

Development of Advanced Materials for Spallation Neutron Sources and Radiation Damage Simulation Code Based on Multi-Scale Model*

Masayoshi Kawai¹, Hiroaki Kurishita², Hiroyuki Kokawa²,

Kenji Kikuchi³, Shigeru Saito³, Seiichi Watanabe⁴,

Toshimasa Yoshiie⁵, Masatoshi Futakawa⁶ and JSPS Grant Team

1. High Energy Accelerator Research Organization (KEK),

2. Tohoku University,

3. Ibaraki University,

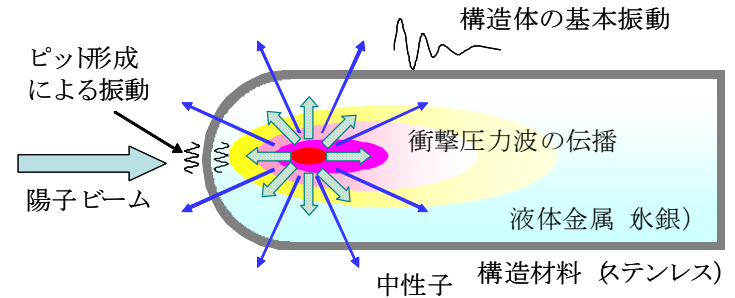
4. Hokkaido University,

5. Kyoto University and

6. Japan Atomic Energy Agency (JAEA)

- Super tungsten with high toughness and R.T. ductility
- GBE stainless steel highly resistant to corrosion and radiation
- Multi-scale model simulation of radiation damage

Objective



Development of materials for the pulsed spallation neutron sources with a MW-power injection of proton beam
And investigation of damage process due to radiation and beam impact

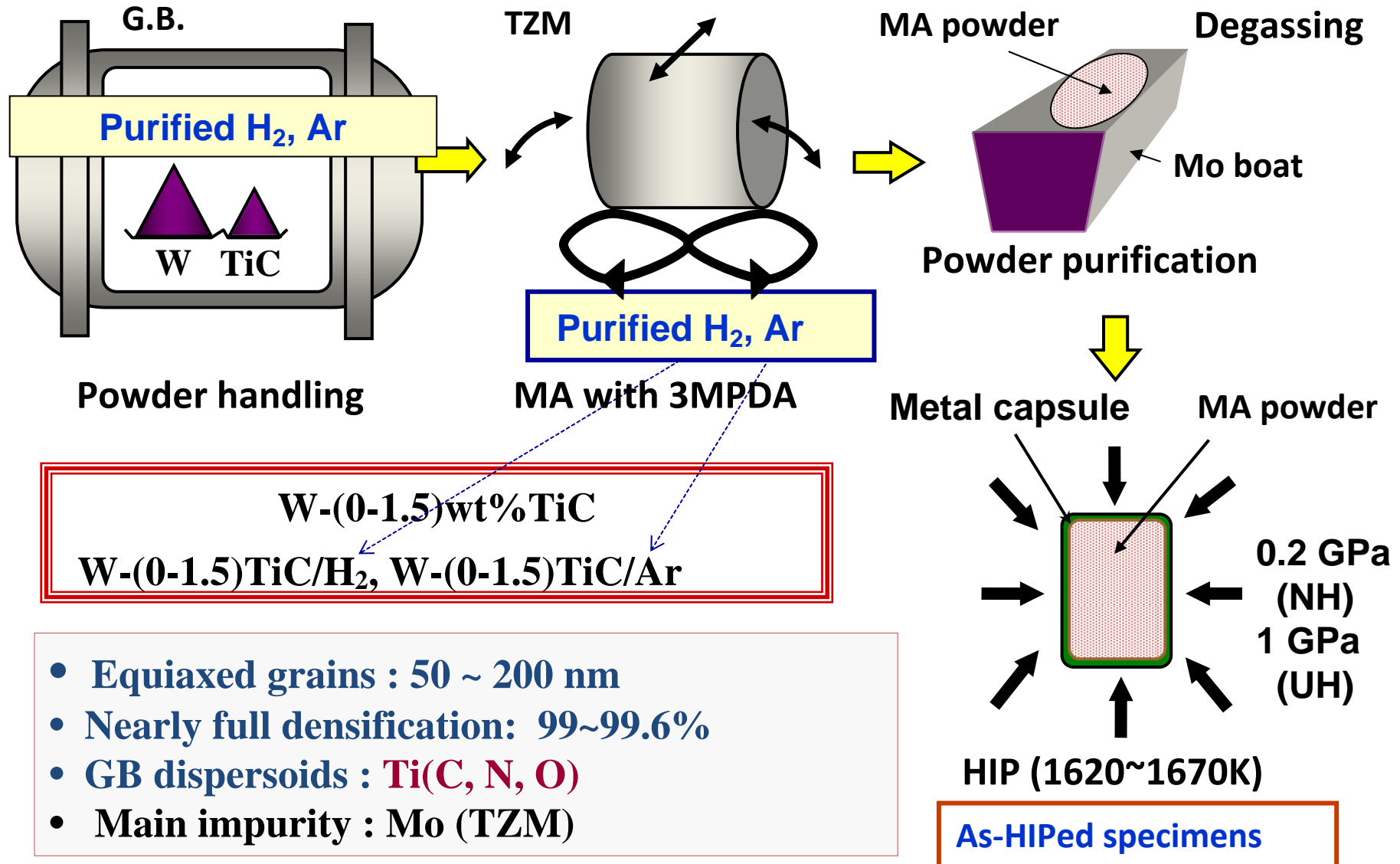
Material Needs for Long-life Source:

- Highly tough tungsten for spallation NS and fusion reactor
- High corrosion- and radiation-resistance SUS (> 10 dpa)

Needs to Radiation Damage Analyses for ADS and pulsed source:
Multi-scale model simulation

Super tungsten with high toughness and R.T. ductility (1)

Processing of UFG W-TiC compacts --- To be presented by H. Kurishita,



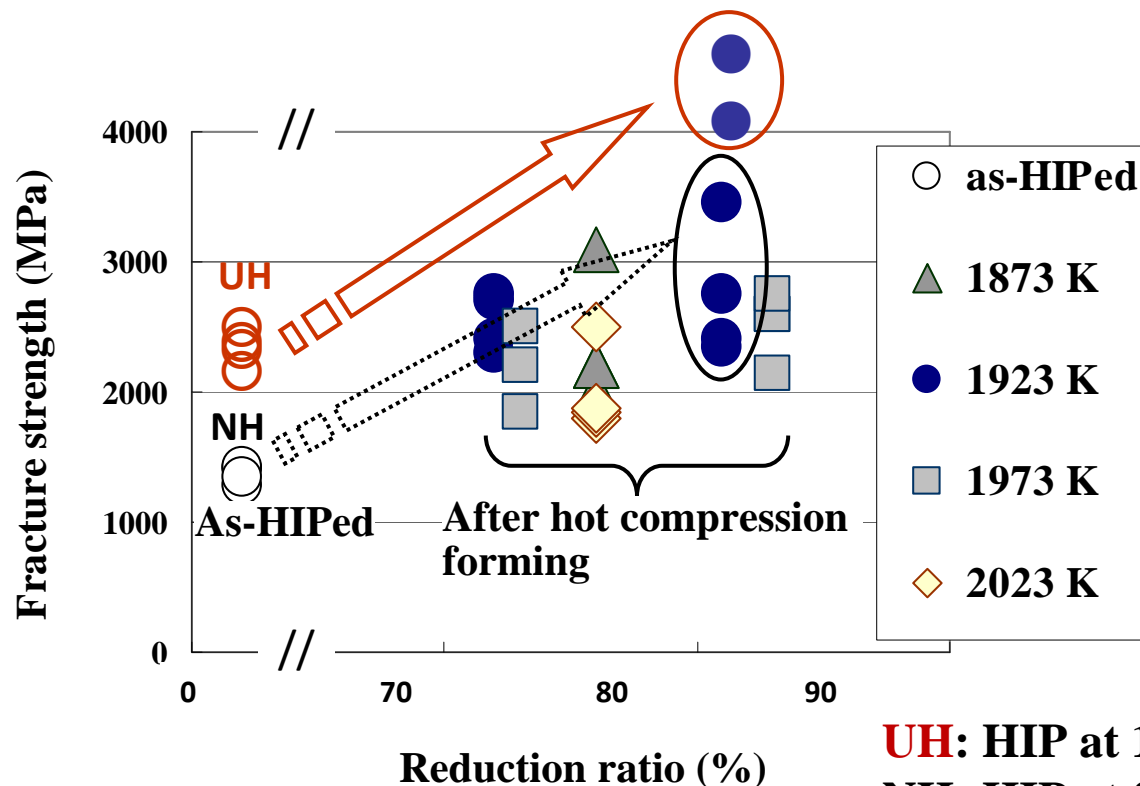
Super tungsten with high toughness and R.T. ductility (2)

Hot compression forming (HCF) in the recrystallized state

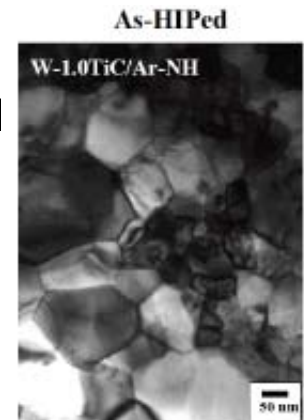
W-(1~1.1)%TiC/Ar: $1\text{GPa} \rightarrow 4.4\text{GPa}$, RT ductility

