

Topics of Plasma Technology (Nuclear Fusion Technology)

Remote Lecture from Japan for MEPHI

December 7, 2016

Michio Yamawaki

(Prof. Emeritus of the University of Tokyo)

Short History of Michio YAMAWAKI

Academics

- 1964.3 Graduated from Nuclear Engineering Department , University of Tokyo
- **1969.3 Graduated from Doctoral Course of Nuclear Engineering, Univ. of Tokyo (Dr. Eng.)**

Jobs or Nominations

- 1969.4 Research Associate, Department of Nuclear Engineering, Univ. of Tokyo
- 1974.7 Associate Professor
- **1987.4 Professor at Univ. of Tokyo (managed Nuclear Fusion Engineering Lab. for 10 years)**
- **2003.3 Retired from Univ. of Tokyo**
- 2003.4 Honorary Researcher at Japan Atomic Energy Research Institute (JAERI, later **JAEA**)
- 2003.4 Guest Professor at Tokai University
- 2003.5 Professor Emeritus of Univ. of Tokyo
- 2005.4 Technical Advisor at Japan Nuclear Energy Safety Agency (Governmental)
- **2010.10 Professor at Univ. of Fukui (Research Inst. of Nuclear Engineering)**
- **2015.12 Guest Professor at MEPHI**
- 2016.6 Chair of Steering Committee of Nuclear Systems Association, Japan Atomic Industrial Forum

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1. Introduction

**2. International Thermonuclear Experimental Reactor (ITER)
and Broader Approach (BA)**

3. Fusion Materials Irradiation Facility

4. Future Plan for Rokkasho

5. Tritium Permeation Barrier

6. Summary

1. Introduction

2. International Thermonuclear Experimental Reactor (ITER)

and Broader Approach (BA)

The Way to Fusion Energy

JT-60

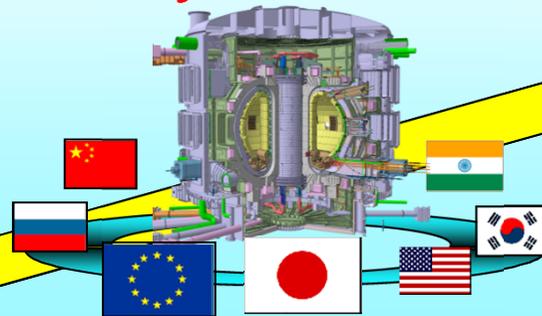
**Breakeven condition
($Q > 1$)**



$Q^{eq} = 1.25$
 $T_i = 45 \text{ keV}$

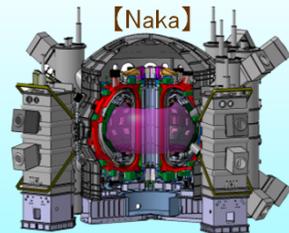
ITER

**Burning plasma
($Q > 10$, 500MW, 300-500 s)
Feasibility of fusion energy**

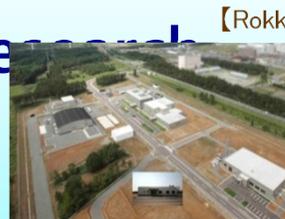


Support ITER

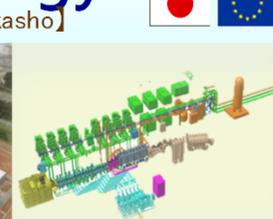
**Broader Approach in the
field of fusion energy
research**



**Satellite
Tokamak JT-
60SA**



**Int'l Fusion
Energy Res
Center**



**IFMIF/E
VEDA**

DEMO



**Electric
Power
Generation**

Practical use

**Complement
ITER**



Current Status of ITER Construction



Headquarters building completed in October 2010

ITER site on 30 April 2014
in Saint-Paul-les-Durance (Gadarashe)

Tokamak complex construction
(Width 87m, Length 123.6m, Depth 17m)



PF coil assembly building (width 45m,
length 252m, height 17m;
completed in Feb. 2012)

ITER test convoy in Sep. 2013
800-ton trailer (width 9m, height
10.4m, length 38m)



Broader Approach for Realization of Fusion

BA Activities

- (1) Taking Initiative of Fusion Research
- (2) Development of Fundamental Fusion Technology
- (3) Human Resource Development

DEMO

Demonstration of Fusion Power Plant

ITER : Demonstration of Scientific and Technological Feasibility of Fusion Energy

*Q = 10
DT Burning 300-500s*

Broader Approach Activities

Rokkasho, Aomori

IFERC

IFMIF/EVEDA

Naka, Ibaraki

Satellite Tokamak

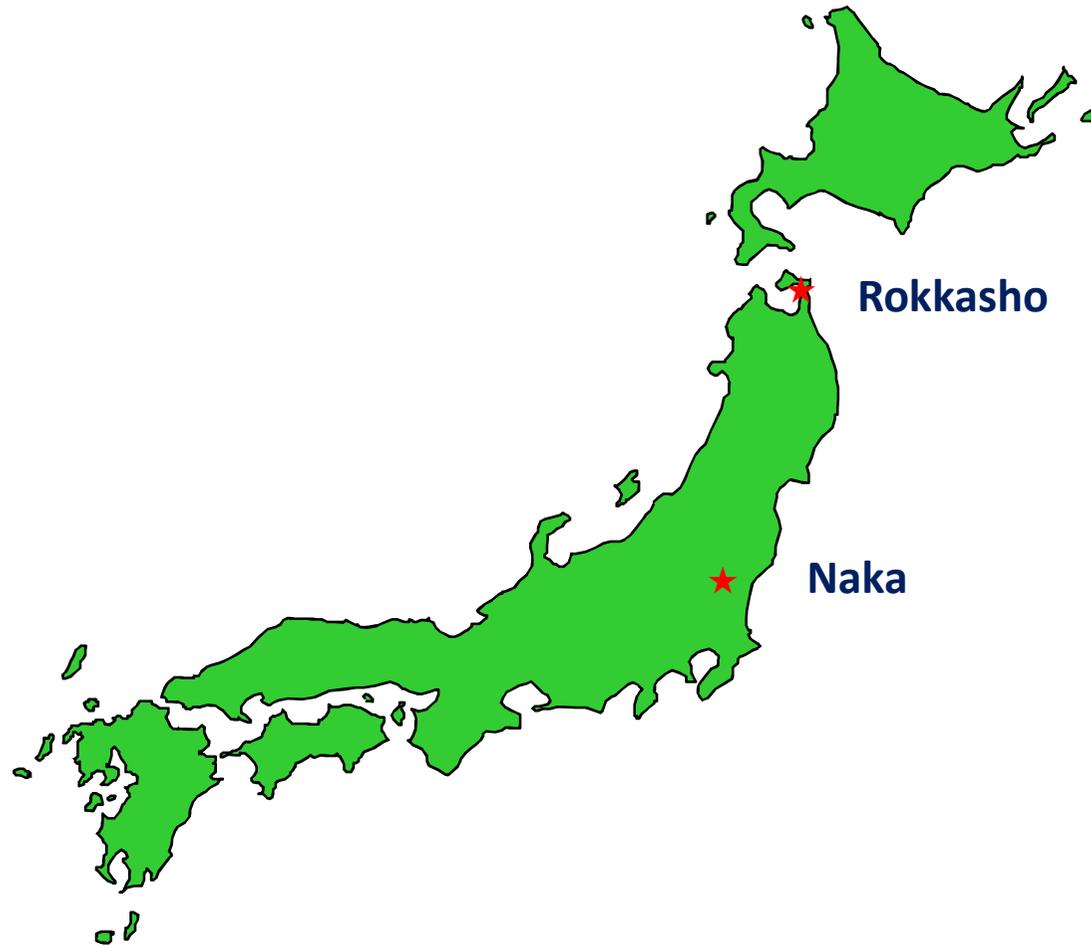
JT-60

*Q = 1.25
Ti(0) = 45keV*

Fusion Technology

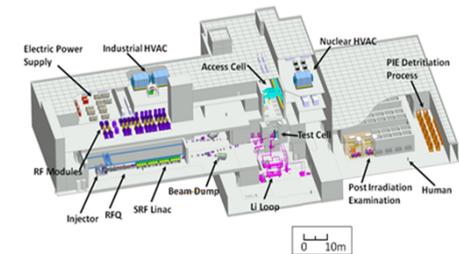
*Material Blanket
R&D (Coils, VV, Heating)*

Rokkasho and Naka Sites of JAEA

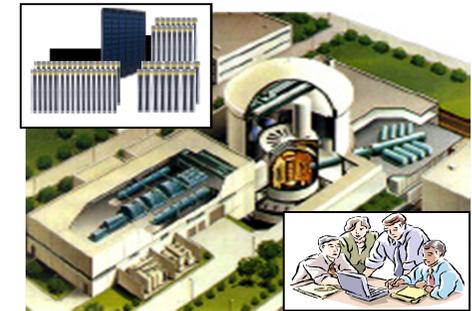


Broader Approach Activities comprise three Projects

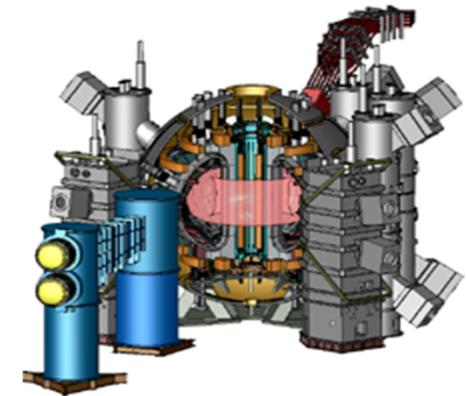
1) Engineering Validation and Engineering Design Activities for the International Fusion Materials Irradiation Facility (**IFMIF/EVEDA**:2007-2017)



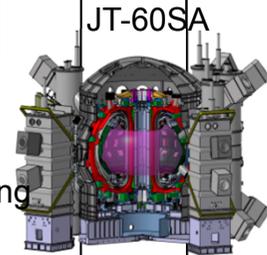
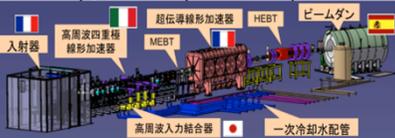
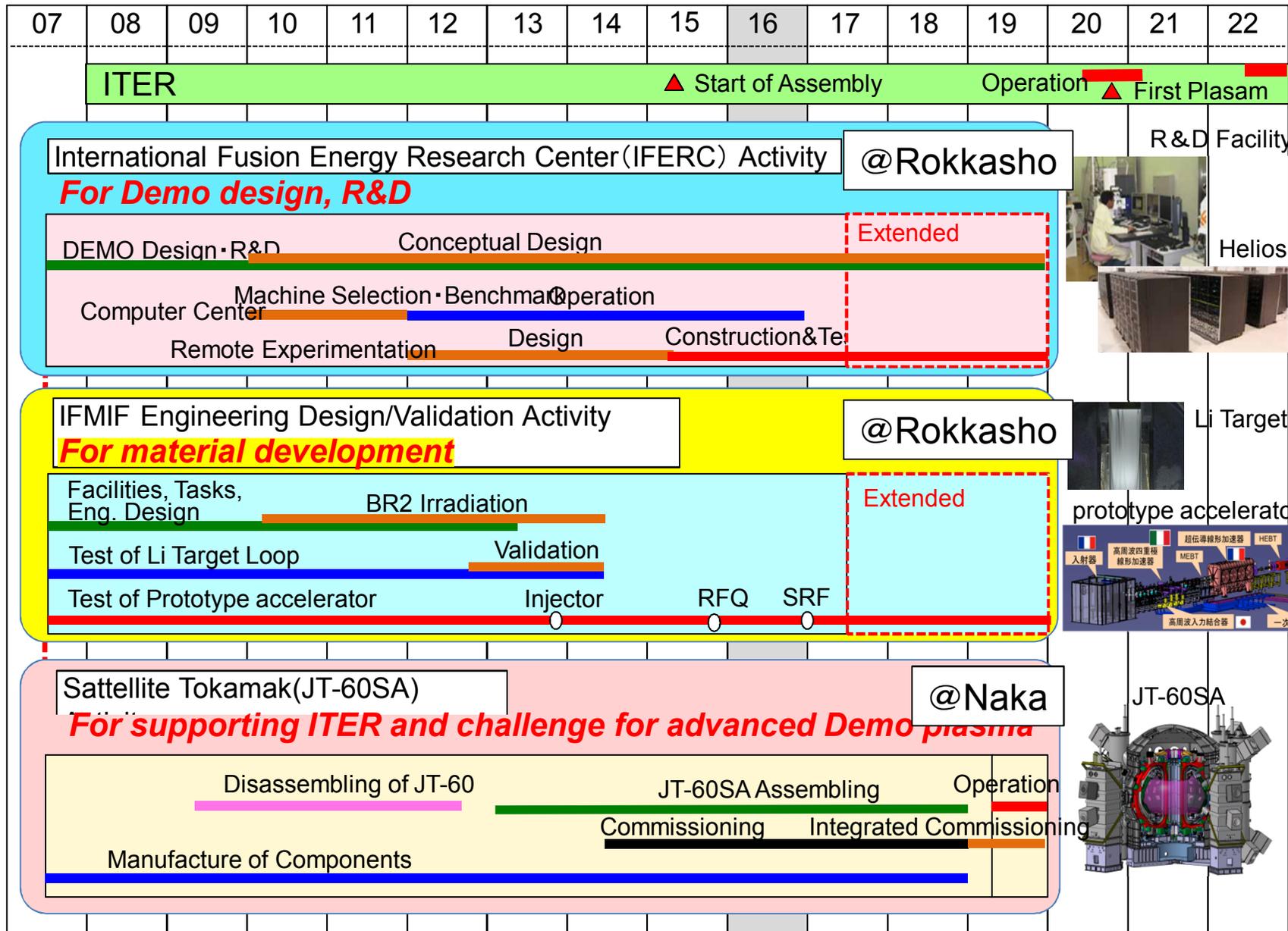
2) International Fusion Energy Research Centre (**IFERC**:2007-2017),
a) DEMO Design and R&D coordination Centre
b) Computational Simulation Centre
c) ITER Remote Experimentation Centre

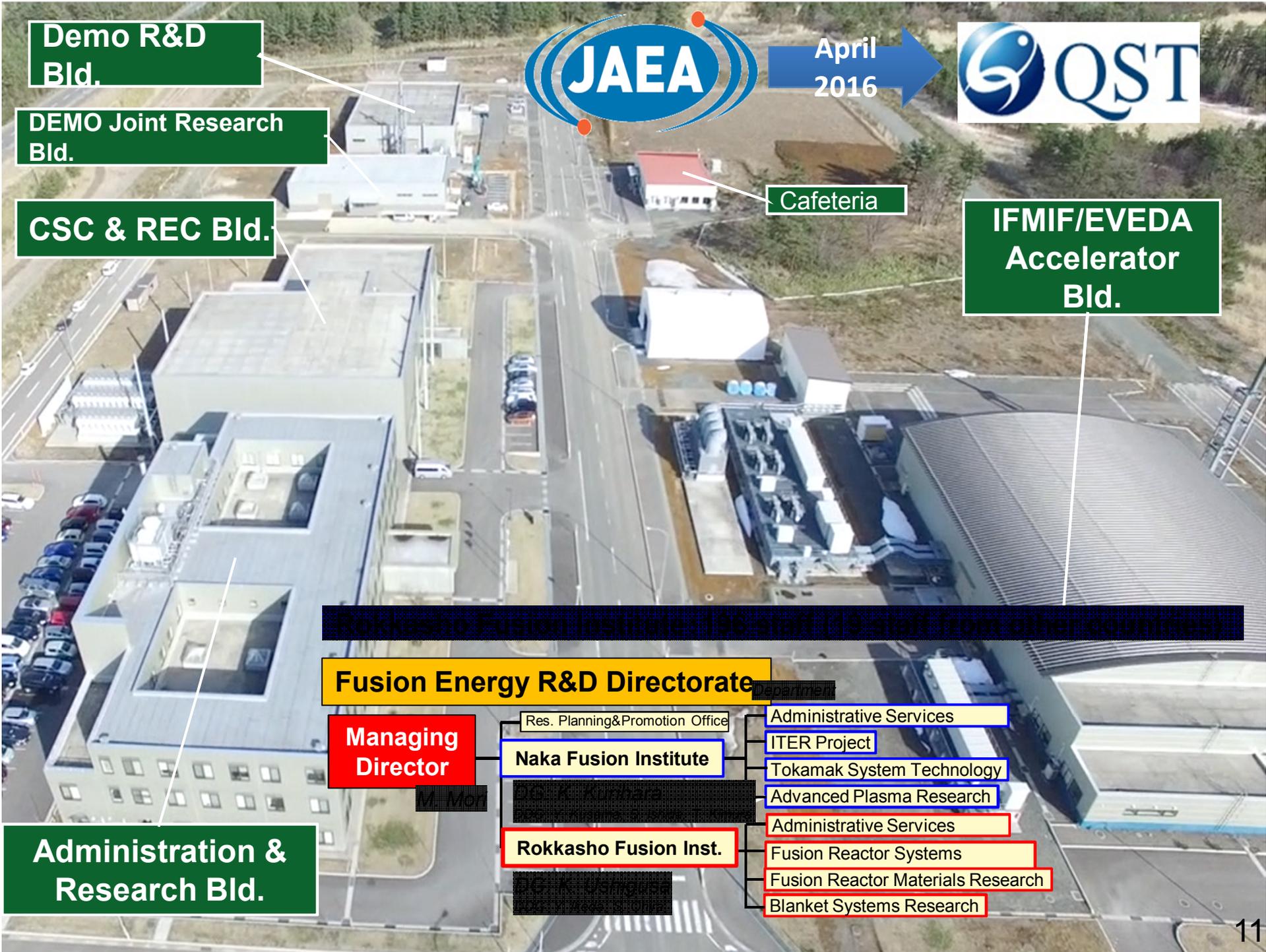


3) **Satellite Tokamak Programme** (2007-2019)
Participation to upgrade of JT-60 Tokamak to JT-60SA and its exploitation.



