Materials database and facilities needed

[and how to use them]

at
8th IAEA DEMO PROGRAMME WORKSHOP

August 31st 2022

Vienna International Centre, Vienna, Austria

Eberhard Diegele

with lots of direct input from
Gerald Pintsuk, FZ Jülich, Germany
Michael Rieth and Ermile Gaganidze, KIT, Germany

views from JP/US and EU colleagues
ideas from Hiroyasu Tanigawa

A guideline formulated for this WS reads

Understand the state of art and existing gaps

Therefore, start

‘Summary’

In lieu of an “Introduction”

Fusion Materials Development Path

Facilities needed

The summary
Taken from an old presentation at ICFRM [n]

Performance under component specific loading - Stage IV

Facility Beyond FNS& ITER ?

Qualified materials, full demonstration of performance - Stage III

14 MeV neutrons or fusion specific n-spectra   >>>   FNS/ IFMIF

To some extend (validation/falsification) ITER-TBM

Demonstration of performance limits - Stage II

Fission reactors (MTR of next generation, at best >10dpa/a)

(FNS)

Materials “Design” - Stage I

Microstructure – Analysis tools
[SANS, TEM, ATP, FIB] sorry for the TLAs

Fission reactors (MTR)
Multi-ion-beam facilities

Complementary Modelling [development and validation]
essential at each stage

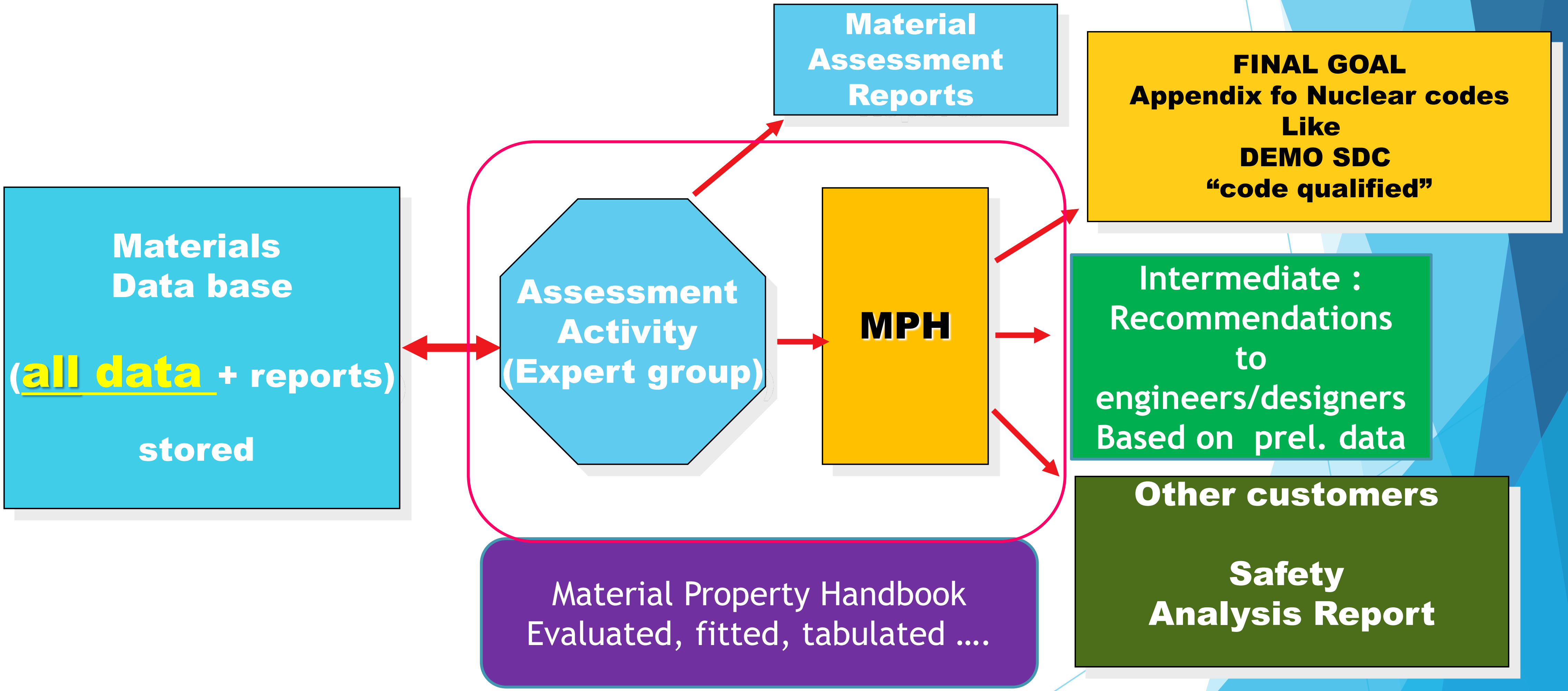
Plus specific facilities
This depends on selection of design choices

Def: FNS Fusion Neutron Source
MTR: Material Test Reactor

Now start the journey to arrive at this summary

Do it like mathematicians – with a “definition”

Definition and for Clarification: “Data base – MPH – Code”



Materials
Data base

(all data + reports)

stored

Assessment Activity (Expert group)

Material Assessment Reports

MPH

FINAL GOAL
Appendix fo Nuclear codes
Like
DEMO SDC
“code qualified”

Intermediate :
Recommendations
to
engineers/designers
Based on prel. data

Other customers

Safety
Analysis Report

Material Property Handbook
Evaluated, fitted, tabulated ….

Modified from a viewgraph by V. Barabash, >10 years old

The “data base” is not the final objective
It is a 1st step in a process

Needs strategy, care, attention, planning
Traceability, reliabity, QA, …

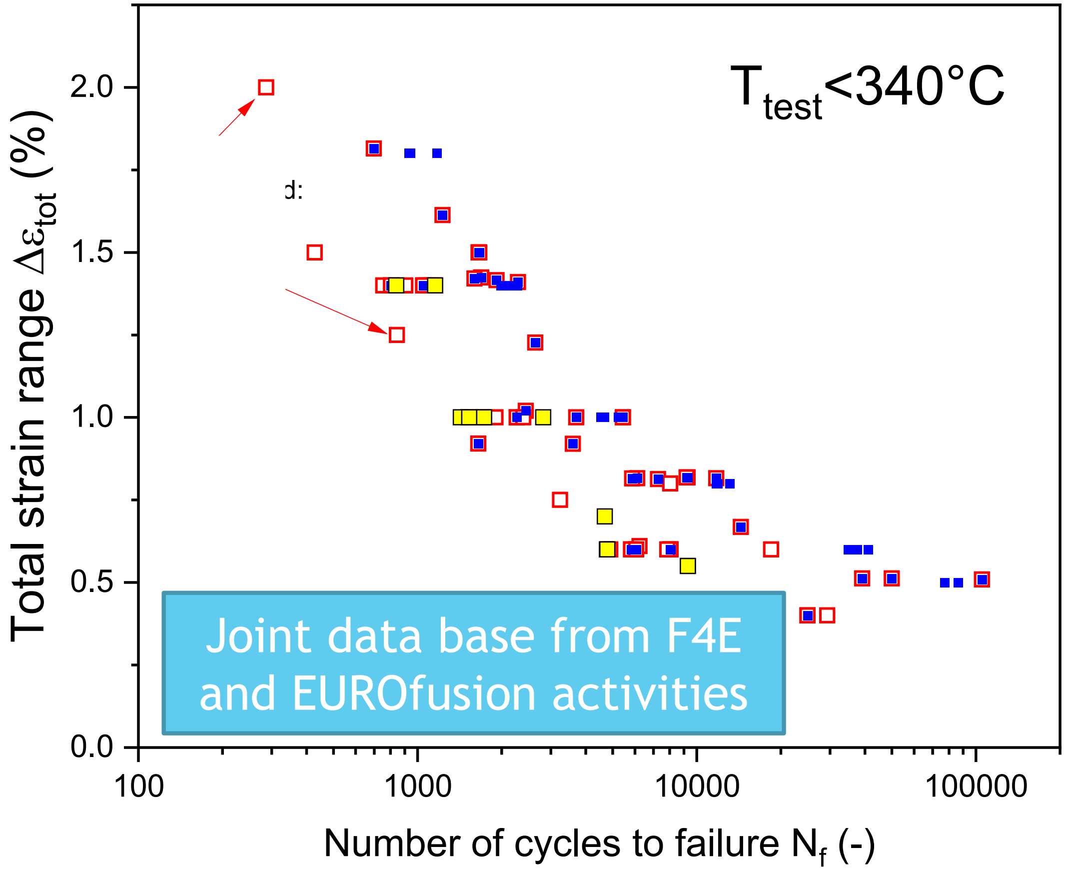
and as many trips [*and I experienced during my travel to Vienna*]

There is a
Detour

An example: From Data Base to MPH

[part of the EUROfusion WP 2022
Credit G.Pintsuk and E. Gaganidze]

EUROFER-97 low cycle fatigue [LCF] properties



Joint data base from F4E and EUROfusion activities

Data base

Many single results

“unordered crowd”

LCF properties - assessment – > elimination process

Non official **EUROFER** batch[es]

Non base material

Duplication of entries

Non standard heat treatment

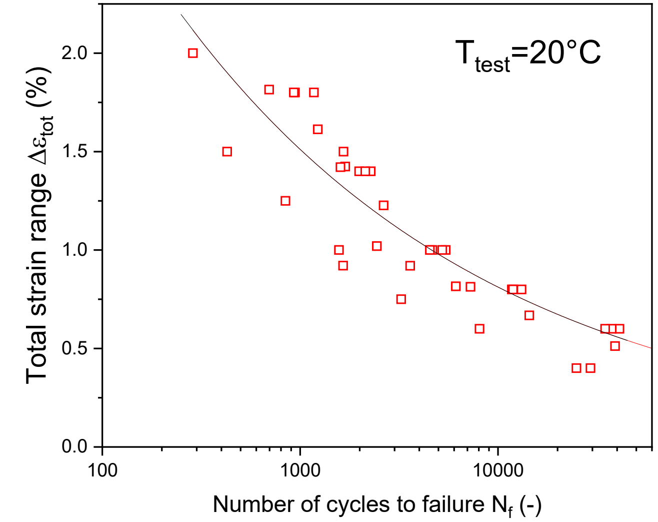
Non standard loading - R-value *[ratio min/max load]*

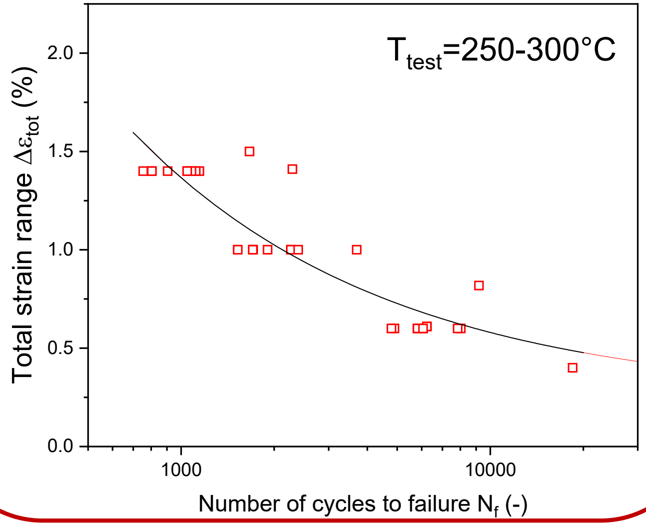
Non standard test geometry, too small dimensions [*]

