Development of Dedicated Models and Databases for Elucidating Fuel Degradation Mechanism

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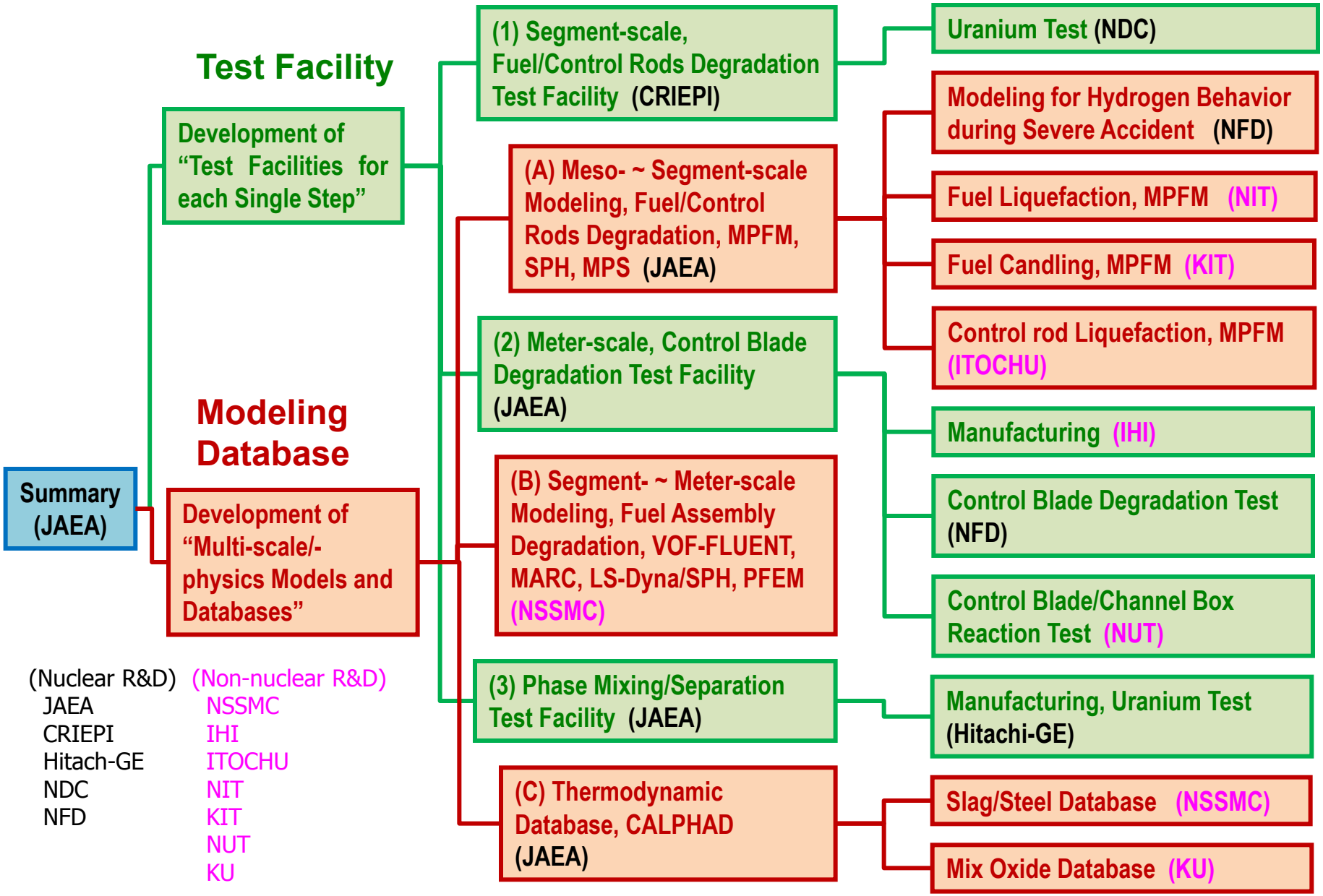
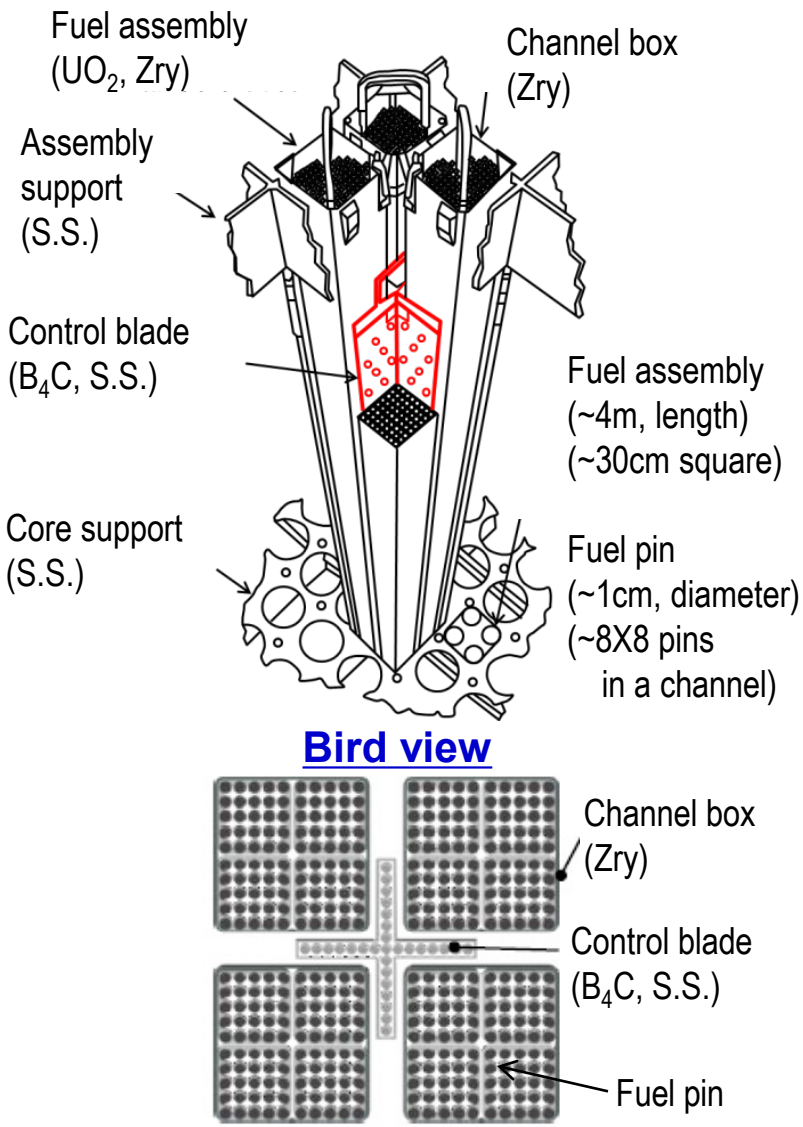
Background, Motivation

- ✔ Development of **"Multi-scale/-physics Models"** and **"Thermodynamic Database"** for detail understanding of **"Fuel Degradation Mechanism"** in nuclear severe accident in Japan. (like US, Europe, Russia, Canada,,,)
- ✔ Dedicated modeling is also proper theme for encouraging next generation nuclear scientists. (they need worthwhile R&D theme except for Fukushima issues)
- ✔ A METI (ministry of economy, trade, industry) project started in JFY-2012, by collaborating with **"Non-nuclear"** institutes, universities, and companies. (, since they have excellent knowledge on steel manufacturing, and physical/chemical condition in blast furnace is rather similar in nuclear severe accident.)