Schedule of BA Three Projects





Demo R&D Bld.

DEMO Joint Research Bld.

CSC & REC Bld.

Administration & Research Bld.



April 2016



Cafeteria

IFMIF/EVEDA Accelerator Bld.

Fusion Energy R&D Directorate

Managing Director

Res. Planning & Promotion Office

Naka Fusion Institute

Administrative Services

ITER Project

Tokamak System Technology

Advanced Plasma Research

Rokkasho Fusion Inst.

Administrative Services

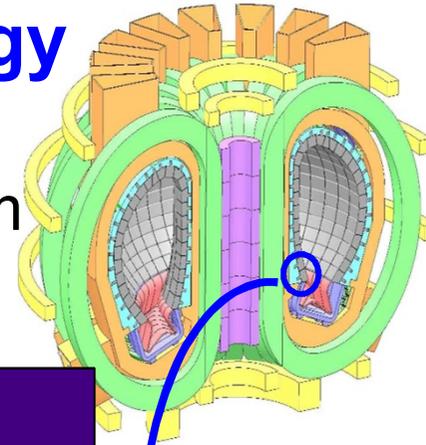
Fusion Reactor Systems

Fusion Reactor Materials Research

Blanket Systems Research

BA-R&D on Nuclear Technology for DEMO Reactor

Five R&D subjects for DEMO Blanket from 2007 to 2017 (extension to end of 2019)



Breeding Blanket

1. RAFM (Reduced Activated Ferric Martensite)

Structural material for DEMO Blanket

4. Tritium Breeder



Li_2TiO_3
1 mm diameter

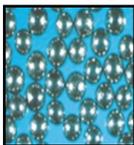


2. SiC/SiC

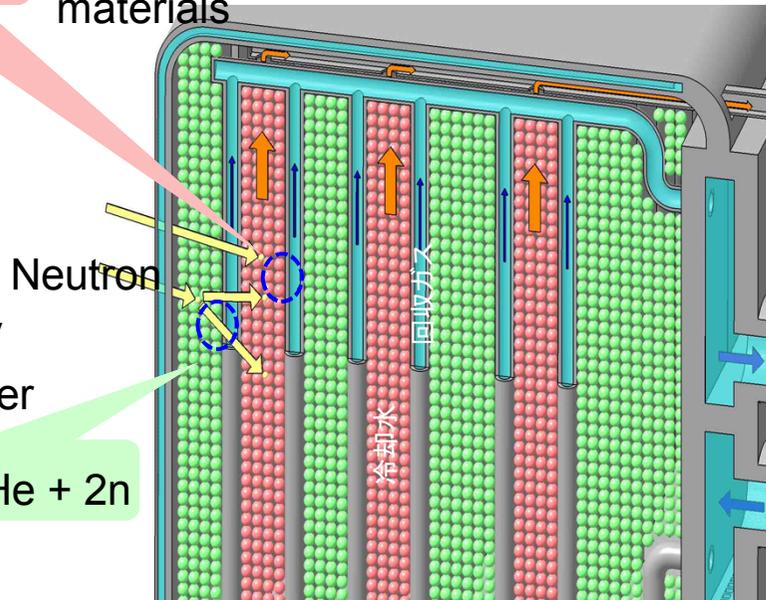
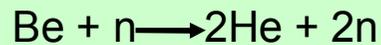
Advanced functional materials

3. Tritium Technology

5. Neutron Multiplier



Be_{12}Ti , Be_{12}V
1 mm diameter



Recovery of tritium

Coolant outlet
325°C

Coolant inlet
290°C

International Fusion Energy Research Center (IFERC) Activity

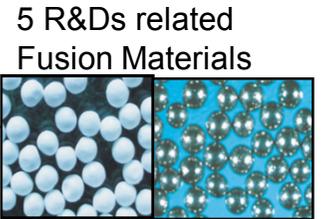
IFERC

DEMO Design



- 40 Technical Meetings
- Joint Analysis of key elements and Safety
- Intermediate Report in 2015
- Join 80 JA scientist

DEMO R&D

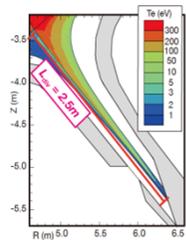


- 5 R&Ds related Fusion Materials
- Advanced neutron multiplier
- Tritium Breeder
- Reduce Activation Ferritic Steel
- SiC/SiC
- Tritium Diagnostics and Control

Computer Simulation



- 1.23 Pflops from Jan. 2012
- Extended by 0.2 Pflops from 2014
- About 4 years
512 papers,
1549 conference reports
- About 600 EU-JA users



ITER Remote Experimentation



- Construct from 2015
- Data Transportation Test from end of 2016

R&D for RAFM: Qualification as a structural material

- Manufacturing and joining technologies -

Manufacturing technology

Reproducibility of F82H in real scale production was demonstrated.

- 20 tons F82H was produced by an electric arc furnace, and the various properties of plates were proved to be equivalent or better compared to those of the past heats.
- Issues : Qualification of all parts form (tube, pipe).

Joining technology

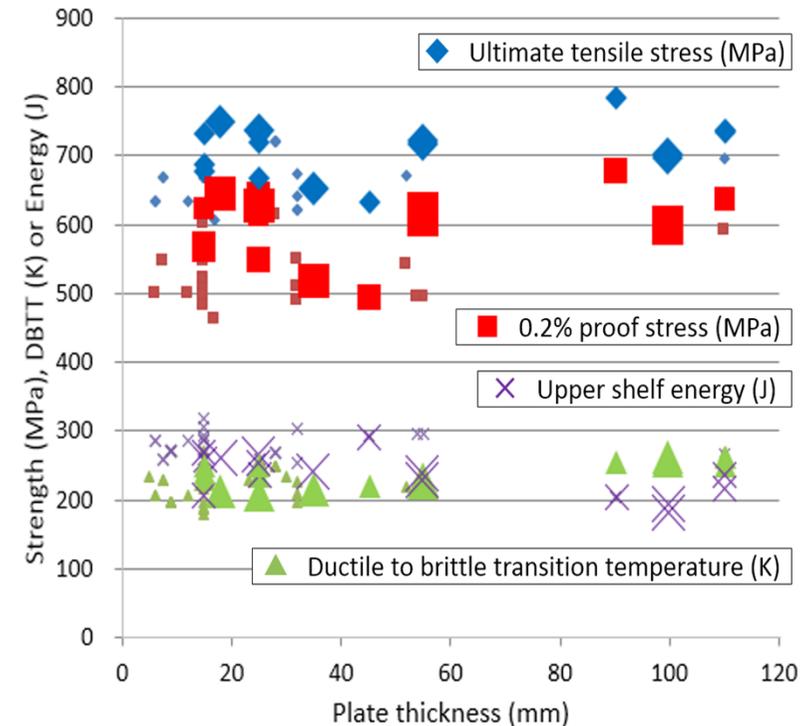
Solid joining technology corresponding to the blanket design, together with inspection technology, was also demonstrated.

- Over 100 m weld length per a single blanket were required to be qualified, and decent TIG and EB weldability along with good (low) crack sensitivity has been proven.

Issues : Assurance criteria of sound HIP joint.

- Selection of the best joining technology for the highly irradiated weldment.

Ref: ASME BPVC Section II PartD
Appendix5



Tensile and Charpy impact properties of various heats of F82H plates plotted against the plate thickness. Larger symbols stand for the data points of F82H fabricated in BA activities.

R&D on SiC

Manufacturing and characterization

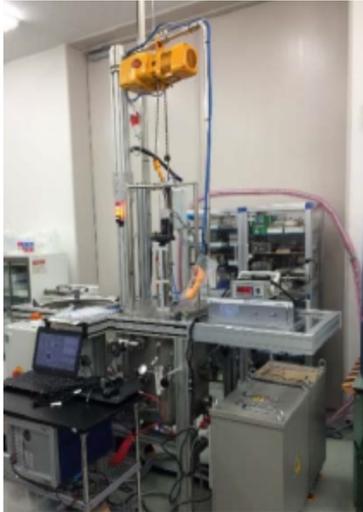
For functional structure applications in the advanced blanket system, e.g., flow channel.

Material data of nuclear grade SiC/SiC

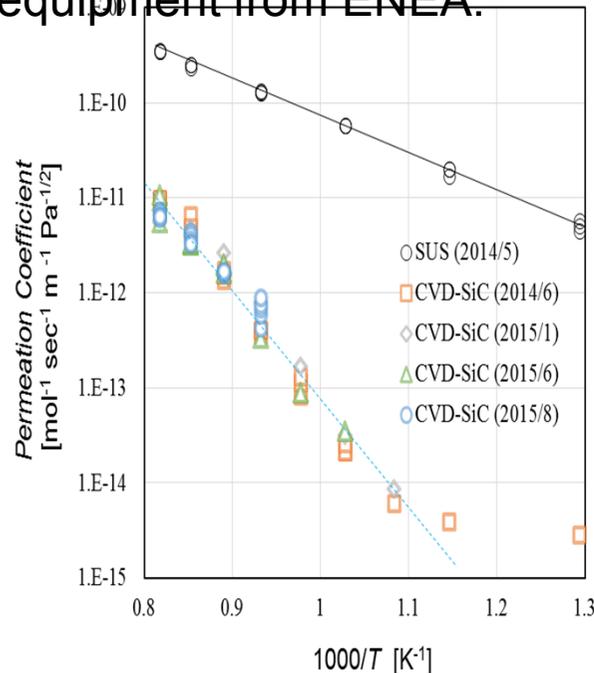
Tensile test, neutron irradiation, etc.

Compatibility with materials in a

Tests for Pb-Li compatibility of NITE SiC/SiC composite and CVD SiC at using the equipment from ENEA.



The deuterium permeability of CVD-SiC was measured.

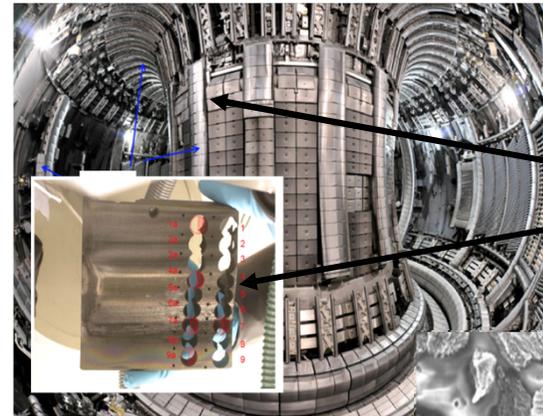


R&D on Tritium Technology

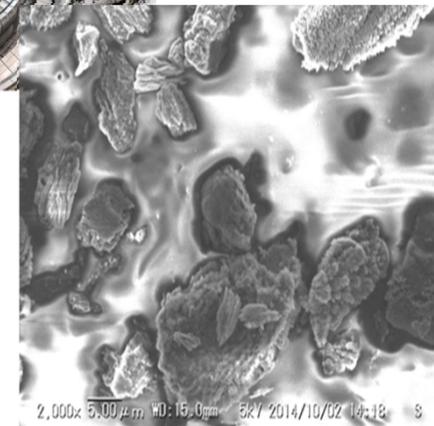
Basic Tritium data (permeation, retention, etc.) of several key materials (e.g., RAFM, W)

Tritium Durability Test with organic compounds, stainless steel (induced by T-beta and radicals.).

Analysis of JET tiles (Evaluation of amount of tritium in tiles and dust etc.,)



tungsten coating on carbon tile and on beryllium

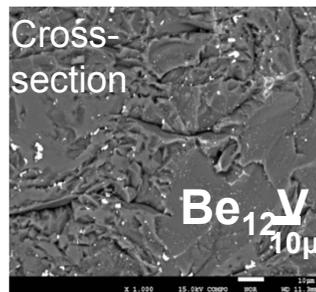
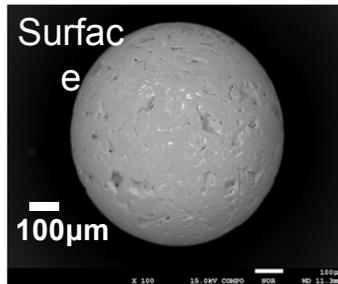
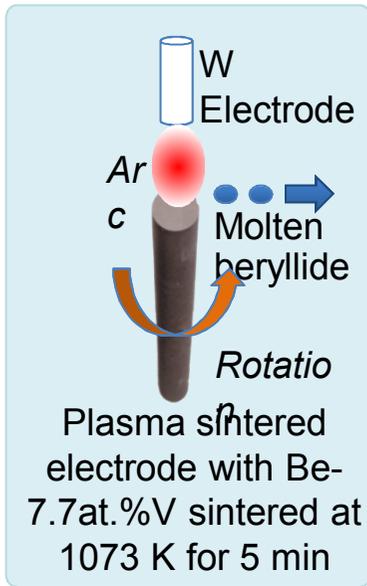


Example of JET dust sample photograph with scanning electron microscopy.



R&D on Neutron Multiplier

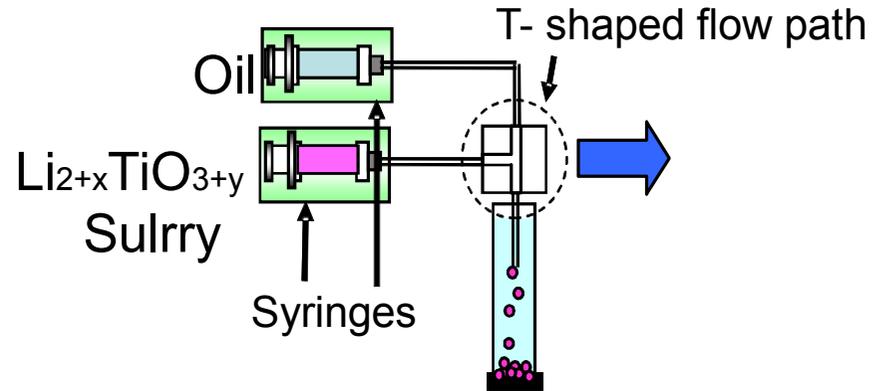
A new beryllide granulation process that combined processes with a plasma sintering method and REM (Rotating Electrode Method) was developed. $Be_{12}V$ pebbles were successfully made.



- $Be_{12}V$ single phase pebbles demonstrated a lower reactivity than Be pebbles.
- H_2 generation ratio of $Be_{12}V$ is two orders of magnitude less than that of Be.