Condition

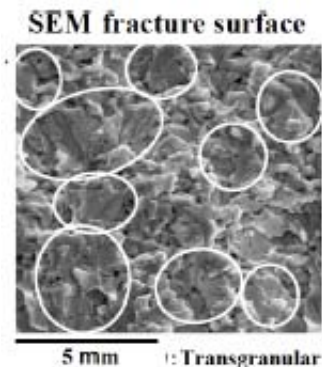
1873 ~ 2023K : $\sigma_f = 60 \sim 160 \text{ MPa}$, $m = 0.3$, $\varepsilon_t > 160\%$



As-HIPed
(Before HCF)



After HCF

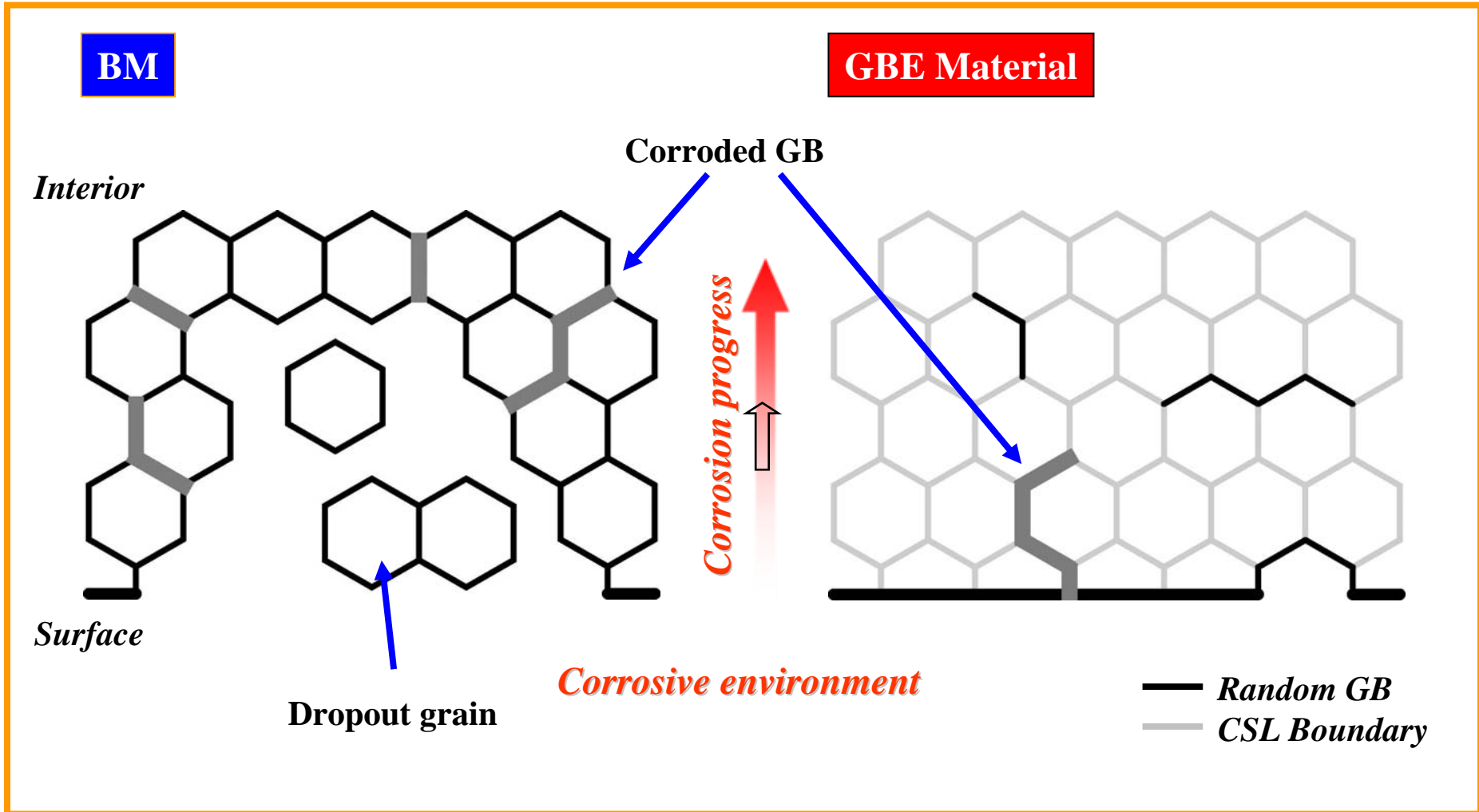


Recent activities on GBE materials (1)

Comparison of Corrosion Scheme between BM and GBE Material

BM: Cr_{23}C_6 precipitation at random GB \rightarrow Depletion of Cr content \rightarrow Easily corroded

GBE material: Increase low-energy GB(CSLB) and suppress sensitization \rightarrow IGCC resistance

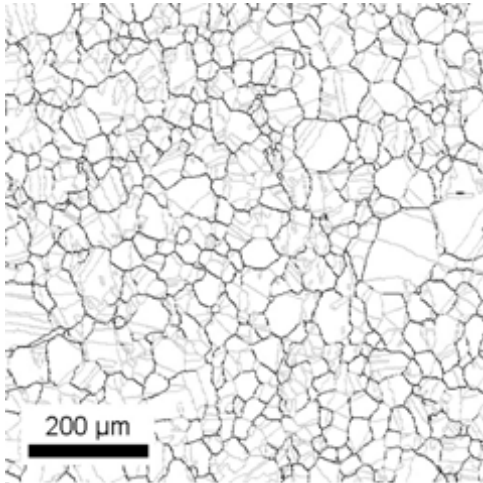


Recent activities on GBE materials (2)

Development of GBE 304SS

OIM Map (粒界性格分布)

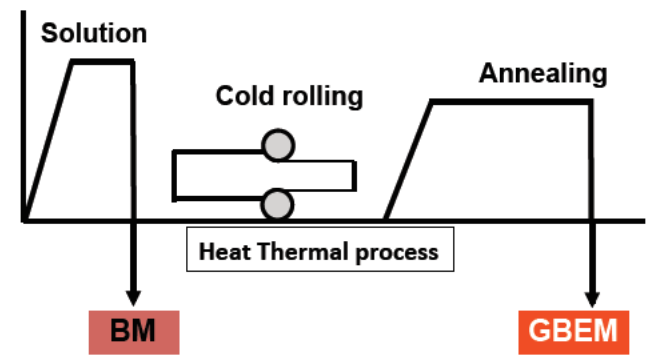
304 BM



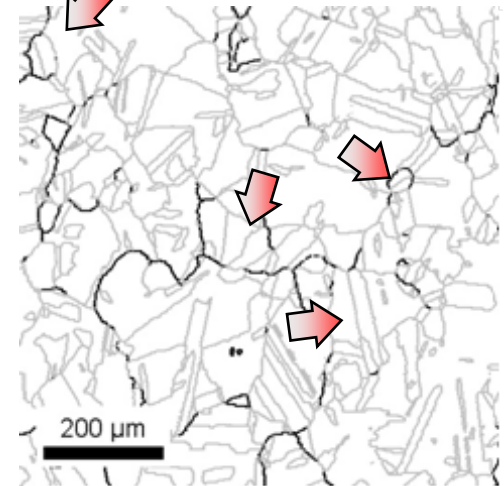
CSL%: 63%



— Random GB (high energy)
— CSLB (low energy)



304 GBEM



CSL%: 87%

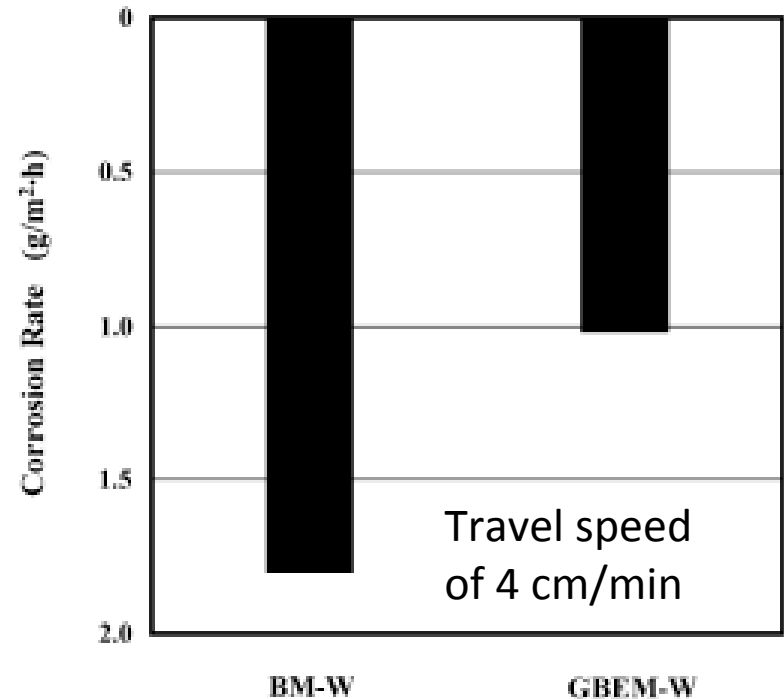
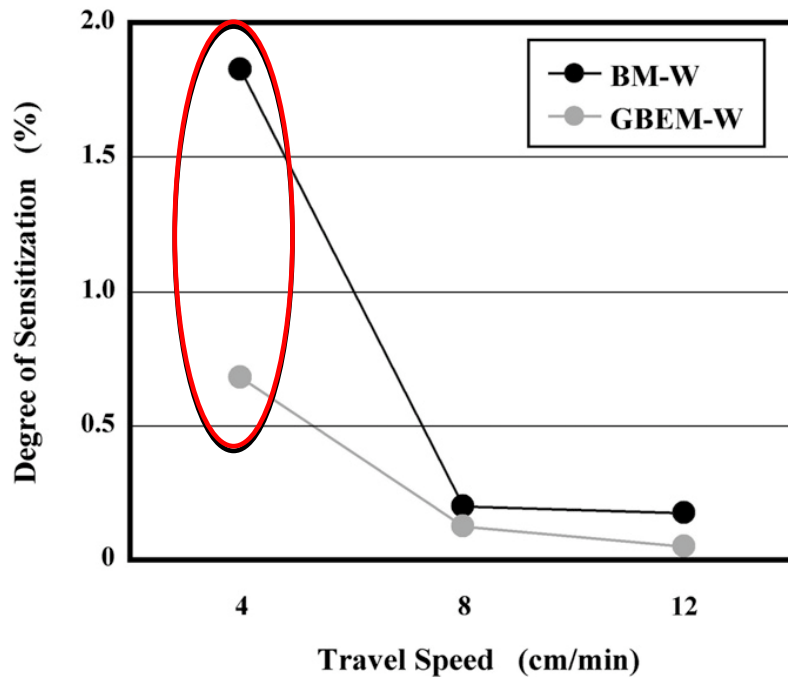
GBE 304 SS