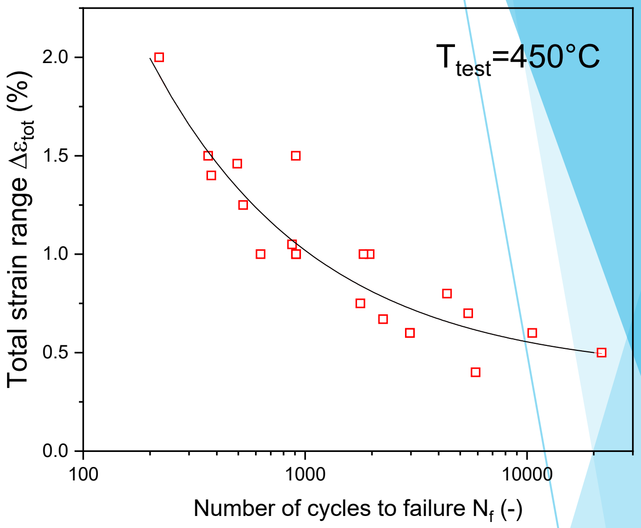
Grouping in T-windows

[*] this added here for completeness

Assessment of the LCF properties – as to be implemented in MPH







Langer's equation

$$\Delta\boldsymbol{\varepsilon}_{tot} = A \cdot N_f^L + C$$

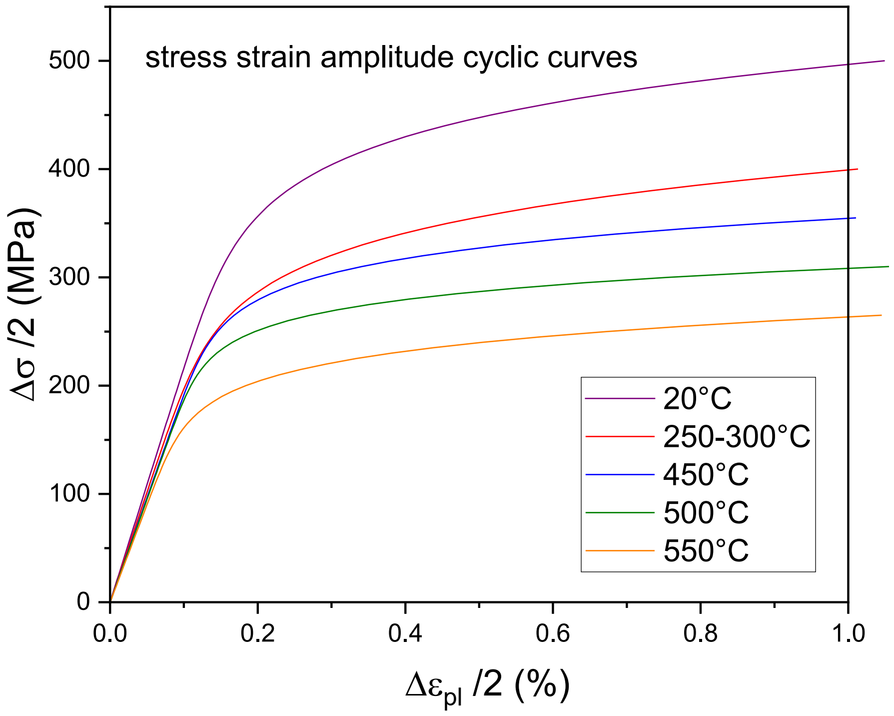
Newly fitted paramters
A,L,C
enter the EUROfusion **MPH**

Assessment of the LCF properties – as to be implemented in RCC-MRx

Cyclic stress vs strain curves

$$\boldsymbol{\Delta\sigma = K \cdot \Delta\varepsilon_{pl}^{m}}$$

$$\Delta\varepsilon_t(\%) = 100\left(\frac{\Delta\sigma}{E}\right) + \left(\frac{\Delta\sigma}{K}\right)^{1/m}$$



No single, indiduell values
Fitted curves, formulae, tables

This small detour is also to give credit to [the very few] specialists.
In fact, they are as precious as multi-million facilities

Data needed

Typical loading conditions in Breeding Blankets

Data needed

Fundamental
- **Strength**
- **Ductility**
- **[Fracture] Toughness**

Basic
- **LCF Low cycle fatigue**
- **Creep**
- **Fatigue-creep interaction**
- **Fatigue crack growth**

Elementary
… many others that are needed for design rule development
... Influence of environment [other than neutron]
…. Non mechanical [thermal, chemical, physical, magnetic….]

Data are needed under various conditions [T, load, …]

Data are needed for non-base material [welds, joints, interface..]

Data needed for order of [half] dozens of welds, *widely overlooked*, may become the most expansive part and extensive part of a qualification programme

EUROfusion MPH
Excess of 30
chapters/subchapters

Look into the future
"one" FNS facility
Might be not sufficient

Typical BB Loading Conditions

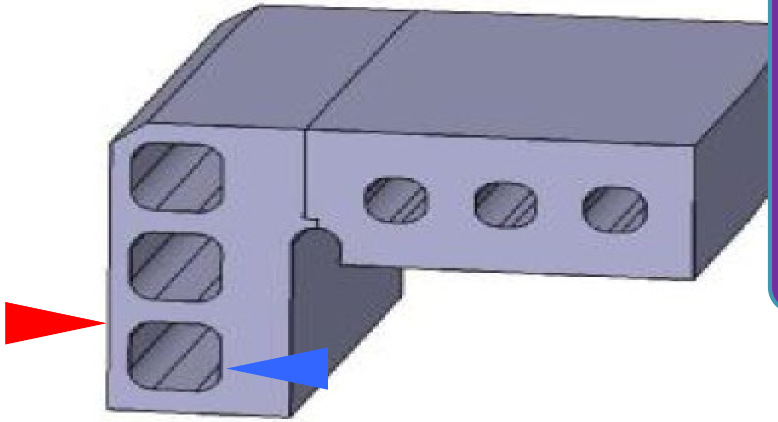
Water Cooled option -WCLL ~300/510°C

- Concern are typically LT properties

Helium Cooled options - HCBP ~340/550°C

> Concern are typically HT properties

Objective:
To address typical features
Needed for presentation



Specifity
Steep gradients
Thin-walled first wall
Concern fracture of
undetected small cracks
QA/NDE & MATERIALS

First Wall
Typical fusion spectrum
Highest n-energy up to 14 MeV
High He generation rates
" typical fusion-n-spectrum"

Rear wall
displacement damage
drops typically up to 2 orders
He generation up to 3 orders
n-spectrum is "fission like"

Various n-spectra at different locations

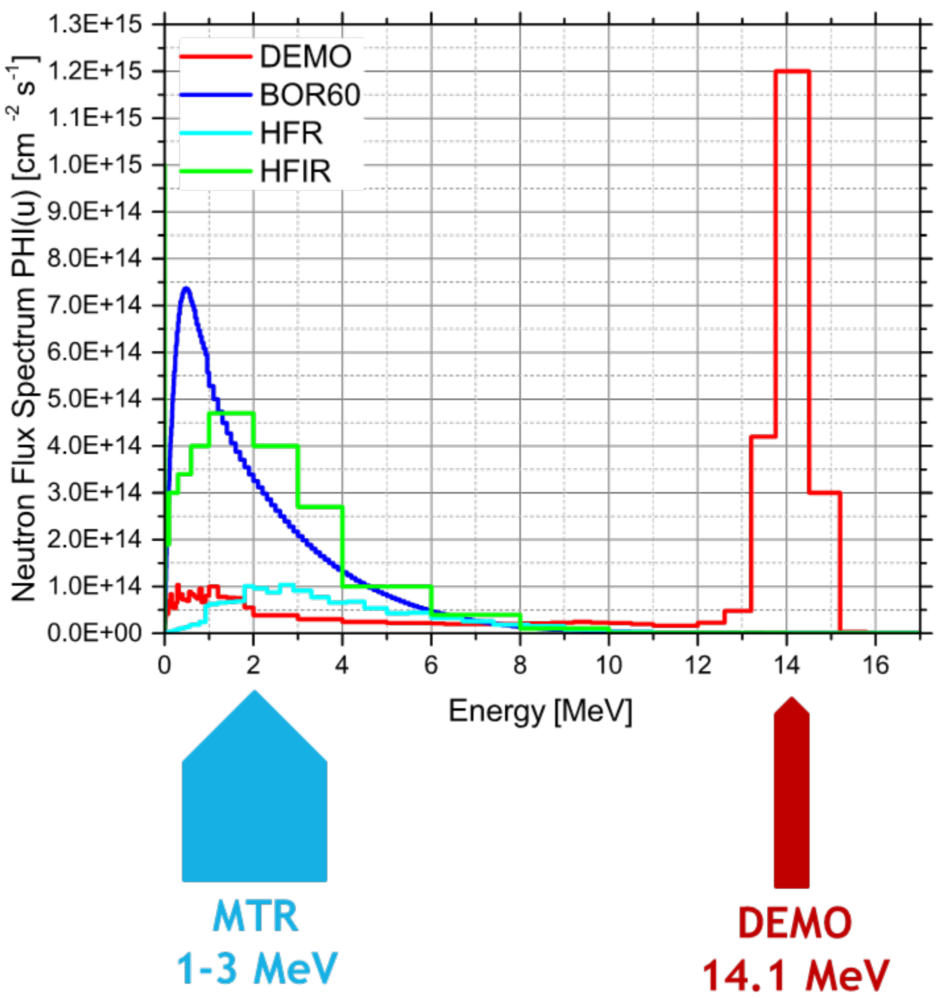
Immediate conclusion:

Any facility built to characterize structural materials under irradidation needs flexibility to adapt for properties and temperature windows

Displacement damage

Transmutation damage

- Is it realistic to simulate “DEMO neutrons” by experiments in fission material test reactors?
- Which differences are to expected ?
  - .. A 1st and a 2nd view



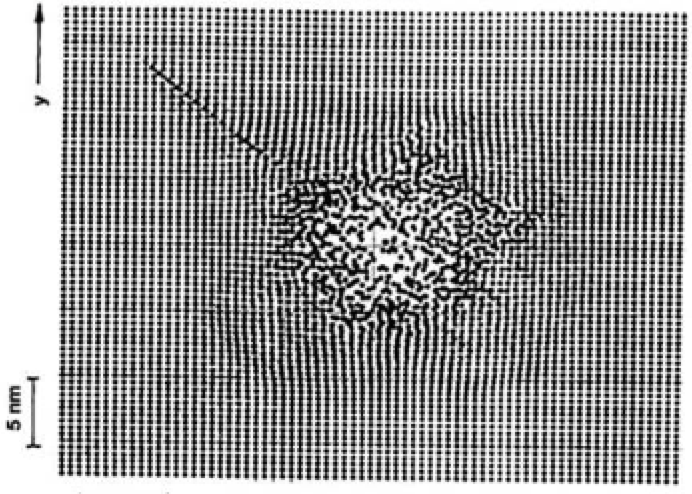
Impact of Neutron Irradiation on Materials

Displacement (Lattice Disorder) & Transmutation

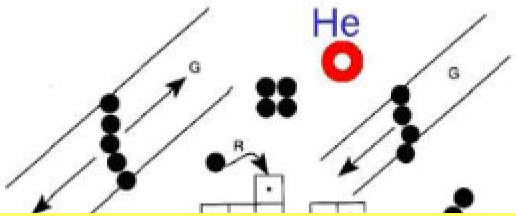
There are 2 elementary reactions

How to solve the He

Displacement Damage („dpa“)