R&D on Tritium Breeder

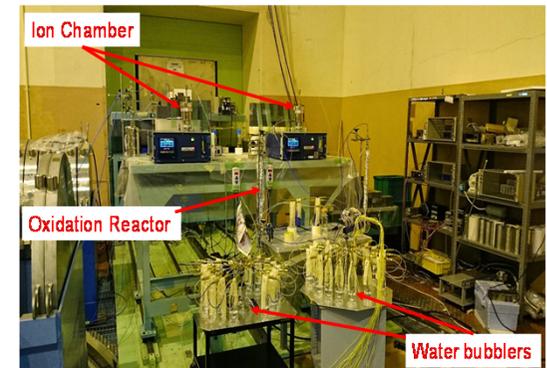
R&D on fabrication and characterization of advanced tritium breeders (**The addition of Li into Li_2TiO_3 10%**)



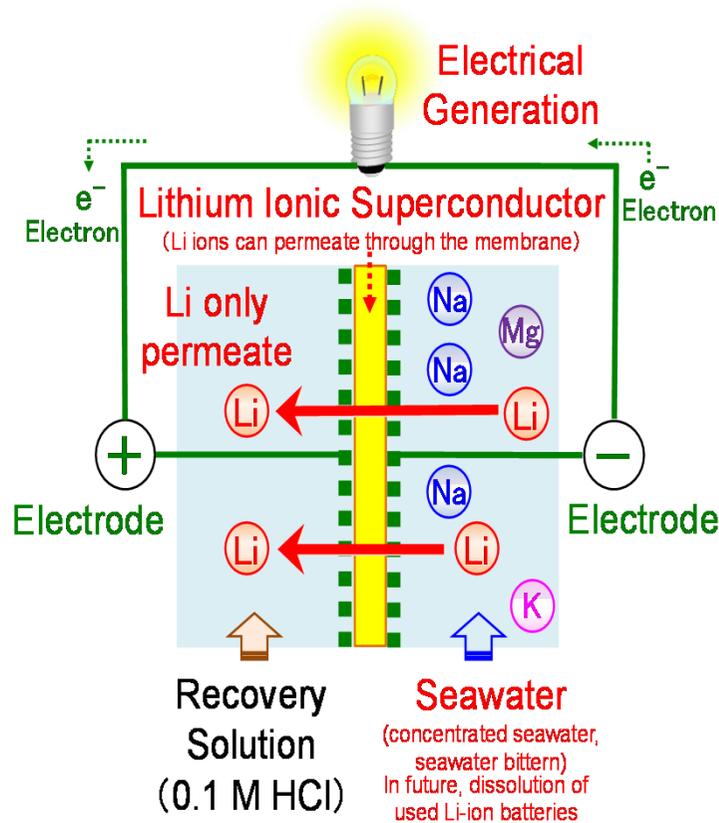
This granulator consisted of two syringes, a T-shaped flow path and an oil-filled container. The size of the gel particles could be controlled by the flow speeds of oil and slurry.

R&D on Tritium release properties

T produced by fusion neutrons was measured. The released amount of HT gas was greater than the released amount of HTO water vapor.

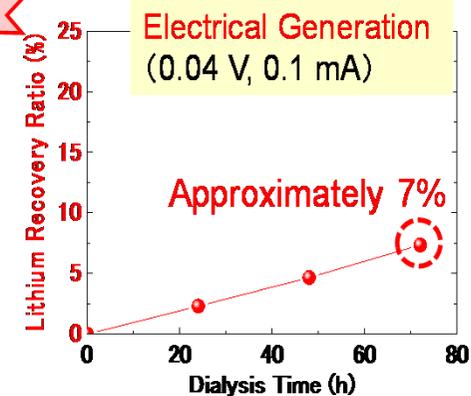


Basic R&D on Li from sea water



Enormous amount of total Li

[Li₂CO₃ is used for tritium breeder in fusion reactor]



- 1) Li only permeates from the negative electrode side to the positive electrode side through a Li ionic superconductor. Li becomes selectively concentrated in a Li recovery solution. Furthermore, electrical power is generated.
- 2) Then, Li₂CO₃ powder, as a raw tritium breeder for fusion reactors, was fabricated by the chemical reaction by adding CO₂.

1. Introduction

2. International Fusion Energy Research Center
Activity

3. Development of Fusion Materials Irradiation Facility

4. Future plan in Rokkasho

5. Summary



Development of Fusion Materials Irradiation Facility

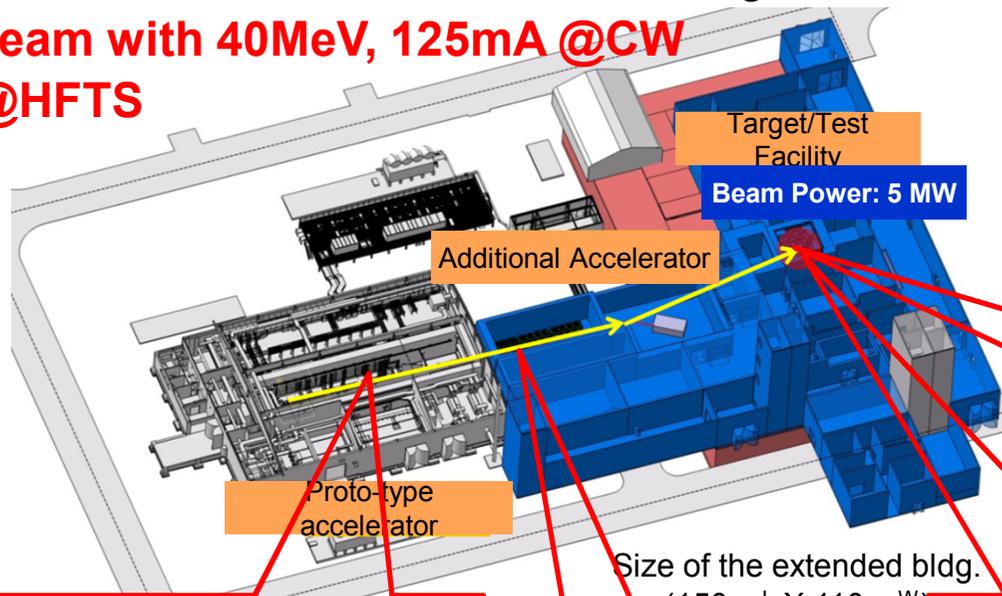
To confirm soundness of fusion material under strong neutron at a DEMO reactor, a strong fusion neutron source, like IFMIF, is required. In Rokkasho, the engineering design and validation tests of key components of IFMIF have been conducted under IFMIF/EVEDA Project of the Broader Approach Activities. As the next step, a neutron source for fusion materials irradiation at the Rokkasho site by utilizing/expanding the

Plan of Advanced Fusion Neutron Source(A-FNS) at Rokkasho

It is almost "half-IFMIF utilizing the facilities used for IFMIF/EVEDA.

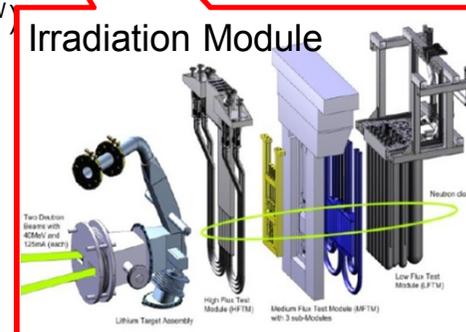
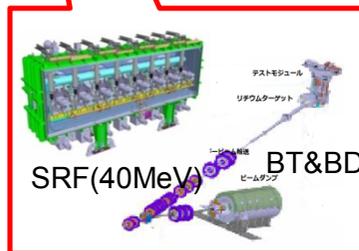
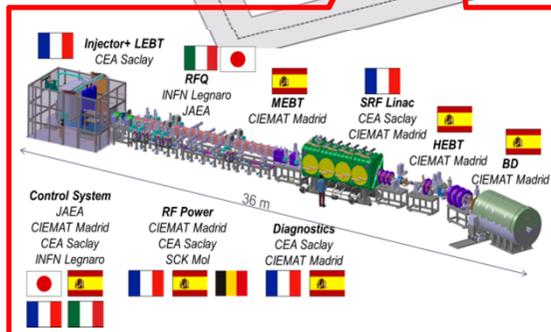
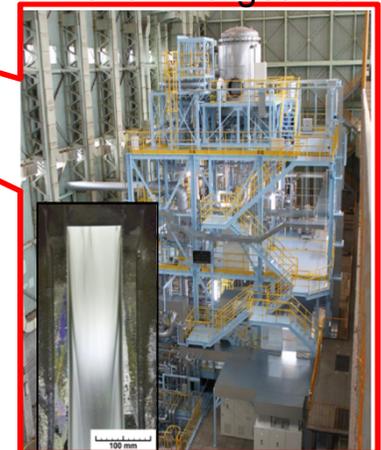
**D⁺ beam with 40MeV, 125mA @CW
n/s@HFTS**

Neutron flux: $S_n \sim 7 \times 10^{16}$



- Peripheral Facilities**
- PIE Facility
 - Tritium Handling Facility
 - Back-end Facility, etc.

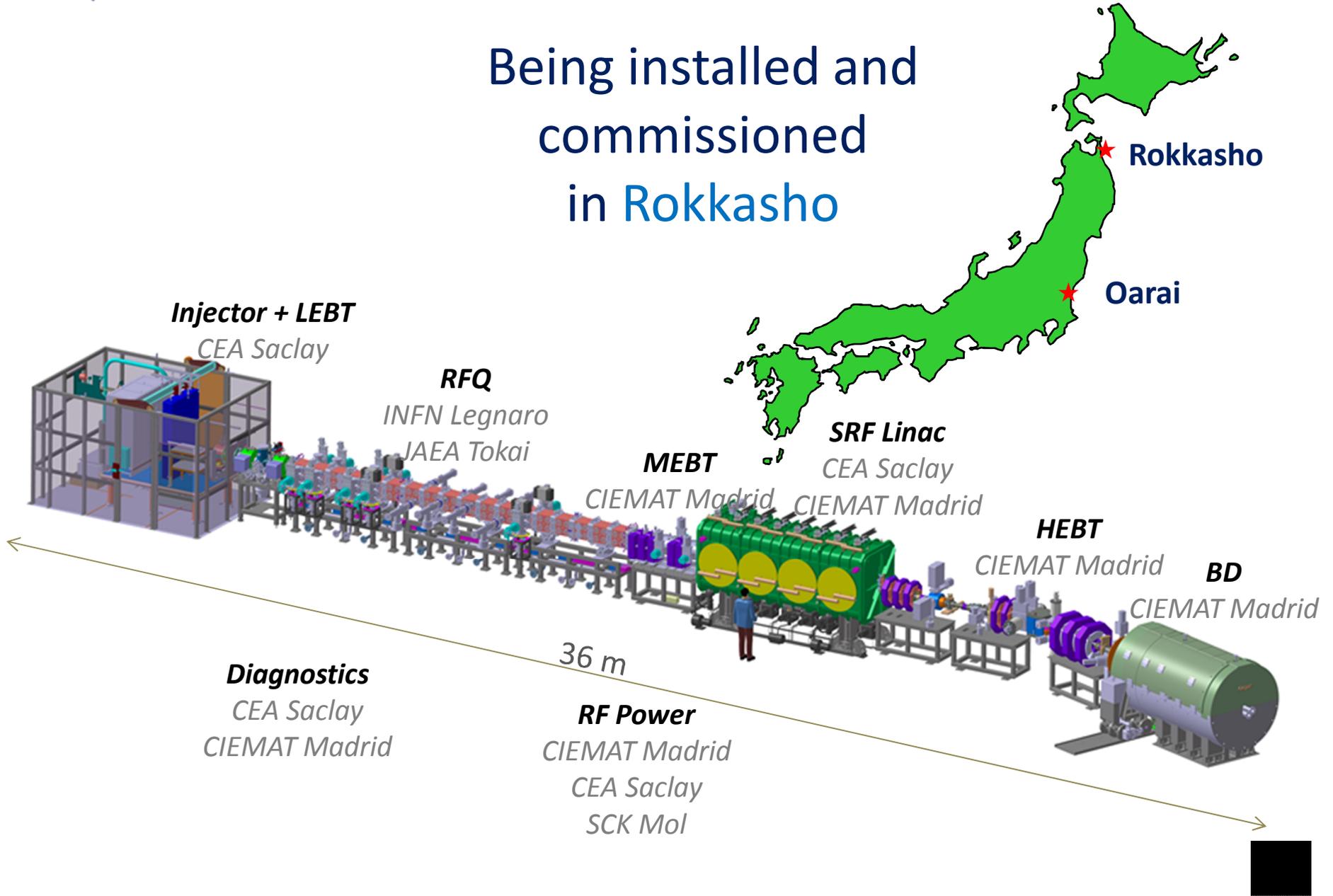
Lithium Target: 20m/





Linear IFMIF Prototype Accelerator - LIPAc

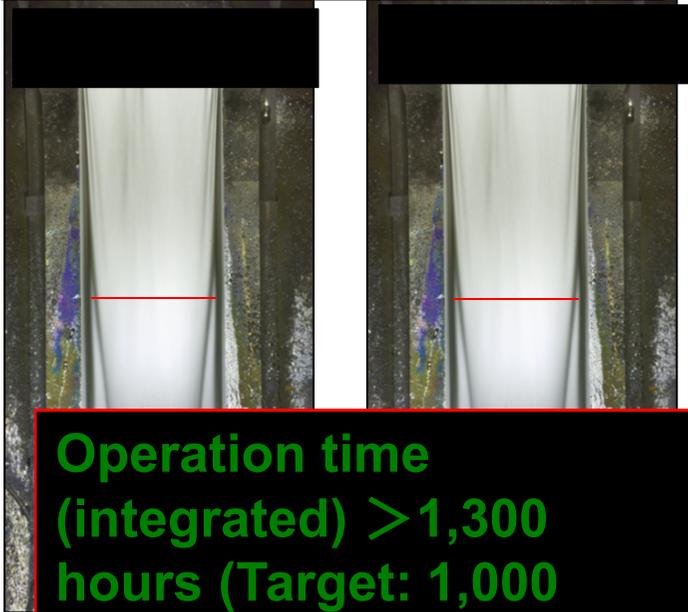
Being installed and
commissioned
in Rokkasho



Lithium Test loop development in IFMIF/EVEDA

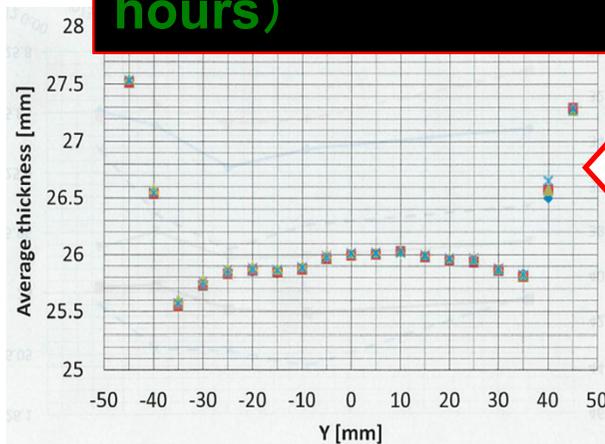
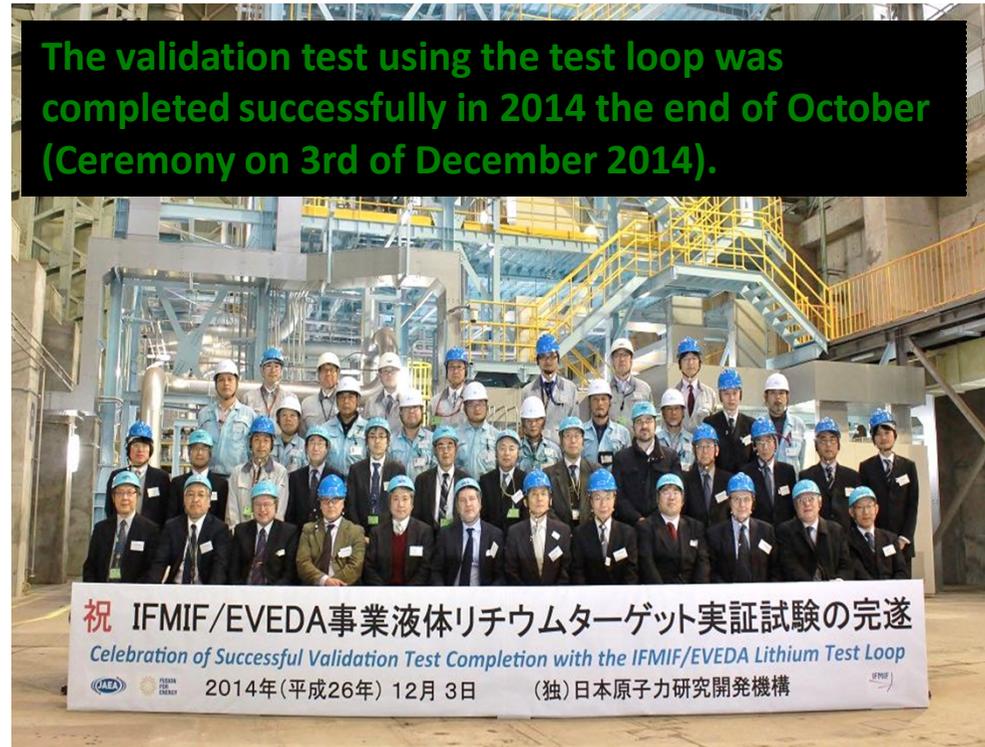
BA Activities

Validation of long term stability of Li flow for 25 days continuous operation in September 2014.

