DE LA RECHERCHE À L'INDUSTRIE

MATERIALS FOR NUCLEAR ENERGY: FISSION AND FUSION

PHYSICS BASED MODELLING OF THE BEHAVIOUR OF MATERIALS UNDER IRRADIATION

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Mat4Energy, Grenoble, France | 16-18 June 2014

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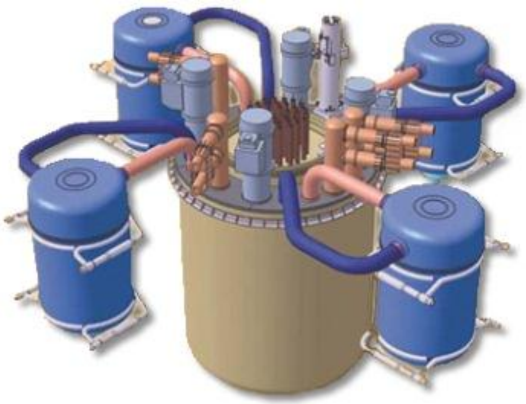
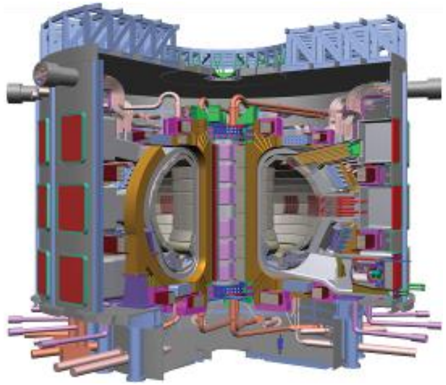
PRESENT AND FUTURE NUCLEAR REACTORS

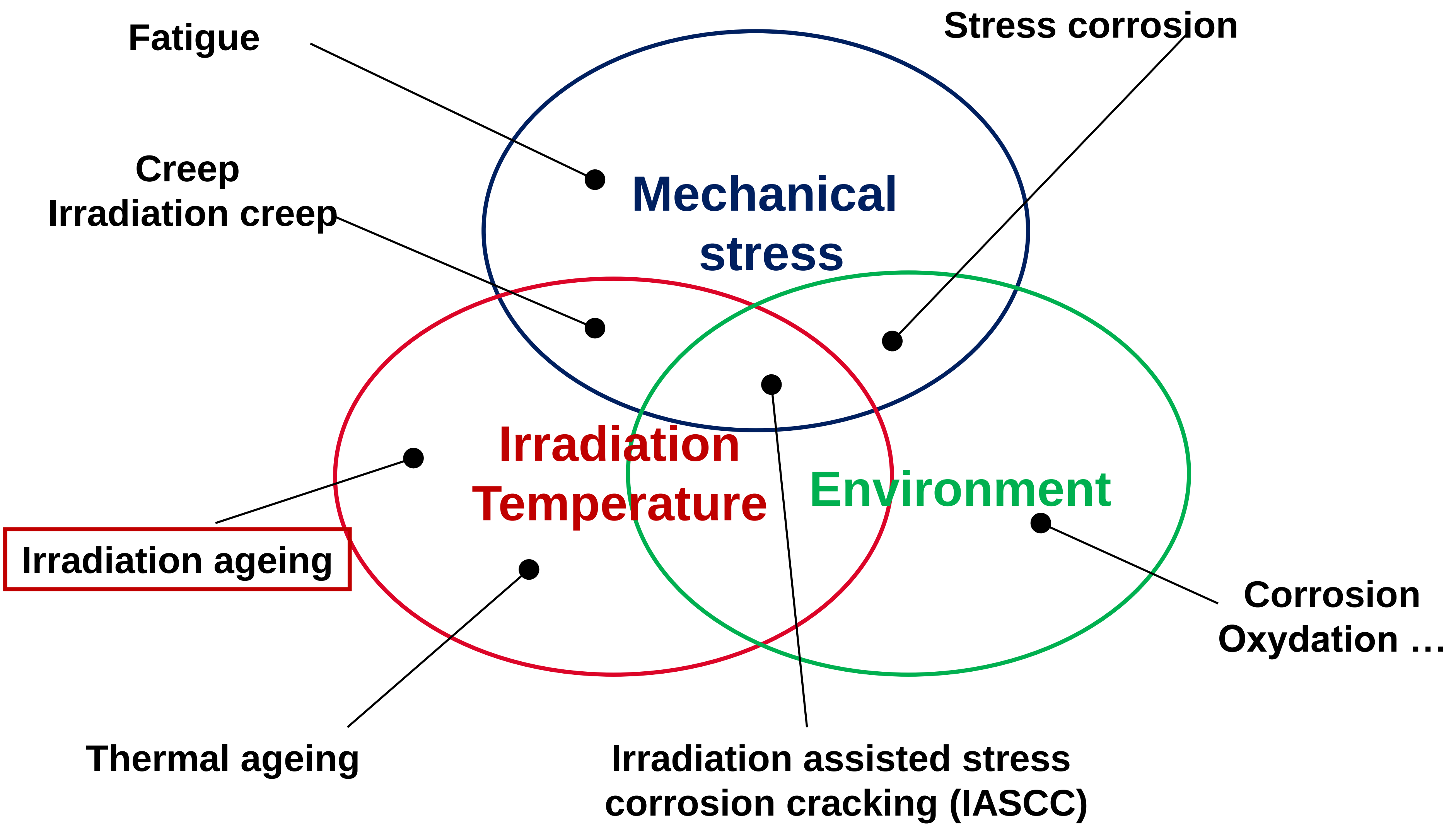




Present

Future

Fission		Fusion
Generation 2&3 (Thermal neutrons)	Gen IV (Fast neutrons)	ITER -> DEMO (14 MeV neutrons)
Coolant and moderator = pressurized water (PWR)	Coolant = liquid sodium (SFR)	plasma
T= 300°C	550°C	T=550°C


Fatigue
Stress corrosion
Creep
Irradiation creep
Mechanical stress
Irradiation
Temperature
Environment
Irradiation ageing
Corrosion
Oxydation …
Thermal ageing
Irradiation assisted stress corrosion cracking (IASCC)

MATERIALS UNDER IRRADIATION AND NUMERICAL SIMULATIONS

WHAT CHANGES IN THE PHYSICS OF MATERIALS UNDER IRRADIATION ?

- **System out of equilibrium**
  - Ballistic jumps vs thermally activated jumps
- **Supersaturation of defects** (vacancies and self-interstitials)

$$c_{v,i} \gg c_{v,i}^{eq}(T)$$

- vacancies ~ quench from high temperature

- self-interstitials become important since $c_i(t=0) = c_v(t=0)$

unlike at thermal equilibrium where $c_i^{eq}(T) \ll c_v^{eq}(T)$ since $H_i^f > H_v^f$

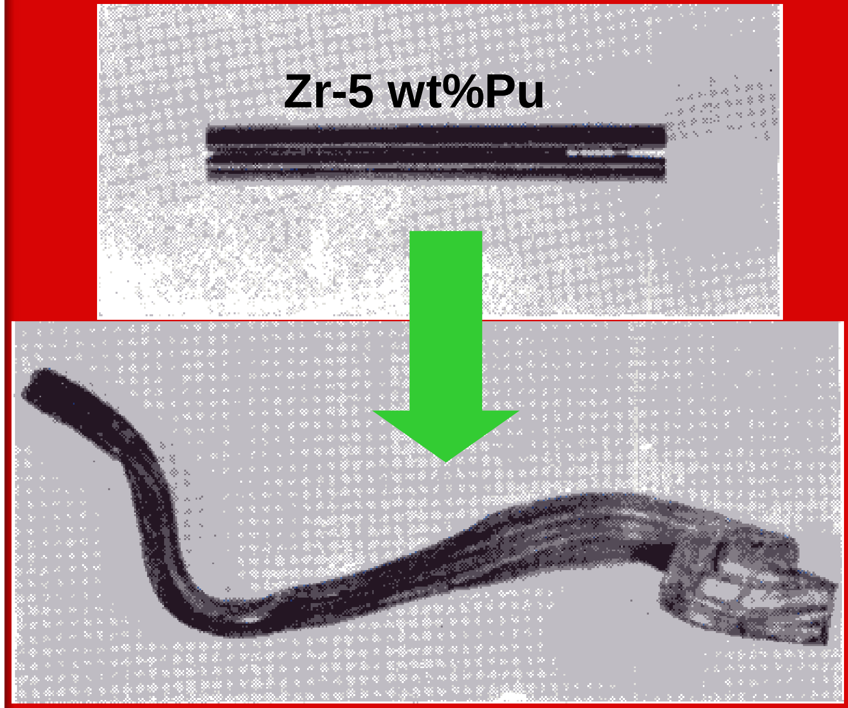
- Irradiation by neutrons: nuclear reactions induce changes in the chemical composition (transmutation) + production of He and H

> - Irradiation changes: structure, chemistry & transport
> - Inherently multiscale problem:
>   - In size: from atoms to components
>   - In time: from picoseconds to centuries
>
> => Key role of numerical simulations