Nuclear Reactions (e.g. He)

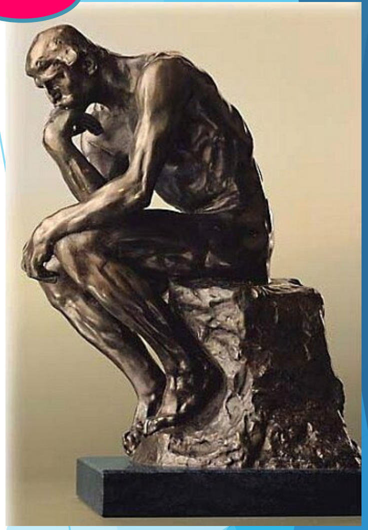


Inelastic reactions (Gaseous Transmutation)

- Generation of H(ydrogen)
- (n)+ N(uclei) - > (p) + Ñ + e
- Generation of He(lium)
- (n) + N(uclei) - > (alpha) + N’

Measure “dpa”
displacement per atom

Measure
[appm – atomic parts per million]



This is the origin of many worries

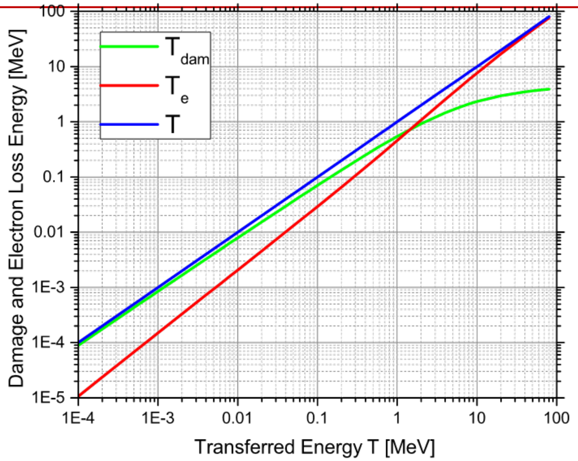
To know for the moment:
He/dpa or H/dpa [generation rates]
are <u>measures for the neutron-spectrum</u>

Rule of thumb for F(irst) W(all):
~40 times more He in fusion
~10 appm He/dpa
~10 dpa/full power year
at 1 MW/m2 n-wall load**

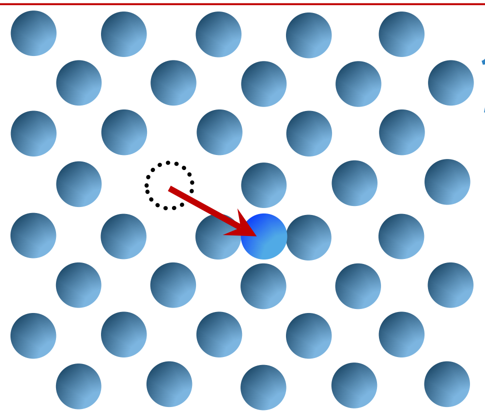
Displacement Damage (NRT) - Norgett-Robinson-Torrens

4 slides from M. Rieth, modified

Threshold energy E_d to displace an Fe atom from its lattice position
+ principle of linear momentum

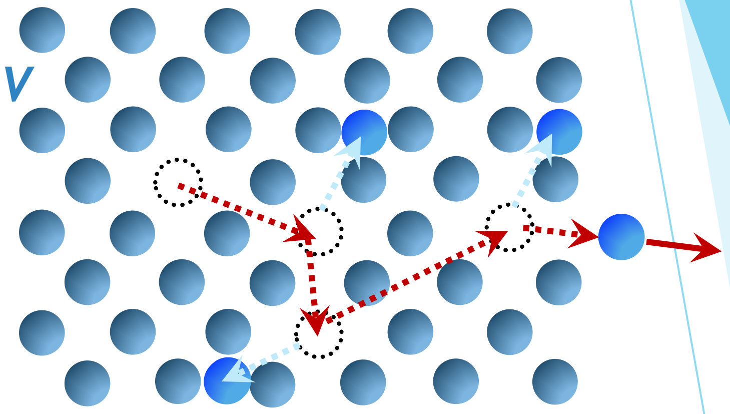


$$T_{dam} = T - T_e$$



If $T_{dam} \approx E_d$ then there is 1 displacement = 1 frenkel pair (vacancy + interstitial)

for iron
E_d = 40 eV



If $T_{dam} > E_d$ the number of displacements N_d (frenkel pairs) can be calculated

T_{dam} = 1 keV → N_d = 10
T_{dam} = 10 keV → N_d = 100
T_{dam} = 95 keV → N_d = 950 (MTR)
T_{dam} = 530 keV → N_d = 5300 (DEMO)

Too simplistic

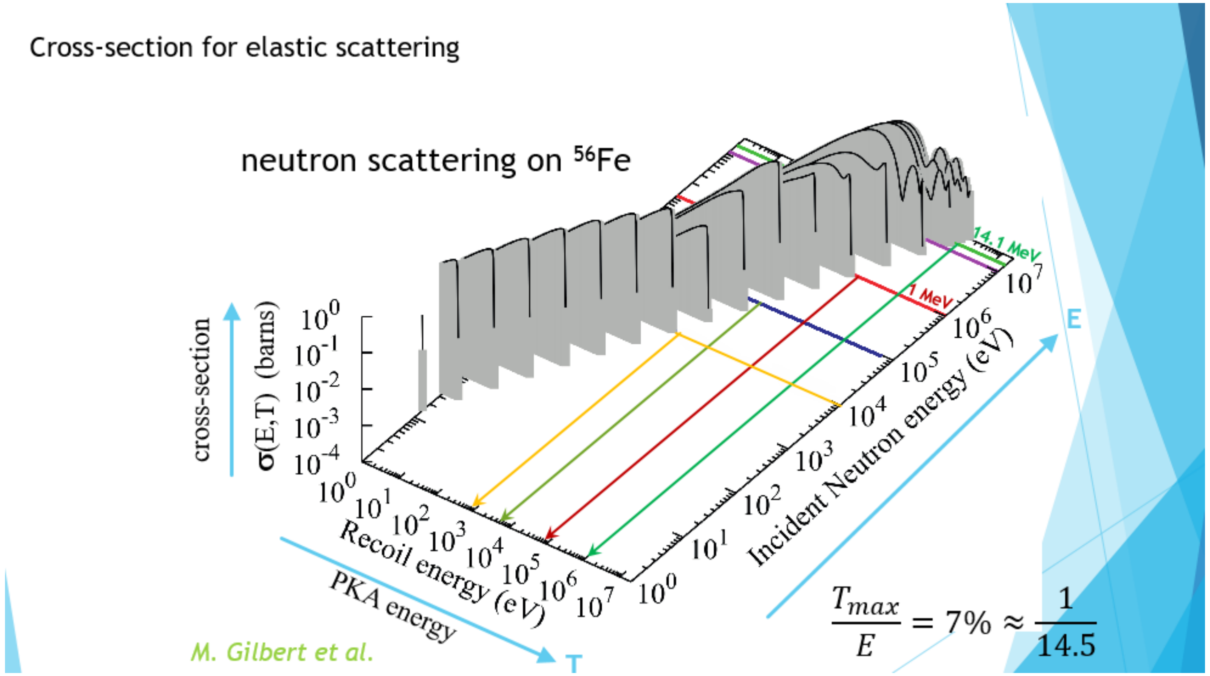
	MTR		DEMO (peak)
Neutron energy E	1 MeV	2 MeV	14.1 MeV
Transf. energy (average) T	35 keV	70 keV	490 keV
Damage energy (average) Tdam	**24 keV**	**44 keV**	**220 keV**
Displacements	**240**	**440**	**2200**

14.1 MeV DEMO neutrons produce 5-10 times more displacements compared to MTR neutrons

?

BUT

Displacement Damage – beyond “rule of thumb”



Displacement Damage Calculation (dpa), falting to integrals

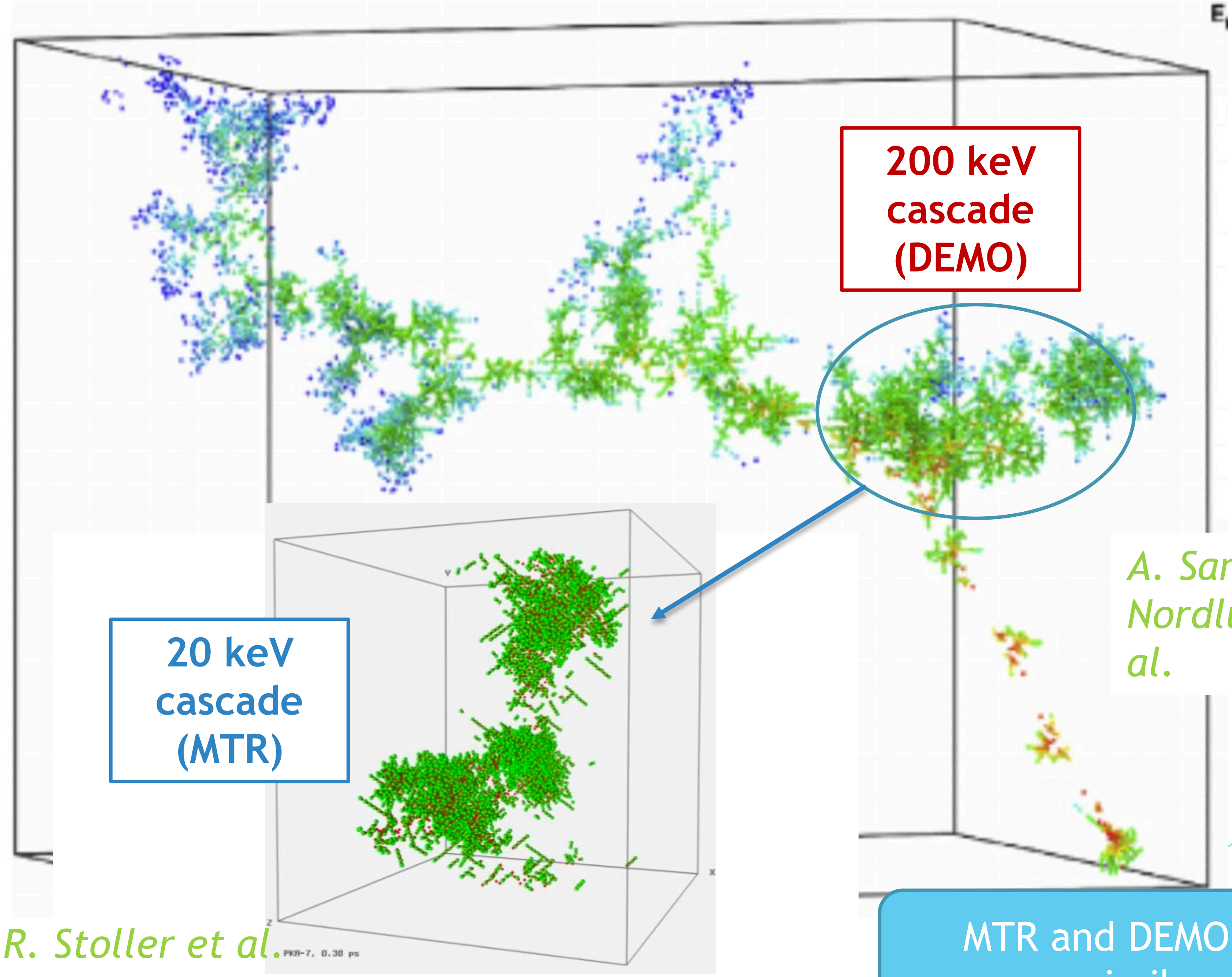
$$\sigma_D(E) = \int_{E_d}^{T_{max}} \frac{\partial \sigma(E, T_{dam})}{\partial T_{dam}} N_d(T_{dam}) dT_{dam}$$