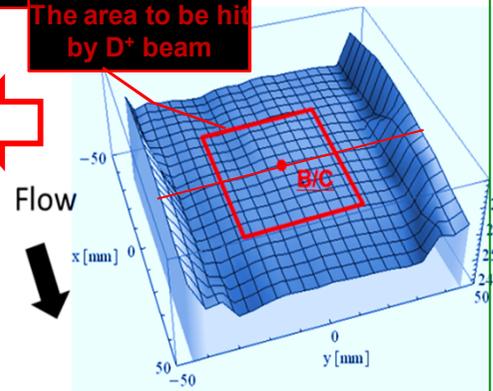


Operation time (integrated) > 1,300 hours (Target: 1,000 hours)

The validation test using the test loop was completed successfully in 2014 the end of October (Ceremony on 3rd of December 2014).



The area to be hit by D⁺ beam



To confirm the flow (surface) stability, a new measurement method using a laser was developed, which enable us to perform 3D measurement. Using this new technique, periodical measurements were made and it was proven that the stability achieved can satisfy its requirement (wave height ± 1 mm or less).

Progress of IFMIF/EVEDA Prototype Accelerator

BA Activities

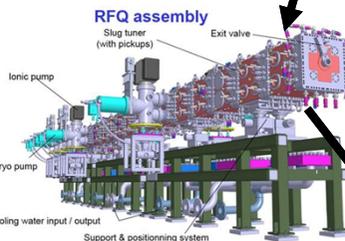
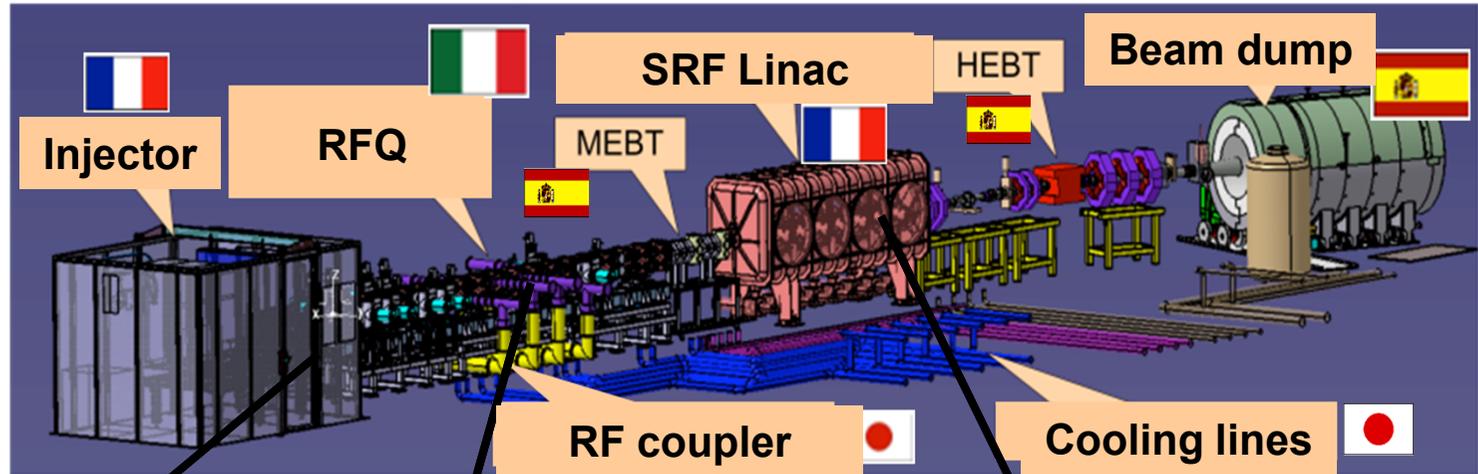
(LIPAc)

- As the first step of the validation test of the IFMIF/EVEDA Prototype Accelerator, the injector and its peripheral systems have been installed. The beam commissioning was started in November 2014 and now proton (H+) beam (100 kV, 125 mA) beam commissioning is in progress.
- Deuteron (D+) beam commissioning will start in July 2015.

For the IFMIF, two accelerators with 40 MeV, 125 mA CS D⁺ beam is needed.

IFMIF/EVEDA Prototype Accelerator (9MeV, 125mA, D+ beam)

Injector



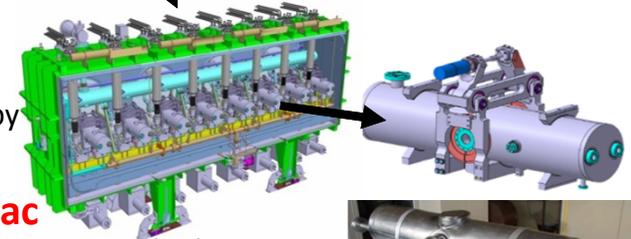
RFQ

Manufactured by
INFN @Legnaro
Italy

SRF Linac

Now it is under licensing process for the Japanese High Pressure Gas Safety Law. As soon as a special approval for the cryo cavity, its manufacture will start.

RFQ was tested in October 2014 and will be delivered to the IFERC site on October 2015.



Prototype cryo cavity

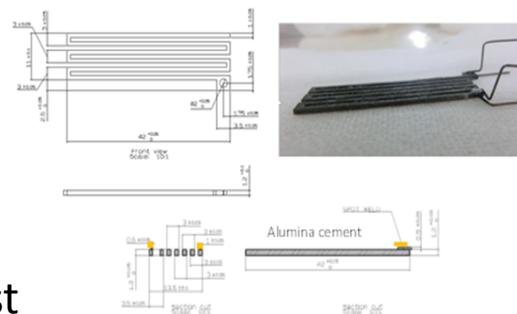
As a part of IFMIF/EVEDA project a gas cooling type high flux test module (HFTM) for the high-temperature irradiation of the IFMIF was developed, and also its performance test and the evaluation of the component equipment of the IFMIF test cell system. **The evaluation test of the electric performance (electric resistance measurement) of W-Re alloy and SiCf/SiC composite which are the candidate materials for the temperature control of the IFMIF, was carried out in Belgian Reactor 2 (BR-2) operated by SCK-CEN in JFY2014.**



BR-2 reactor (left) and the capsule for test of HFTM

In BR-2, we performed the evaluation test of the electrical properties (electrical resistance measurement) under the high-temperature irradiation of W-Re alloy and SiCf/SiC composite which are the candidate materials for the temperature control of the HFTM.

As a result of about 0.1 dpa irradiation test under the temperature condition of 600° C in the 1st cycle, the electric resistance value of W-3% Re alloy increased very moderately and the increase rate was $3.3 \times 10^{-3} \Omega / \text{dpa}$. On the other hand, the electric resistance value of SiCf/SiC composite moderately decreased with the passage of the irradiation time, and the decrease rate was $0.42 \Omega / \text{dpa}$.



BR-2 SiC/SiC composite test

plate (left) and W-3%Re alloy test plate

2. International Fusion Energy Research Center Act

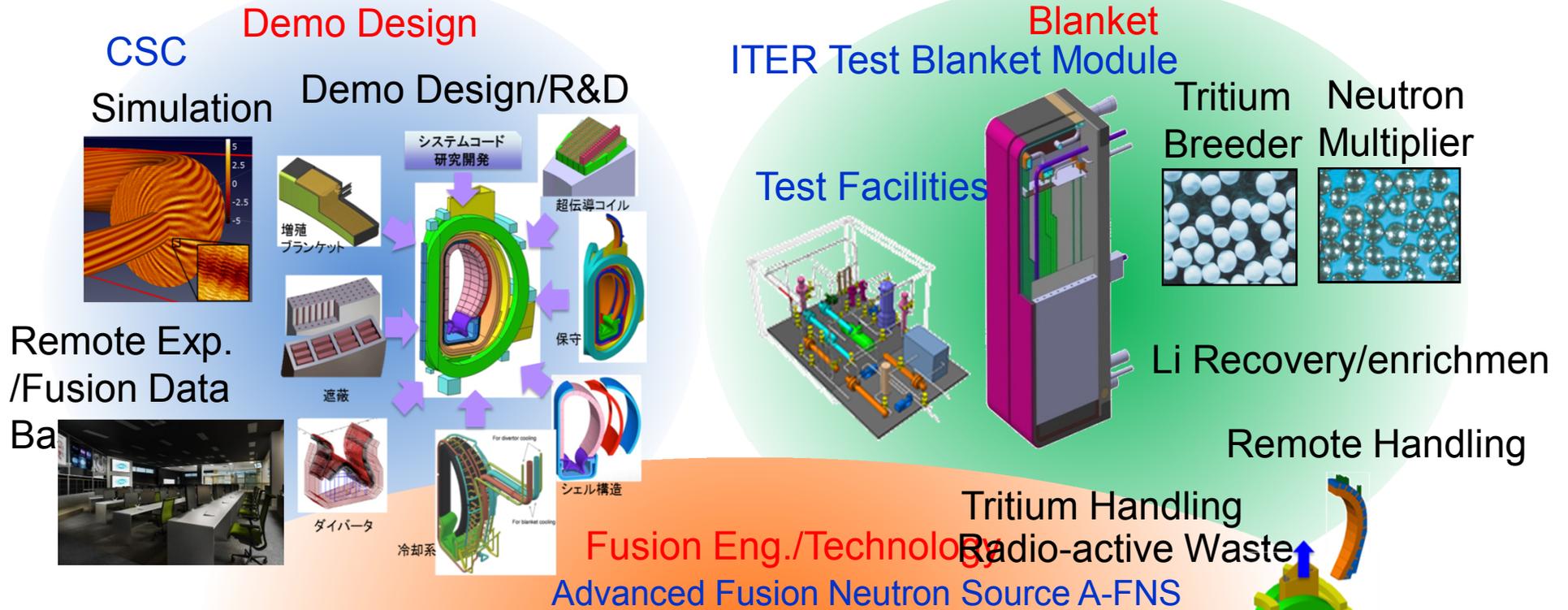
3. Development of Fusion Materials Irradiation Faci

4. Future plan in Rokkasho

5. Summary

Fusion Demo Frontier in Rokkasho

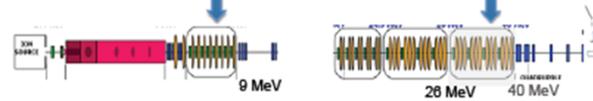
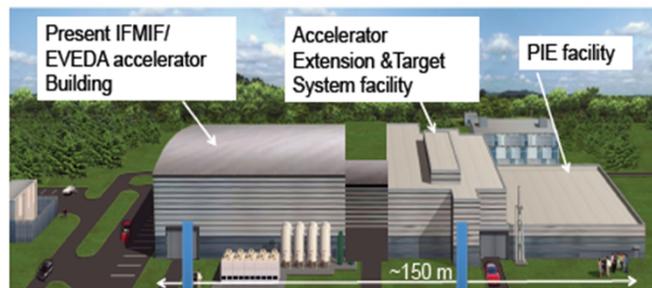
JA Core Site for Fusion Engineering & Technology using/expanding Facilities developed in BA activities



Structural Materials F82



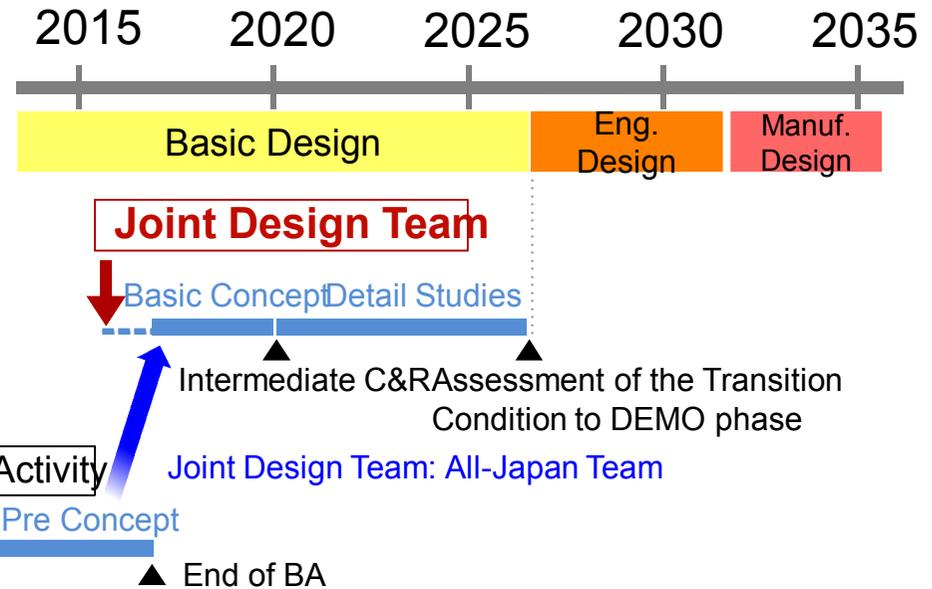
Advance Materials SiC/S



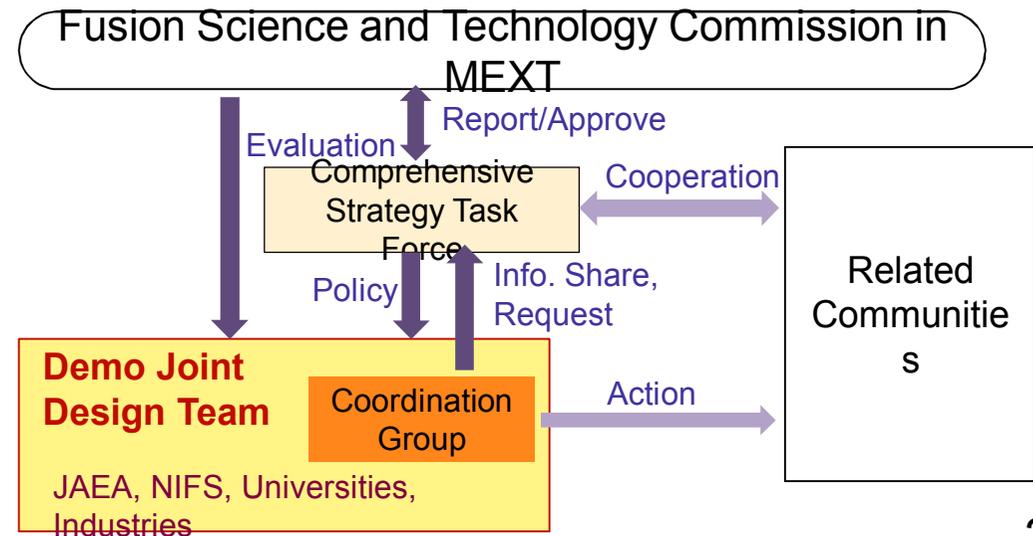
DEMO Joint Design Team

From 1st June 2015, the DEMO Joint Design Team started its activity in Rokkasho Fusion Institute.