Dimensional changes

SWELLING

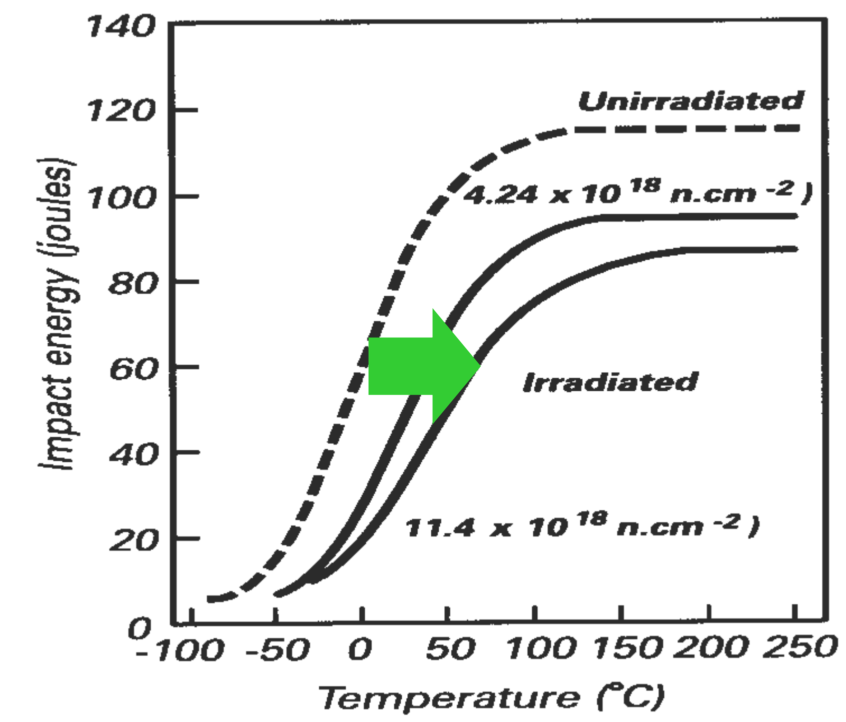
GROWTH



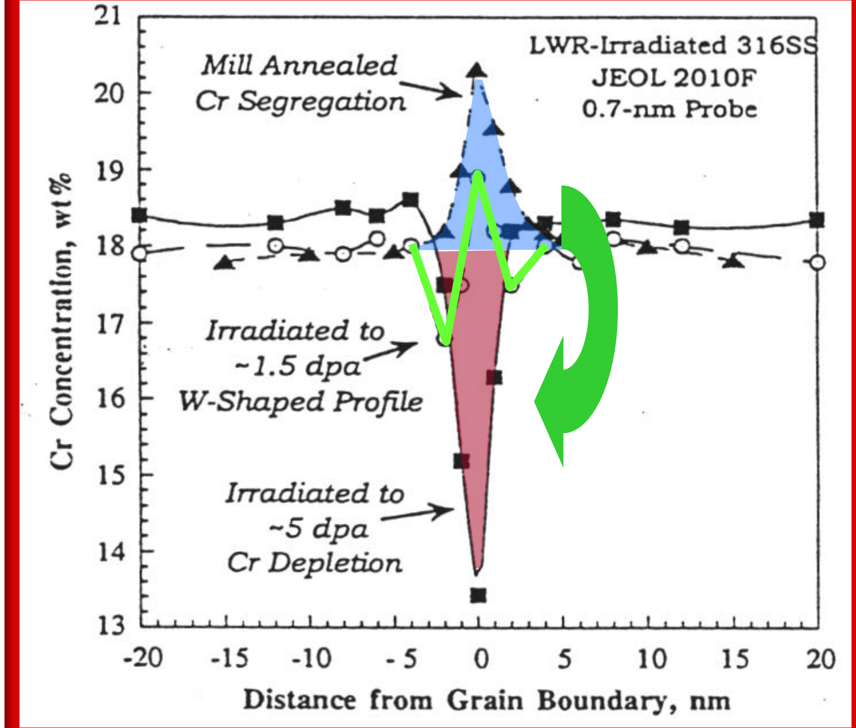
J.A. Horak et al.(1961)

AGEING OF MATERIALS UNDER IRRADIATION (2/2)

EMBRITTLEMENT



SEGREGATION



Bruemmer et al., JNM (1998)

IRRADIATION CONDITIONS OF COMPONENTS IN NUCLEAR REACTORS

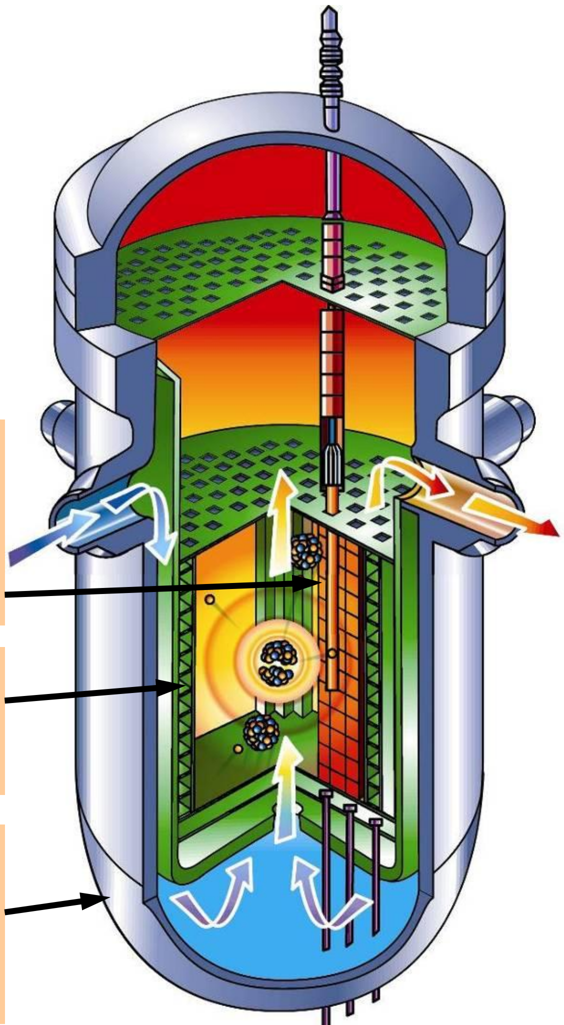
Measure of damage:
dpa = displacement per atom

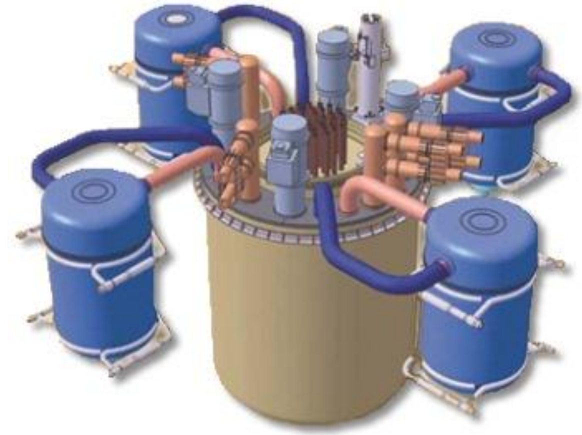
T= 300°C

fuel cladding
5 years
10 dpa

internals
100 dpa

vessel
60 years
0.2 dpa

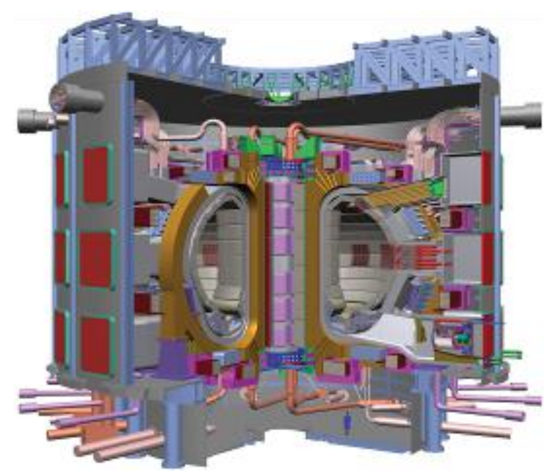




~ 550°C
~ 200 dpa

Generation IV
(fast neutron reactors)