Damage cross-section

$$\frac{dpa}{s} = \int_{E_{min}}^{E_{max}} \sigma_D(E)\, \Phi(E) dE$$

Damage rate (dpa/s)

Cascade MD [molecular dynamics] Simulation



200 keV cascade (DEMO)

20 keV cascade (MTR)

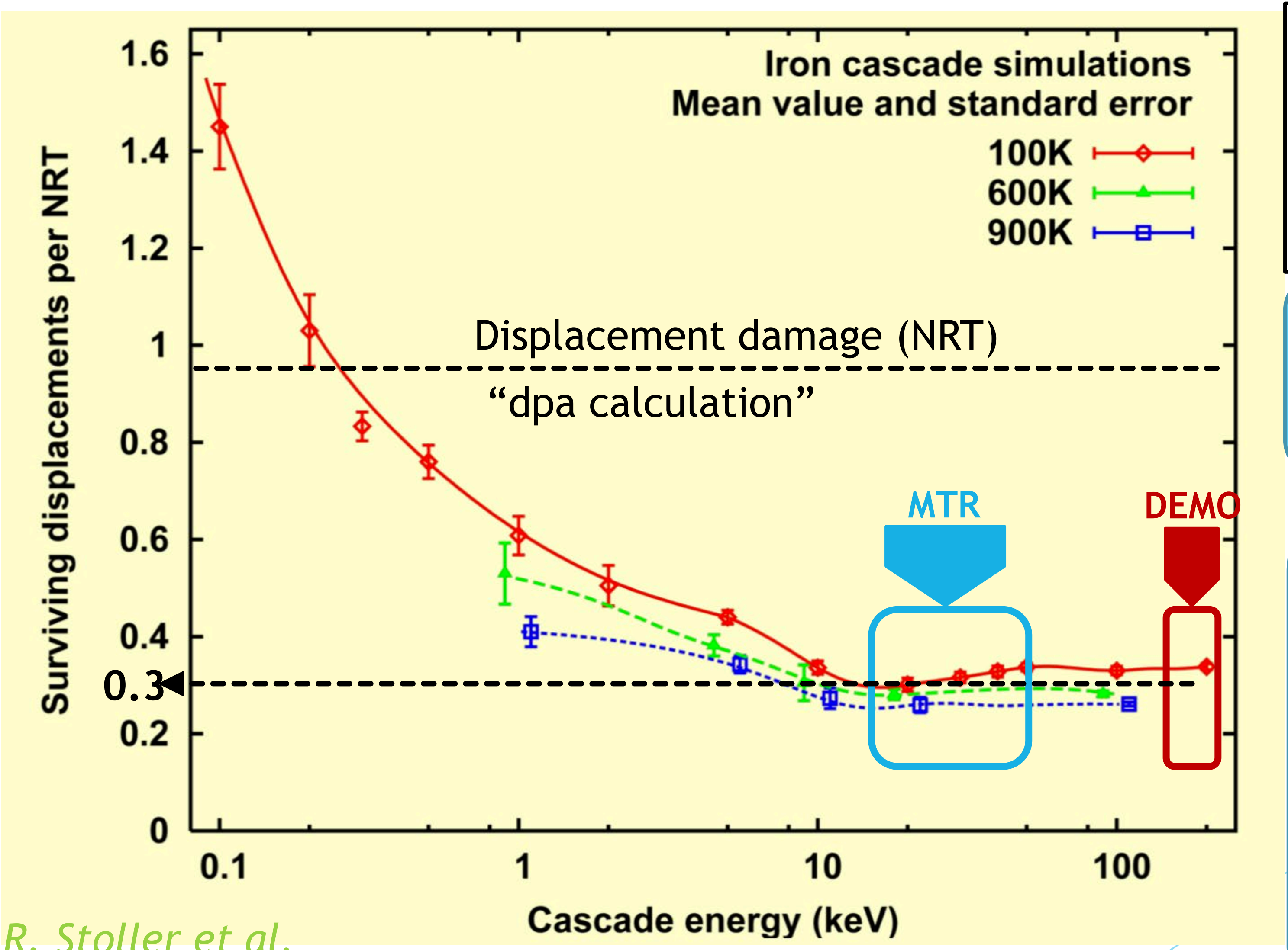
R. Stoller et al.

A. Sand, K. Nordlund et al.

MTR and DEMO cascades decay in similar subcascades

Surviving defects

In the "absence" of transmutation fission displacement damage is "similar" to fusion n-irradiation



R. Stoller et al.

- Also confirmed by *L. Malerba et al.* and others
- Experimentally confirmed by *S. Zinkle et al.* and others

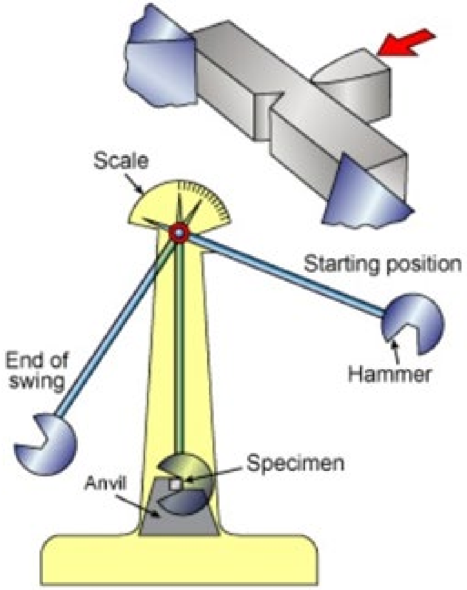
The NRT picture to calculate is not fully true

The PARADOX / SURPRISE the dpa approach (even if it doesn't mirror reality) is still applicable to the MTR simulation of DEMO neutrons *in terms of "cascade damage"*, there are no major differences to expect!

MTR irradiation deliver is a good approximation for fusion irradiation displacement damage

Example

Impact properties under n-irradiation

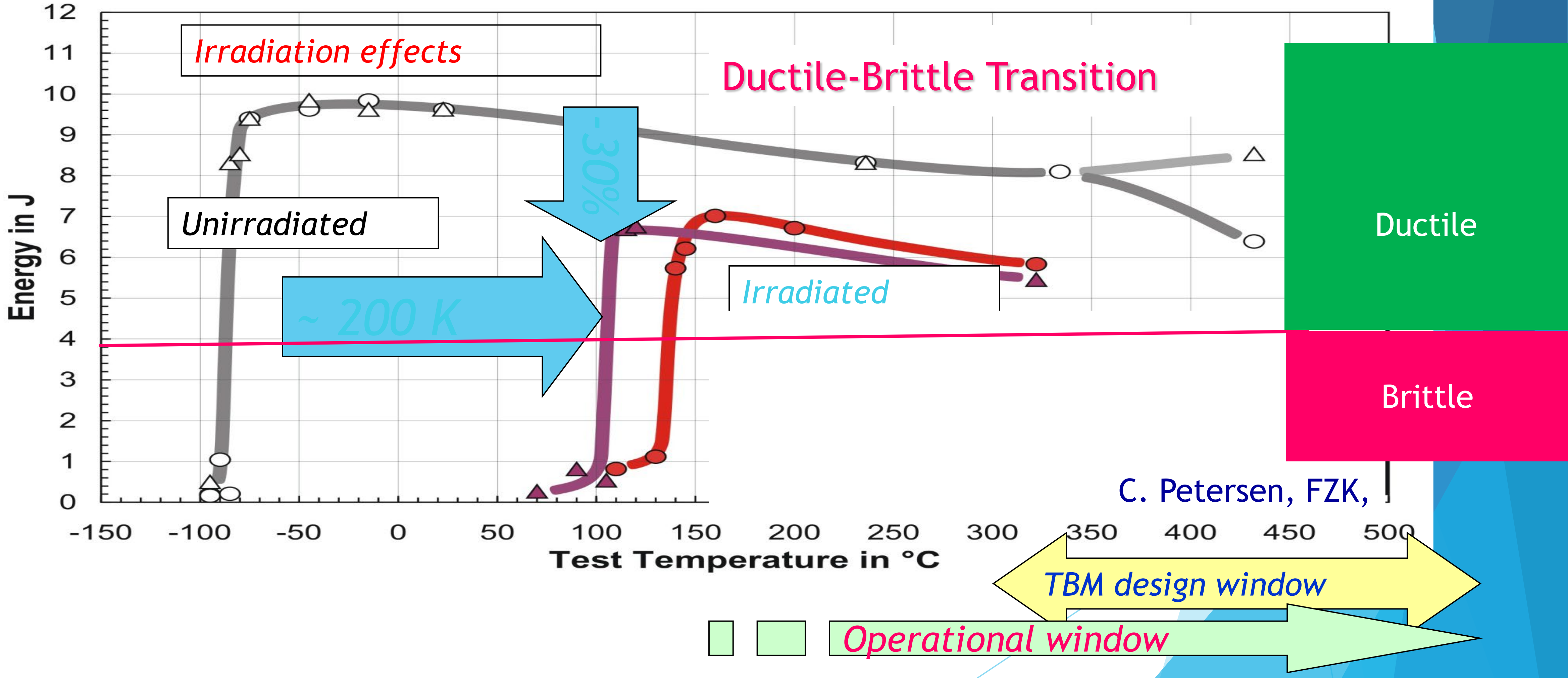


Briefly:

Degradation of Impact Properties under Neutron Irradiation

Bcc steels become brittle if irradiated,
For EUROFER most pronounced below ~ 330°C