Joint Design Team:
 Full Time : 18staffs
 Part Time: 34staffs
 from JAEA, NIFS, Universities,
 Industries



First Meeting at 18th June, 2015



DEMO R&D Facilities

- Completion of world top level facility handling **Tritium, RI with γ emission, and Beryllium**
- Start of RI handling, development of fabrication technology of Beryllide pebbles

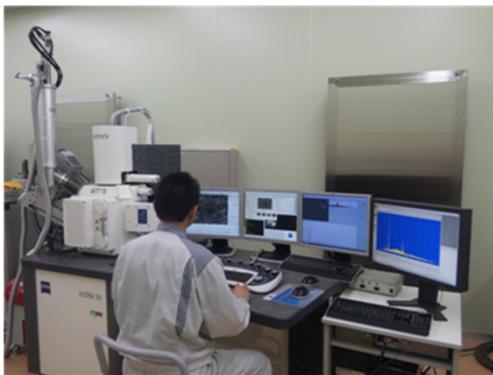
Glove box for Tritium handling



Start of RI handling

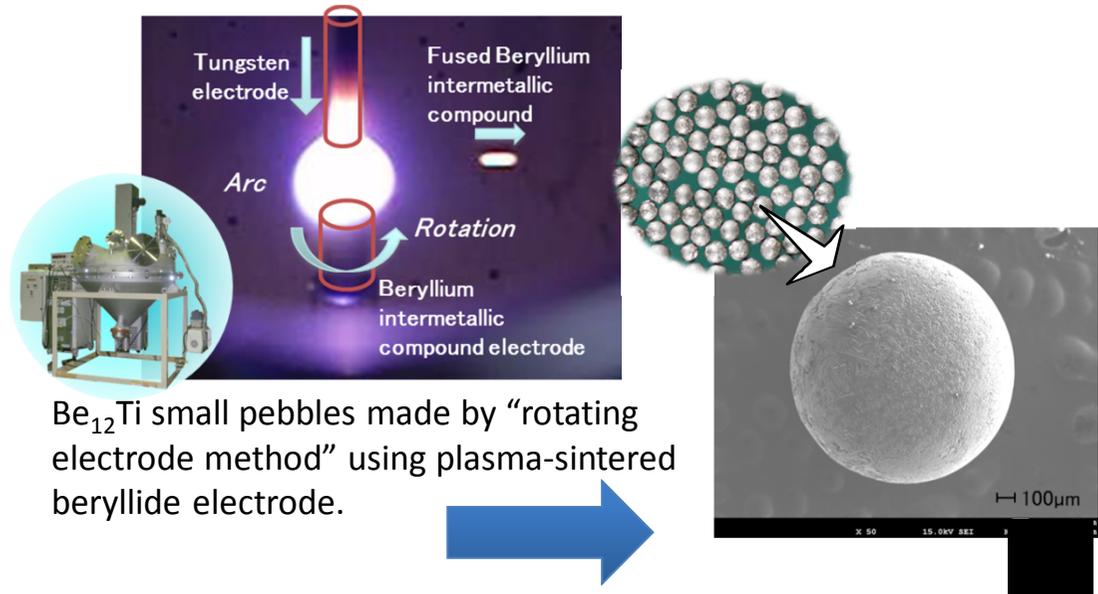
- Licensing of RI area (2012/2)
- Bringing Tritium (2012/3, 38GBq)
- Erosion test of stainless steel by Tritium

Micro-structure analysis



High-performance FE-SEM/μ-EDS

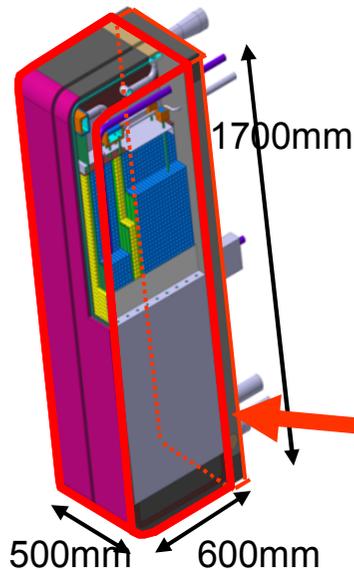
Beryllide pebble fabrication by rotating electrode method using plasma-sintered beryllide electrode



Be₁₂Ti small pebbles made by “rotating electrode method” using plasma-sintered beryllide electrode.

Blanket Development

Test Blanket Module for ITER



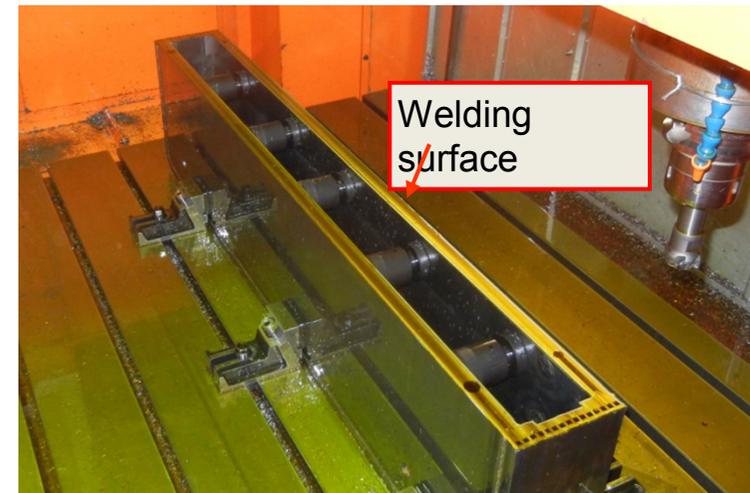
Pressure Test
For cooling
channel
@18.5MPa

Pressure test of Full-size
Back-Plate Mock-up

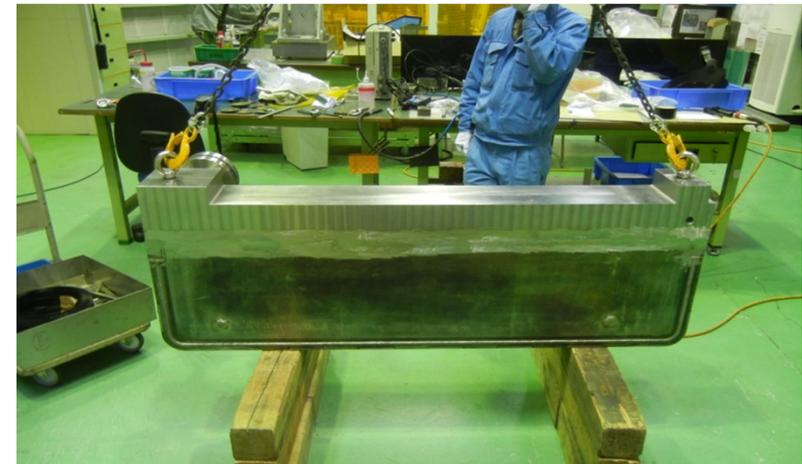
Manufactured Full-size back-plate for ITER Test Blanket Module(TBM) using Reduced-activation ferritic steel F82H and completed pressure test of Back-plate Mock-up at 18.5MPa. By welding the back-plate to side-wall Mock-up, Completed to manufacture Full Box Mock-up of ITER TBM. Verified soundness of welded structure by

Heavy irradiation test
on structural Material
⇒US-Japan
Collaboration

R&D of structural material, breeding
material, neutron multiplication
material
⇒R&D on BA Project

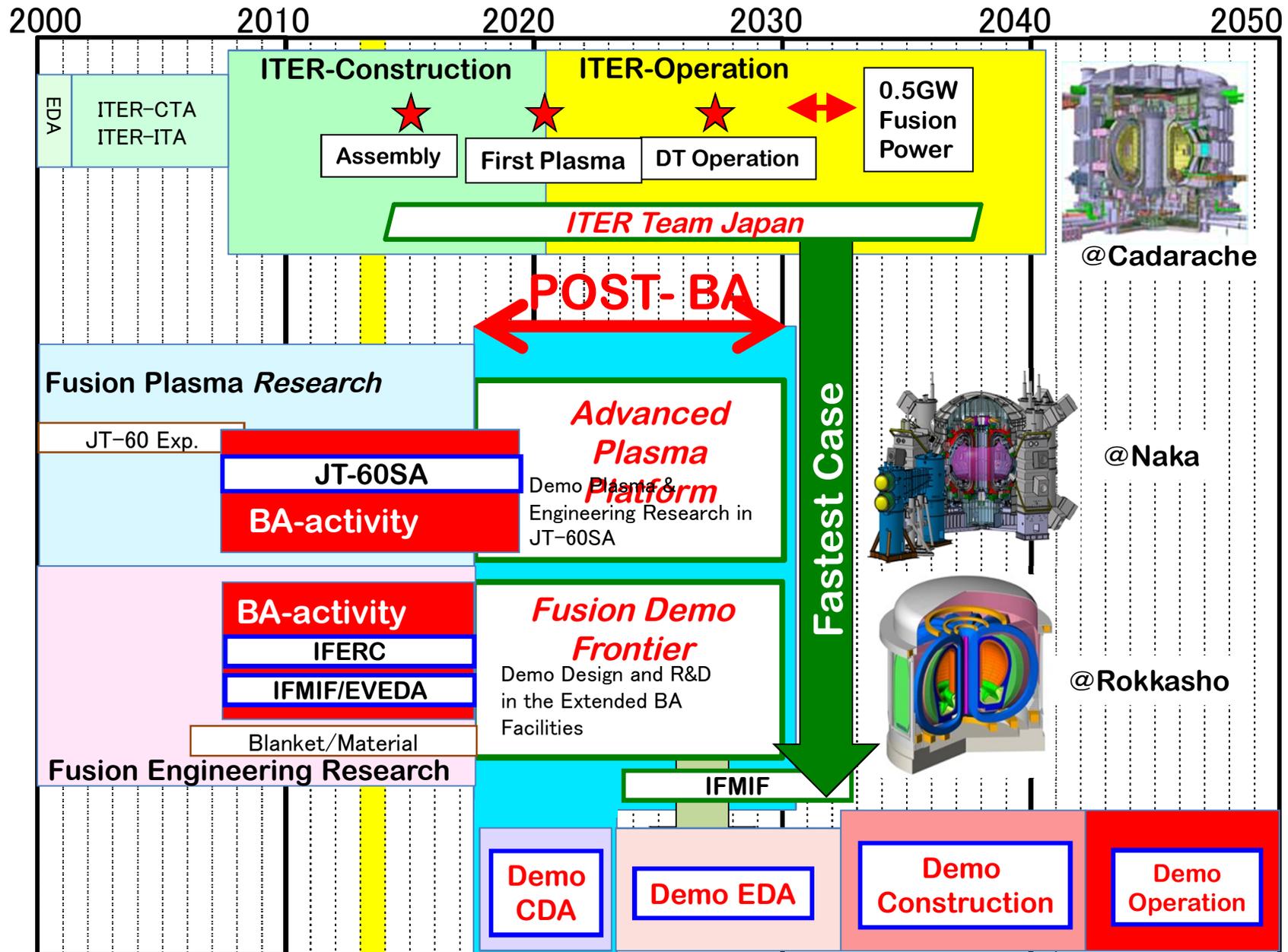


Process welding surface in Side-wall Mock-up



Full Box Mock-up of ITER TBM

JAEA Plan* toward Demo Reactor



* Consistent with the general roadmap shown in the policy paper issued by the Atomic Energy Committee of

Another Topic

- 5. Experimental and computational approaches to the elucidation of hydrogen isotope permeation in erbium oxide coatings for tritium permeation barrier (T.Terai et al., Univ. of Tokyo)**

Tritium permeation barrier in fusion devices

Most metals for structural materials of fusion reactors (Fe, V, Ti, etc.) has high permeability of hydrogen isotopes.

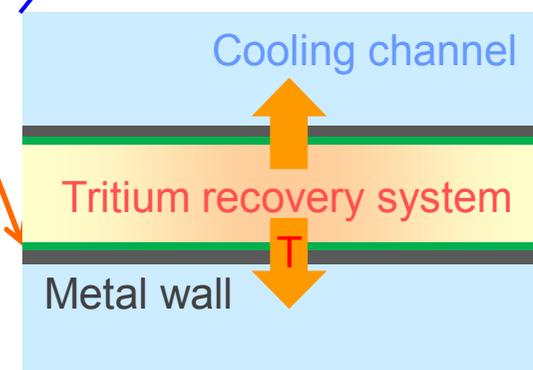
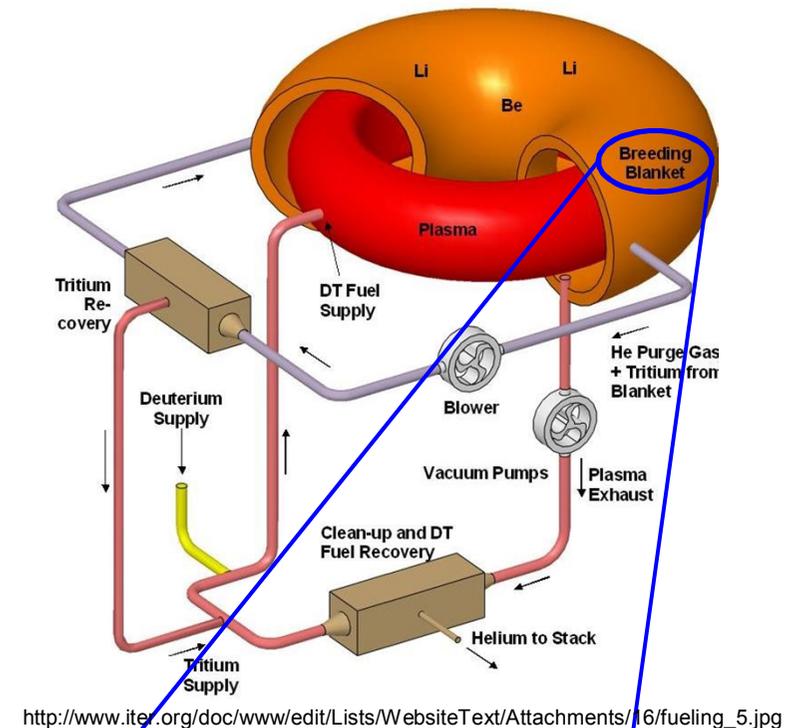
→ Tritium permeation through the structural materials in fuel systems causes:
crucial fuel loss / radiological problems.

Tritium Permeation Barrier (TPB)

TPB coatings have been investigated since 1970's with **ceramics**.

Requirements

- ◆ High permeation reduction factor (PRF)
 $PRF = J_{uncoated} / J_{coated} > 10^2 - 10^3$
- ◆ Compatibility with blanket materials
- ◆ Thermal durability, irradiation resistance, accessible fabrication process, etc.



Erbium oxide coatings as TPB

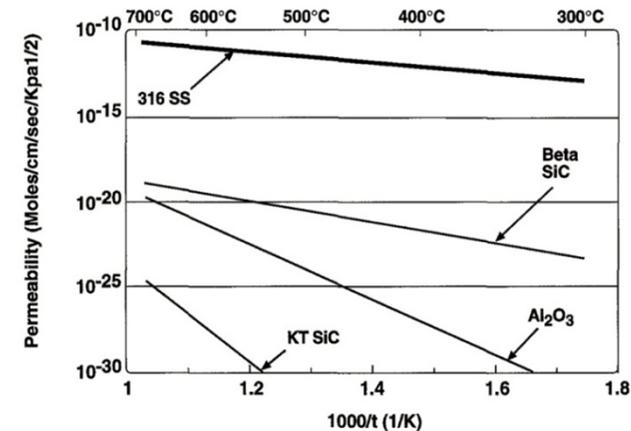
Problems of TPB coating research

- ✓ Much higher permeability than bulks
- ✓ 4 orders of magnitude **scattered data**

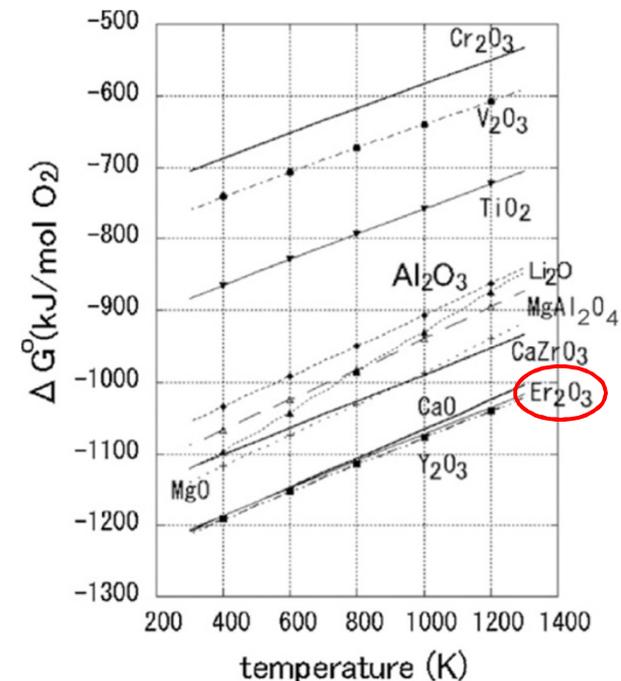
Erbium Oxide (Er_2O_3)

- Originally selected as an **electrical insulating coating**
- High thermodynamic stability
- Compatibility with liquid Li
- Lower crystallization temperature ($< \text{Al}_2\text{O}_3$)

In this presentation, the decade-long study on the elucidation of hydrogen isotope permeation mechanism in Er_2O_3 coatings through experimental and computational approaches is reviewed.