Project Members



Aims of Dedicated Modeling



Fuel Assembly Configuration of BWR.

✔ Dedicated modeling to understand **"Fuel Degradation Mechanism for Each Single Physical/Chemical Step"** of severe accident.

ex.) progress in liquefaction at the interfaces between UO_2/Zry or B_4C/S.S.

✔ Multi-scale/-physics modeling to predict **"Overlap Phenomena or Intermediate Situation"** on fuel assembly degradation.

ex.) difference on degradation among fuel, control blade, and channel box.

✔ Furthermore, to evaluate the tendency for **"what may happen in various hypothetical conditions"**.

ex.) in which area or way degraded fuel solidified, according to accident scenarios.

Role of Member Institutes for Modeling

Fuel Pin

NSSMC
(Segment Degradation)

KIT
(Candling)

NIT
(Liquefaction)
(Diffusion)

Fuel Assembly

NSSMC
(Assembly Degradation)

Control Blade

CTC
(Liquefaction)

NSSMC
(Segment Degradation)

JAEA
(Solidification)

Core Support

JAEA
(Segment Solid/Melt)

NSSMC
(Core Support Degradation)

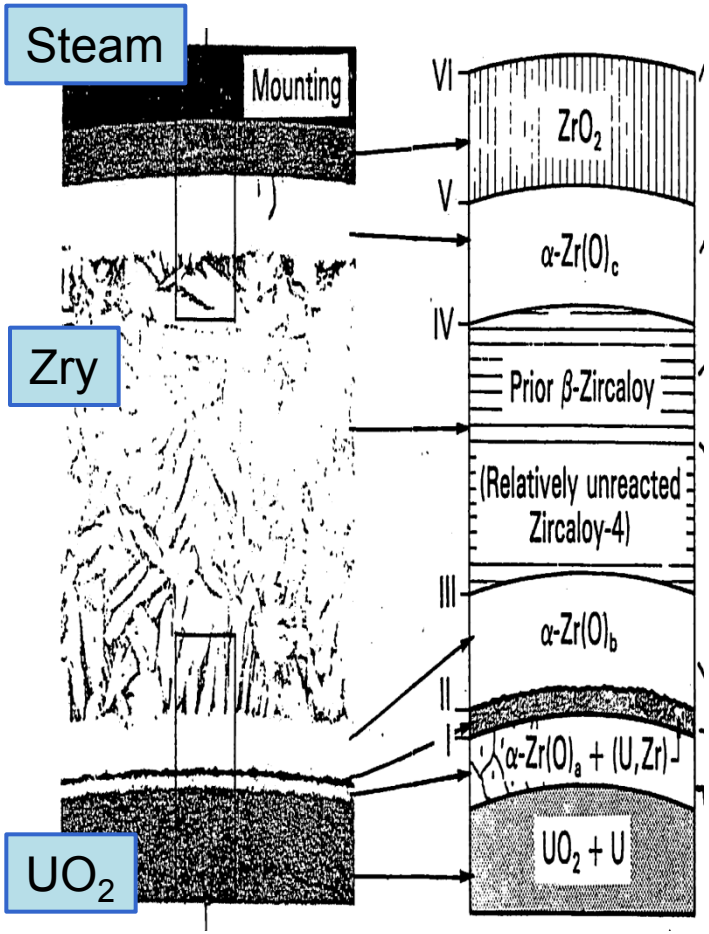
Thermodynamic Database

JAEA
(Degraded Fuel,

NSSMC
(MCCI)

Fuel Assembly Configuration of BWR

Meso-scale Modeling for Material Interface



Schematic image of layer formation "just before liquefaction" of Zry-cladding. (at ~2173K)

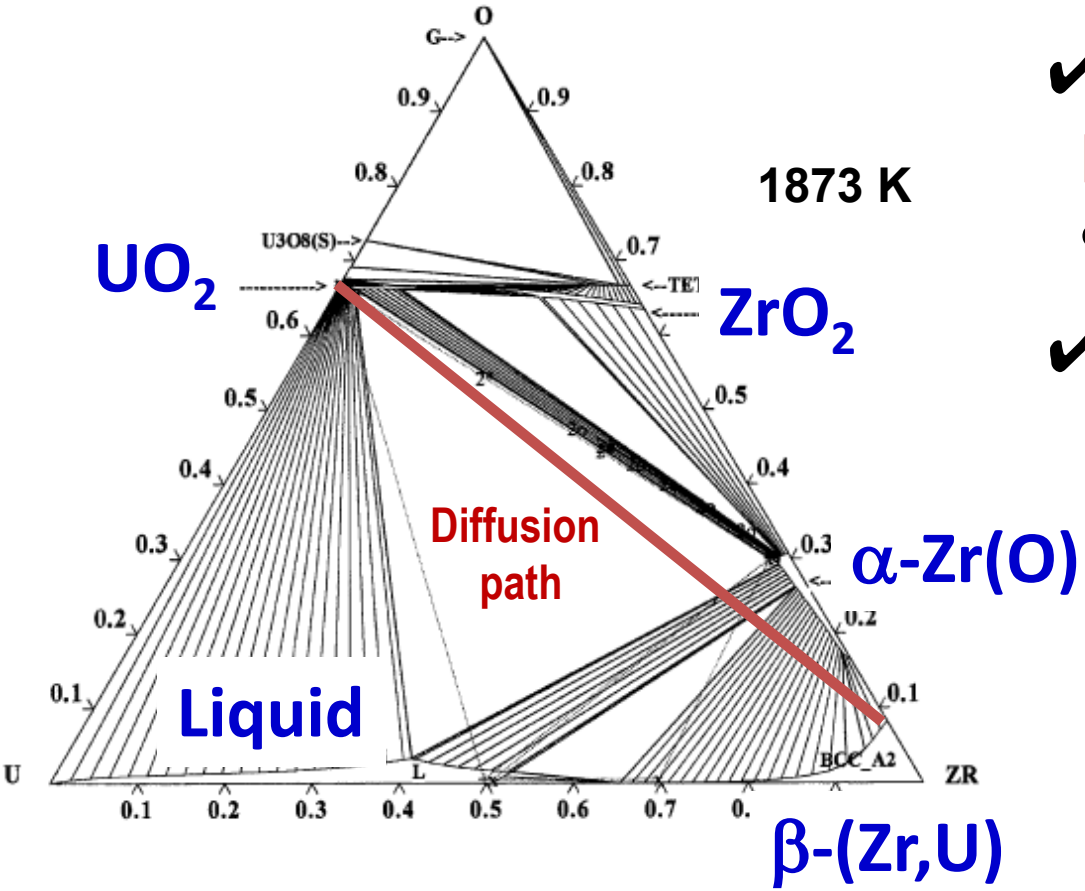
(P. Hofmann et al.)

