated Materials

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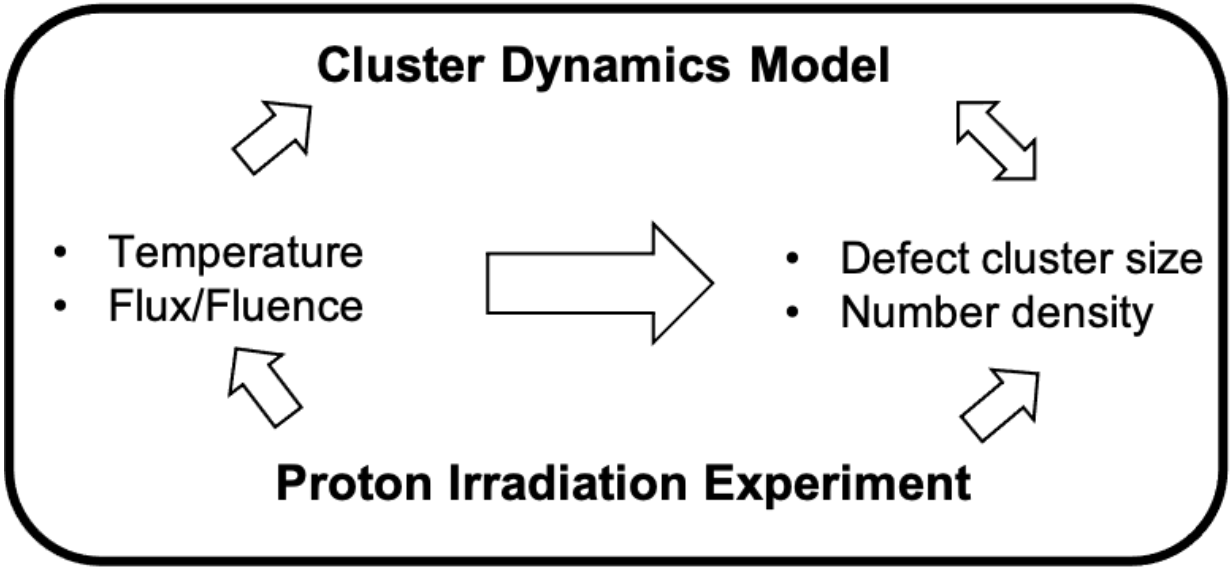
Simulation Tools for Modeling Radiation Damage in Materials

Summary and Future Work

Summary and Future Work

- Cluster Dynamics model has been built to predict the microstructure evolution in the irradiated Be metal.



- More physical processes would be involved: the size-grouping method for large cluster and diffusivity of defect clusters.
- Experimental data will be performed to validate the CD model.

COMPUTATIONAL MATERIALS GROUP

Faculty

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* Lane Schultz * Lin Lin
* Shuguang Wei * Shuxiang Zhou
* Tianyu Ma * Tomonori Baba
* Vrishank Jambur * Wei Li
* Yeqi Shi * Yipeng Cao
* Yu-chen Liu * Zhuohan Li

Undergraduate Students

* 25+ students involved in Informatics Skunkworks
https://skunkworks.engr.wisc.edu/

Informatics Skunkworks

Thank you for your attention!

Computational Materials Group