Hydrogen permeabilities of ceramic bulks [1].



Gibbs free energy of metal oxides [2].

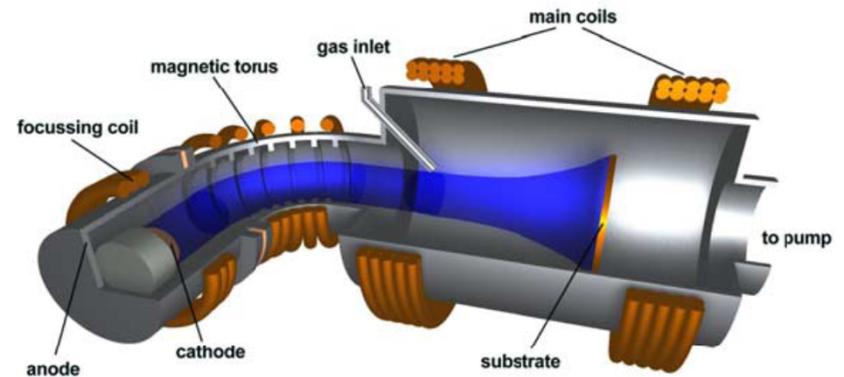
[1] G.W. Hollenberg, et al., *Fusion Engineering and Design* 28 (1995) 190–208.

[2] T. Muroga, et al., *Fusion Engineering and Design* 85 (2010) 1301–1306.

Fabrication methods

(1) Filtered vacuum arc deposition (VAD)

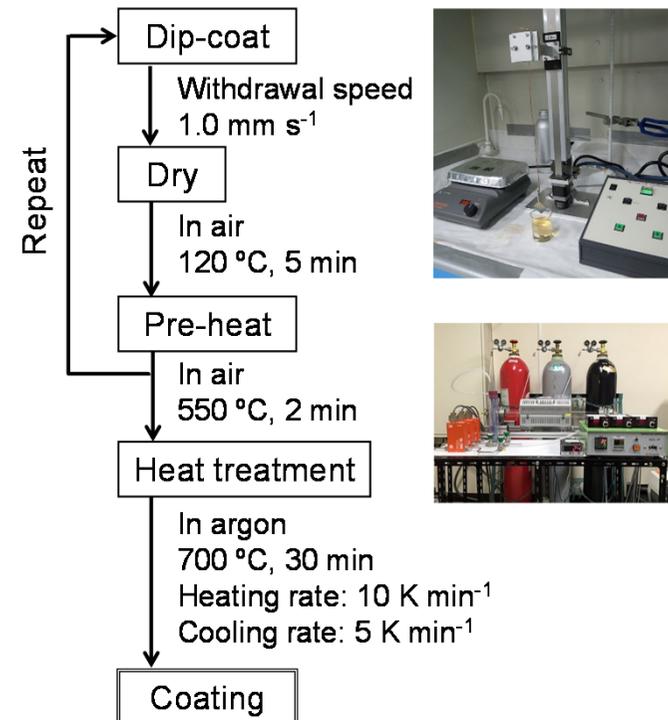
- A physical vapor deposition method
 - Good adhesion on substrates
 - Low impurity
 - Coating thickness: 1–3 μm
- Clarification of permeation mechanism



Vacuum arc deposition device (IPP-Garching).

(2) Metal-organic decomposition (MOD)

- Ability to coat on complex-shape substrates
 - Potential to apply plant-scale fabrication
 - Coating thickness: 0.1–0.3 μm (adjustable by repeating the coating process)
 - Other ceramic coatings (Y_2O_3 , ZrO_2 , etc.) can be prepared using precursors
- Development of practical applications

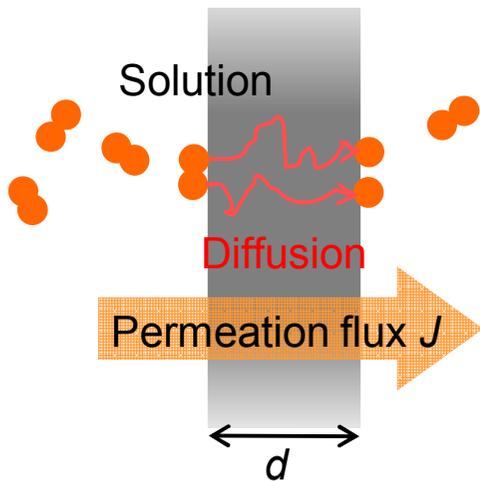


MOD process (dip coating).

Characterization

Gas-driven permeation formula

Permeation = Solution × Diffusion

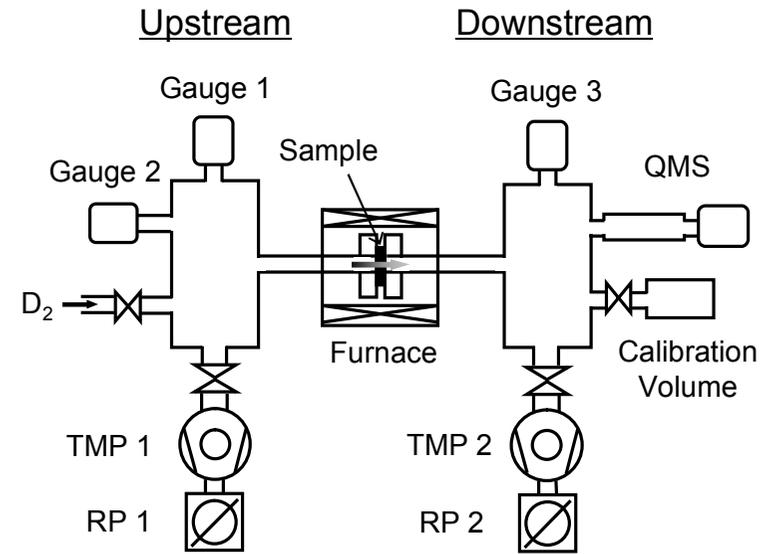


Richardson's law

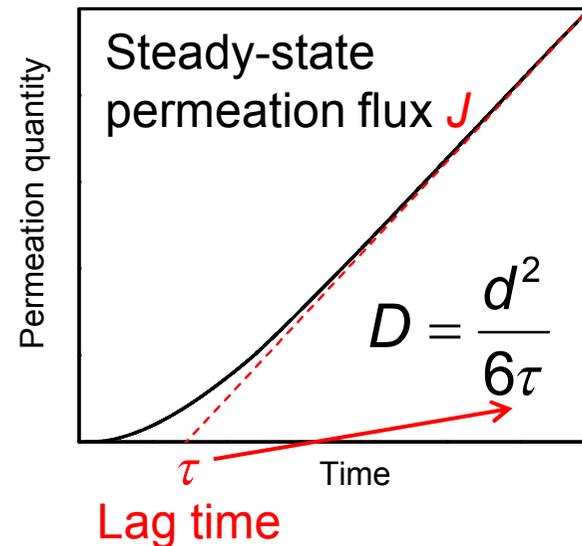
$$J = \underbrace{K_S D}_{P} \frac{\Delta p^n}{d}$$

$$P = P_0 \exp\left(-\frac{\Delta H + E_D}{RT}\right)$$

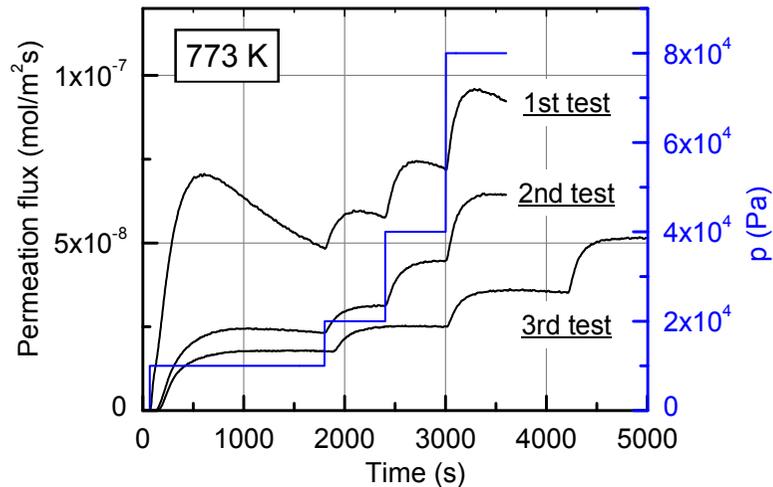
- J : Permeation flux
- D : Diffusivity
- p : D_2 partial pressure
- ΔH : Solution heat (enthalpy difference)
- E_D : Activation energy of diffusion
- K_S : Sieverts' constant
- P : Permeability
- d : Sample thickness



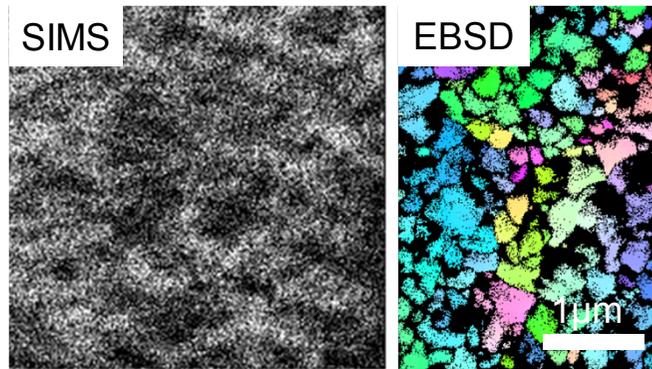
Gas-driven deuterium permeation apparatus.



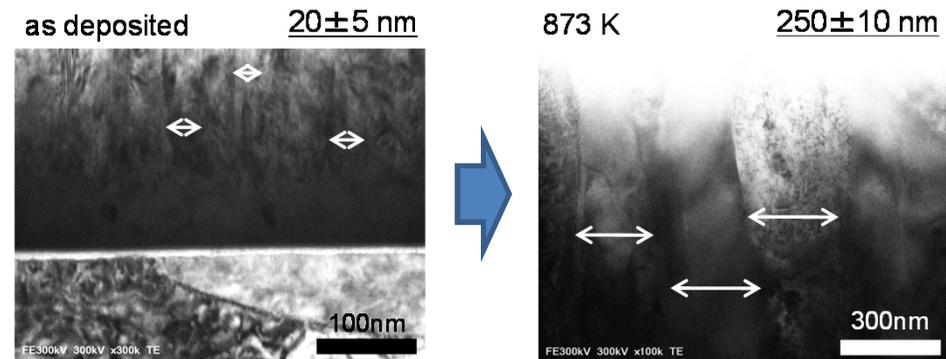
Permeation mechanism in VAD coating



Temporal change of deuterium permeation flux of VAD- Er_2O_3 coating deposited at R.T.



Deuterium distribution of the VAD coating surface after deuterium introduction (left) and grain structure of the coating (right).



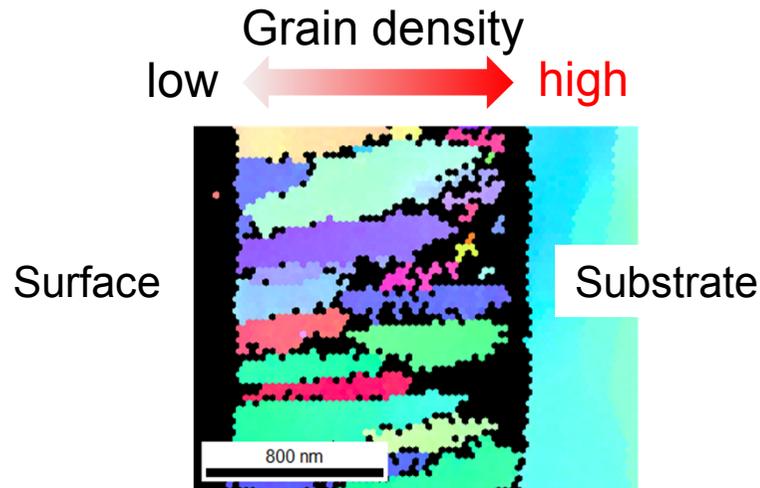
Cross-sectional bright field TEM images of the VAD- Er_2O_3 coating before and after permeation tests.

- In spite of fixed driving pressures, deuterium permeation flux decreased at the beginning of the permeation tests.
- The crystal grain of the coating grew depending on the test temperature.

Grain growth ⇔ High TPB efficiency

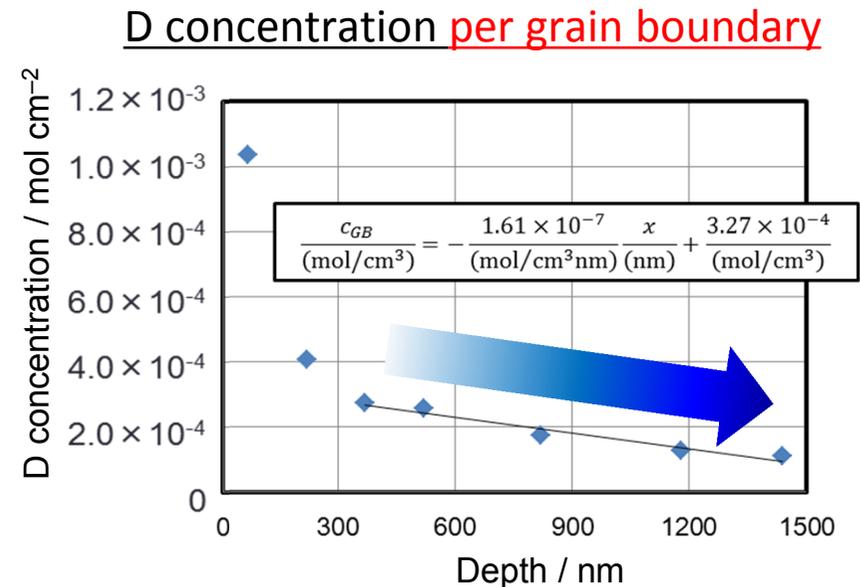
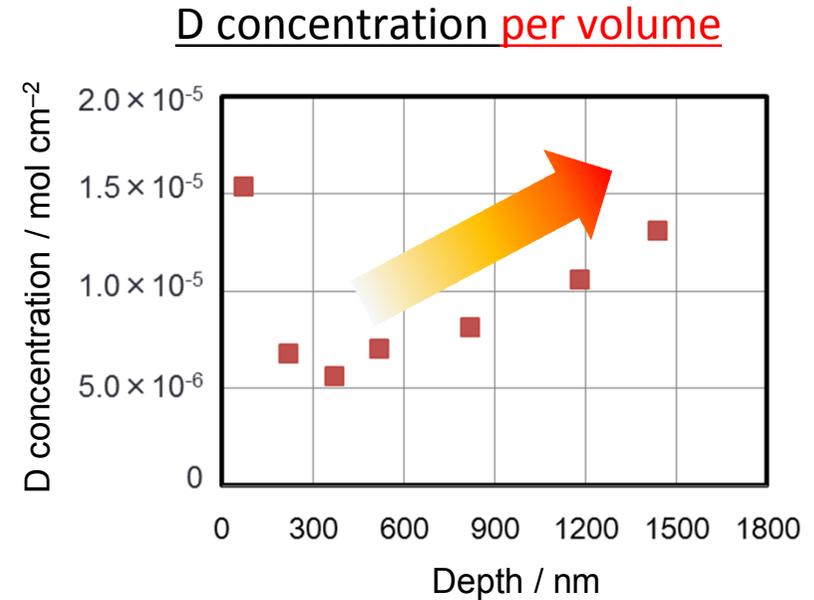
Deuterium permeation through the coating is dominated by **grain boundary diffusion** rather than lattice diffusion.

Permeation mechanism in VAD coating



Grain orientation of the cross-section of the Er_2O_3 coating using electron back scattering diffraction (EBSD).