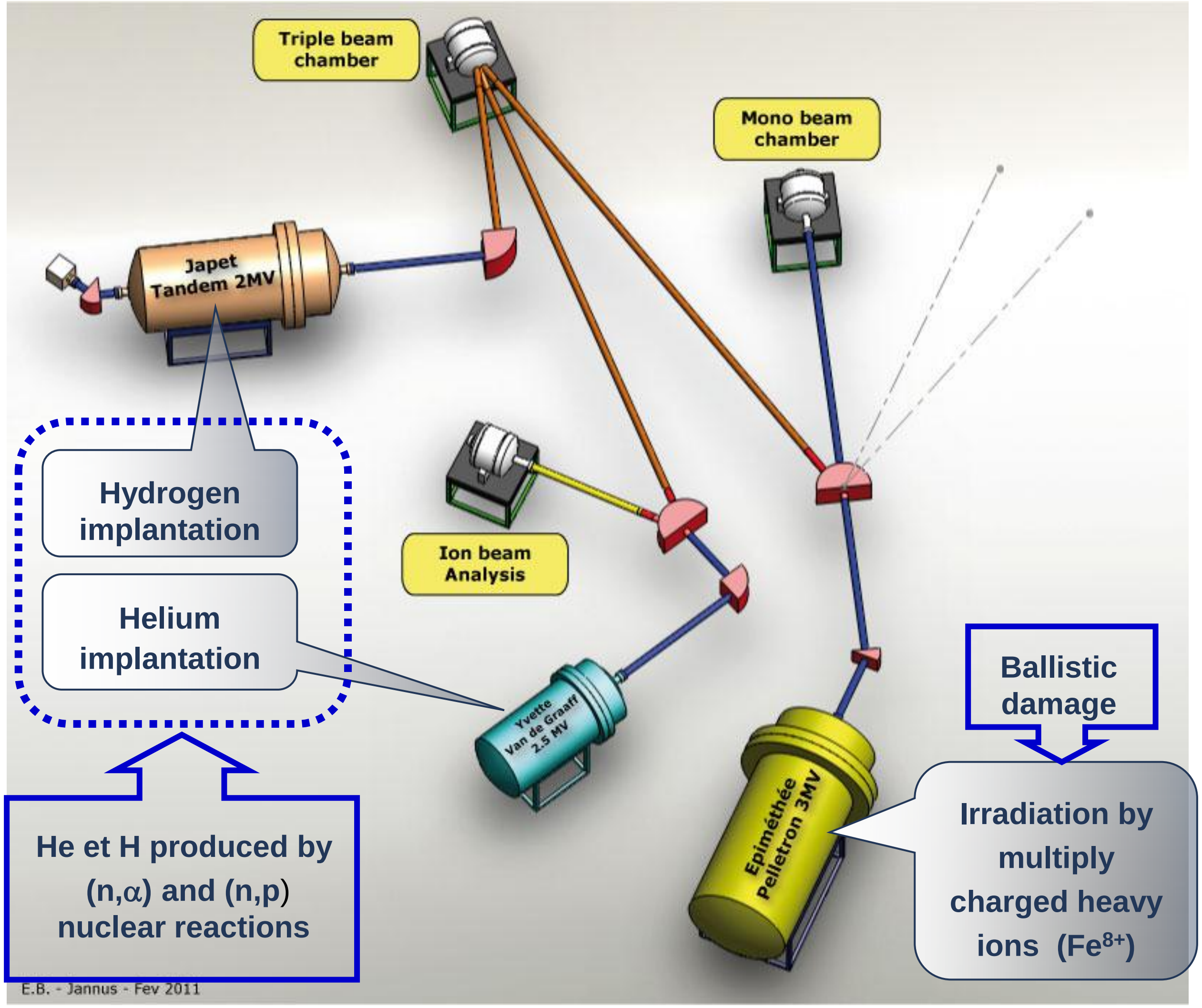
Reactor:
~ 550°C
~ 150 dpa
~10 appm He/dpa
~ 45 appm H/dpa



Fusion devices

USING IONS TO MIMIC THE EFFECT OF NEUTRONS

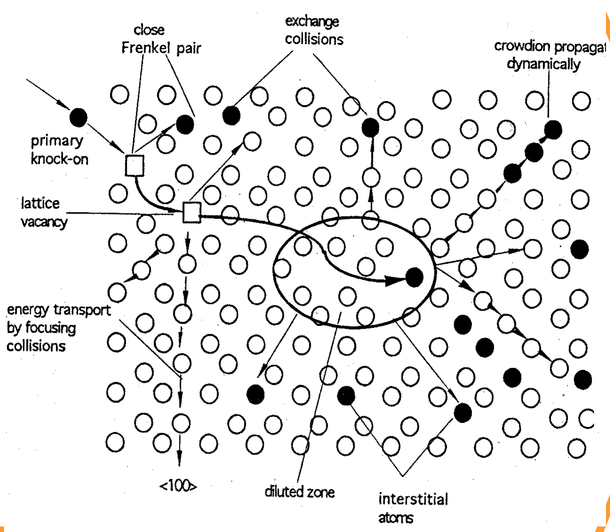
The Jannus-Saclay triple beam facility

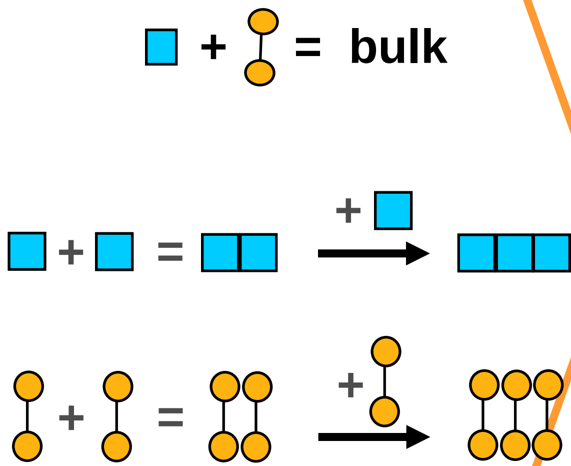


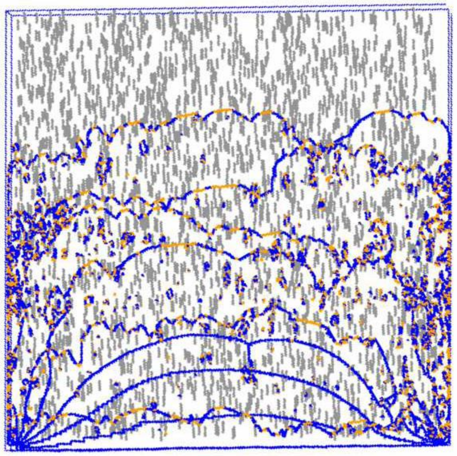
Advantages:
- Faster (~10 dpa per day)
- Cost
- Well controlled conditions
- Samples are not activated

Limitations:
- Implantation depth (~1μm)
- Mechanical tests
- ion/neutron transferability

