Multiscale modeling of radiation damage in materials

材料照射損傷のマルチスケールモデリング研究

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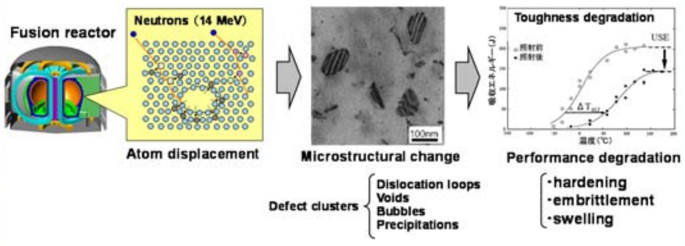
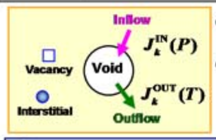
The necessity of prediction of material behavior during irradiation

- The fist wall materials in a fusion reactor suffer from high energy neutron bombardment.
- This causes microstructural changes of the materials, resulting in degradation of the materials' performance.

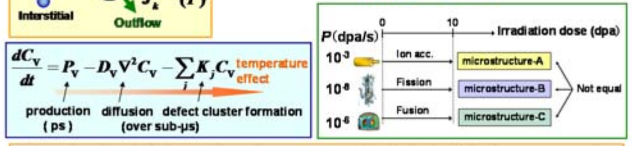


For a reliable fusion reactor, material behavior during irradiation, "radiation damage", should be accurately predicted.

How to predict radiation damage in fusion environment (3/3)



- Microstructural change is caused by defect cluster formation.
- Growth of a defect cluster is determined by balance between inflow and outflow of point defects.

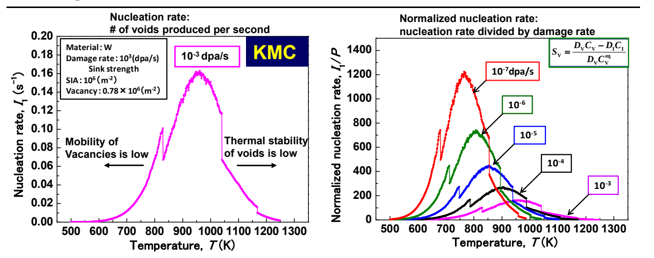


Microstructural change is a phenomenon in defect diffusion process, in which temperature is very important parameter.

- Damage rate P(dpa/s), helium gas production rate (appm He/s)
- Temperature, sink strengths, ･･･

For estimation of microstructural change in fusion environment, it is necessary to understand the relationship between irradiation field and microstructural change, "Irradiation correlation".

Damage rate & temperature dependence of void nucleation

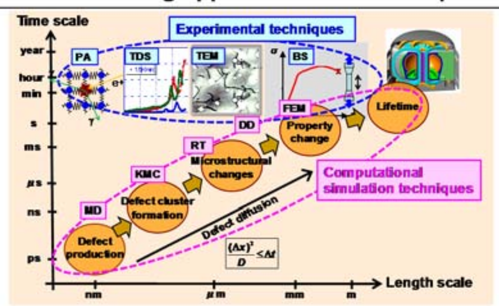


Void nucleation has a peak temperature.

- All curvatures should be completely matched without damage rate.
- With increasing damage rate, peaks shift to high temperature side.

Damage rate dependence is important for void formation.

Multiscale modeling approach of irradiation processes

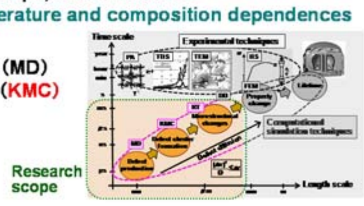


- Temporally and spatially multiscale phenomena.
- Complementary use of those evaluation techniques is necessary.
- Microstructureal change is a key of the prediction of property change.

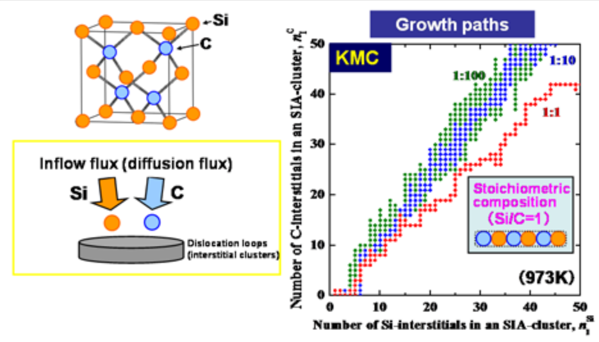
Objectives & procedures

Theoretical modeling of microstrucural change in material during irradiation for a description of irradiation correlation.

- **Materials**
  - ･Metals: Tungsten (W), iron (Fe)
  - ･Ceramics: Silicon carbide (SiC)
- **Target**
  Modeling of defect cluster nucleation taking into account of multiscale feature of radiation damage
  ※Voids, dislocation loops, helium bubbles
  ※damage rate, temperature and composition dependences
- **Main procedures**
  - ･Molecular dynamics (MD)
  - ･Kinetic Monte-Carlo (KMC)
  - ･Rate theory (RT)



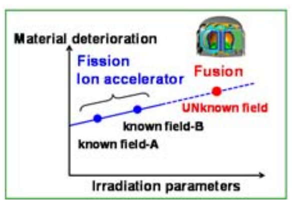
Composition dependence of dislocation loop nucleation in silicon carbide (SiC) during irradiation



Composition dependence is also important for defect cluster formation in a multi-component material.