- An average grain boundary density at a certain depth was estimated using the grain structure information.
- D concentration per grain boundary showed a linear depth profile corresponding to Fick's law.
- Estimated diffusivity
D depth profile: $1.7 \times 10^{-15} \text{ m}^2 \text{ s}^{-1}$
Permeation data: $1.8 \times 10^{-15} \text{ m}^2 \text{ s}^{-1}$

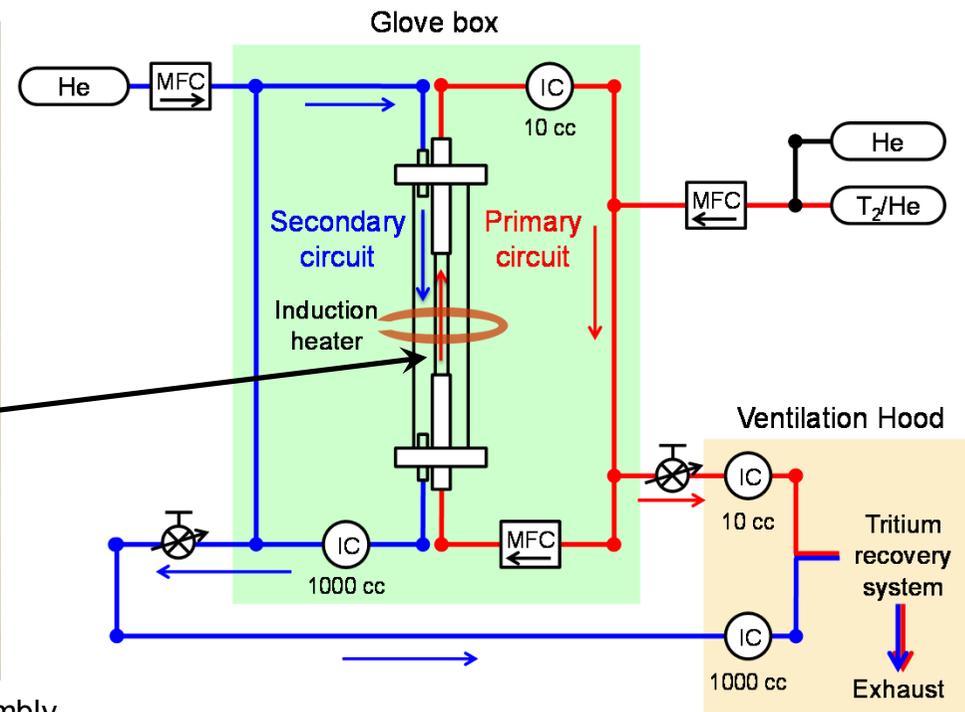


Permeation mechanism in MOD coating

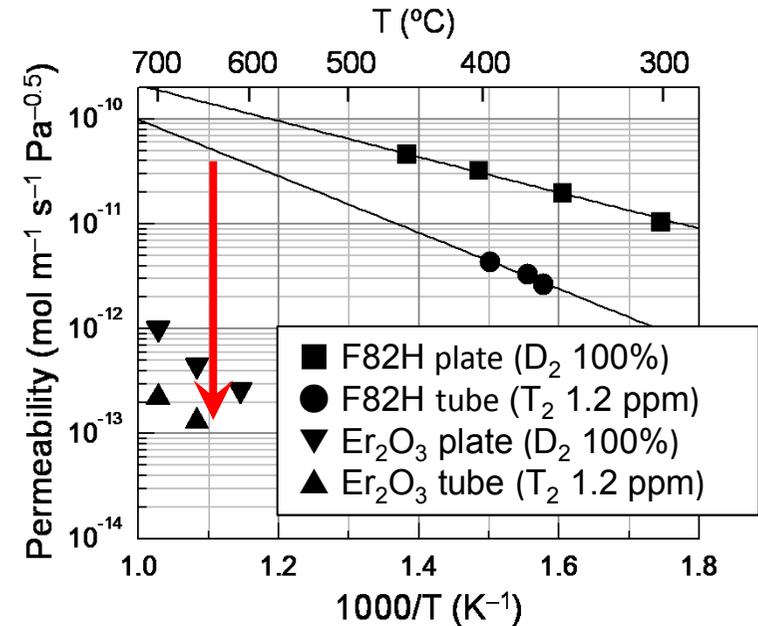
Tritium permeation experiments on F82H and Er_2O_3 -coated F82H tubular samples were carried out with **low partial pressure tritium (1–100 ppm / 0.1–10 Pa)** in the framework of Japan-US TITAN collaborative program.



Sample assembly (Er_2O_3 -coated)



Tritium permeation system

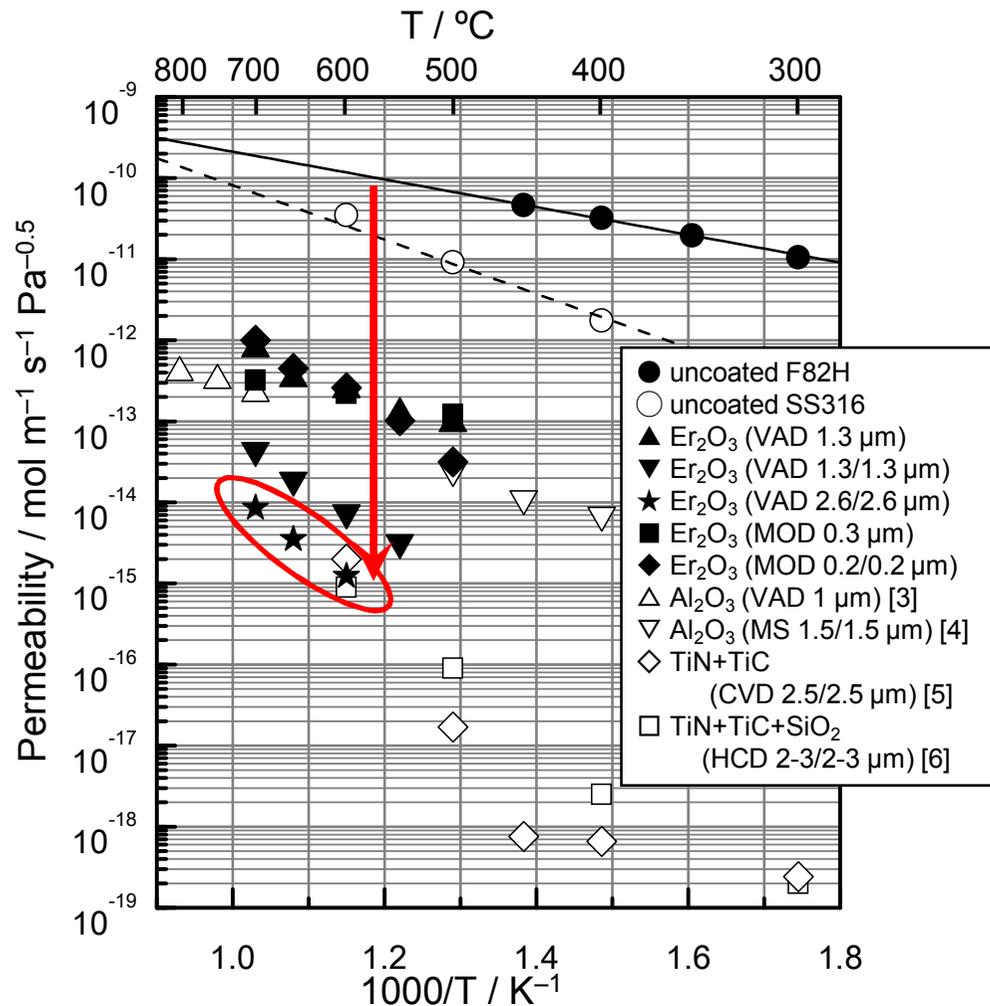


Comparison of tritium/deuterium permeability of uncoated and coated F82H plates and tubes.

The PRF comparable with those of VAD coatings was confirmed with the MOD coating prepared on F82H tubular substrates.

Details in: T. Chikada, *et al.*, *Journal of Nuclear Materials* 442 (2013) 533–537.
T. Chikada, *et al.*, *Fusion Engineering and Design* 89 (2014) 1402–1405.

Summary of hydrogen permeability



Comparison of deuterium permeabilities obtained in our study (filled) and references [3–6] (open).

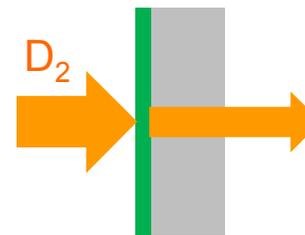
- [3] D. Levchuk, *et al.*, *Journal of Nuclear Materials* 328 (2004) 103–106.
- [4] E. Serra, *et al.*, *Journal of Nuclear Materials* 257 (1998) 194–198.
- [5] C. Shan, *et al.*, *Journal of Nuclear Materials* 191–194 (1992) 221–225.
- [6] Z. Yao, *et al.*, *Journal of Nuclear Materials* 283–287 (2000) 1287–1291.

Er₂O₃ coatings showed PRFs of more than 10³ by both VAD and MOD methods.

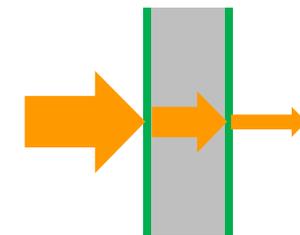
→ Uniform coatings without pores or cracks were fabricated.

A series of experiments achieved **the world largest PRFs (10⁴-10⁵)** by **both-side-coated** samples at > 600 °C.

One-side coated



Both-side coated



The number of permeation steps is important to reduce the hydrogen permeation flux.

Modeling of hydrogen permeation

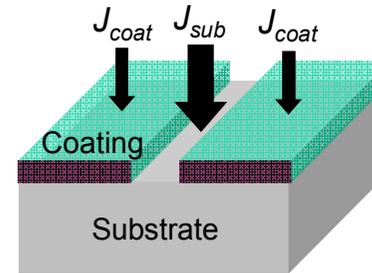
Surface coverage model and grain boundary diffusion model were combined in order to evaluate the response to each parameter.

$$J(\theta, S_a) = \underbrace{(P_{gb} S_a) \frac{p^{0.5}}{d_{coat}} \theta}_{\text{Coated region}} + \underbrace{P_{sub} \frac{p^{0.5}}{d_{sub}} (1 - \theta)}_{\text{Uncoated region}}$$

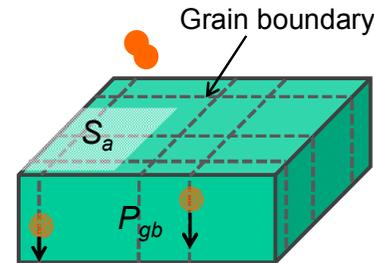
→ Large permeation reduction cannot be expected by the coatings with large crystal grain **if surface coverage is low.**

First priority is **surface coverage**

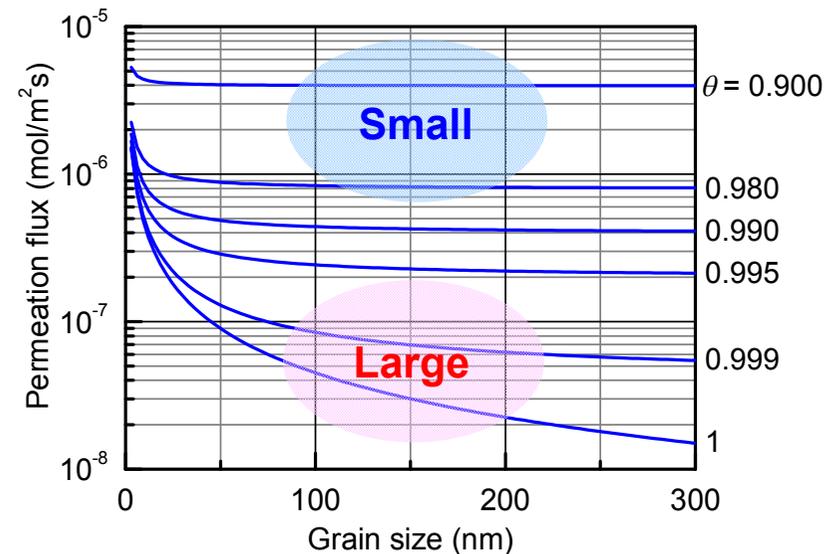
→ Materials and fabrication methods with lower S_a and P_{gb} should be selected afterwards



d_{coat} : Thickness of coating
 P_{sub} : Permeability of substrate
 d_{sub} : Thickness of substrate
 p : Driving pressure
 θ : Surface coverage

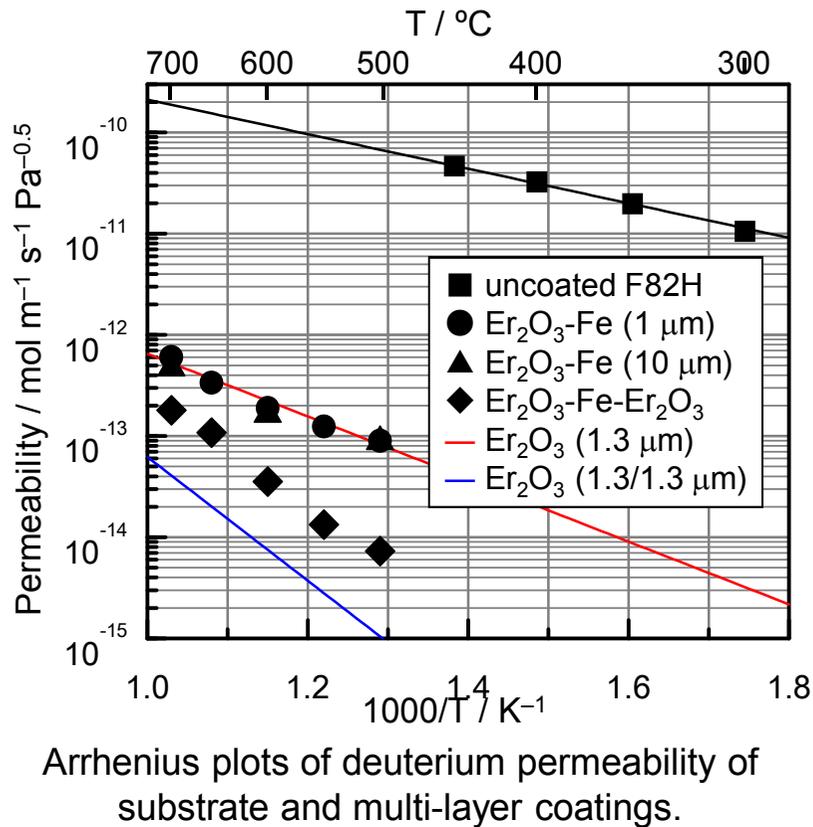


P_{gb} : Permeability through grain boundary
 S_a : Grain area density



Relationship between permeation flux and grain size of the VAD coatings with different surface coverage (1.3 μm -thick coating, at 500 °C, and 8.00×10^4 Pa)

Recent topics (1) Potential of multilayer coatings



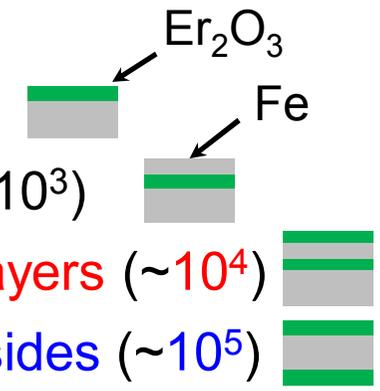
PRFs

Single Er_2O_3 layer ($\sim 10^3$)

\approx Er_2O_3 -Fe two layers ($\sim 10^3$)

< Er_2O_3 -Fe- Er_2O_3 three layers ($\sim 10^4$)

< Er_2O_3 coating on both sides ($\sim 10^5$)