32 dpa, 332°C, ARBOR
(fission) irradiation

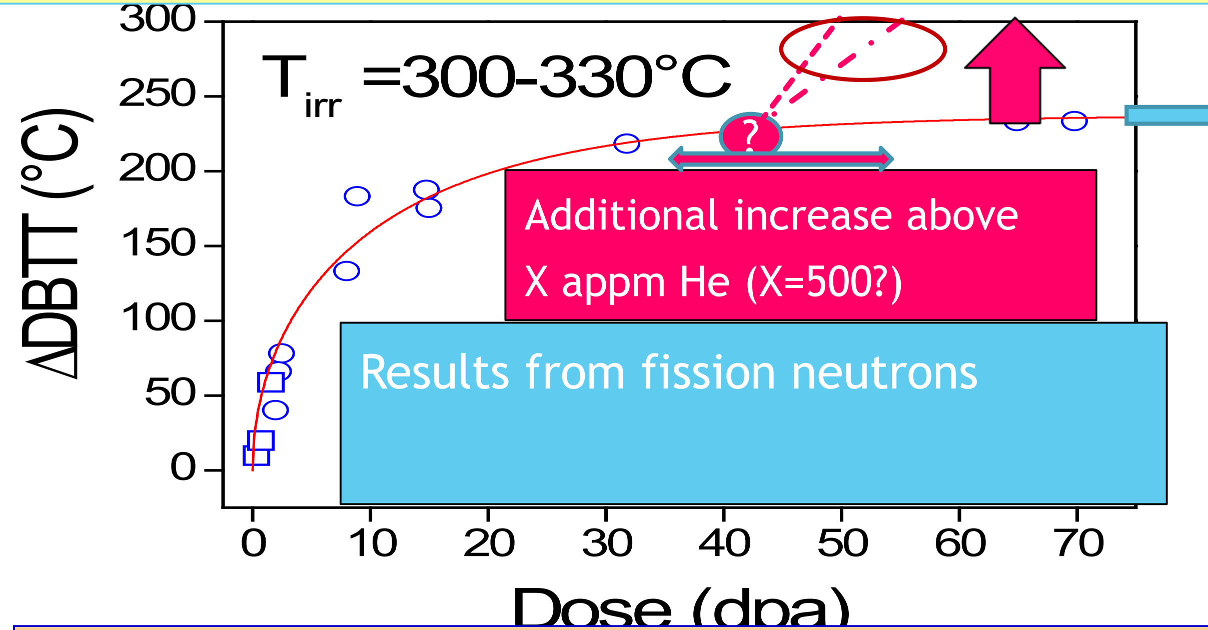


C. Petersen, FZK,

Briefly

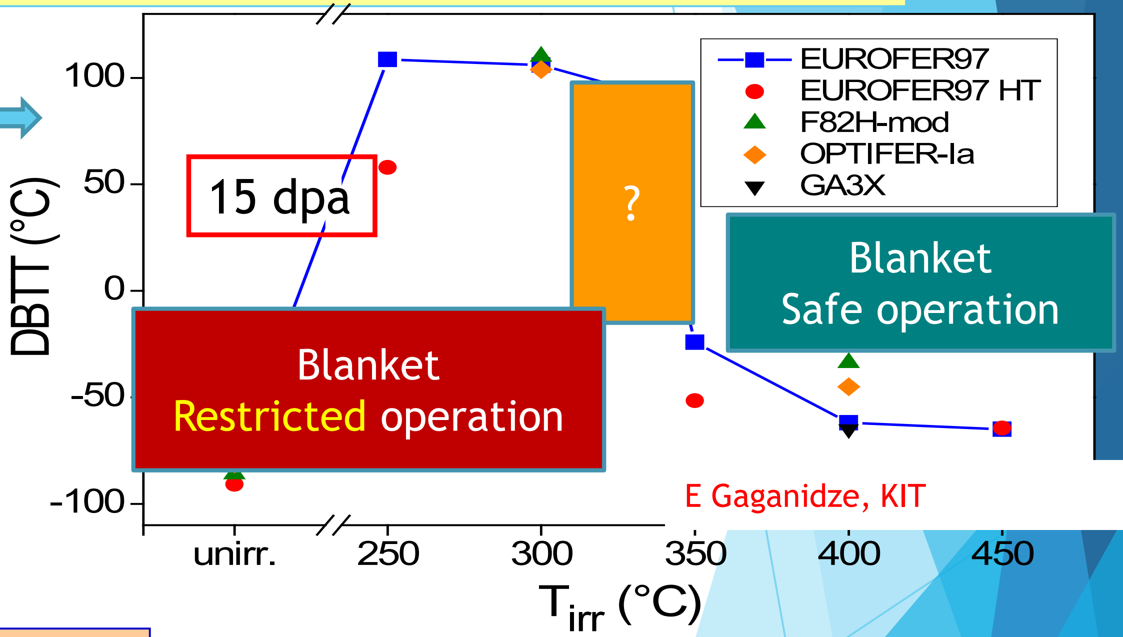
Ferritic-Martensitic Steels Embrittlement (ductile-brittle-transition)

Bcc steels become brittle if irradiated,
For EUROFER most pronounced below ~ 330°C



Additional increase above X appm He (X=500?)

Results from fission neutrons



Blanket
Restricted operation

Blanket
Safe operation

E Gaganidze, KIT

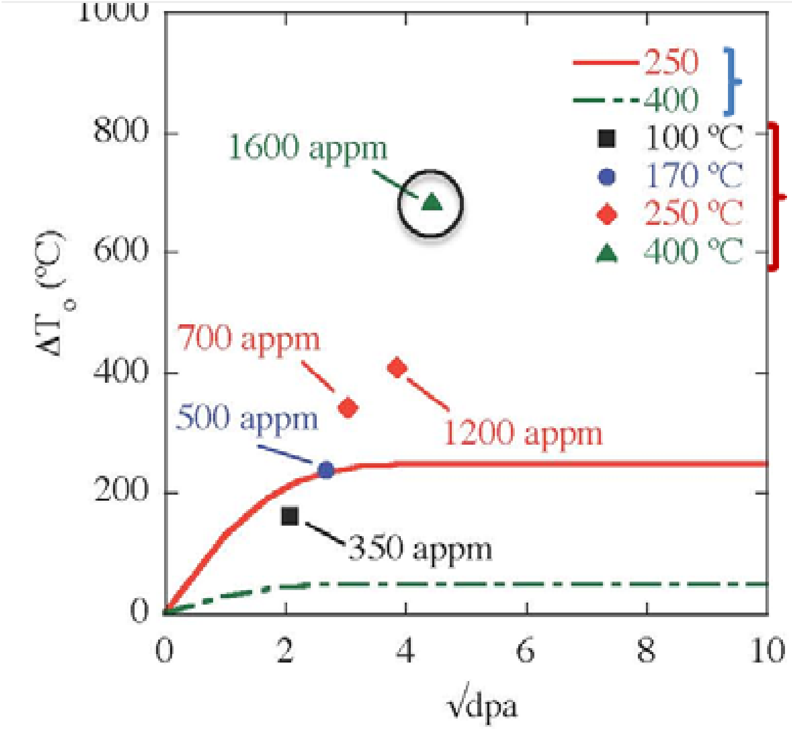
In MTR irradiation - effect of translutation is missed
[btw: it does as well exist in tensile - but most serious in toughness]
Known: there is an effect of Helium
Unknown: threshold and amount? > needs fusion n-spectra

Under some conditions
The effect is not negligible - rather dominating

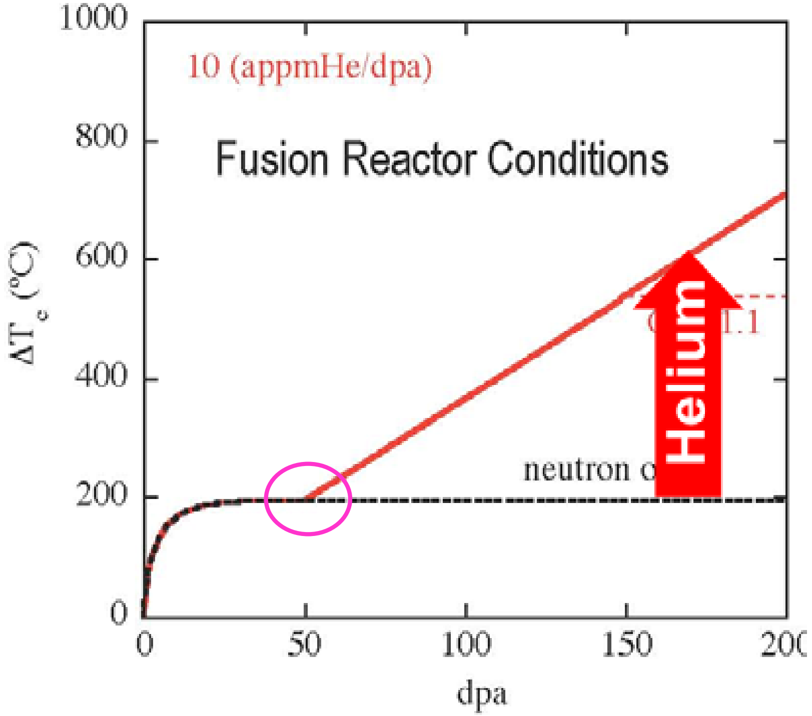
- T_{irr} ≤ 330°C: *strong embrittlement*
- T_{irr} ≥ 350°C: moderate *embrittlement*

Effect of "Addional" He from transmutation [on DBTT]

Btw: the effect of transmutation was already discussed 30 years ago and there was evidence



Fission [Be-doped material]
and spallation neutron irradiation



R. Kurtz (SOFT-26)

Prediction by modeling

onset unknown
slope unknown

And this within targeted operation of BB

Still not sufficient to motivate for a dedicated
FNS fusion neutron source ?

How to “simulate” 14 MeV n-damage

Options

- Fe-54
- Spallation
- Be-doping

Simulate He-effects

Fe-54:

Nuclear reaction: Fe-54(n,a)Cr-51

- 6% in natural iron

there were some attempts, but

- with Fe54, the He/dpa is only increased by some factor 6-8 compared to fission n-spectra and still some factor 3-4 short to He/dpa of 10 appm/dpa
- there is only a small market and it is extremely expensive [2005 for 250k €, EFDA got 400g – *the material was stored in a safe*]

"Nice" for scientific studies. Not applicable for material qualification programme

Spallation

- The energy spectrum is very harsh [factors higher than fusion neutrons]
- **There is "additional" transmutation of alloying elements**
- **Works at "low temperature"**

"Nice" for scientific studies. Not applicable for material qualification programme

B-doping

$n + {}^{10}B \rightarrow {}^{4}He + {}^{7}Li$

- Has been used in some irradiation campaigns [ARBOR in Bor-60, Russian reactor]
- Minor issue: B-burn-up early and no constant He/dpa over life …..
- And a major issue …..

B-doped RAFM Steels, 15-16 dpa neutron irradiation at 250 °C


EUROFER, <10 appm He, <1 appm He/dpa

EUROFER-type, 415 appm He, 28 appm He/dpa

EUROFER-type, 5800 appm He, 387 appm He/dpa

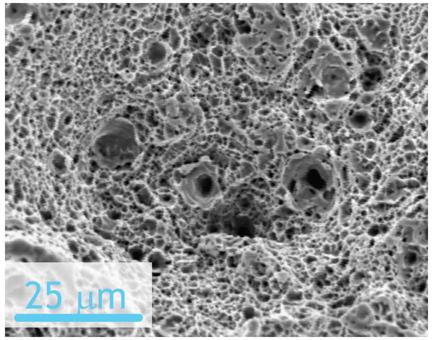
Development of He-bubbles

E. Materna-Morris, et al.
JNM 386(2009)422

.. Then the second look

EUROFER Steel - the second look to B doped material

EUROFER, <10 appm He

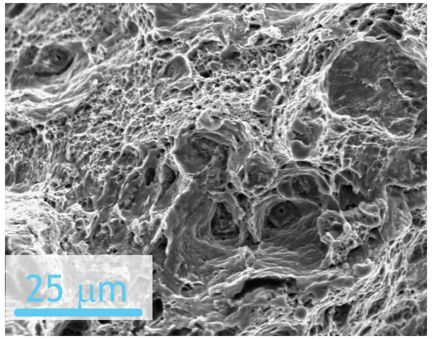


M. Klimenkov et al., Micron 46 (2013) 51–56

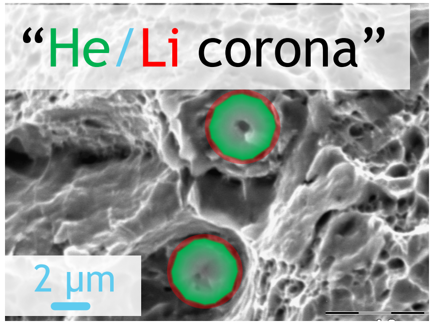
M. Klimenkov et al, J. Nucl. Mater. 462 (2015) 280-288

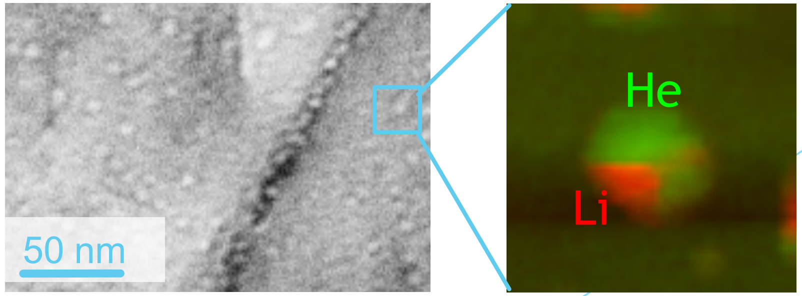
- KIT: first direct observation of Li clusters
- database on dpa/He effects
- ^{10}B-doping: He and Li effects cannot be decoupled.