- ✔ to understand **"physical/chemical mechanism of layer formation and liquefaction"**, based on thermodynamic knowledge, with progressing diffusion of elements and transformation of phases.
- ✔ to construct **"meso-scale model"** for UO_2/Zry and B_4C/S.S.
- ✔ to construct **"robust model"**, easy to refer various experimental observations, and easy to multi-physics/-scale model.

MPFM

Thermodynamic database : NUCLEA (tentatively)

Base MPFM for UO_2/Zr Interface



U–Zr–O isotherm.

✔Base **"U-Zr-O diffusion path model"** developed as one-dimension model.

✔5-Phases taken care of:

- UO_2 (fluorite)
- α-Zr(O) (hcp)
- β-(Zr,U) (bcc)
- Liquid
- ZrO_2

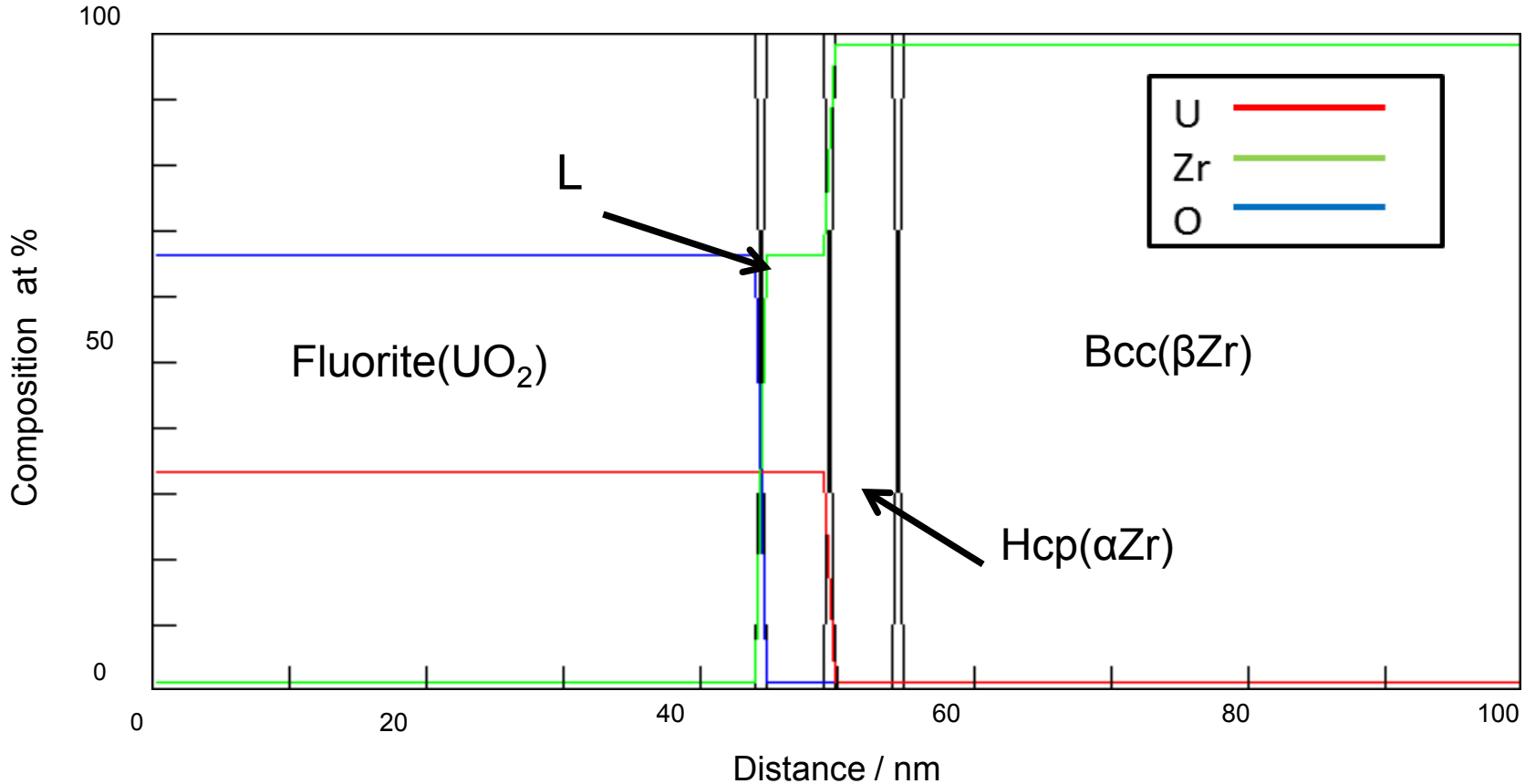
・Concerns

In which condition liquefaction starts?

Meta-stable spinodal observed?

Calculation for Evaluating Liquefaction

✔ Hypothetically, initial liquid(L) and Hcp(αZr) given in UO_2/Zr diffusion path at 1773 and 1873 K.



Initial composition profile

UO_2/β-Zr diffusion couple with thin layers (L and α-Zr)

(1773K)