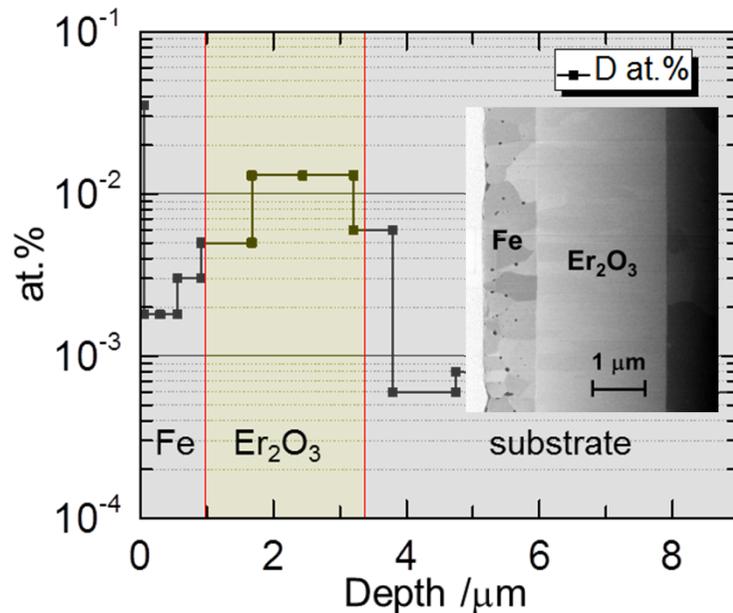
Activation energy of permeation

Temperature dependence of permeability showed an intermediate slope between single or two layer and both-sides coated samples. ($E_p \sim 100 \text{ kJ mol}^{-1}$)

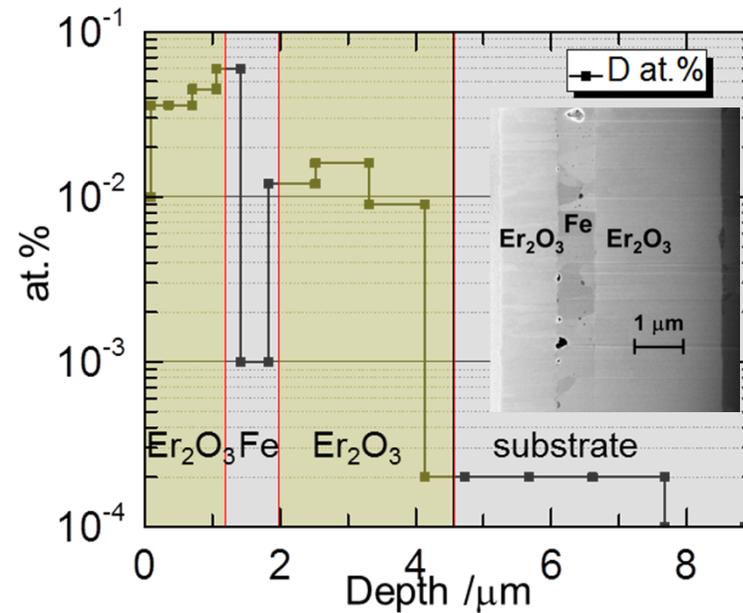
- Two diffusion barriers of Er_2O_3 coatings were contributed **independently** to the decrease of permeability in comparison with the single-layer coating.
- Permeation behavior was affected by recombination process on **back surface**.

Recent topics (1) Potential of multilayer coatings

D₂ pressure: 80 kPa / Exposure temperature: 600 °C



Deuterium depth profiles for Er₂O₃-Fe coating.



Deuterium depth profiles for Er₂O₃-Fe-Er₂O₃ coating.

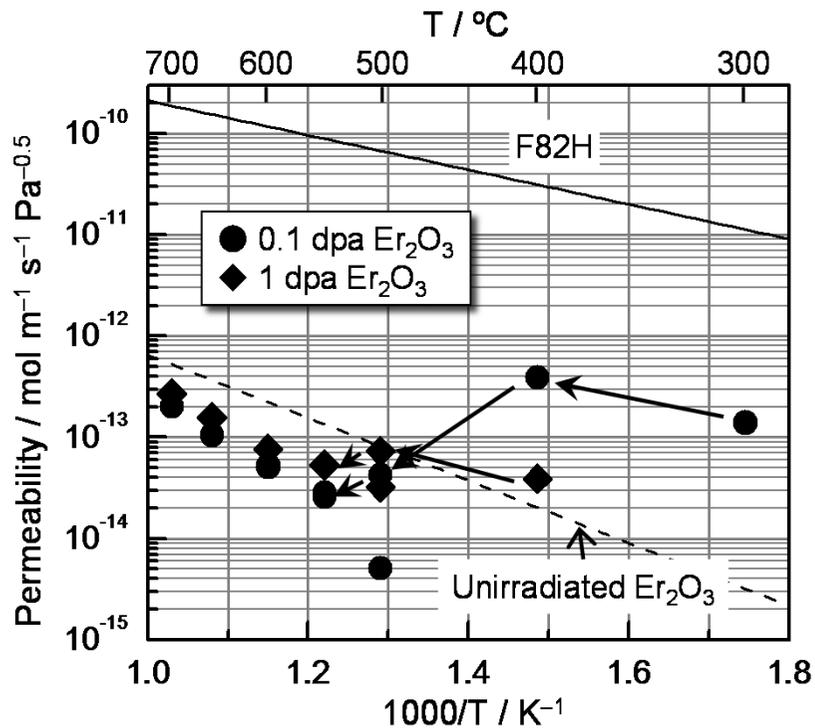
Two-layer coating

- ❑ Deuterium permeation was dominated by grain boundary diffusion.
- ❑ Lower D retention than the Er₂O₃ single layer coating would be attributed to **the lower D solubility in the Fe layer.**

Three-layer coating

- ❑ Total D retention was **three times higher** than the Er₂O₃-Fe coating due to **the surface Er₂O₃** and **two Er₂O₃ layers.**

Recent topics (2) Irradiation effect on permeation



Arrhenius plots of deuterium permeability of damaged Er_2O_3 coatings.

Irradiation condition

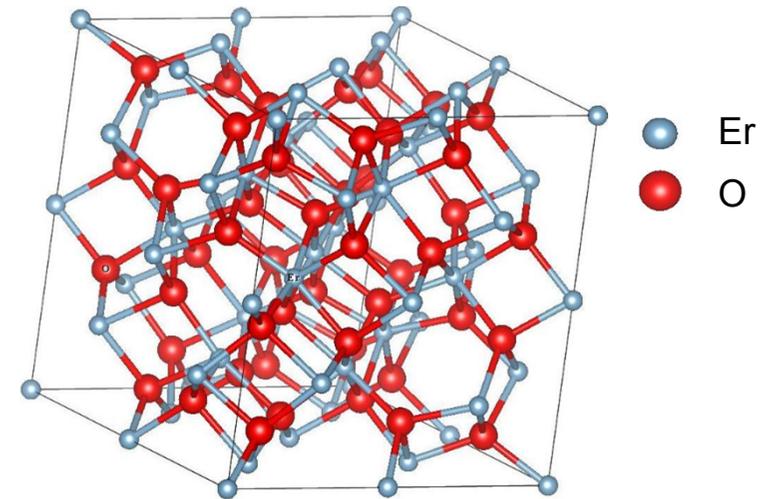
- Energy/Ion species: 6.4 MeV Fe^{3+}
- Flux: $2.1 \times 10^{15} \text{ m}^{-2} \text{ s}^{-1}$
- Fluence: 1.8×10^{18} , $1.8 \times 10^{19} \text{ m}^{-2}$
- Sample temperature: 600 $^\circ\text{C}$

- ❑ Heavy-ion irradiation was applied to simulate neutron irradiation because the damage distributes throughout the Er_2O_3 coating.
- ❑ The damaged samples showed lower deuterium permeabilities and higher activation energy of permeation than the unirradiated Er_2O_3 coating.
 - ➔ The ion irradiation under elevated temperature contributes to the modification of the grain structure of the coating by irradiation damage introduction and recovery.
- ❑ Observation of grain structure and irradiation defects is ongoing.

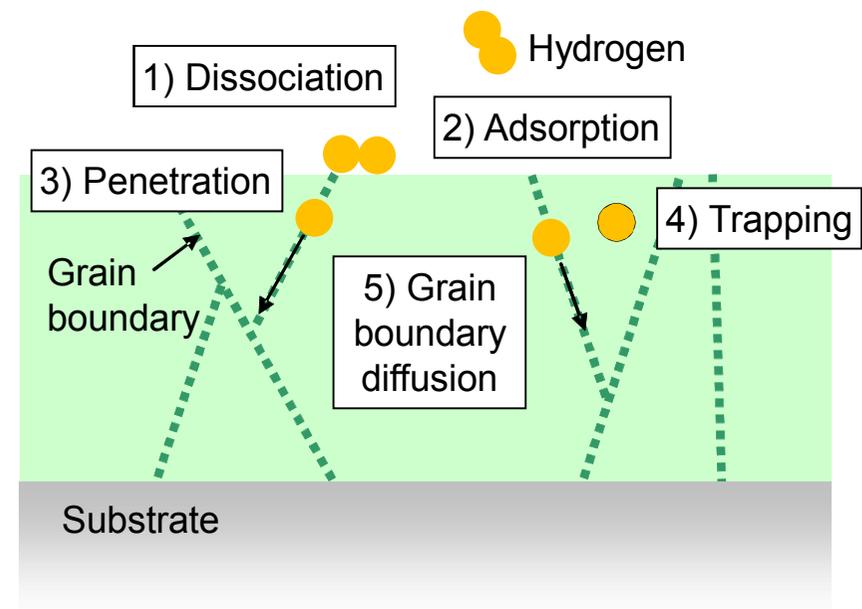
Calculation of microscopic hydrogen behavior

Microscopic behavior of hydrogen migration in Er_2O_3 is investigated using **density functional theory DFT** and **molecular dynamics MD**.

- Elemental steps in hydrogen permeation:
 - 1) dissociation at surface,
 - 2) adsorption,
 - 3) penetration from surface to bulk,
 - 4) diffusion in the bulk,
 - 5) interaction with vacancy, and
 - 6) diffusion along grain boundary, were simulated.
- Energetic values such as activation energy of diffusion E_D and heat of solution ΔH were calculated on Er_2O_3 with/without defects and grain boundaries.



Conventional cubic-phase Er_2O_3 cell (Er:32, O:48).
 $a = b = c = 10.55 \text{ \AA}$, $\alpha = \beta = \gamma = 90^\circ$



Calculation conditions

Quantum mechanics and density-functional theory (DFT)

Schrödinger equation

$$\hat{H}\Psi(x, t) = E\Psi(x, t)$$

Code: Vienna Ab initio Simulation Package (VASP 5.2.12)

- GGA-PBE pseudopotential
- Cut-off energy: 500.0 eV
- Nudged elastic bond (NEB) and zero-point-energy (ZPE) correction.

Slab: 2×2×1 supercell (240 atoms)
+ vacuum region (12 Å),
2×2×1 K-points.

Bulk: Conventional cell (80 atoms),
4×4×4 K-points.

Molecular dynamics (MD) simulations

Interatomic potential

(Lennard-Jones, Buckingham etc.)

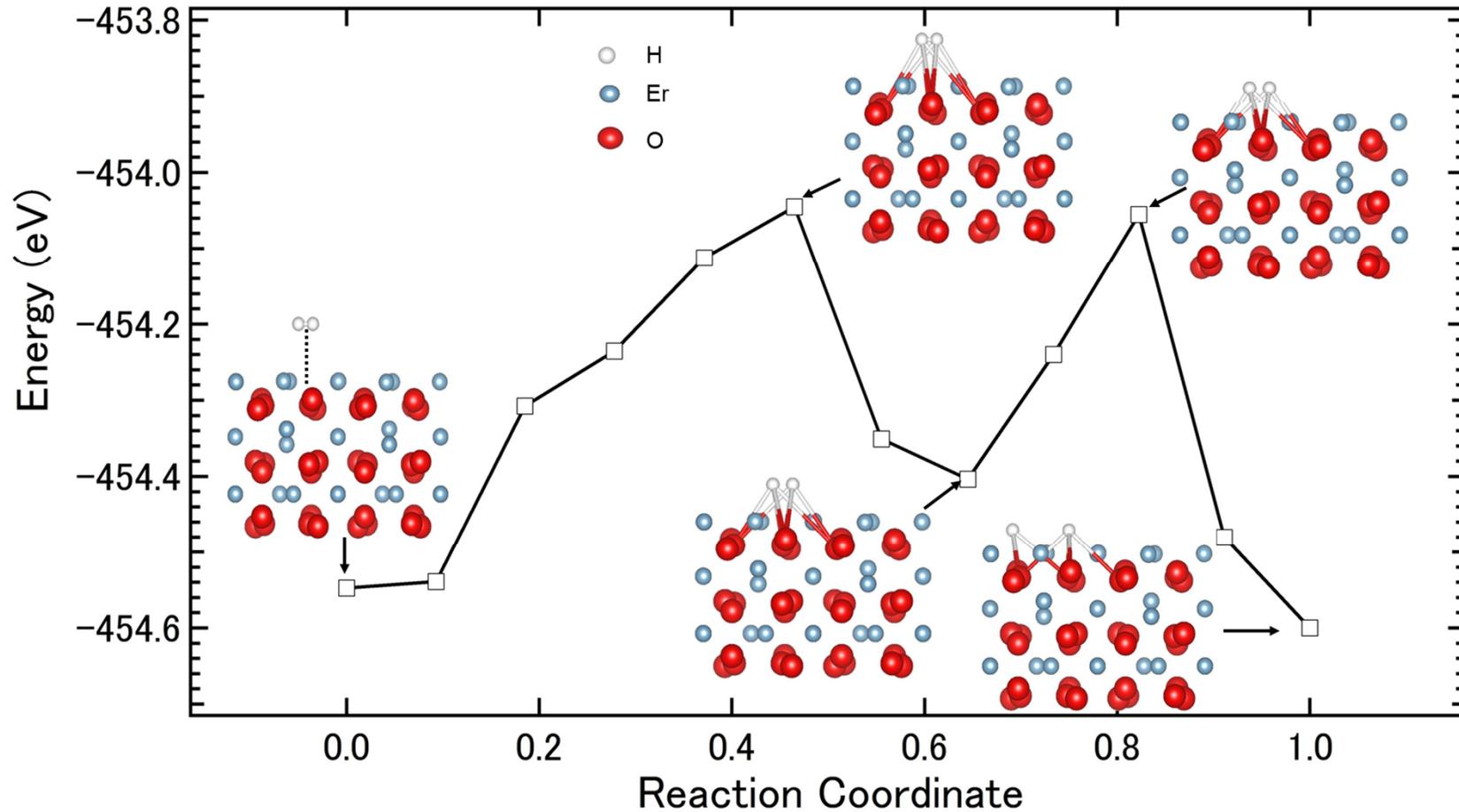
Code: LAMMPS (2013/05)

- Mean square displacement (MSD), diffusivity (D) and activation energy of diffusion (E) were calculated using pairwise potentials.

Interatomic potentials applied for MD calculations

| Pair | A_{ij} (eV) | ρ_{ij} (Å) | C_{ij} (eV Å ⁶) |
|-------|---------------|-----------------|-------------------------------|
| Er-Er | 0 | 0 | 0 |
| Er-O | 1678.21 | 0.33781 | 10.34 |
| O-O | 9547.96 | 0.21916 | 32 |
| H-Er | 0 | 0 | 0 |
| H-O | 396.3 | 0.23 | 0 |
| H-H | 0 | 0 | 0 |

Dissociation of hydrogen molecule



- Dissociation energy of 0.5 eV was determined by NEB method.
- The small H₂ dissociation energy confirms the permeation regime obtained by the experiments (atomic diffusion in Er₂O₃).

Summary and future prospects (Tritium Barrier Study)

Experimental and computational studies on hydrogen permeation mechanisms in Er_2O_3 coatings have been reviewed.

- Er_2O_3 coatings prepared by VAD and MOD showed 3–5 orders of magnitude lower deuterium permeability than uncoated RAFM steel.
- Key parameters (surface coverage and grain density) were examined with experiments and simplified models.
- Hydrogen permeation behaviors for multi-layer and radiation-damaged coatings will provide a more detailed permeation mechanism.
- Computer simulations revealed elemental steps of hydrogen permeation through Er_2O_3 single crystal with and without vacancies and grain boundaries.
- The experimental and computational approaches are conforming over discrepancies.

Overall Summary

- In the Rokkasho Fusion Institute established in 2009, many activities based mainly on the Broader Approach Agreement have been conducted.
- In the IFERC activities, that for the Computer Simulation Centre and the DEMO Design and R&D Centre, a lot of achievements have been obtained.
- For development of Fusion Materials Irradiation Facility, engineering design and validation activities for IFMIF have been conducted in Rokkasho, which will be inherited beyond the current scope of the IFMIF/EVEDA Project.
- For development and construction of DEMO, the federal planning is now being reviewed and re-examined due to delay of ITER, but key R&D items will be carried out in Rokkasho.

Thank you for your attention !