How to predict radiation damage in fusion environment (1/3)

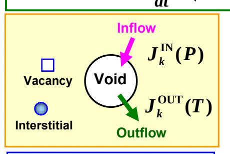
- Irradiation data has been obtained from alternative irradiation facilities such as existing *material testing reactors* and *ion accelerators*.
- Extrapolation of the irradiation data to those in fusion reactor environment is required.
- Methodology to theoretically interpret the irradiation data should be developed.



Model of defect cluster formation

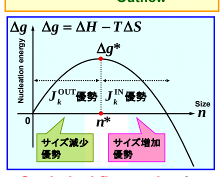
Growth or shrinkage are determined by the net flux of point defects.

Growth rate $\frac{dn}{dt} = \left(J_V^{IN} - J_V^{OUT} - J_I^{IN} + J_I^{OUT}\right)$



Influx of point defects into a cluster $J_k^{IN} = \alpha D_k C_k \quad (k = V, I, ...)$

Outflux of point defects from a cluster $J_k^{OUT} = \alpha D_k C_k^{eq} \quad (k = V, I, ...)$



Statistical fluctuation is needed for nucleation.

$$D_k = \frac{1}{6}\lambda^2 z \nu_0 \exp\left(-\frac{E_m^k}{k_B T}\right)$$

← Migration energy of a point defect

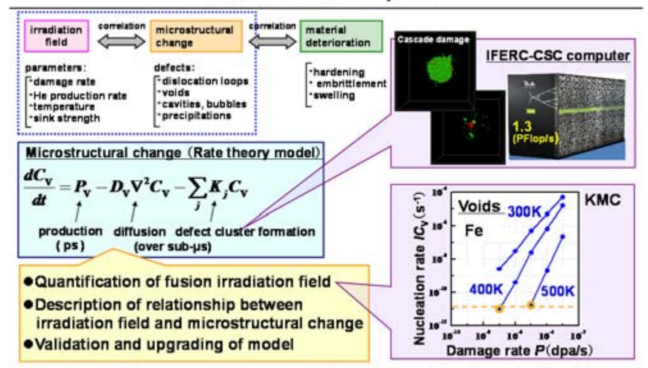
$$C_k^{eq} = \exp\left(-\frac{E_B^{cluster-k}}{k_B T}\right)$$

← Binding energy of a point defect to a cluster

Input parameters:
- Defect energies ← MD calculations
- Defect concentrations ← RT analysis

Nucleation model based on Monte-Carlo technique is developed.

Future research plan



- Quantification of fusion irradiation field
- Description of relationship between irradiation field and microstructural change
- Validation and upgrading of model

An *irradiation correlation model* to interpret the irradiation data will be developed, which is required for prediction of radiation damage in fusion reactor.

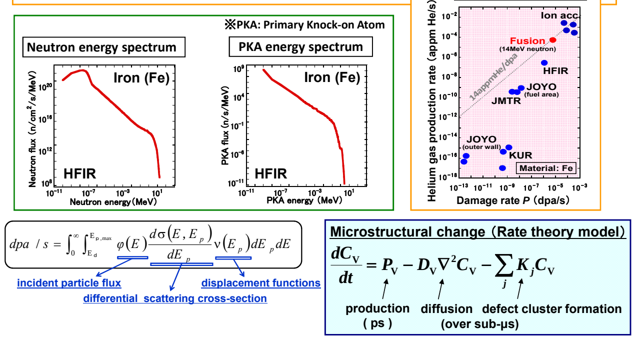
How to predict radiation damage in fusion environment (2/3)

Remarkable difference between irradiation facilities (irradiation fields) is defect production by atomic displacement.

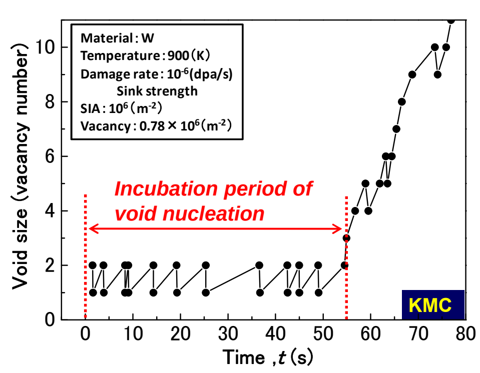
- Damage rate P(dpa/s), helium gas production rate (appm He/s)
- Temperature, sink strengths, ･･･

dpa: displacement per atom

※PKA: Primary Knock-on Atom



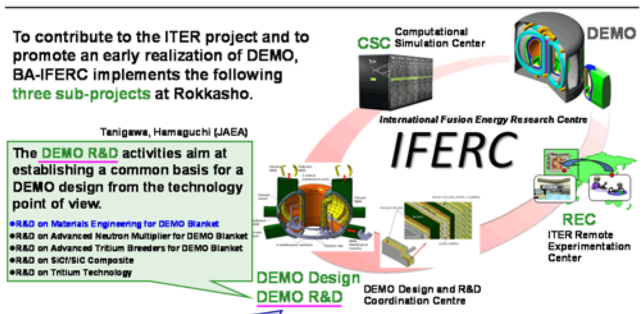
Void nucleation simulation: Kinetic Monte-Carlo (KMC) technique



Our research in the BA-IFERC activities

To contribute to the ITER project and to promote an early realization of DEMO, BA-IFERC implements the following three sub-projects at Rokkasho.

The DEMO R&D activities aim at establishing a common basis for a DEMO design from the technology point of view.



Main task of R&D on Materials Engineering for DEMO Blanket, ~2017

Task 1	Optimization of fabrication technology
Task 2	Irradiation effects on mechanical properties and microstructure
Task 3	Basic engineering for material property and structural design interface