MULTISCALE ASPECT OF MATERIALS UNDER IRRADIATION







10 ps ; (10-100 nm)^3

10^3 s ; (10-100 μm)^3

Primary damage

Molecular Dynamics
Simulations of displacement cascades

Defect population evolution

Kinetic models:
Monte Carlo, cluster dynamics

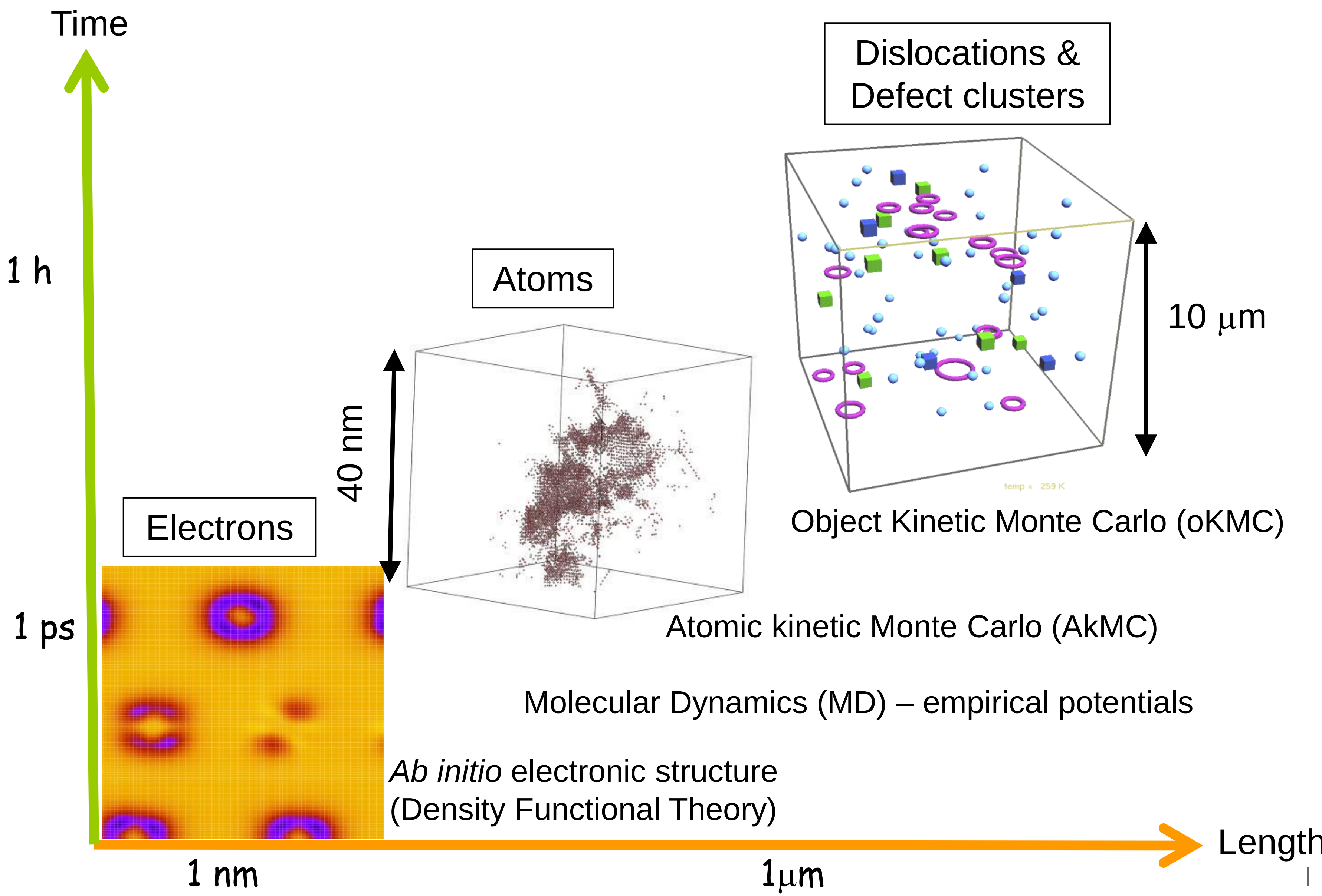
Consequences on materials properties

Mechanical properties:
Dislocation Dynamics

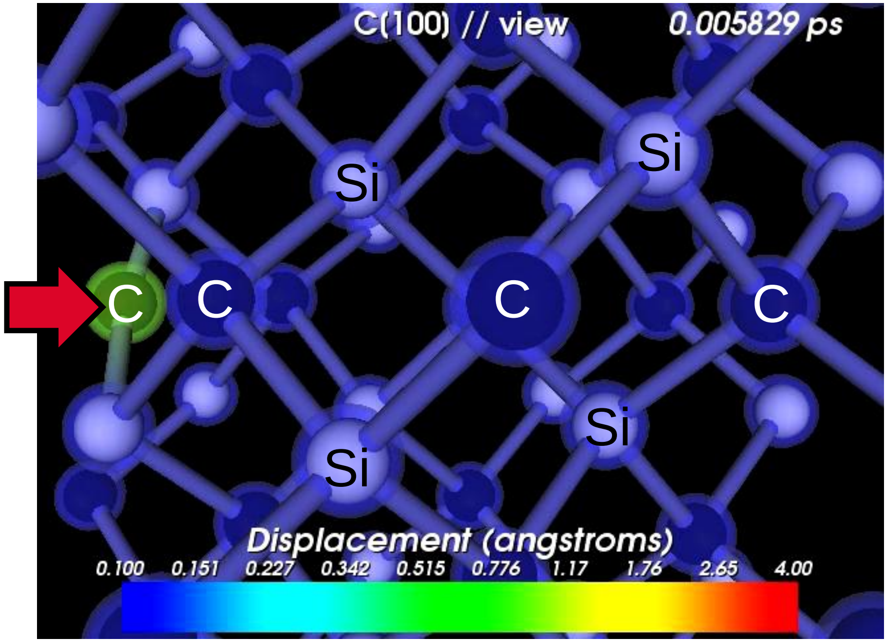
Defect properties :
ab initio calculation

Dislocation properties
Molecular Dynamics

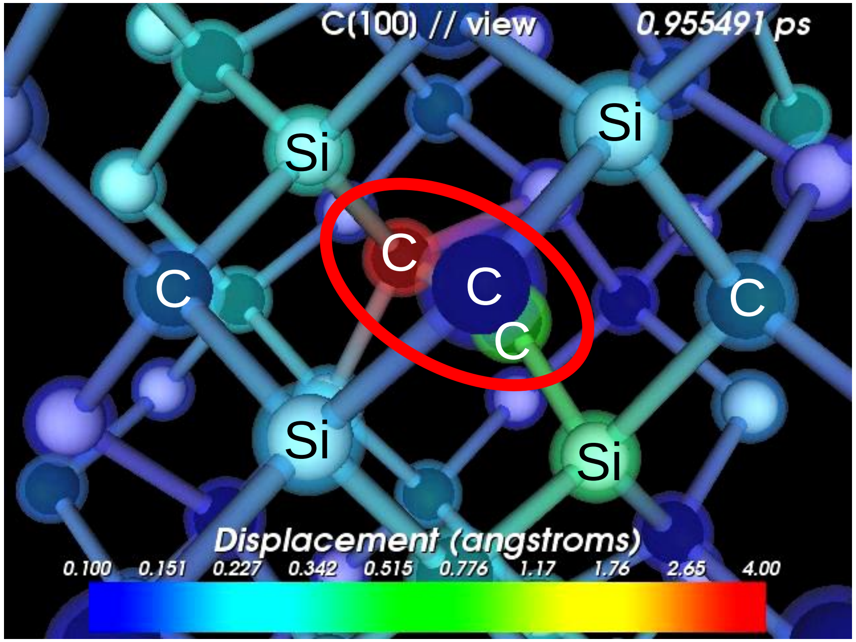
MULTISCALE MODELLING TOOLBOX



AB INITIO MD SIMULATION OF THRESHOLD DISPLACEMENT ENERGIES IN SIC



t = 0.006 ps



t = 1 ps

G. Lucas and L. Pizzagalli, PRB (2005)

MD SIMULATION OF DISPLACEMENT CASCADES

Movie: courtesy of A. Calder and D. Bacon, The University of Liverpool, UK

- Deviations from the « NRT rule »

Number of defects

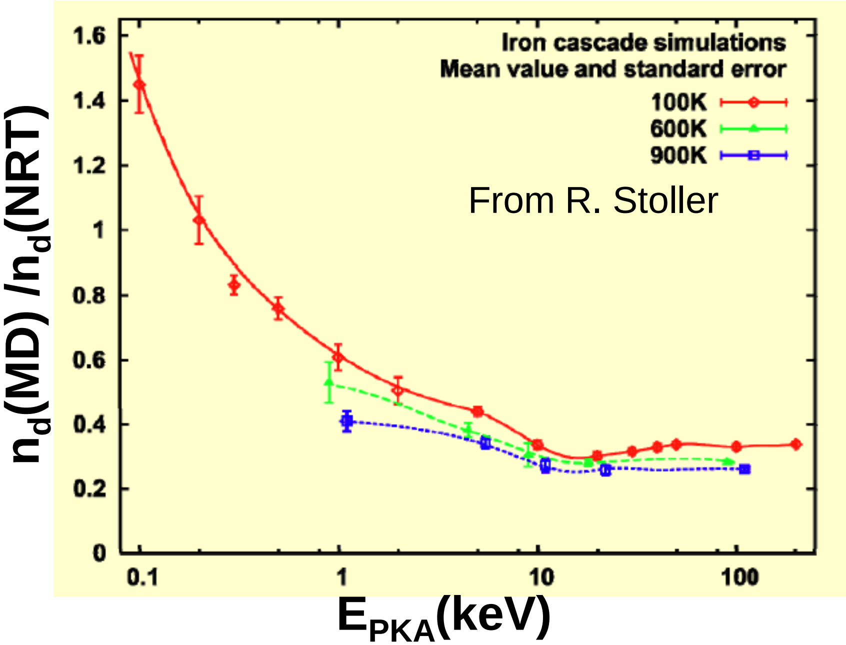
$$n_d = 0.8 \frac{E_{PKA}}{2E_d}$$

Primary knock-on atom energy

Threshold displacement energy

Norgett, Robinson and Torrens (1975)

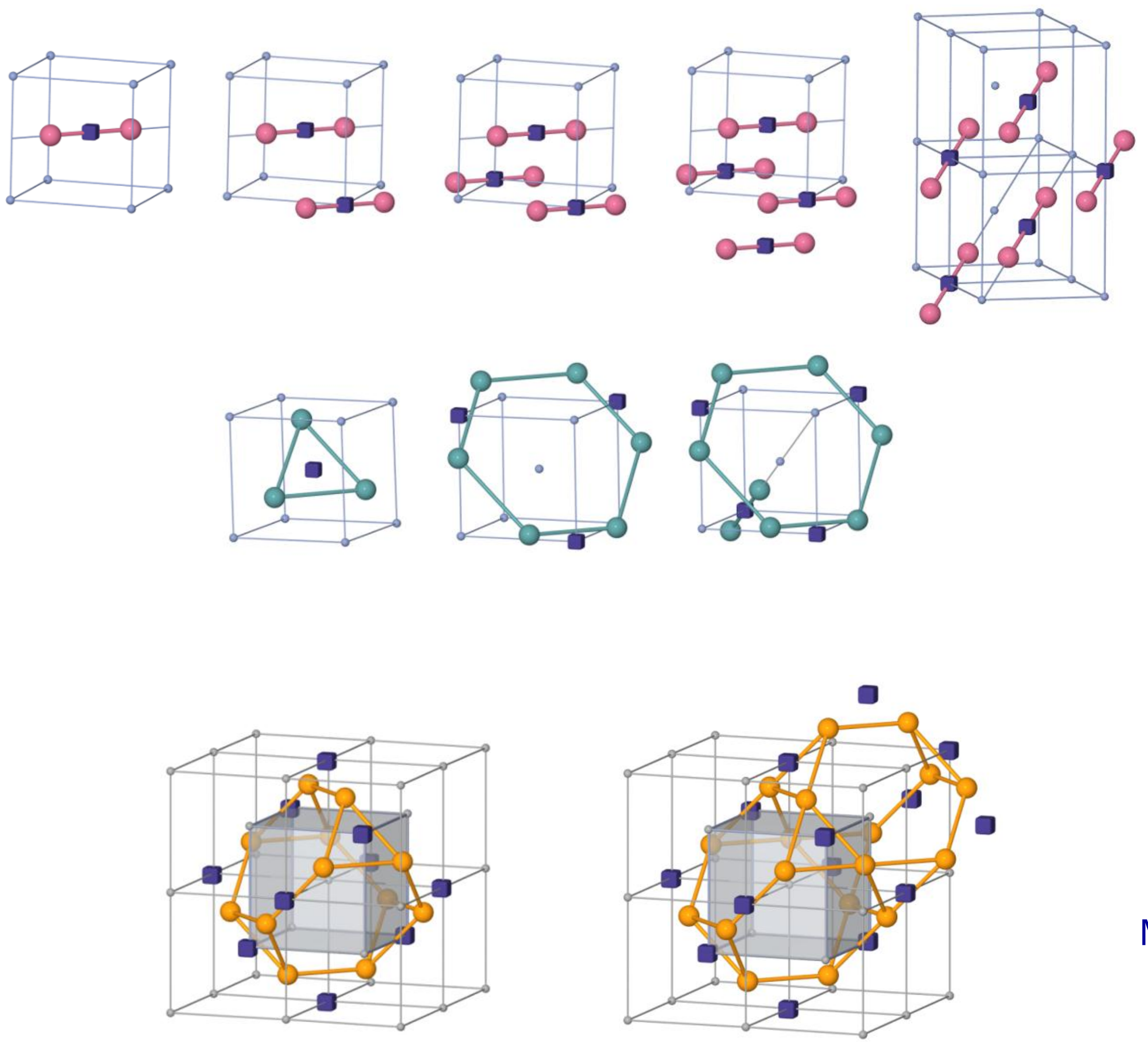
- n_d non-linear in E_{PKA}
- at high energies: n_d ~1/3 NRT