EUROFER-type, B-doped, 415 appm He



n + ^{10}B → ^{4}**He** + ^{7}**Li**
range of He (1.0 MeV): 1.6 µm
range of Li (1.8 MeV): 2.0 µm

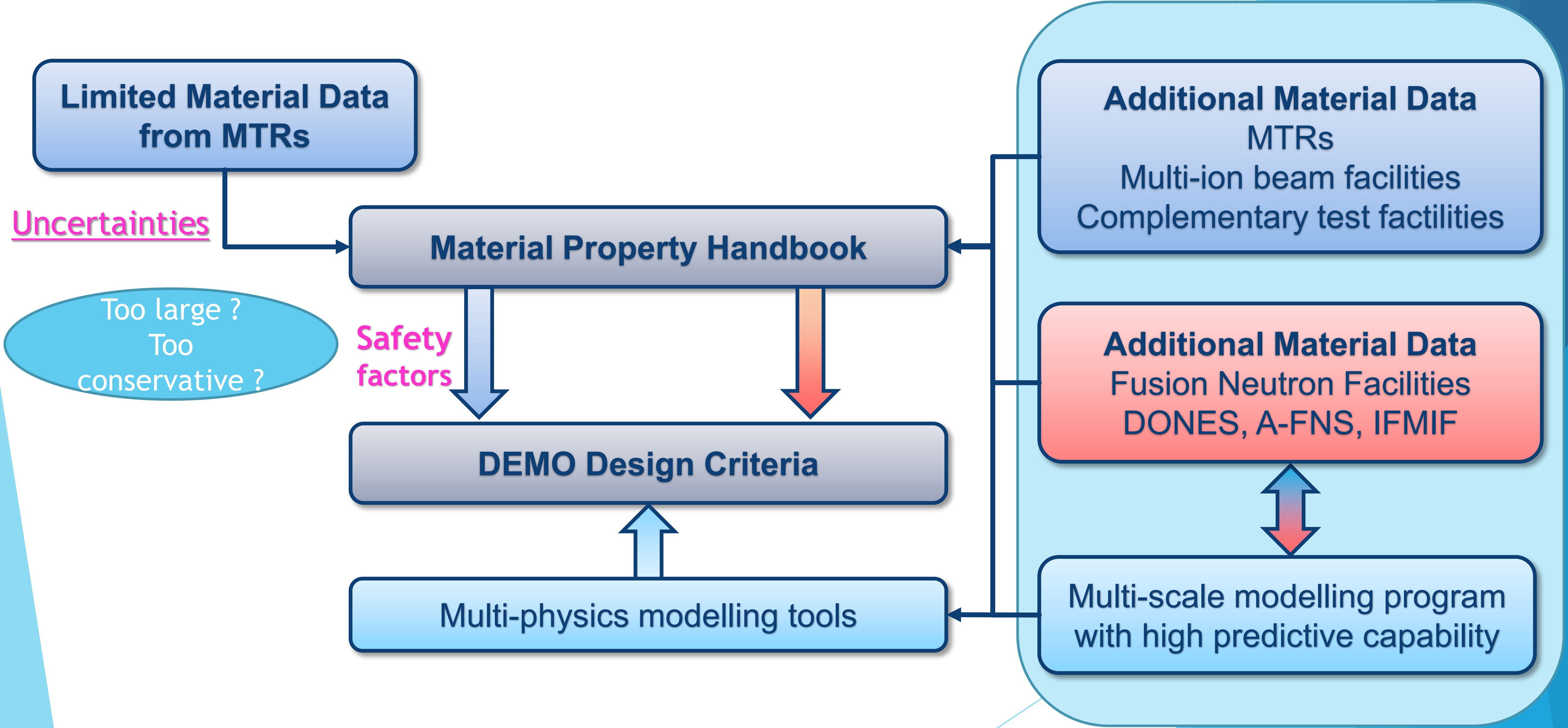




Strategy to qualify materials under fusion n-spectra

- INCOMPLETE without proper knowledge on transmutation effect
- [only He was discussed for simplicity, but H is a concern in welds/joints]

Irradiation Data Base - Actual Status vs. Planning [example EU]



Limited Material Data from MTRs

Uncertainties

Material Property Handbook

Too large ?
Too
conservative ?

Safety
factors

DEMO Design Criteria

Multi-physics modelling tools

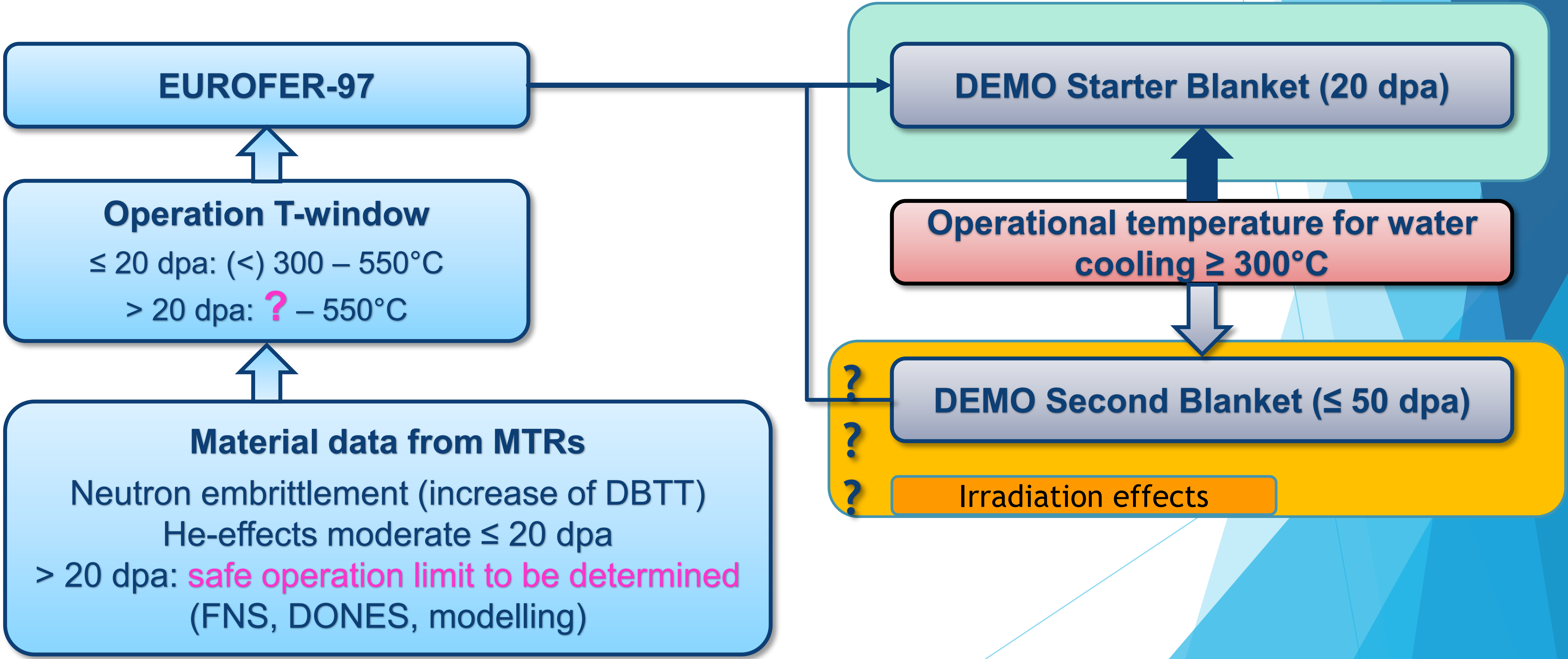
Additional Material Data
MTRs
Multi-ion beam facilities
Complementary test factilities

Additional Material Data
Fusion Neutron Facilities
DONES, A-FNS, IFMIF

Multi-scale modelling program
with high predictive capability

Actual Limits on RAFM operation (Example)

The strategy for design and licensing structures is driven by material performance limits and constraints in knowledge.



EUROFER-97

Operation T-window

≤ 20 dpa: (<) 300 – 550°C

> 20 dpa: ? – 550°C

Material data from MTRs

Neutron embrittlement (increase of DBTT)

He-effects moderate ≤ 20 dpa

> 20 dpa: safe operation limit to be determined (FNS, DONES, modelling)

DEMO Starter Blanket (20 dpa)

Operational temperature for water cooling ≥ 300°C

DEMO Second Blanket (≤ 50 dpa)

? ? ?

Irradiation effects

Strategy to qualify materials under fusion n-spectra

The silver bullet

✓ Need for FNS [IFMIF, DONES..] demonstrared/agreed!

- Need for a smart strategy involving MTR and FNS

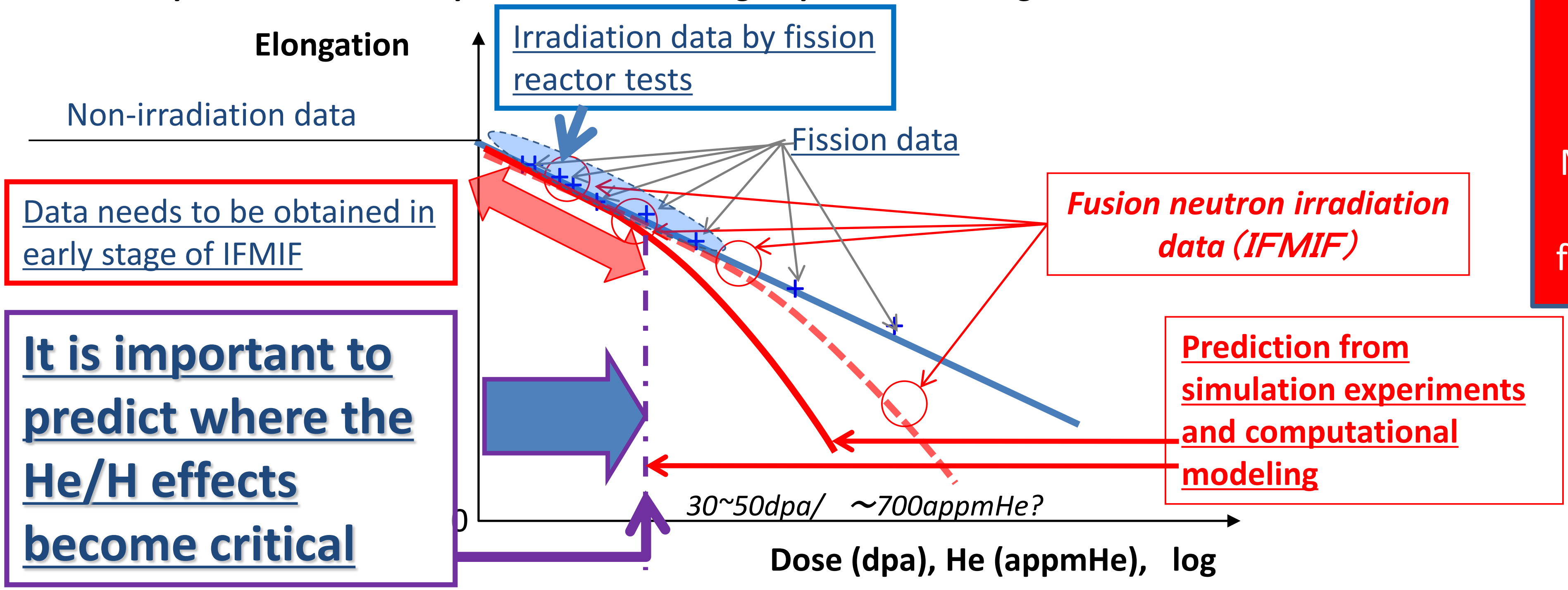
Strategy of the fusion neutron irradiation effect prediction technique development

Fusion neutron irradiation data cannot be acquired until IFMIF will be in operation

✓The initial DEMO design target should be within the range where fusion neutron irradiation data is no too far off from the data trend obtained from fission irradiation experiments.