Highly-dense CSLB + Discontinuous random GB
(BM:63% → GBEM:87%) (⇨ break)

Corrosion rate was reduced by a factor of 4

Recent activities on GBE materials (3)

Comparison of Degree of Sensitization (DOS) in the HAZ and the Corrosion Mass Loss between the Welded BM and GBEM.

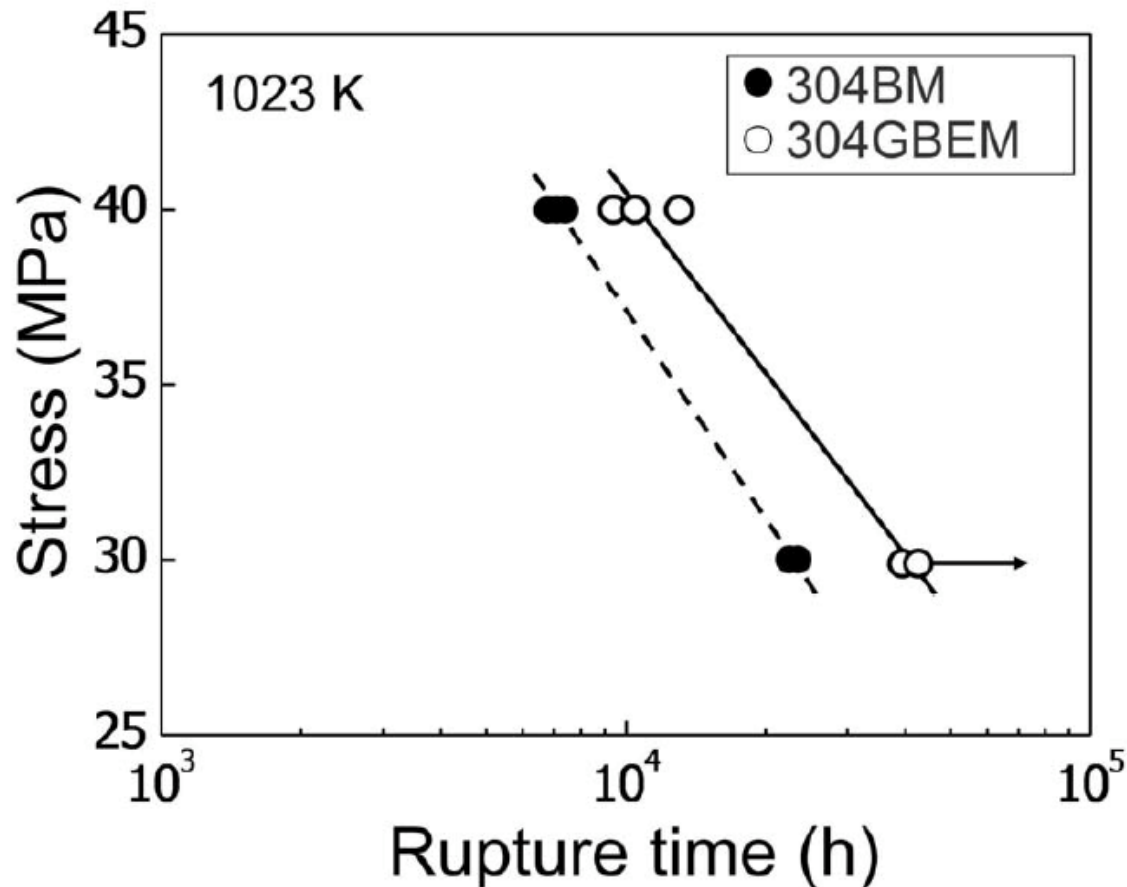


The corrosion rate of the weld-decay region in the GBEM-W was about half of that in the BM-W.

The corrosion rate in the GBEM-W should be much smaller than half of that in the BM-W, considering that the Streicher-tested specimen consisted of the whole weldment including other non-sensitized parts.

Recent activities on GBE materials (4)

Creep Test of SUS304 at 1023 K



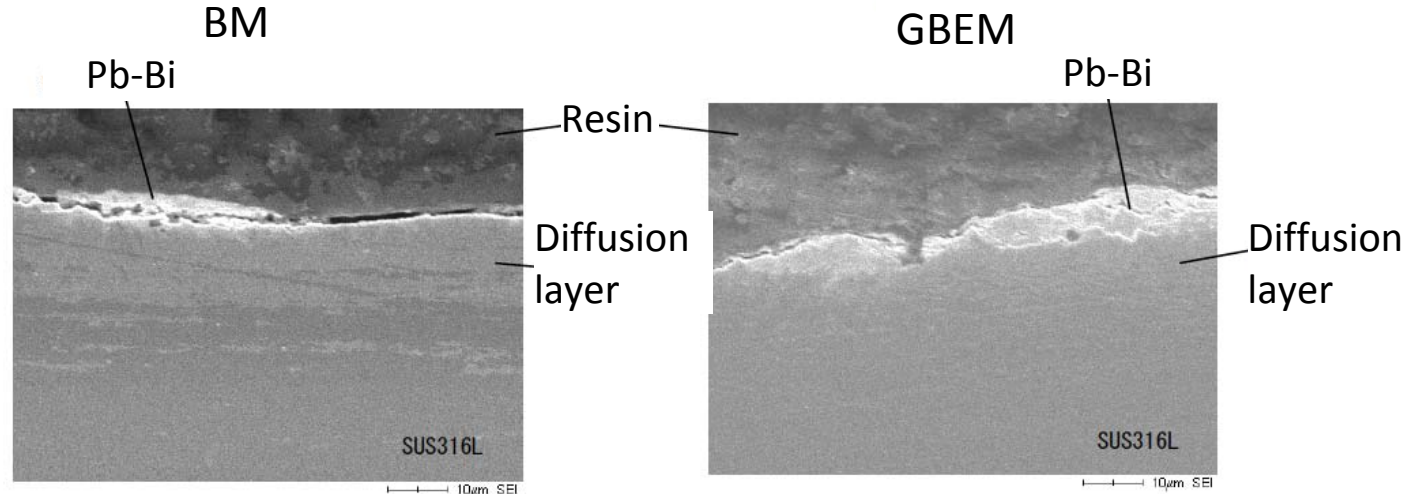
CSL has a possibility to suppress a grain boundary sliding.

Rupture time of 304GBEM was 1.5 times larger than that of 304BM.

Recent activities on GBE materials (5)

--- Presented by S. Saito, 10/19 13:55 in IWSMT-10

Erosion test of BM and GBEM in Pb-Bi Flow



Polished 316L BM: remarkably eroded



Pb-Bi flow

500μm

Polished 316L GBEM

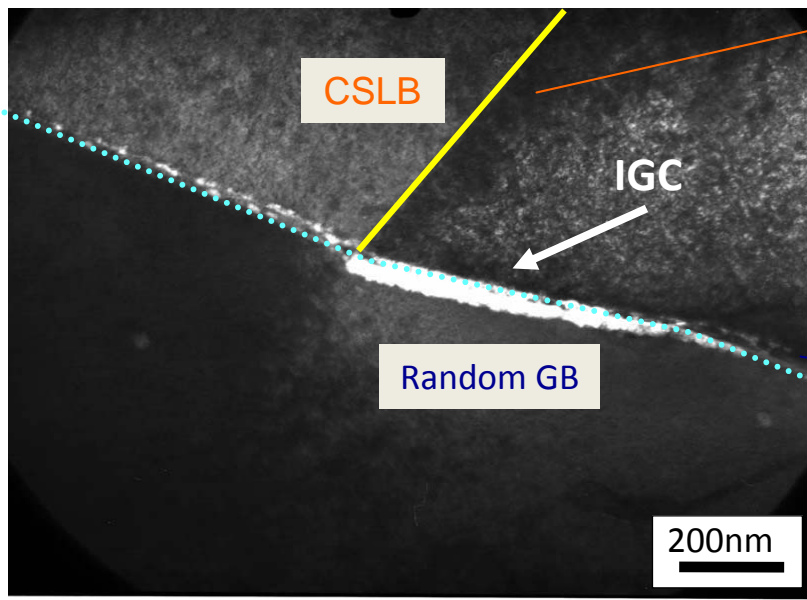


Recent activities on GBE materials (6)