- The real number of displaced atoms that have moved from their lattice sites can be ~ 10-100 times higher
- About 50% of the defects are clustered

  -> major difference between irradiation by electrons and by neutrons or high energy ions
- Structure of cascades: vacancies at the center and interstitials at the periphery

Structure of Interstitial clusters in Fe revisited by DFT calculations



Parallel dumbbells

FW et al.; NIMB (2005)

Triangle and rings

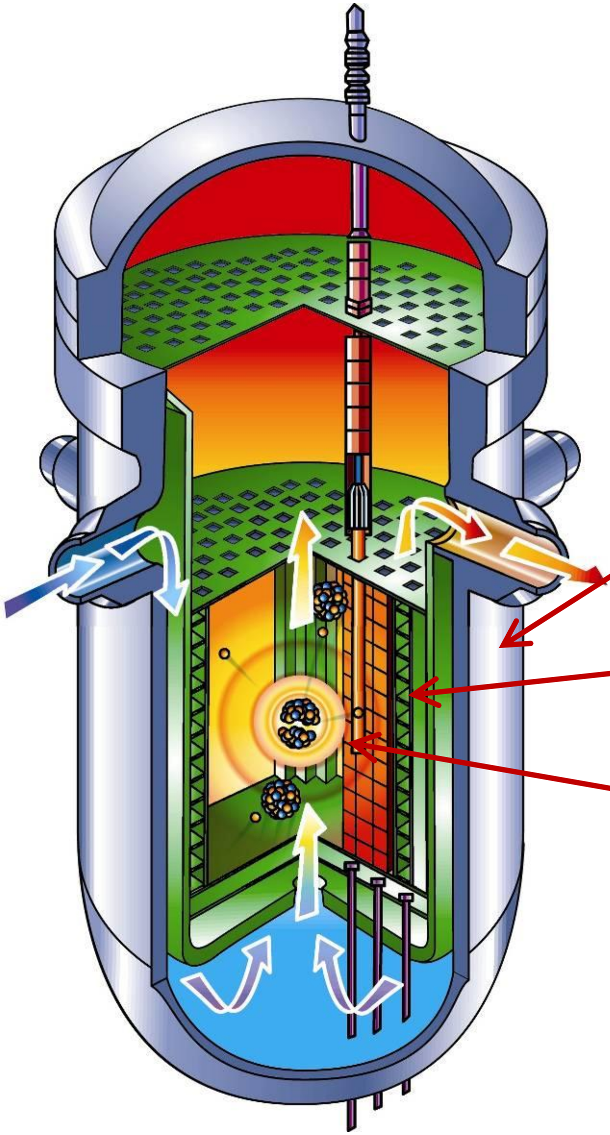
D.A Terentyev et al.
Phys. Rev. Lett. (2008)

3D Laves phase structure

M. C. Marinica, FW, J-P Crocombette
Phys. Rev. Lett. (2012)

MATERIALS ISSUES IN PRESENT REACTORS (FISSION – PWR – GEN 2&3)

MATERIALS ISSUES IN NUCLEAR REACTOR COMPONENTS



Ageing of nuclear power plants

Life limiting component
=> Pressure Vessel (irreplaceable)

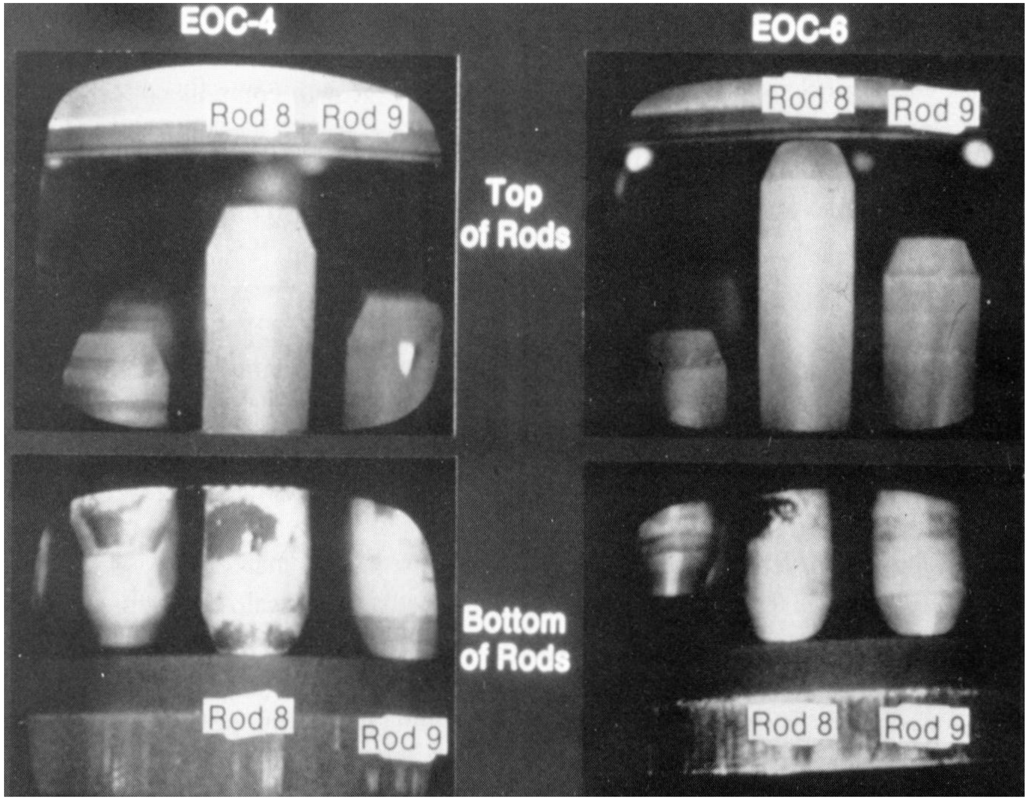
Availability limiting components
=> Internals (replaceable)

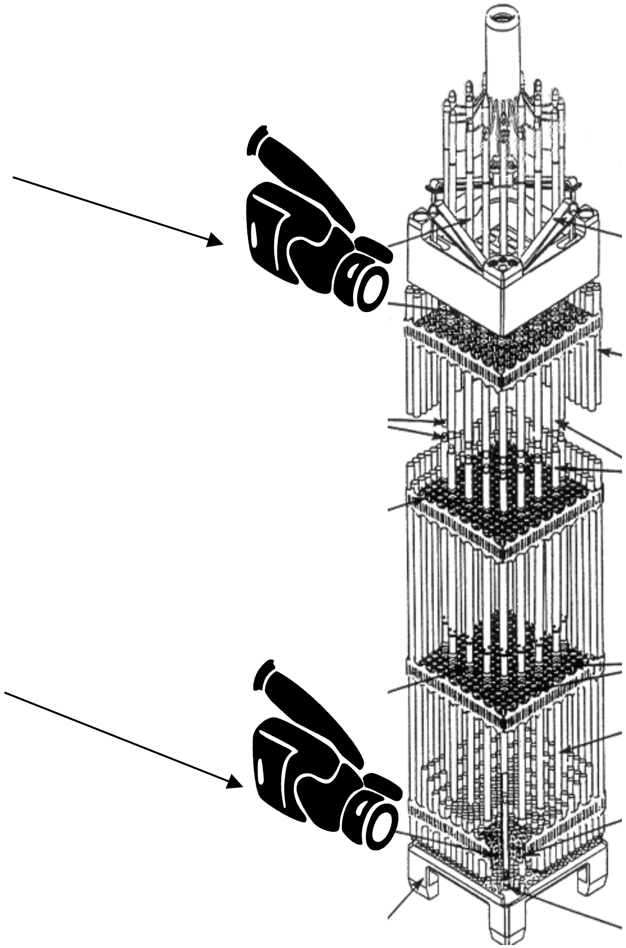
Fuel consumption limiting component
=> Fuel cladding (consumable)

CONSUMABLES:

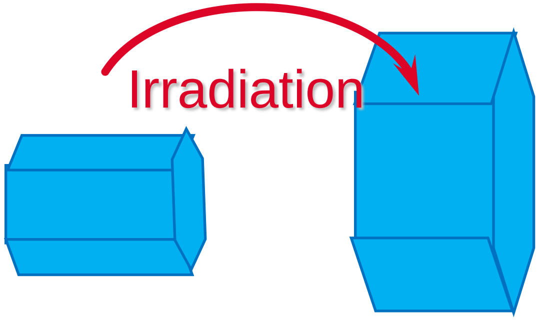
FUEL CLADDINGS

GROWTH OF ZIRCONIUM FUEL CLADDINGS

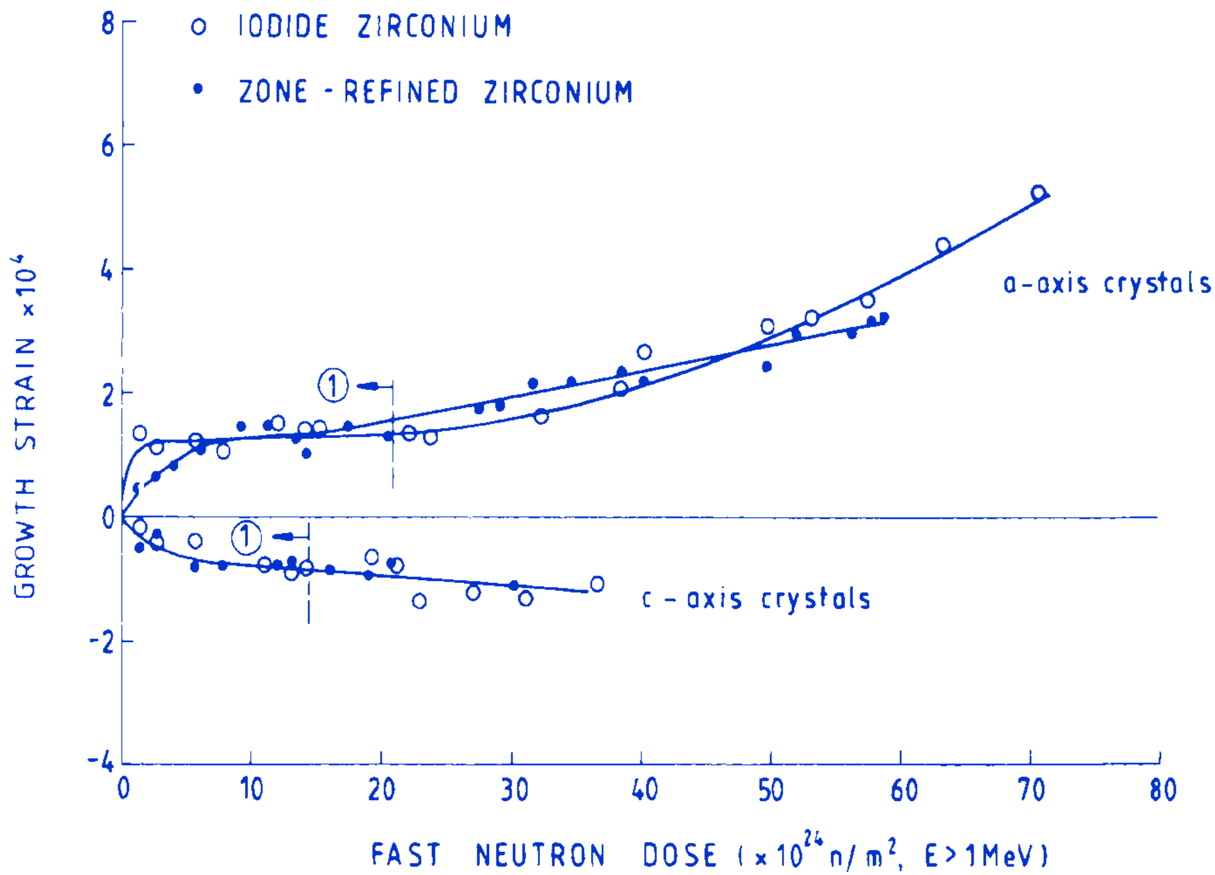




Zr: hexagonal close packed
(hcp) structure
Extension ⊥ <c>
Contraction // <c>



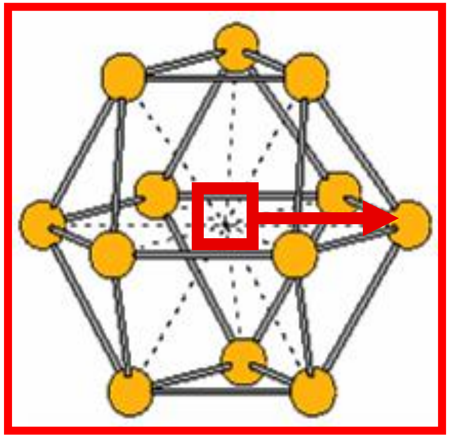
GROWTH OF ZR SINGLE CRYSTALS



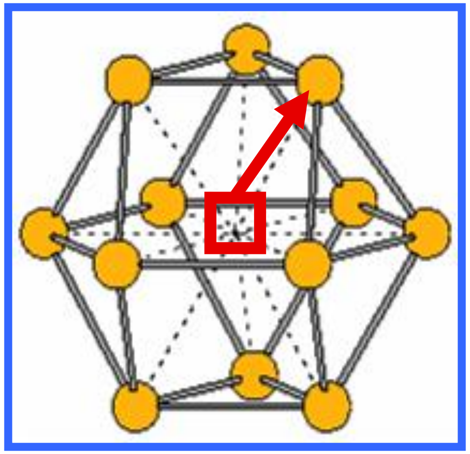
Carpenter (1981)

POINT DEFECTS IN THE HCP STRUCTURE

- **<u>Vacancy</u> : 2 migration paths**



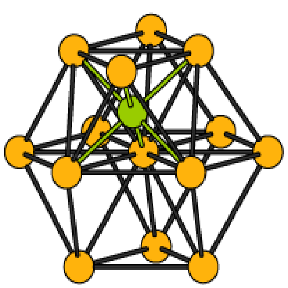
Basal migration



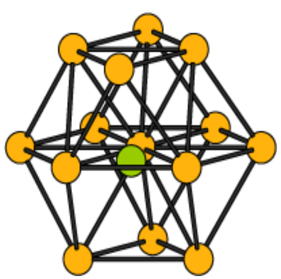
Non-basal migration

⇒ **May yield to diffusion anisotropy**

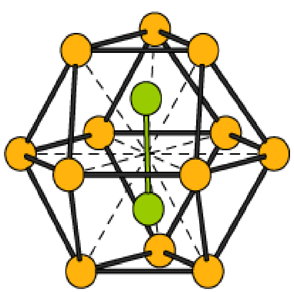
- **<u>Self-interstitials</u>: 6 configurations with similar formation energies according to DFT calculations**



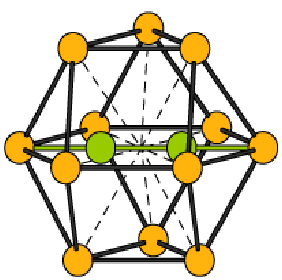
O



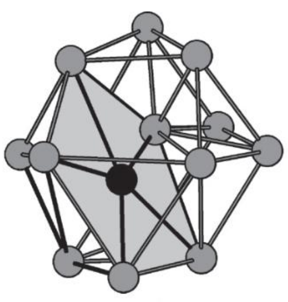
BO



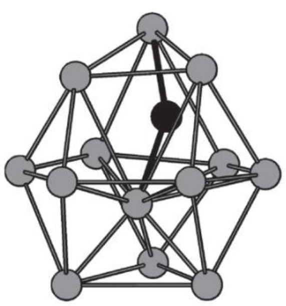
S



BS



BC'

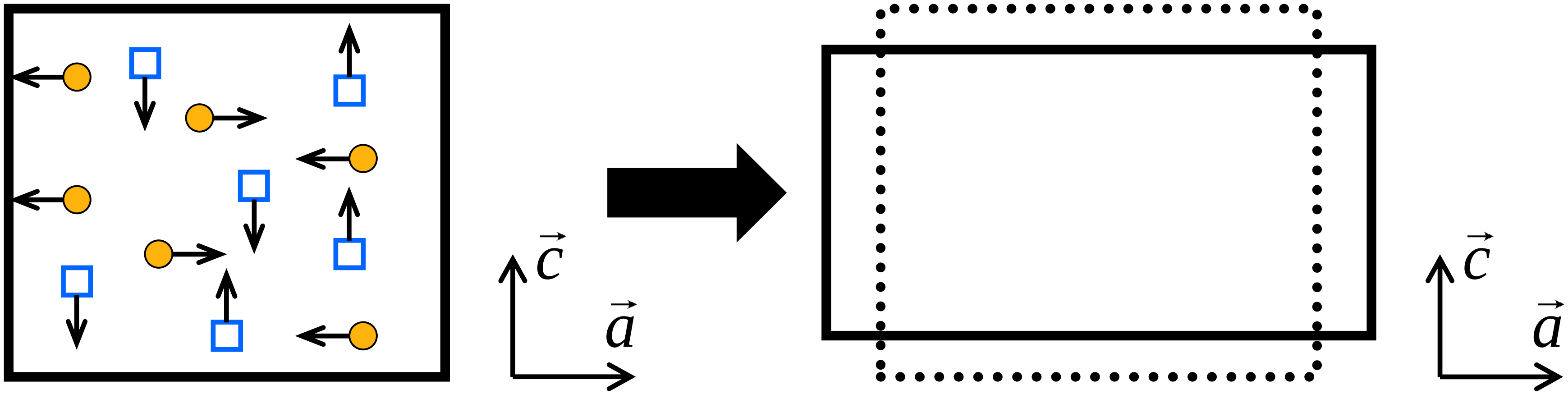


C'

G. Vérité et al. Phys. Rev. B 87, 134108 (2013)

Diffusion Anisotropy Model for irradiation growth

→ **Based on the hypothesis of Differential Anisotropy Diffusion of point defects**

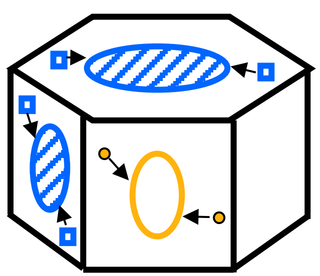


vacancy: migration selon c

Self-interstitials: migration plan basal

→ **Problem: not compatible with DFT data (at T=0K)**

- **Role of loops ?**



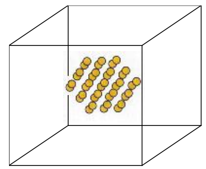
REPLACEABLE:

INTERNAL STRUCTURES

Radiation effects on austenitic stainless steels

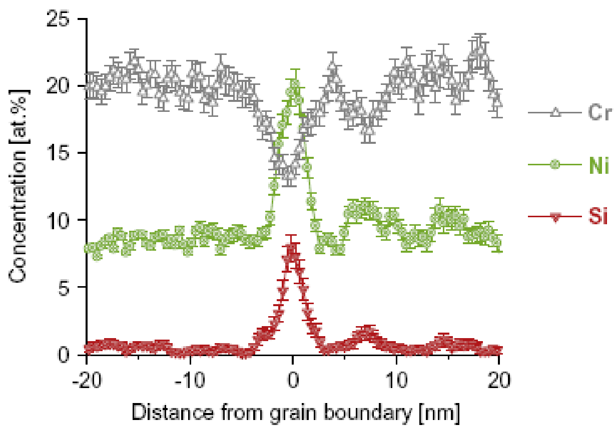
Consequences on mechanical properties and sensitivity to IASCC

Dislocation loops



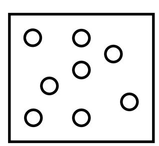
HARDENING
IRRADIATION CREEP
LOCALIZATION-CHANNELLING
TOUGHNESS DECREASE

Segregations at grain boundaries :



INCREASED SENSITIVITY TO SCC (IASCC)

Cavities, helium bubbles…:



POTENTIAL SWELLING

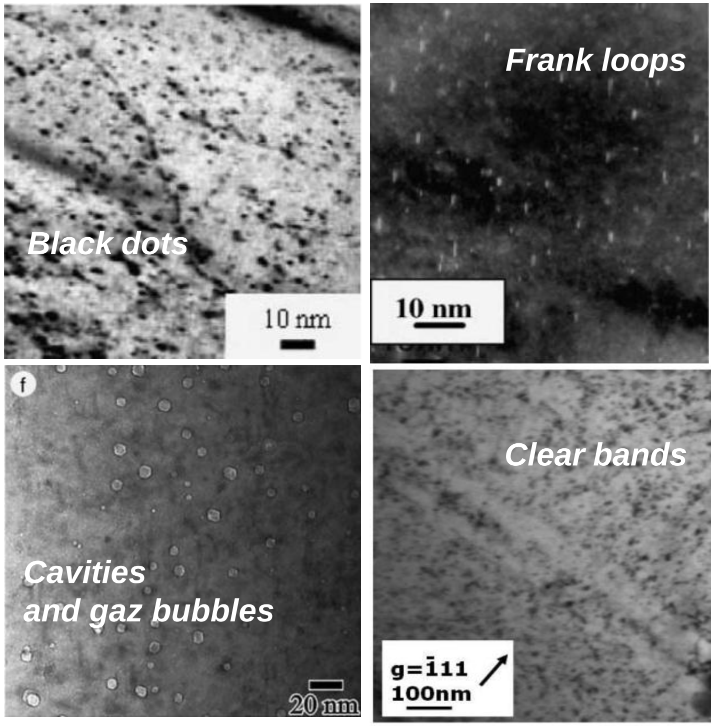
Radiation effects on austenitic stainless steels

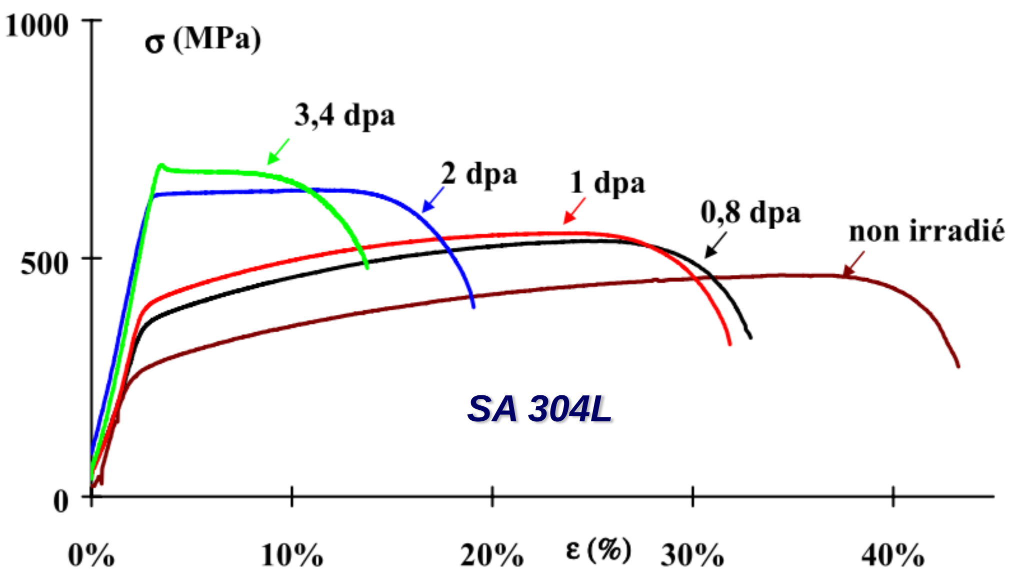
Microstructural evolutions

- Evolution of the initial dislocations network
- Irradiation defects: black dots, Frank loops, cavities and precipitates
- Formation of « Clear band » (under deformation)

Modification of mechanical properties

- Hardening (increase of yield stress)
- Loss of ductility
- Softening (yield drop + localization of deformation in « cleared channels)
- Decrease of fracture toughness





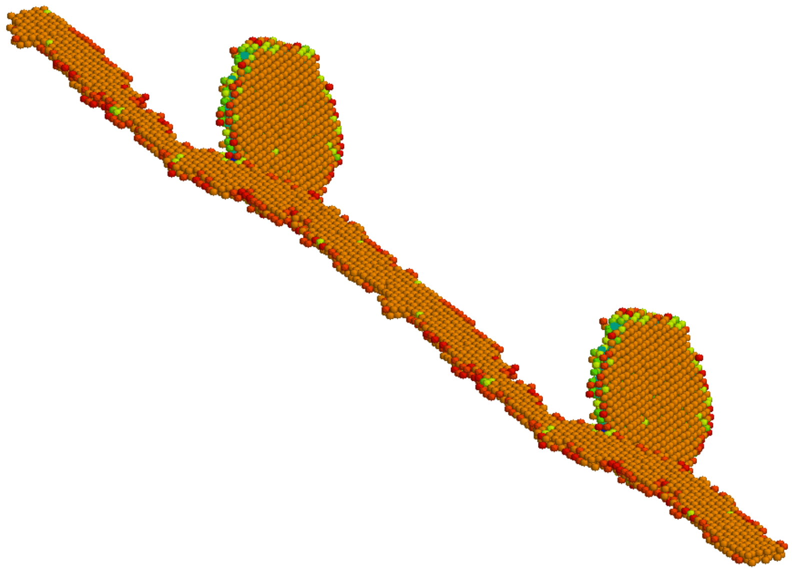
[Pokor (2003)]