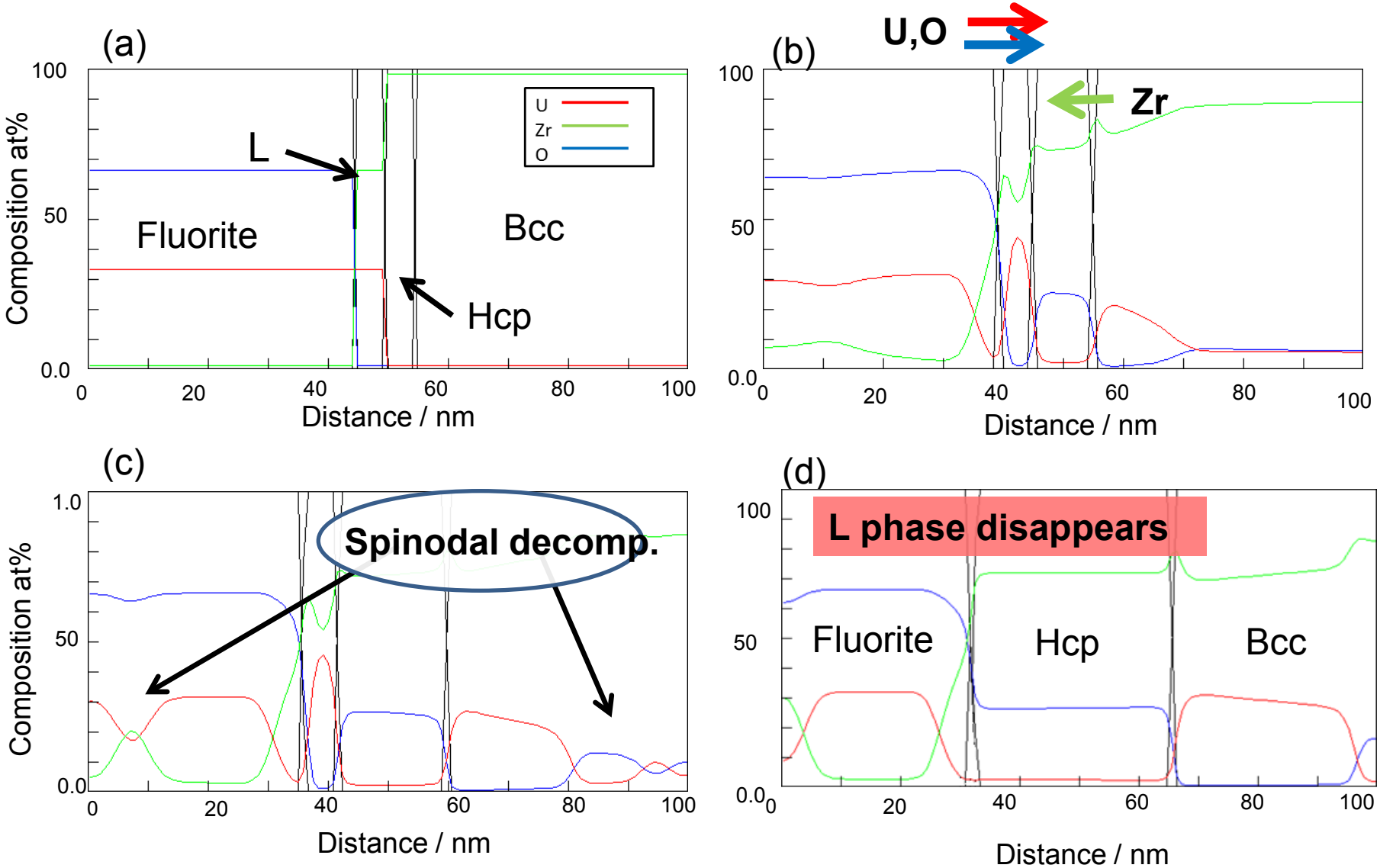


Fig. Simulation result of diffusion couple (1773 K)

(a) t'=0, (b) t'=1 × 10^6, (c) t'=4 × 10^6, (d) t'=7 × 10^6

(1873K)

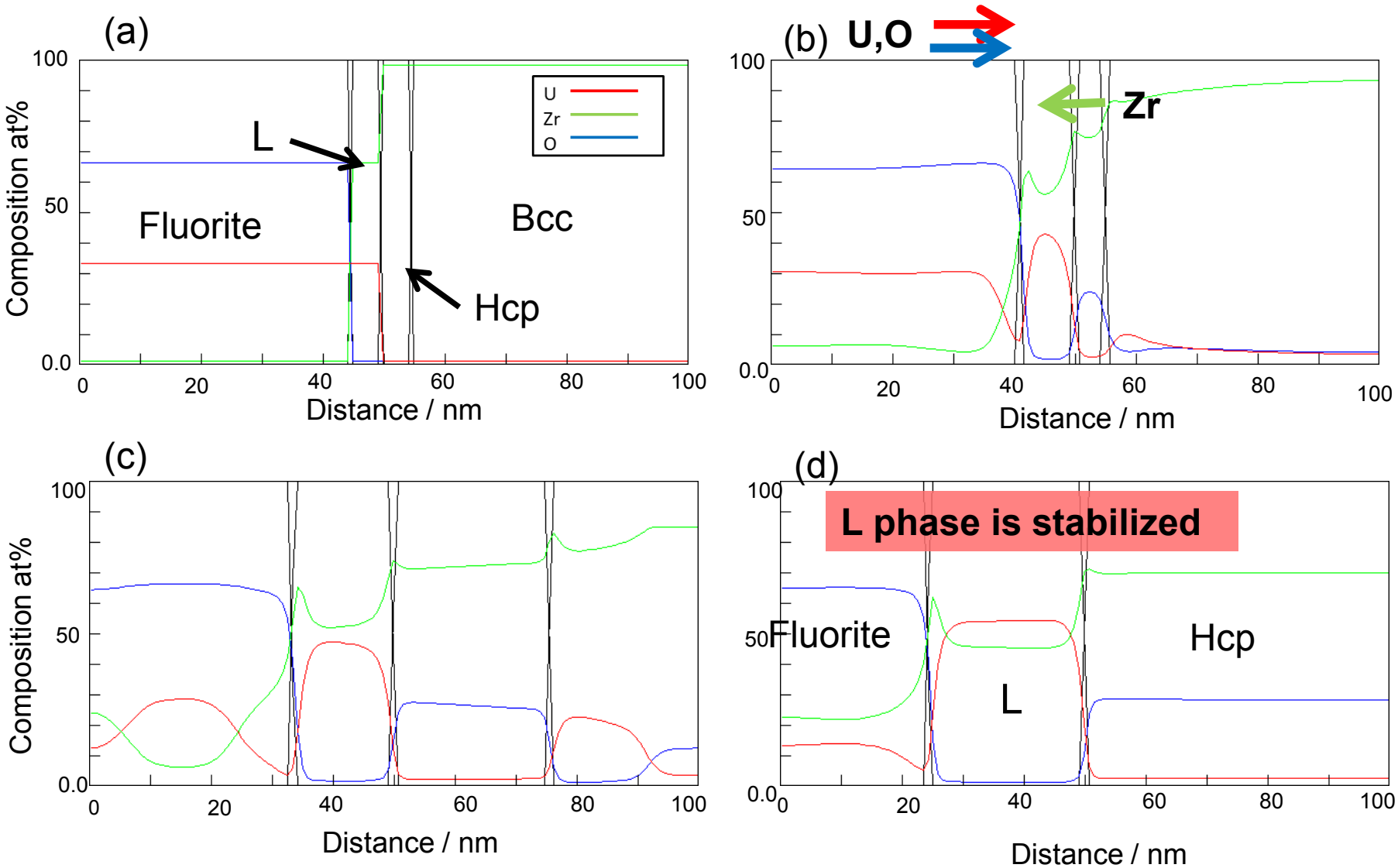
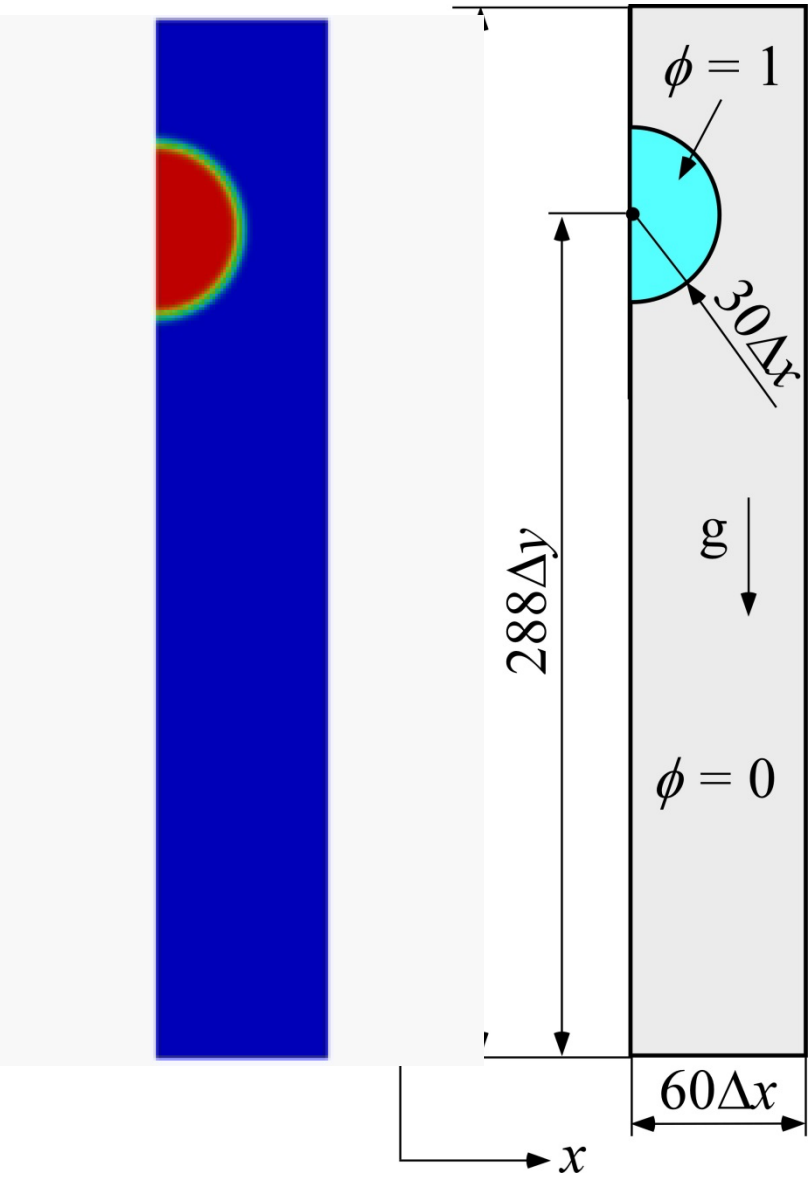