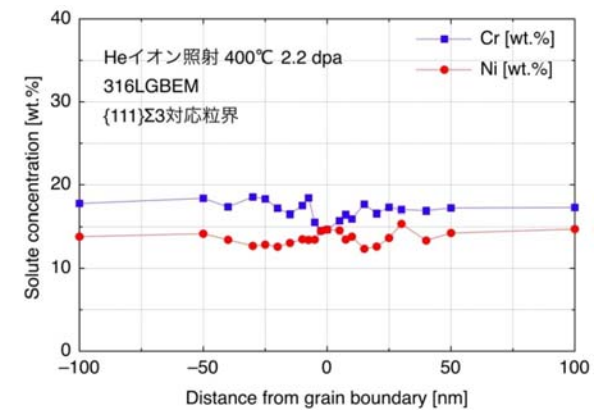
Beam Irradiation Experiments

- ◎ High voltage electron microscope (L-HVEM) with a function of multi-beam irradiation by electron, ion and laser
 - Electro-etching in 10% oxalic solution

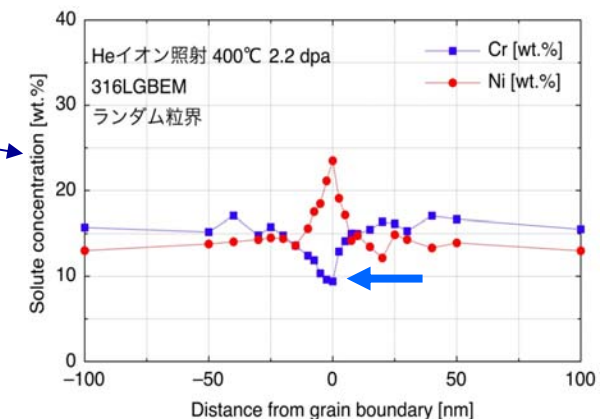
Observation of micro-structure after etching



Scare segregation



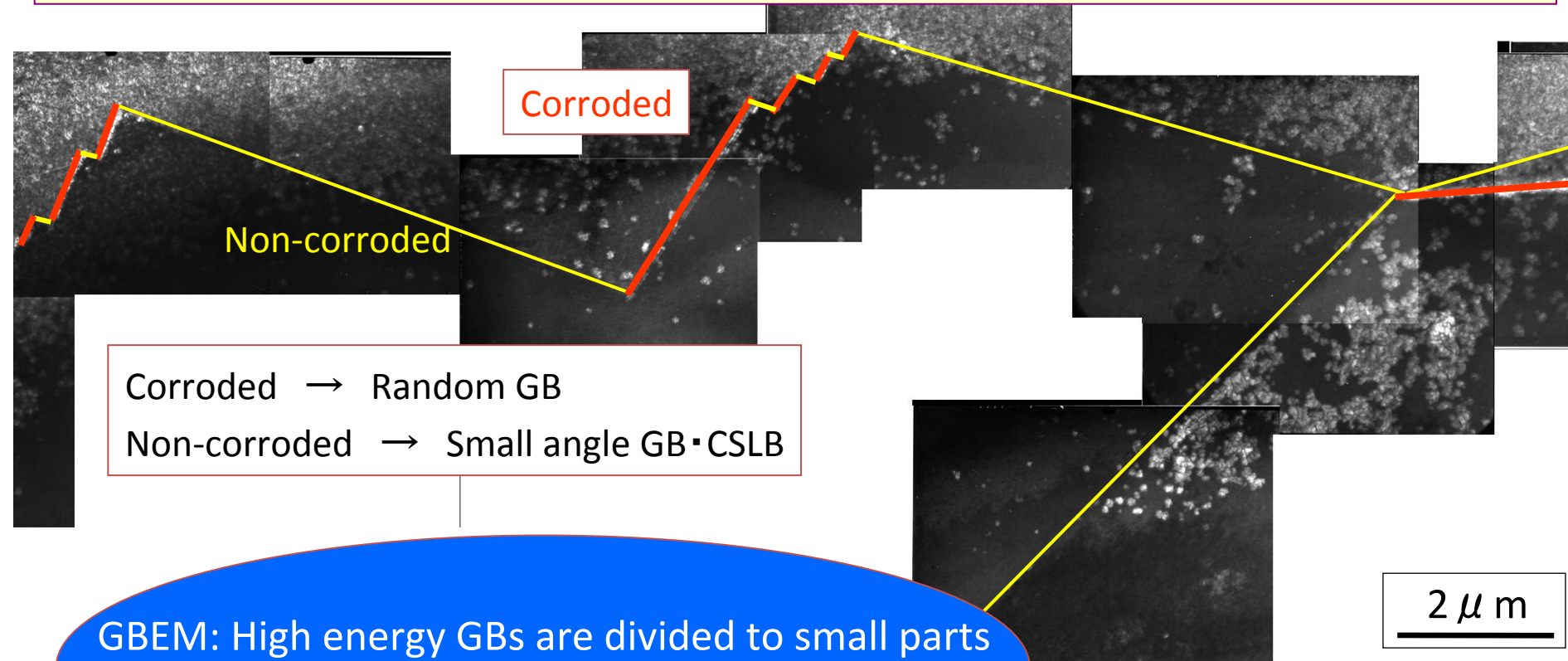
Cr depletion down to 12%



Recent activities on GBE materials (8)

CLS's: Dividing into parts of IGC network

SUS316GBEM: He ion irradiation (400°C, 2.2dpa) + Electroetching (10% oxalic solution)



GBEM: High energy GBs are divided to small parts
→ High inter-granular corrosion resistance

MULTI-SCALE MODELING OF IRRADIATION EFFECTS IN SPALLATION NEUTRON SOURCE MATERIALS

Toshimasa Yoshiie¹, Takahiro Ito², Hiroshi Iwase³,
Yoshihisa Kaneko⁴, Masayoshi Kawai³, Ippei Kishida⁴, Satoshi Kunieda⁵, Koichi
Sato¹, Satoshi Shimakawa⁵, Futoshi Shimizu⁵, Satoshi Hashimoto⁴, Naoyuki
Hashimoto⁶, Tokio Fukahori⁵, Yukinobu Watanabe⁷, Qiu Xu¹, Shiori Ishino⁸

¹Research Reactor Institute, Kyoto University

*² Department of Mechanical Engineering, Toyohashi University of Technology
High Energy Accelerator Research Organization*

Osaka City University

⁵Japan Atomic Energy Agency

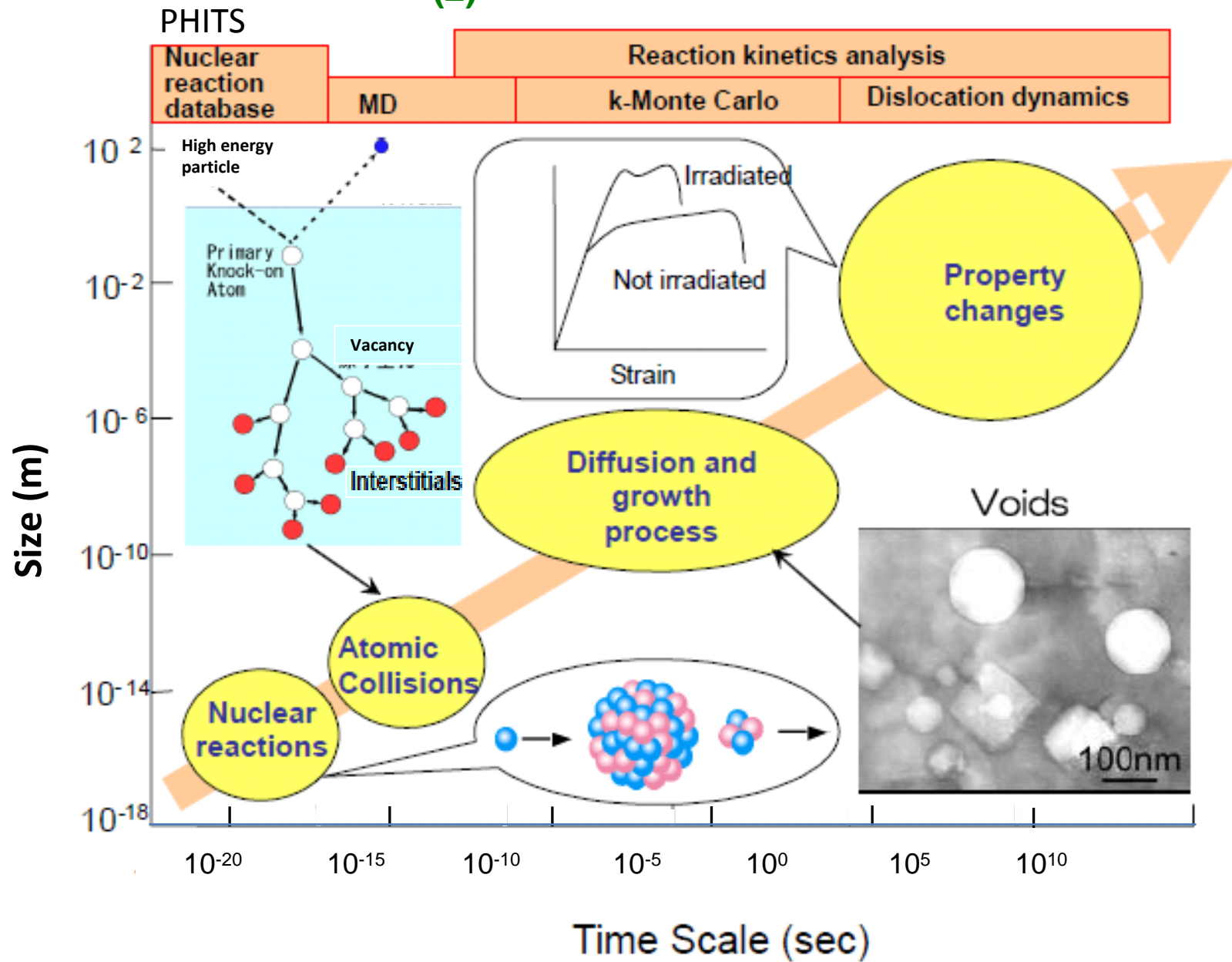
⁶Hokkaido University

⁷ Kyushu University

⁸Univerity of Tokyo

- **Nuclear reactions and electronic excitaion:** PHITS, PKA energy spectrum
- **Atomic collision :** MD, k-Monte Carlo, Subcascade analysis.
- **Damage structure evolution :** Reaction kinetic analysis
- **Mechanical properties changes :** Discrete dislocation dynamics