- ***Accumulation of "rich" fission irradiation database within above range would be essential.***
- ***It is critical to characterize and estimate materials performance under high does fusion neutron irradiation using simulation experiments and computational modeling to predict the range***

Information from FNS IFMIF/DONES Does only "work" with MTR data base And support from modelling



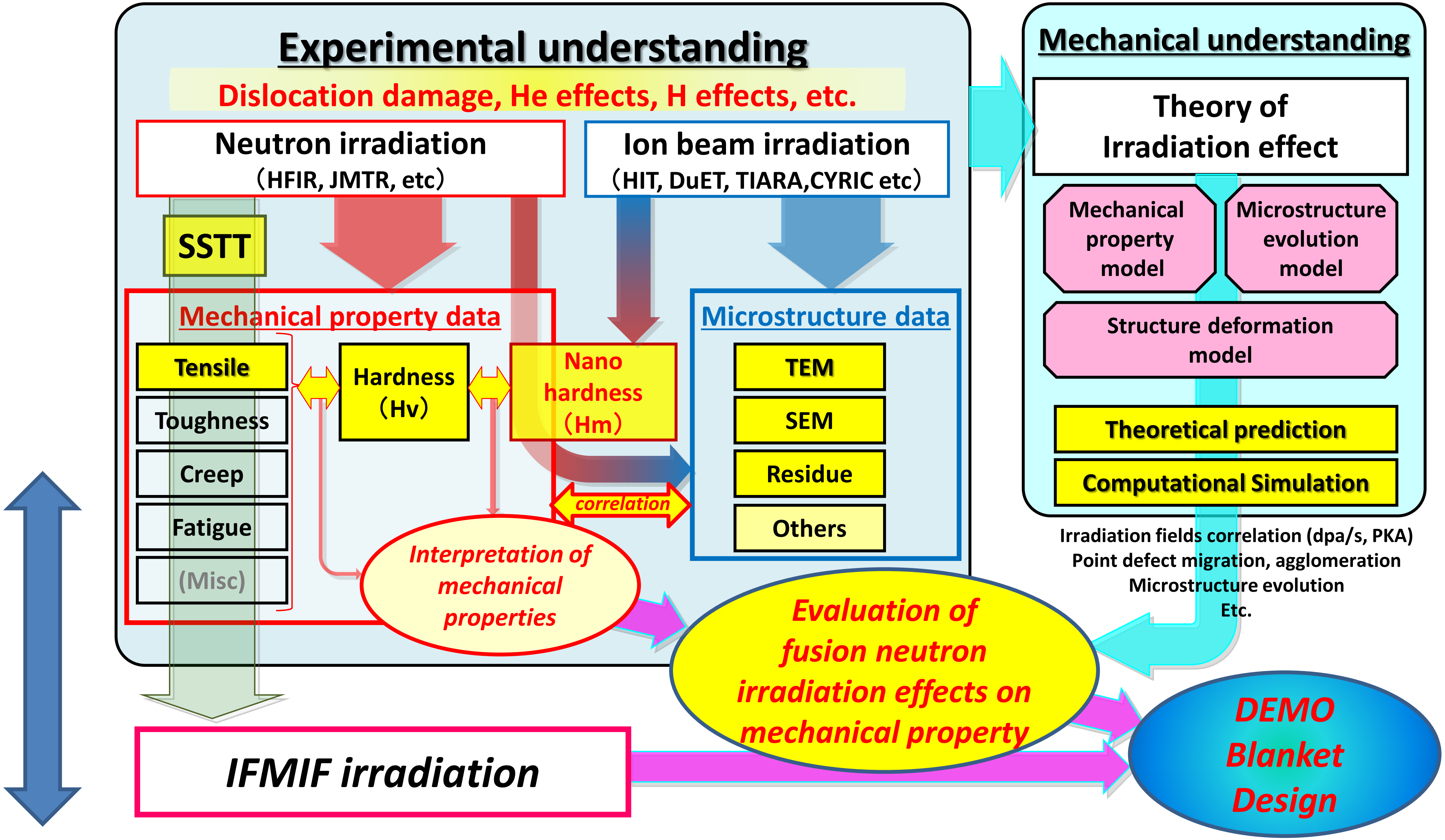
Data needs to be obtained in early stage of IFMIF

It is important to predict where the He/H effects become critical

Prediction from simulation experiments and computational modeling

Prediction of fusion neutron irradiation effect

Strategy on the estimation of fusion neutron irradiation effects



Experimental understanding

Dislocation damage, He effects, H effects, etc.

Neutron irradiation
(HFIR, JMTR, etc)

Ion beam irradiation
(HIT, DuET, TIARA,CYRIC etc)

SSTT

Mechanical property data

- Tensile
- Toughness
- Creep
- Fatigue
- (Misc)

Hardness (Hv)

Nano hardness (Hm)

correlation

Microstructure data

- TEM
- SEM
- Residue
- Others

Interpretation of mechanical properties

Mechanical understanding

Theory of Irradiation effect

- Mechanical property model
- Microstructure evolution model
- Structure deformation model

Theoretical prediction

Computational Simulation

Irradiation fields correlation (dpa/s, PKA)
Point defect migration, agglomeration
Microstructure evolution
Etc.

Evaluation of fusion neutron irradiation effects on mechanical property

IFMIF irradiation

DEMO Blanket Design

Material-Design-Interaction
Or
The material science / engineering interface

“Design rules”
“Design allowable data”

Approaches towards DEMO Design Rules

Many issues
Facilities may assist
But
In needs a full programme

Existing "fission based" frameworks

- *AFCEN-RCC-MRx, ASME, ITER-SDC ….*
- *Likely are insufficient for many reasons*
  - *Material: historically developed for fcc-steels -> need to adapt to bcc*
    understand that RAFM steels materials are "different" not "worse"
    "high" yield strength – less hardening / plasticity
    cyclical softenimg
  - *Environment: fusion-n-spectrum, magnetic fields, ….*
  - *Challenging (multi-)function of plasma-near components (cool/breed/shield..)*
  - *"Geometry-dimension": large, thin-walled*

Issues

Challenge in itself

- **Are / where are rules too conservation ?**
- **Sparse data base for irradiated materials [even with or just because of] FNS**
- **Uncertainties of in-situ n-irradiation effects [fatigue/creep interaction]**

“Commercial” break in favour of the host

An opportunity to highlight some IAEA activity on SSTT

FNS and or licensing require standardization of SSTT / mandatory

IAEA CRP on SSTT

IAEA Coordinated Research Programme on SSTT

- Small specimen test technique (SSTT) development is indispensable to optimize the use of the small irradiation volume and ***transferability*** of small specimen data [data base -> rules -> to the design of structures for reactor operation].
- Best practices for SSTT are only available to individual laboratories and appear significantly fragmented from a global perspective.
- To mitigate this, the International Atomic Energy Agency (IAEA) launched a Coordinated Research Project (CRP) in 2017 with participants from Europe, Japan, US, and China.

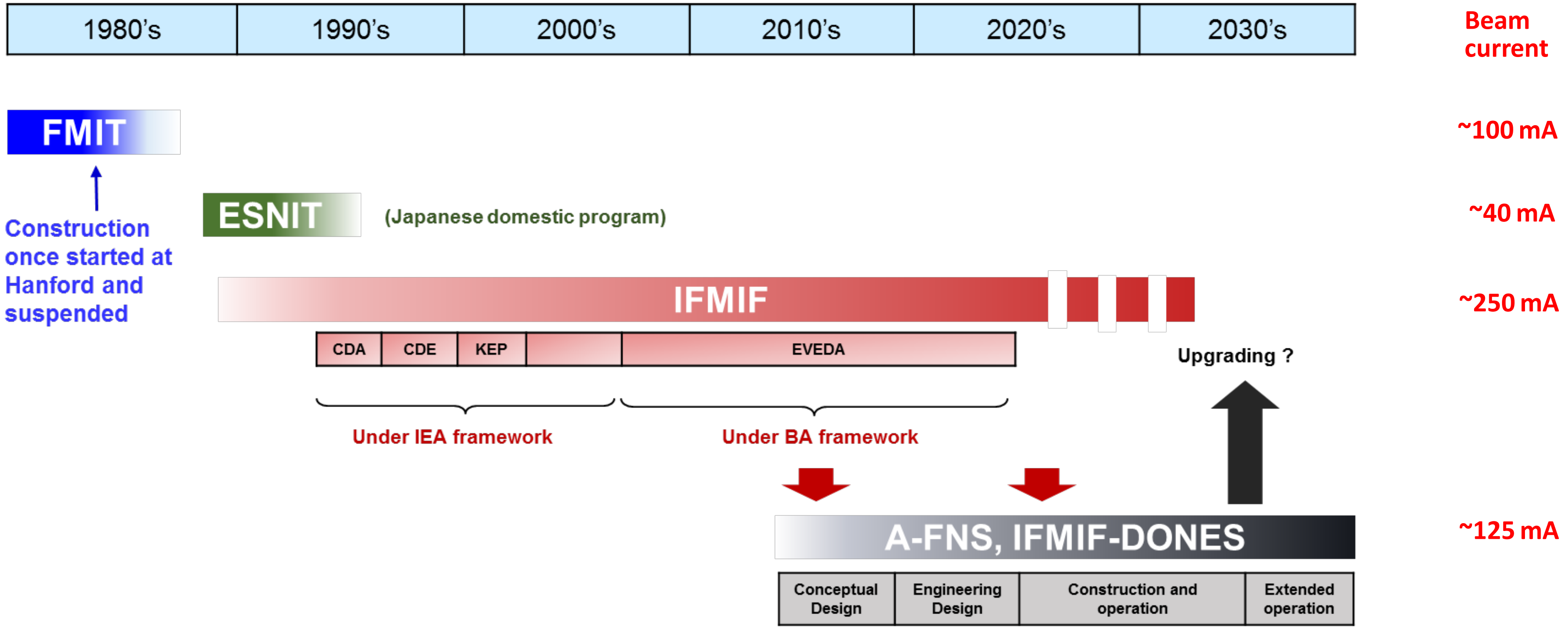
- The overall objective of this CRP was to provide a set of guidelines for SSTT based on common agreed best practices on main material test techniques (tensile, creep, low cycle fatigue, fracture toughness, fatigue crack growth) for reference structural fusion materials (in particular, reduced activation ferritic-martensitic steels) as the first step.
- The CRP includes round-robin-tests under the same agreed conditions and is performed on two materials [F82H and EUROFER].