Fig. Simulation result of diffusion couple (1873 K)

(a) t'=0, (b) t'=1 × 10^6, (c) t'=4 × 10^6, (d) t'=7 × 10^6

Meso-scale Modeling for Candling



Base PFM for droplet move.
(wetting on left wall)

- ✔ to understand physical/chemical mechanism of **"candling of solid/liquid mixture"** of degraded fuel
- ✔ to predict **"rate of droplet falling and droplet solidification"** for UO_2/Zry and B_4C/S.S.
- ✔ to construct **"robust model"**.

PFM and SPH

Boundary conditions

Velocity	$\vec{n} \cdot \vec{v} = 0$
Pressure	$\vec{n} \cdot \nabla p = 0$
Phase – field	$\vec{n} \cdot \nabla \phi = 0$

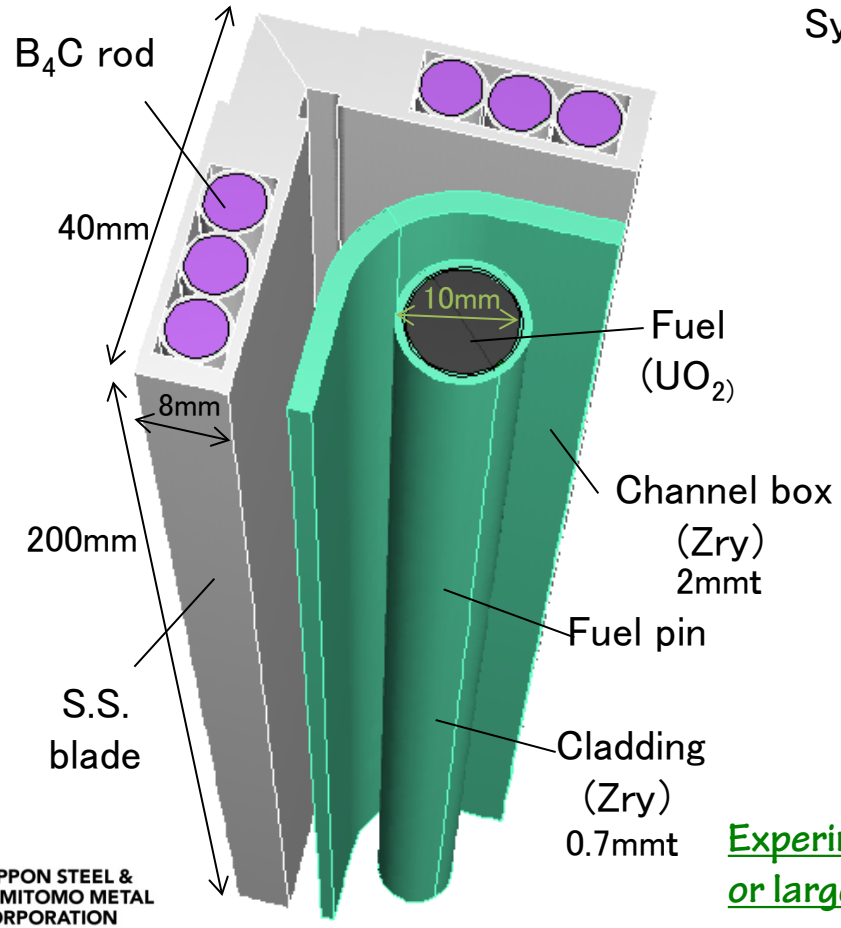
Coupling with MPFM liquefaction model ongoing

Larger-scale Modeling for Fuel Assembly Degradation

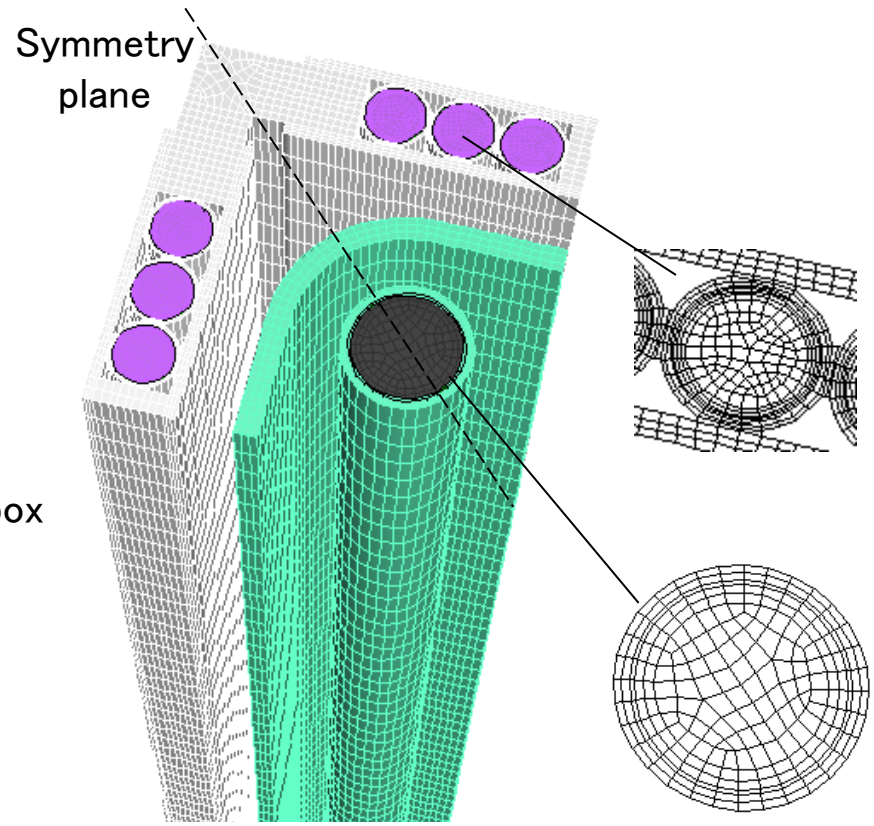
✔ to introduce **"general methods/tools of non-nuclear material modeling"** into **"multi-scale/physics modeling"** for fuel assembly degradation.