Multi-Scale Modeling (2)



Data flow between each code

Nuclear reactions (PHITS code)



Primary knock-on energy spectrum



Atomic collisions (Molecular dynamics)



Point defect distribution



Damage structural evolutions (Reaction kinetic analysis)



Concentration of defect clusters



Mechanical property change (Three-dimensional discrete dislocation dynamics)



Stress-strain curve

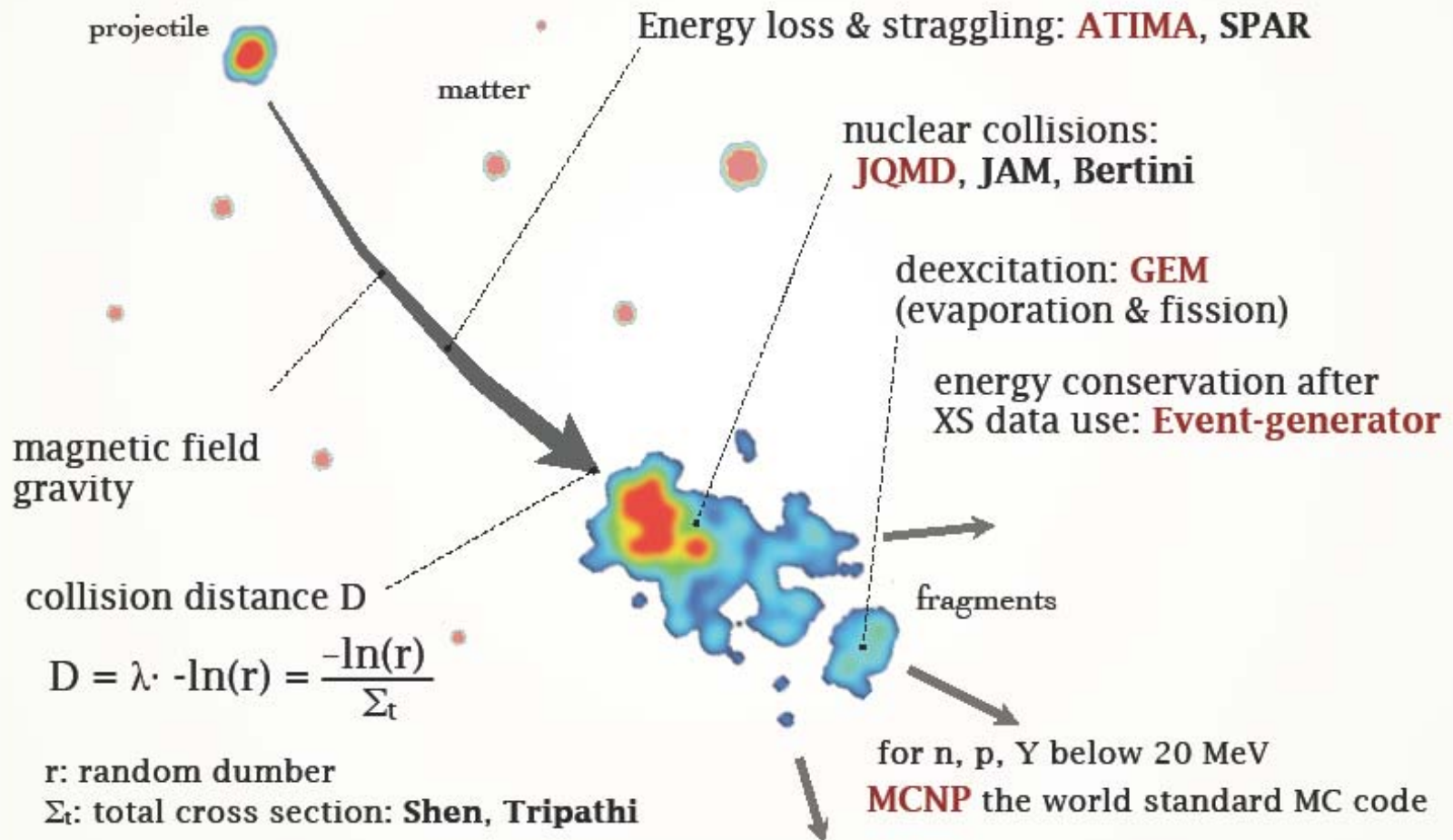
Multi-Scale Modeling

(4)

1. Nuclear Reaction

Nucleation rate of neutrons, photons, charged particles and PKA energy spectrum by them

PHITS (particle and heavy ion transport code system)



Multi-Scale Modeling (5)

PHITS (Particle and Heavy Ion Transport code System) Feature (1): JQMD-1

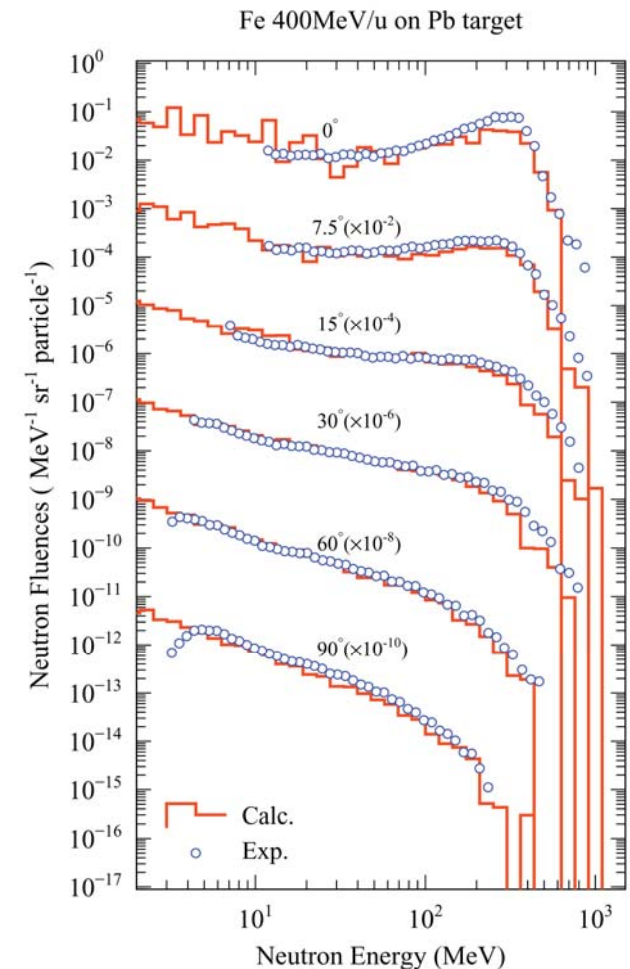
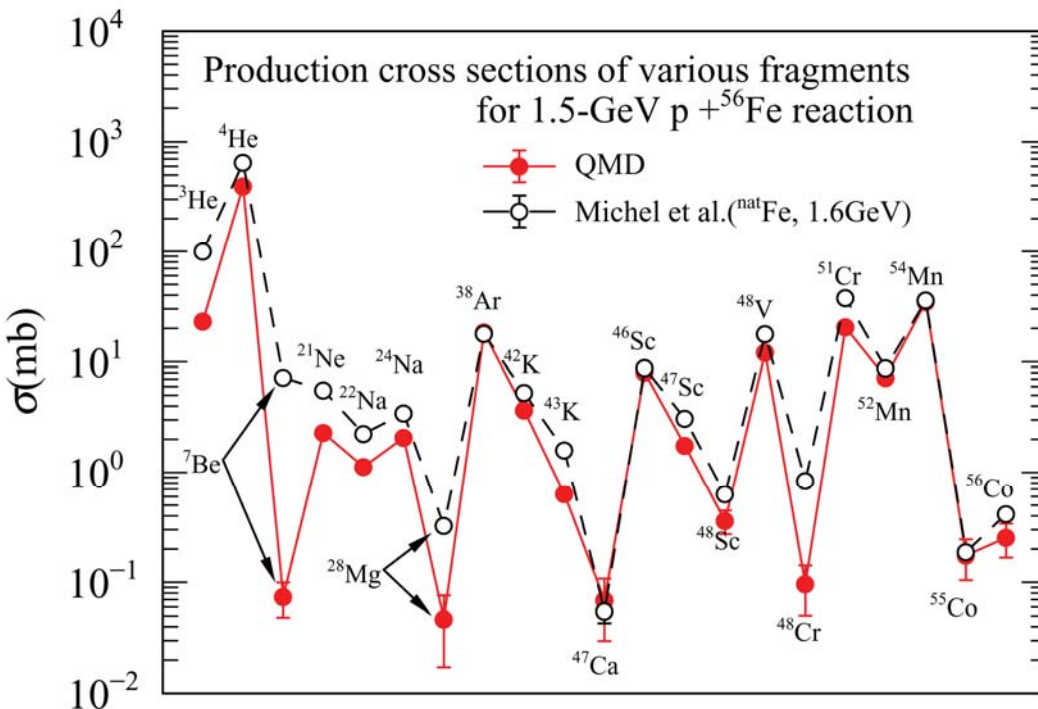
JQMD (Jaeri Quantum Molecular Dynamics) for Simulation of Nucleus-Nucleus Collisions