- The 1st part of the CRP was completed in 2020
- The 2nd part as launched and kick-off meeting will be held December 2022

  With the goal to develop the guidelines so far that they serve as 'supporting documents' for standardization by organizations such as ASME or ISO

FNS History

History of D-Li Neutron Source Design and R&D



1980's | 1990's | 2000's | 2010's | 2020's | 2030's

Beam current

FMIT ~100 mA

Construction once started at Hanford and suspended

ESNIT (Japanese domestic program) ~40 mA

IFMIF ~250 mA

CDA | CDE | KEP | EVEDA

Under IEA framework

Under BA framework

Upgrading ?

A-FNS, IFMIF-DONES ~125 mA

Conceptual Design | Engineering Design | Construction and operation | Extended operation

FMIT (Fusion Materials Irradiation Test Facility, USA) :

Early start of construction was attempted to promote fusion materials development

ESNIT (Energy Selective Neutron Irradiation test Facility, Japan) :

Scientific contribution was emphasized with cost/risk reduction toward staged development

IFMIF (International Fusion Materials Irradiation Facility, International [IEA] but then BA based) :

Largest volume and highest flux have been designed for materials development/qualification

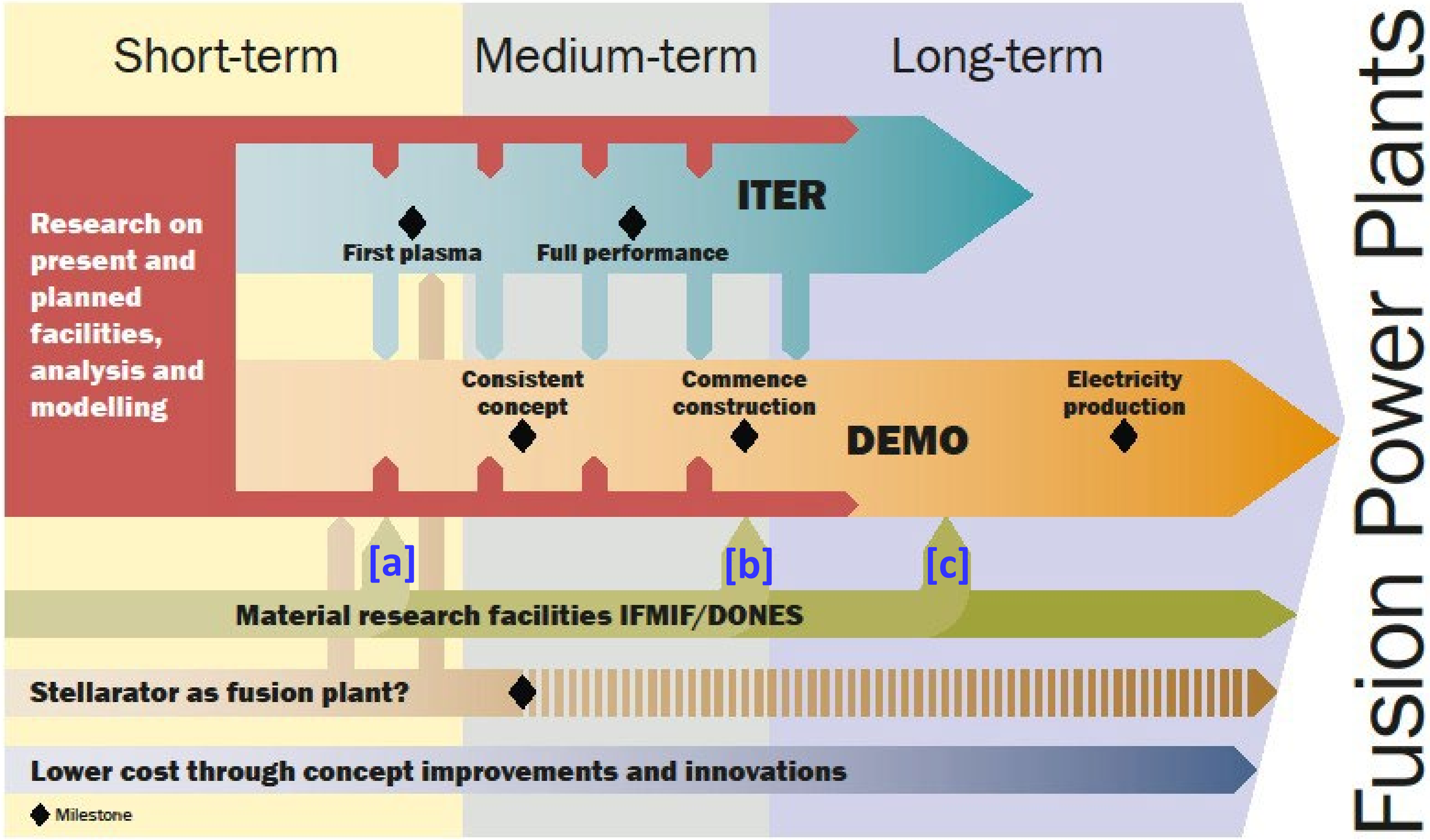
A-FNS, IFMIF-DONES

Timely construction is being planned for materials qualification meeting DEMO schedule

Muroga, Diegele, Möslang, ICFRM-19

EU Roadmap

EUROfusion 2018



Short-term

Medium-term

Long-term

Research on present and planned facilities, analysis and modelling

ITER

◆ First plasma

◆ Full performance

◆ Consistent concept

◆ Commence construction

DEMO

◆ Electricity production

[a]

[b]

[c]

Material research facilities IFMIF/DONES

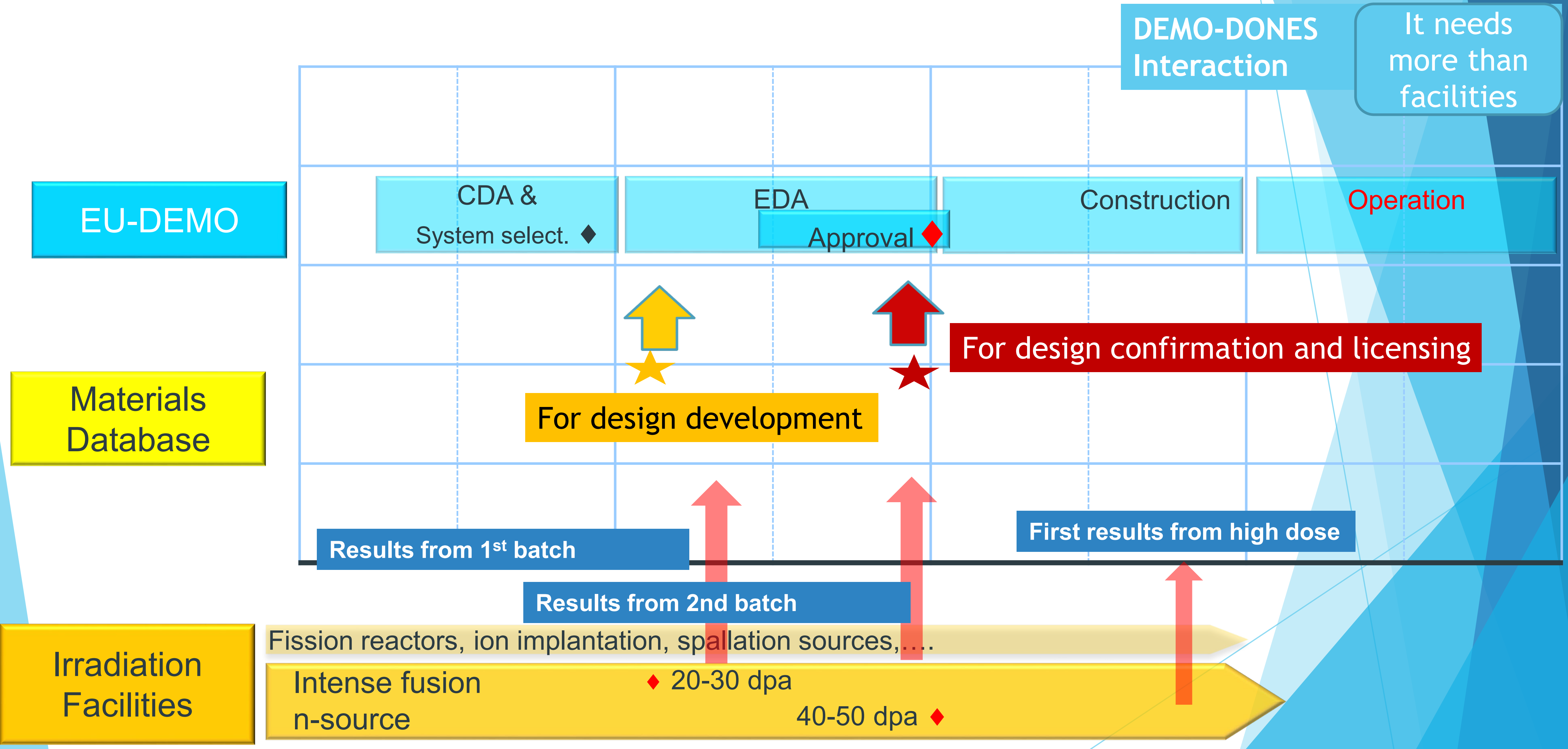
Stellarator as fusion plant? ◆

Lower cost through concept improvements and innovations

◆ Milestone

Fusion Power Plants

Data - when are they needed?....



DEMO-DONES Interaction

It needs more than facilities

EU-DEMO

CDA &
System select. ♦

EDA

Approval ♦

Construction

Operation

For design confirmation and licensing

Materials Database

For design development

Results from 1st batch

First results from high dose

Results from 2nd batch

Irradiation Facilities

Fission reactors, ion implantation, spallation sources,….

Intense fusion
n-source

♦ 20-30 dpa

40-50 dpa ♦

SUMMARY

Fusion Materials Development Path
Facilities needed

Performance under component specific loading Stage IV

Facility Beyond FNS& ITER !

Qualified materials, full demonstration of performance Stage III

14 MeV neutrons or fusion specific n-spectra >>> FNS/ IFMIF

To some extend (validation/falsification) ITER-TBM

Demonstration of performance limits Stage II

Fission reactors (MTR of next generation, at best >10dpa/a)

(FNS)

Materials "Design" Stage I

Microstructure – Analysis tools
SANS, TEM, ATP, FIB

Fission reactors (MTR)
Multi-ion-beam facilities

Complementary Modelling [development and validation] essential at each stage

Plus specific facilities
depends on selection of design choices

Intentionally left open. Expected to be covered with the "facility needed" from BB

Many names
VNS, CTF
Personally in favour

Otherwise likely DEMO is overloaded with objectives

Concern

It appears like in front of a shortage in MTRs

Fusion Materials Development Path
Modelling: Needs / Challenges & Benefits

Stage IV Macroscopic phenomena related to operation (gradients,cycles)

Stage III (Qualification) Modelling (interpretation & transferability of data)

"Transferability" *(correlate data from different irradiation facilities and different conditions). [Mandatory to guarantee licensing]*

Link MTR and FNS irradiation data

Stage II (Demonstration) Modelling of meso to macro-scale phenomena

Aim: Develop theory and models to explain plasticity and fracture (dislocation dynamics / visco-plastic constitutive equations) and in-situ fatigue or creep-fatigue

Benefit: improved design methodologies, improved confidence level in design rules, life prediction.

Stage I: (Materials Design) Basic science complementing empirical approach

Aim: Increase step-wise knowledge on
- stability and evolution of microstructure under irradiation and/or load
- driving mechanisms, time scales, thermodynamic stability criterion.

Challenge: towards predictive capability for alloys.

Benefit: Relationship between processing and microstructure.