➡ VOF/FLUENT/MARC, LS-Dyna/SPH, PFEM etc.

Partial Configuration of Fuel Assembly



Calculation mesh for VOF/FLUENT



Experimental study with similar or larger scale planed

100,000 mesh

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Model Calculation, Preliminary

✔ Manner and Assumption, general manner

- **FLUENT(Finite Volume Method)** : User Defined Function, Non-stable Condition Analysis
- **VOF(Volume of Fluid)** : Free interface analysis, Geo-Reconstruct Method for Interface
- **Immersed Boundary Method** : Solid treated as Fluid with Extremely High Viscosity
- **Radiation Heat Transfer** : DO-model (Discrete Ordinate)
- **Heat Source** : Proportional to Volume Fraction of Each Phase
- **Thermodynamic parameters** : Not Considered in Preliminary Model
- **Volume Change** : Not Considered in Preliminary Model

✔ Procedure

- **Temperature Variation** only calculated in the condition until S.S. attains to melting temperature (time step=1 sec.)
- Then, **variation in fluid and free surface** co-calculated (time step=0.0001 sec.) after liquid phase generated in steel.

✔ Condition

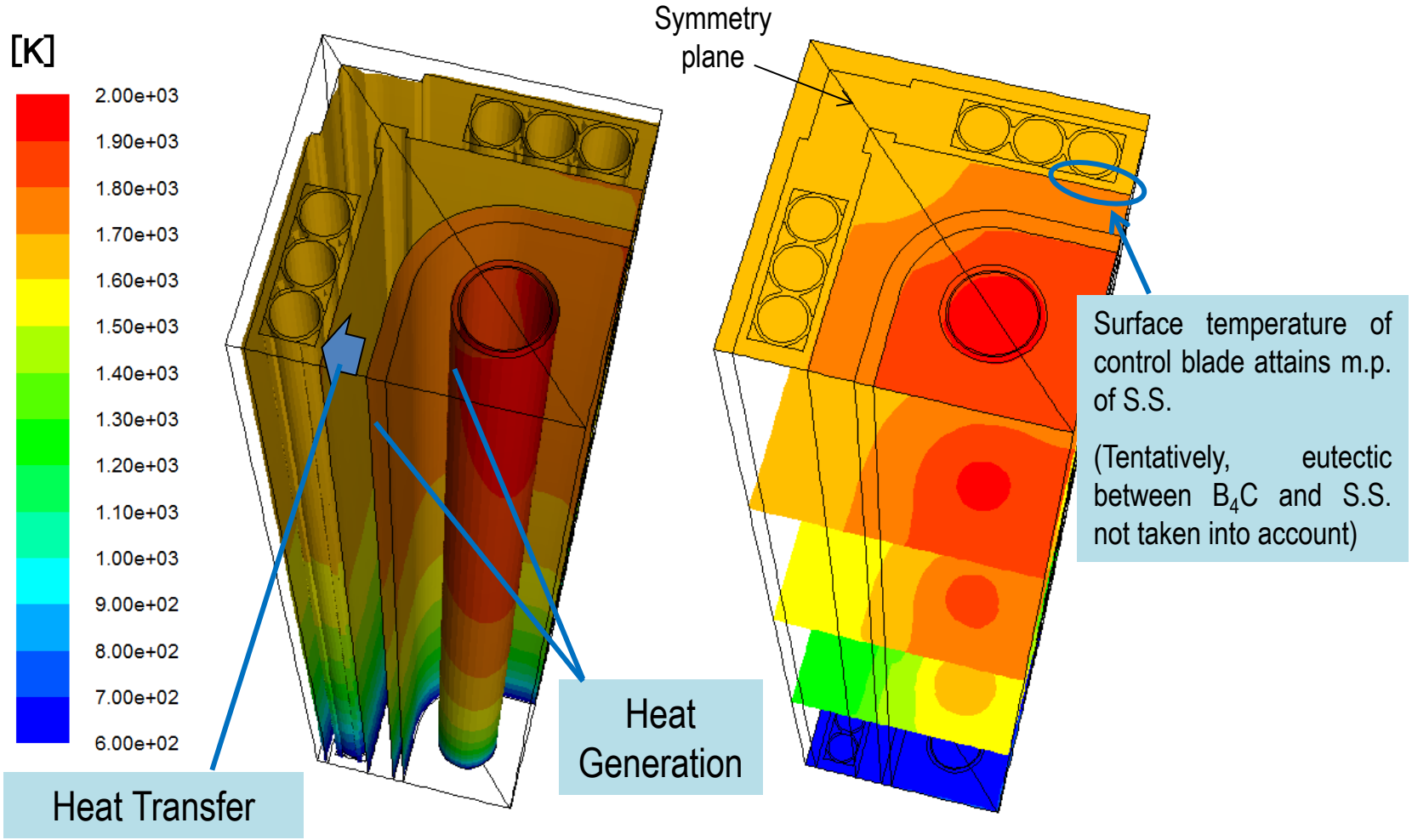
- **Initial Temperature** : 600 K (isothermal)
- **Heat generation from fuel** : 1.53×10^7 W/m^3
- **Heat generation from Zry-oxidation** : (estimated from Cathcart-Pawel Eq.)

  $97\exp(0.0061T)$ W/m^3

- Radiation Heat Transfer only taken into account.

Model Calculation, just before liquefaction

✔ Surface temperature of control blade increasing by heat transfer.