K. Niiita et.al. *Phys. Rev.* **C52** (1995) 2620 <http://hadron31.tokai.jaeri.go.jp/jqmd/>

H. Iwase et.al. *J. Nucl. Sci. Technol.* **39** (2002)

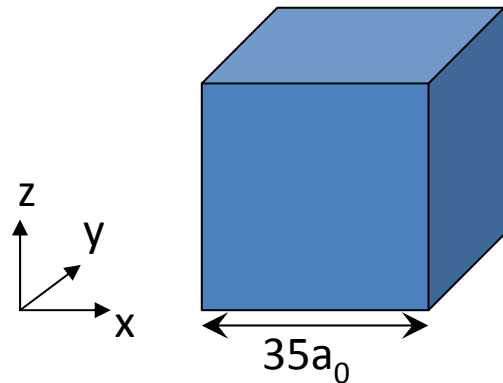
Analysis of Nucleon-Nucleus Collisions by **JQMD** 1142

S. Chiba et.al. *Phys. Rev.* **C53** (1996) 1824, **C54** (1996) 285



2 Atomic Collision Simulation by MD

Calculation Condition



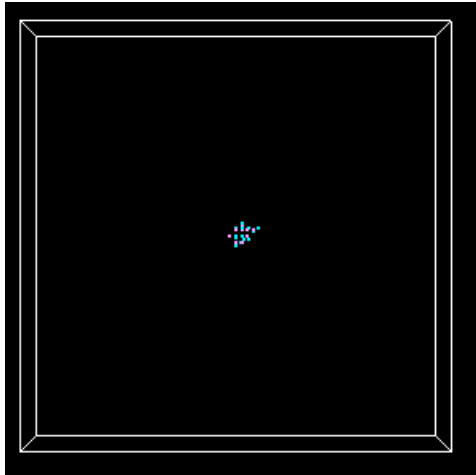
a_0 : lattice constant at
300 K

- Potential model by Daw and Baskes (1984)
- NVE ensemble (i.e., number of the atoms, cell volume and energy were kept constant)
- 35x35x35 lattices (171,500 atoms) in a simulation cell
- Periodic boundary condition for the three directions
- Initial condition : equilibrium for 50 ps, at 300 K, 0 MPa
- PKA energy: 10keV
- MD runs with different initial directions of PKA (none of which were parallel to the lattice vector.)

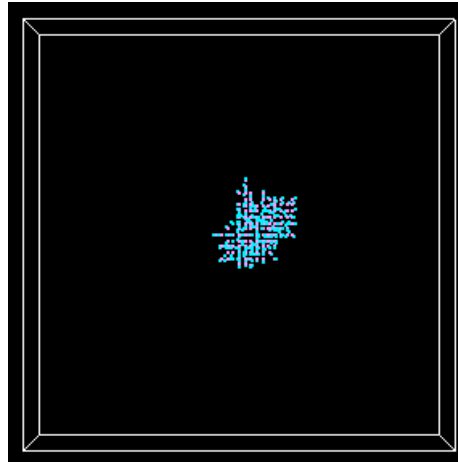
Multi-Scale Modeling (7)

Typical Distribution of Point Defects

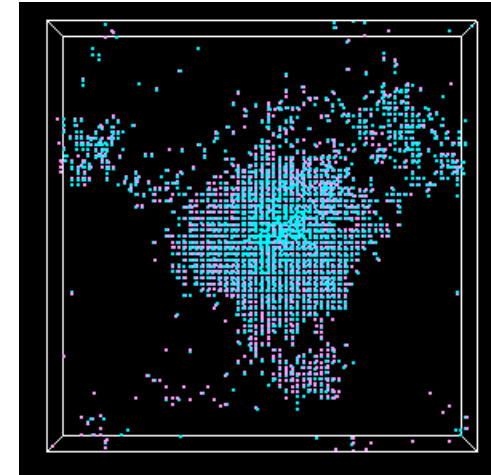
Marble : interstitial atoms, Violet : Vacancy sites



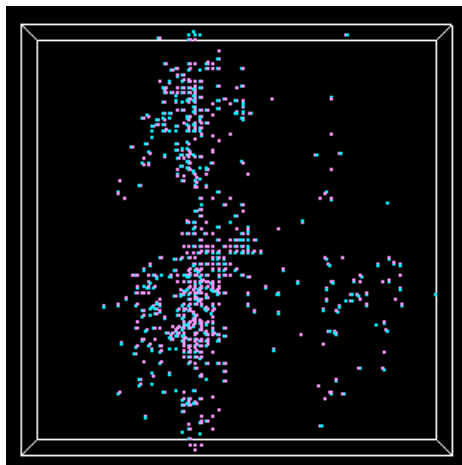
0.006ps



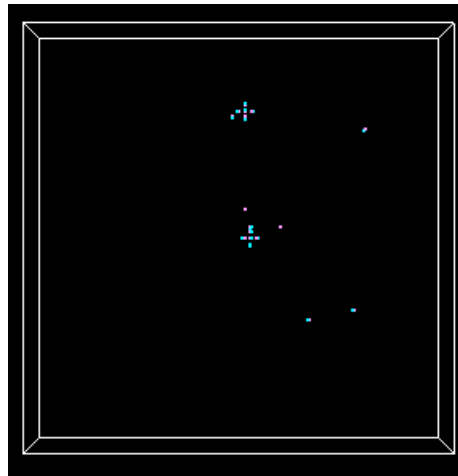
0.025ps



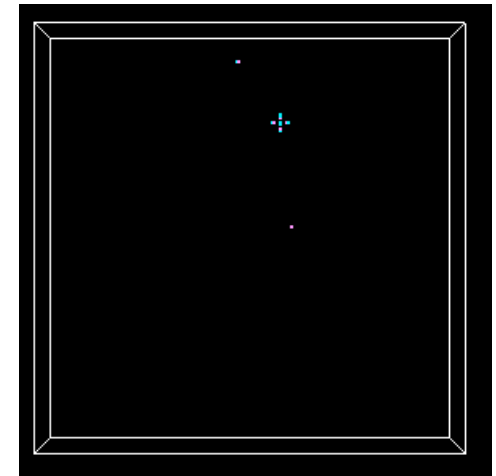
1.132ps



7.395ps



18.40ps



96.38ps

3. Damage Structure Evolution by Reaction Kinetic Analysis

$$\frac{dC_I}{dt} = P_I - 2Z_{I,I}M_I C_I^2 - Z_{I,V}(M_I + M_V)C_I C_V$$

damage production I-I recombination mutual annihilation

$$- Z_{I,IC}M_I C_I S_I - Z_{I,VC}M_I C_I S_V - M_I C_I C_S \dots\dots\dots$$

absorption by loops absorption by voids

annihilation of interstitials at sink

C_I : Interstitial concentration (fractional unit).