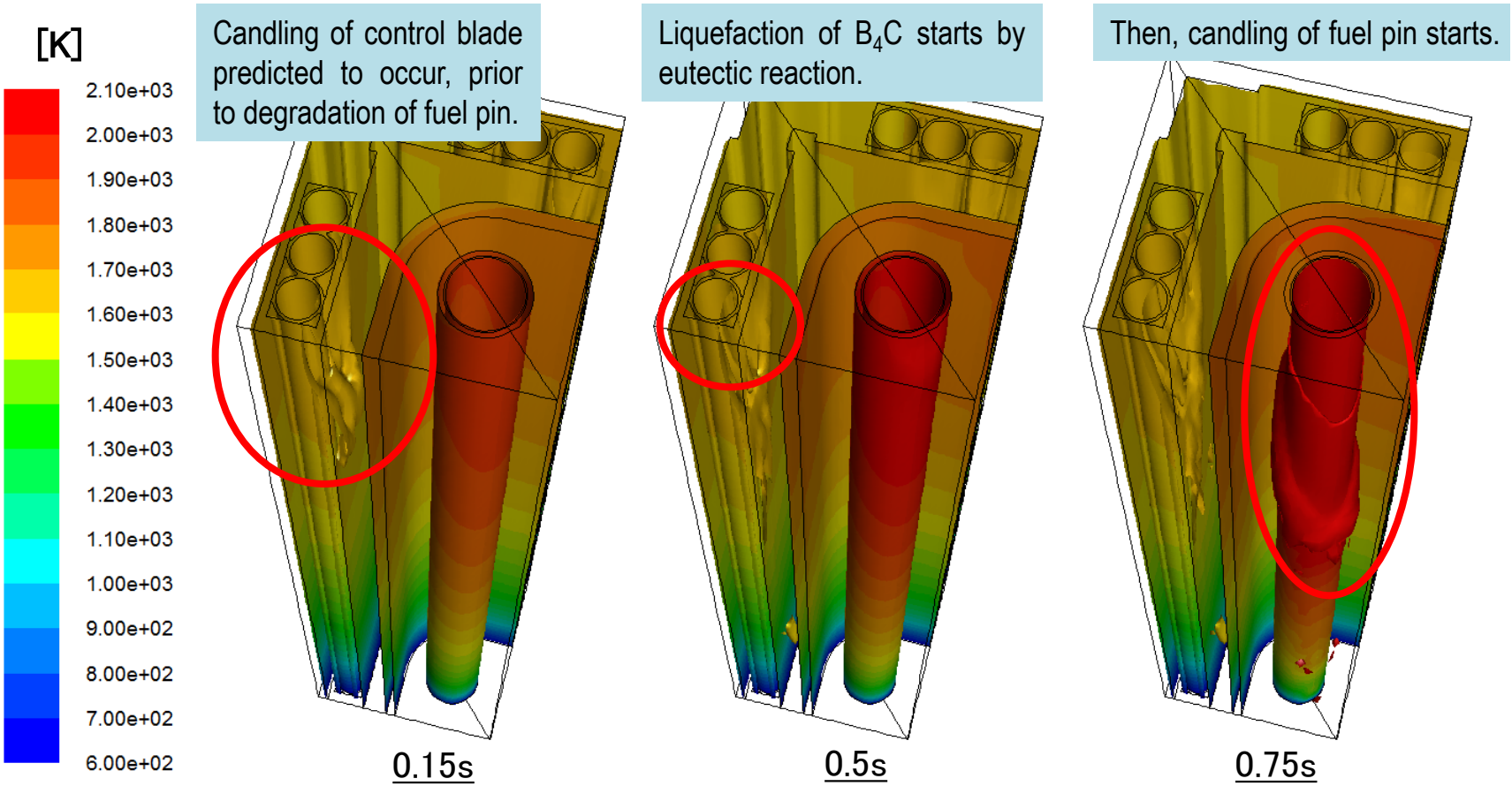


Temperature Variation (700 sec. later)

Model Calculation, start Degradation

✔ **"Degradation of control blade occurs prior"** to that of fuel pin and channel-box, even assuming extremely high temperature increase rate (x10).

✔ Control blade degradation is **"expected to happen more prior",** when considering realistic increase in temperature (~10 K/sec. or less)



Progress in degradation for fuel pin and control blade

(preliminary result, assuming temperature increase rate : 100 K/sec.)

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Thermodynamic Database

✔ Thermodynamic database for **"degraded fuel"** being developed as **"sub-lattice model"**. **"U-Pu-Zr-Fe-O"** being improved, based on Gueneau's database for oxides and Kurata's database for alloys. **"S.S.-B-C-O"** being re-evaluated by collaborating with Prof. Hasebe. **"U-Gd-O"** being developed by collaborating with Prof. Tokunaga.

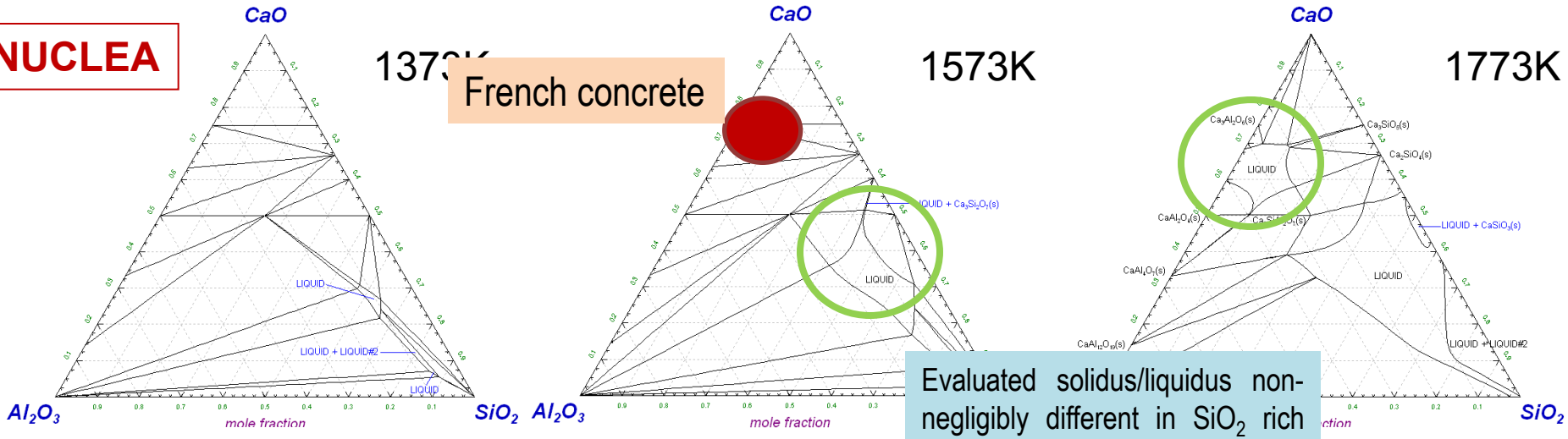
⇒ Base database for modeling of meso-scale fuel degradation, in which variation in $g(O_2)$ should be taken care of.

✔ Thermodynamic database for molten core concrete interaction (**"MCCI"**) being developed as **"quasi-chemical model"** by collaborating with NSSMC.

⇒ Base database for modeling of larger scale interaction among oxide-melt/metal-melt/oxide-solid/metal-solid ex. stratification in mixture, hole-formation of steel, etc.

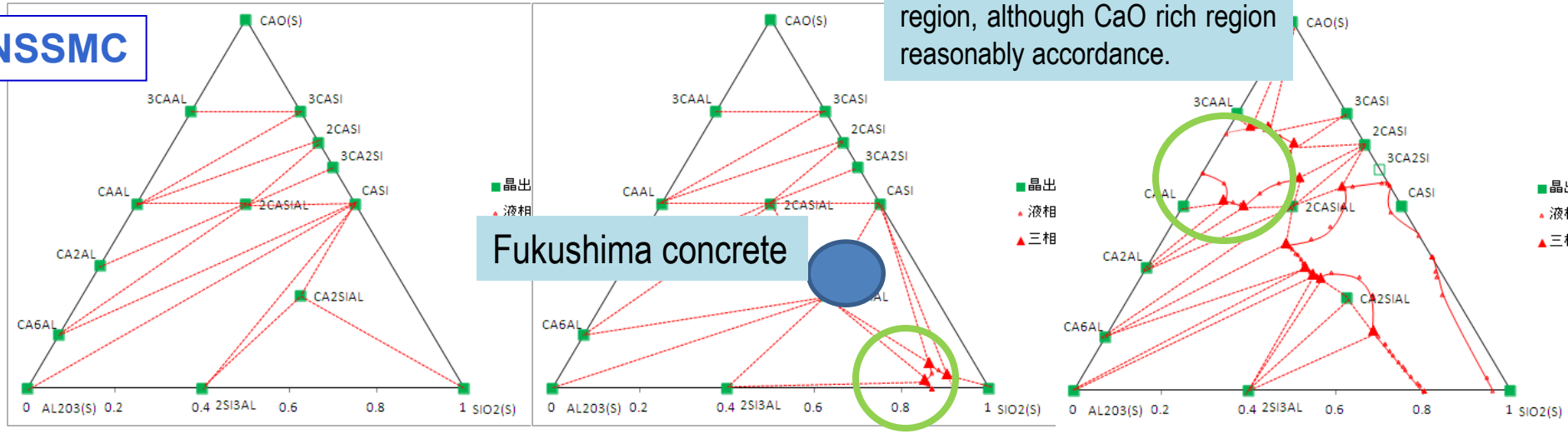
Thermodynamic Database, Concrete

NUCLEA



Evaluated solidus/liquidus non-negligibly different in SiO_2 rich region, although CaO rich region reasonably accordance.

NSSMC



✔ **"NUCLEA"** database suitable for general **"French concrete"** rich in **"CaO"**. On the other hand, **"NSSMC"** database suitable for **"Fukushima concrete"** rich in **"SiO_2-Al_2O_3"**.

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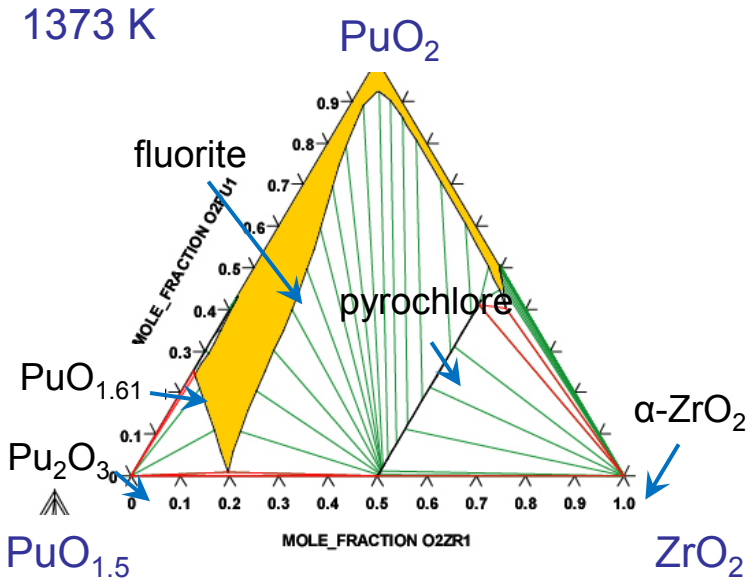
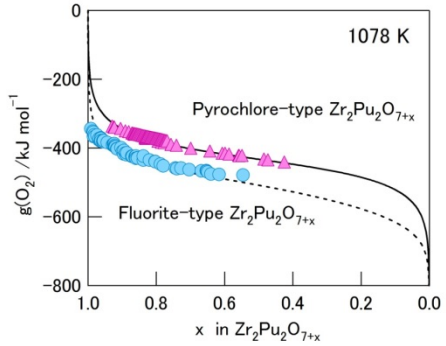
Thermodynamic Database, Degraded Fuel

Pu-Zr-O system

1373 K

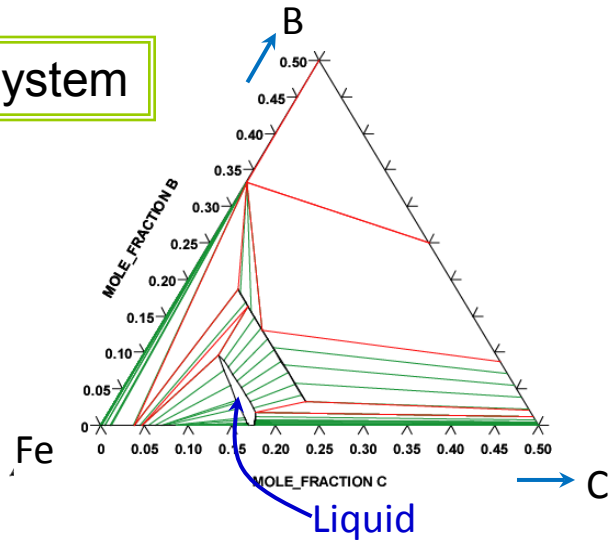


Oxygen potential measurement



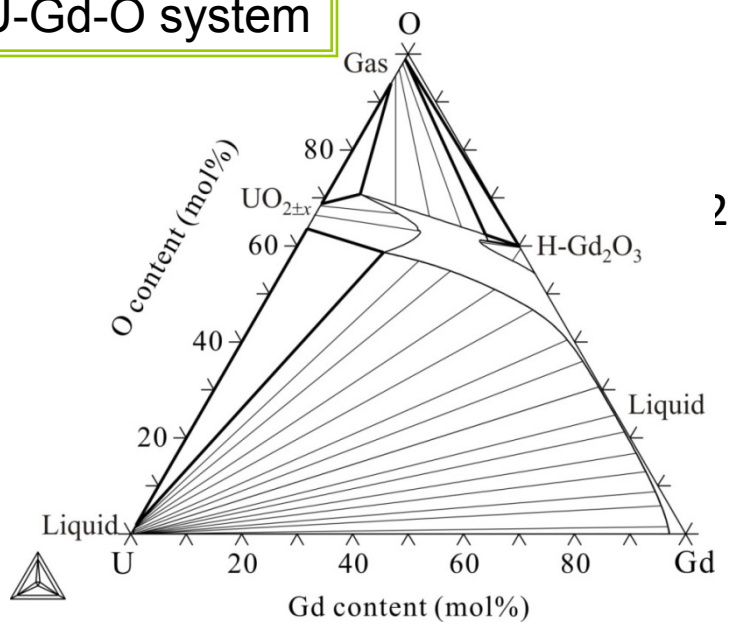
Fe-B-C system

1443 K



U-Gd-O system

2500K)



Summary

- ✔ METI-project started in Japan for multi-scale/physics modeling and databasing of nuclear fuel degradation.
- ✔ Project being performed in a collaboration between nuclear and non-nuclear institutes, universities, and companies
- ✔ Base models like MPFM for U-Zr-O, PFM for droplet falling, and etc. developed in 2012.
- ✔ Various model calculation using conventional methods used in steel manufacturing shows their high potentials for modeling larger scales.
- ✔ Improvement of thermodynamic database ongoing.

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