C_V : Vacancy concentration

Z : Cross section of reaction

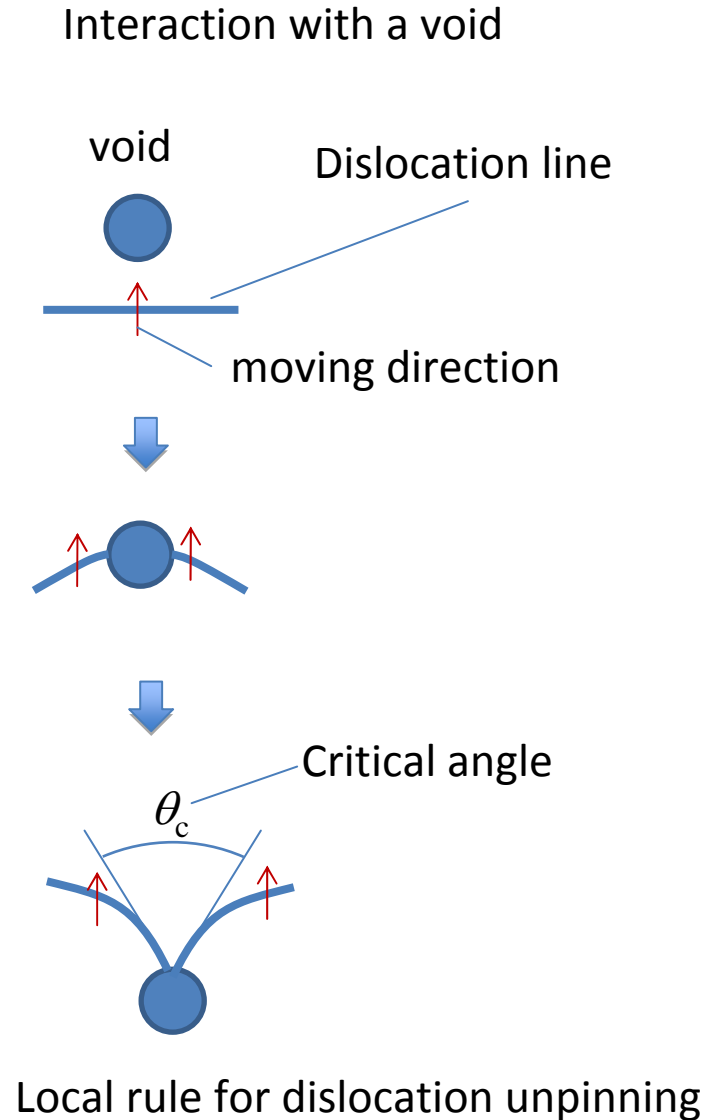
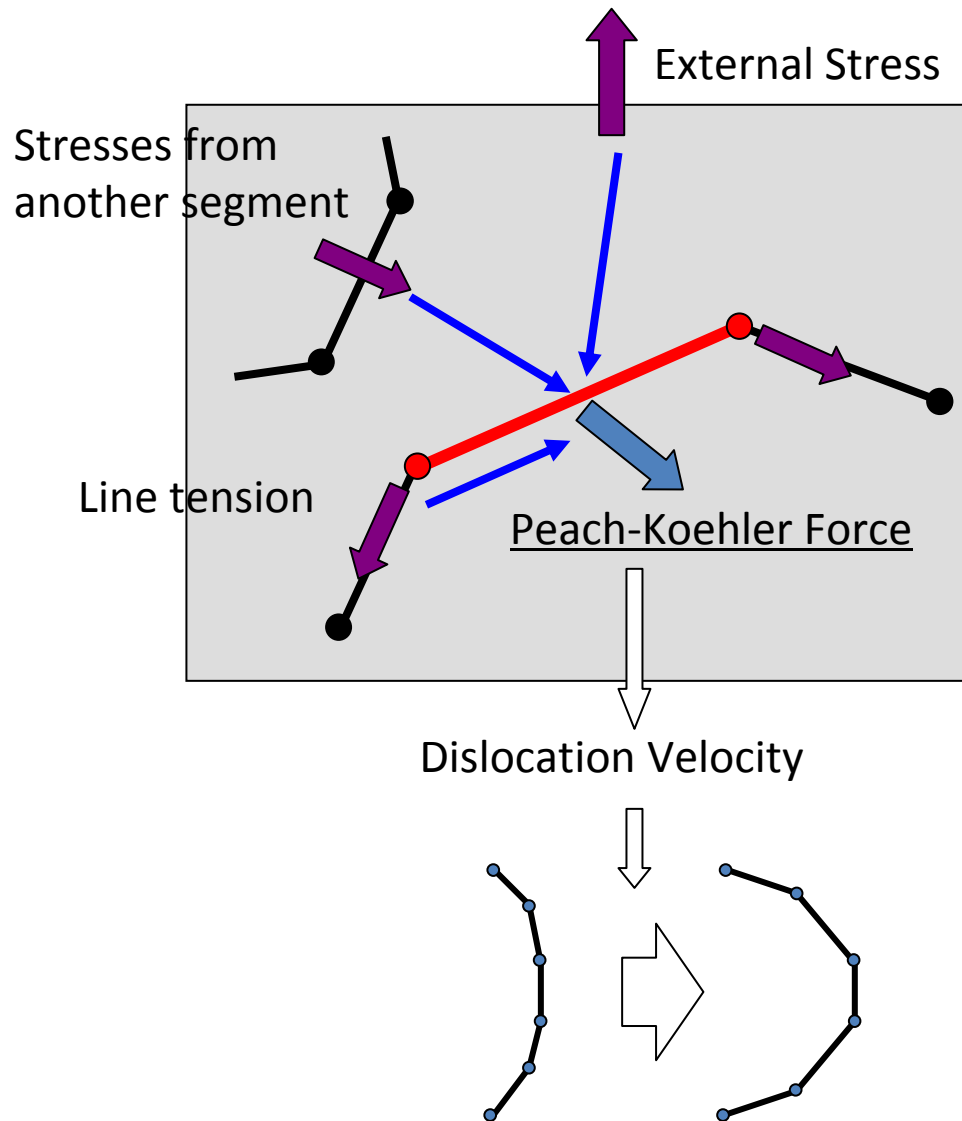
M : Mobility

4. Estimation of mechanical property changes with the 3D-Discrete Dislocation Dynamics code

- Strengths of multilayered structures have been investigated using three-dimensional discrete dislocation dynamics (DDD) simulation.
- The multilayered structure was modeled as a stack of misfit dislocation networks which must exist at an interface between adjoining crystals having different lattice constants.
- Passages of a single mobile dislocation through several kinds of network stacks were simulated.
- The critical stress required for the dislocation passage depended on the dislocation spacing of the network, the number of network sheet and the spacing between network sheets.

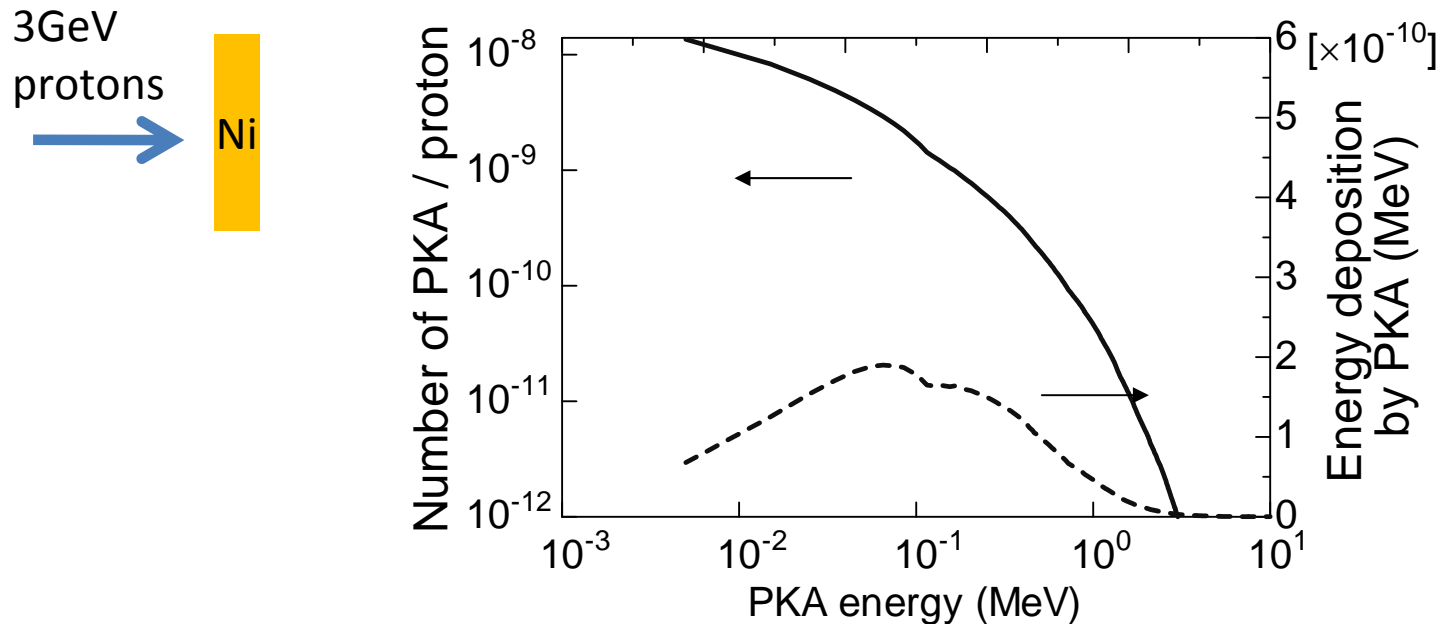
Multi-Scale Modeling (10)

3D-Discrete Dislocation Dynamics Procedure



Sample Calculation in Case of Ni

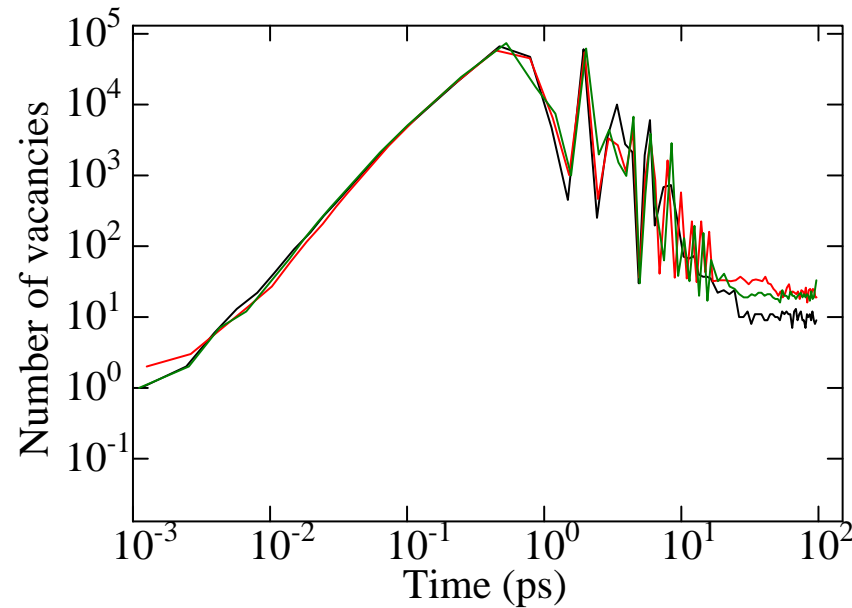
Result of PHITS Simulation



Number of PKA energy (left) and energy deposition by PKA (right) in 3 GeV proton irradiated Ni of 3 mm in thickness.

Results of MD Calculation

Number of
vacancies



- On average 17 vacancies, 17 interstitials were produced.
- Formation of defect clusters is calculated by k-Monte Carlo.
Clusters of three point defects are formed.

Results of k-Monte Carlo under the condition at 423K and 10 dpa:

Formation of vacancy clusters of four vacancies, concentration:
 0.59×10^{-3} ,
Dislocation density: $1.1 \times 10^{-9} \text{ cm/cm}^3$.

Multi-Scale Modeling (13)

Dislocation motion in the crystal with randomly-distributed voids

Normal stress

0MPa

200MPa

300MPa

400MPa

500MPa

600MPa

650MPa

700MPa

750MPa

800MPa

820MPa

840MPa

860MPa

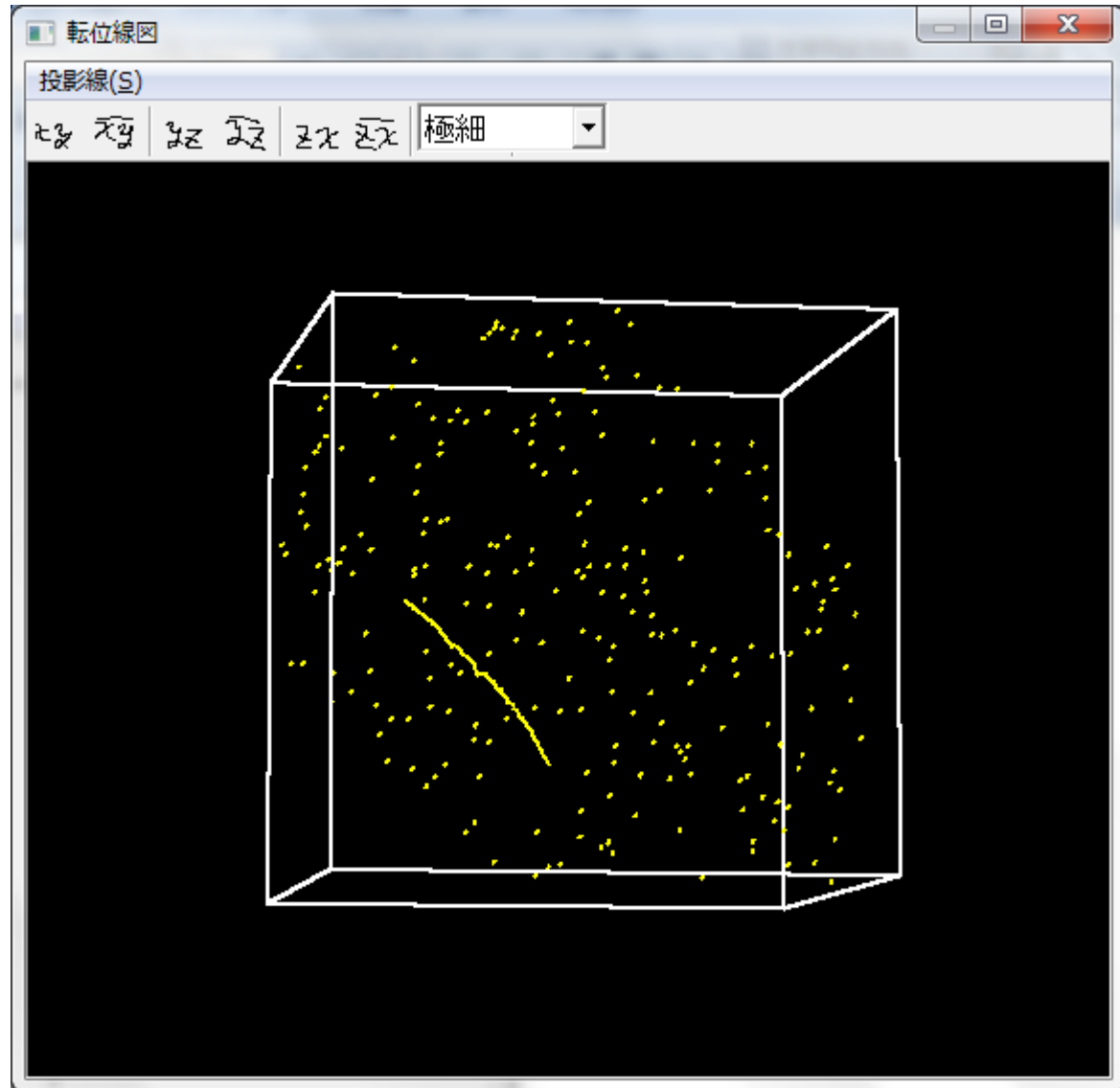
880MPa

900MPa

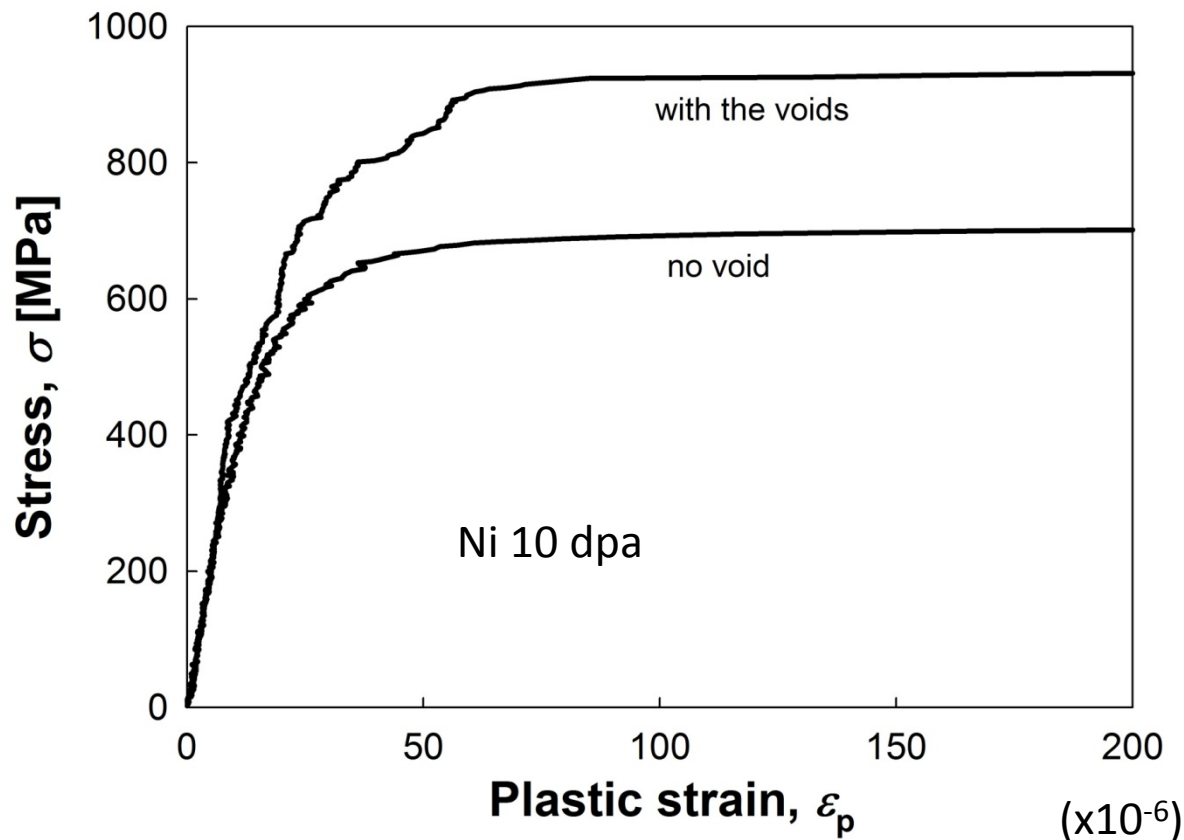
920MPa

930MPa

935MPa



Stress-Strain Curves Calculated with DDD Simulation



Plastic shear strain

$$\gamma_p = A b / V$$

Plastic strain

$$\epsilon_p = \gamma_p S_f$$

A: area swept by a dislocation

b: Burgers vector

V: volume of model crystal

S_f : Schmid factor

Plastic strain is recalculated
such that dislocation density
 $\rho = 1.1 \times 10^{-9} \text{ cm}^{-2}$

Radiation hardening is expressed.

Summary

(1) Development of materials resistant to beam impact and radiation damage

- Successful to develop a remarkably strong nano-structured tungsten with RT ductility by means of MA, HIP and TMT for strengthening weak GBs in the recrystallized state.
- Successful to develop a stainless steel resistant to intergranular corrosion and having a possibility to be strong to radiation damage and high creep resistance, by means of GBE method.
- 316L GBEM was highly resistant to Pb-Bi erosion.

(2) Multi-scale model simulation system has been constructed.

- **Nuclear reactions** : PHITS, PKA energy spectrum
- **Atomic collision** : MD, k-Monte Carlo, Subcascade analysis.
The number of point defects and clusters in the subcascade
- **Damage structure evolution** : Reaction kinetic analysis
Vacancy clusters, Dislocation density
- **Mechanical properties** : Discrete dislocation dynamics
Statistic energy calculation. Stress strain curve
- One-through calculation in case of nickel (typical fcc crystal)
- In future: Improve of parameters and DDD model considering interactions.

Thank you for your attention !

Acknowledgement:

The present work has been performed under the FY2007 to FY2011 JSPS Scientific Research Grants categorized to “S” project, No. 19106017 entitled with “Comprehensive study on material damage mechanism by experimental and theoretical methods and development of materials for high-energy quantum-beam fields”.