DEFECT DISLOCATION INTERACTION

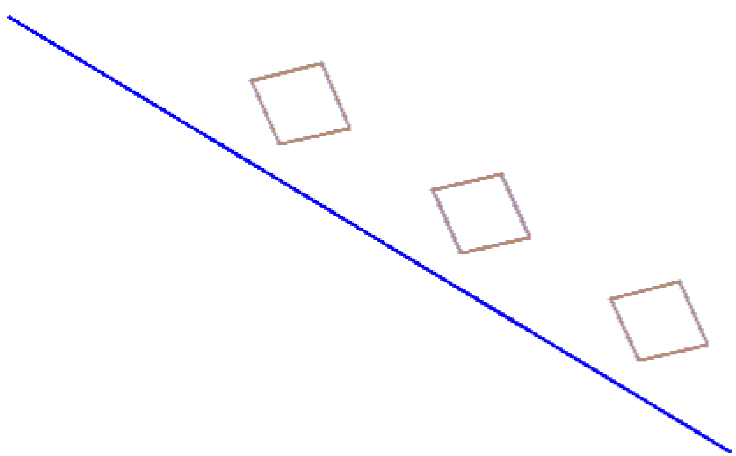
T. Nogaret et al. (2007)
INPG & CEA

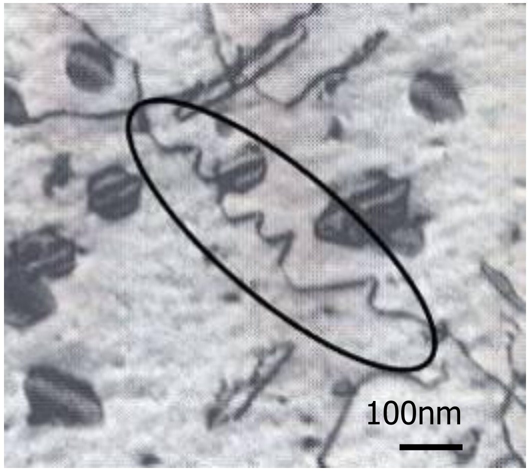
Molecular Dynamics

Screw dislocation – Frank loop

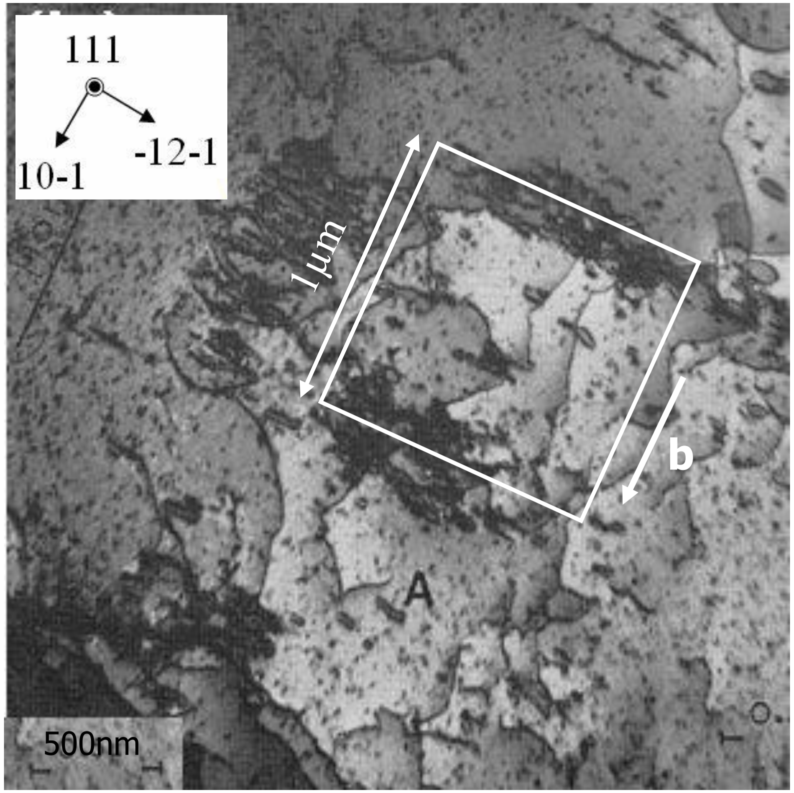


Dislocation Dynamics

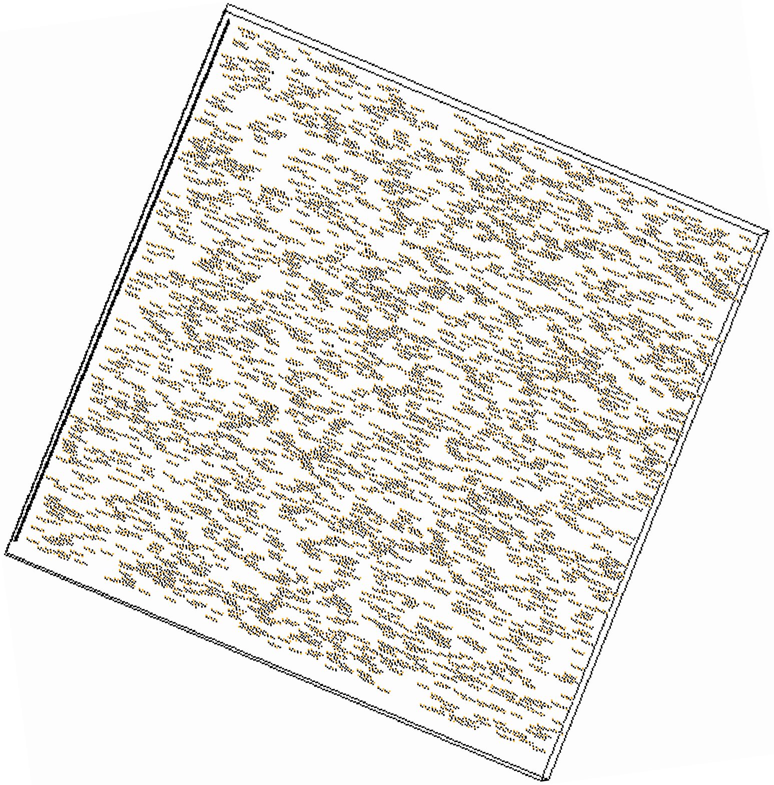




COLLECTIVE BEHAVIOUR OF DISLOCATIONS



Clear band formation [Sharp, 67]



Dislocation dynamics

T. Nogaret et al. (2007)
INPG & CEA

IRREPLACEABLE:

VESSEL

REACTOR PRESSURE VESSELS

- Dimensions:

  10x5 m, thickness = 23 cm

- Ferritic steel composition:

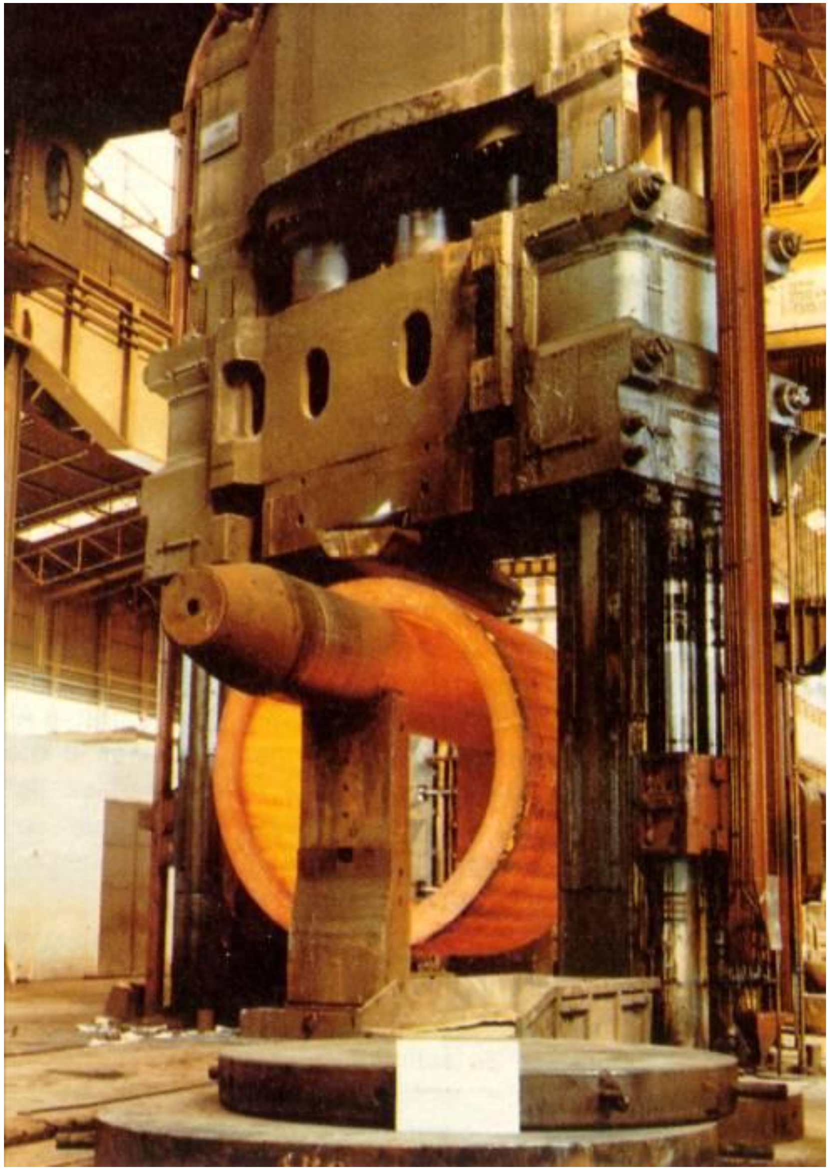
Solutes (%):

C	Mn	Ni	Mo	Cr	Si
<0.2	1.4	0.6	0.5	<0.25	0.2

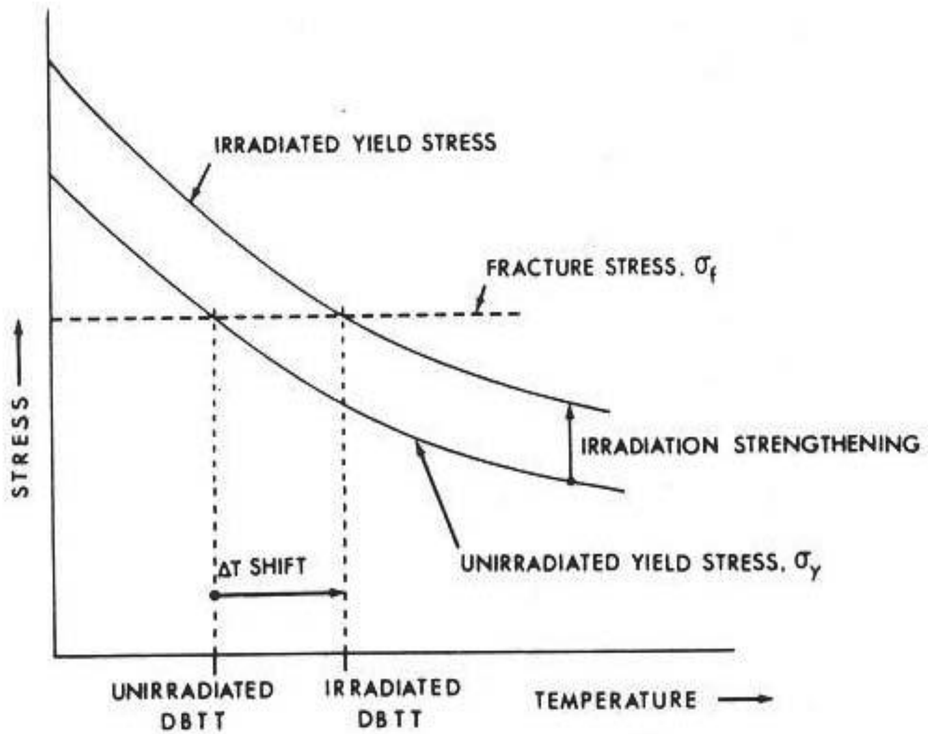
impurities (ppm):

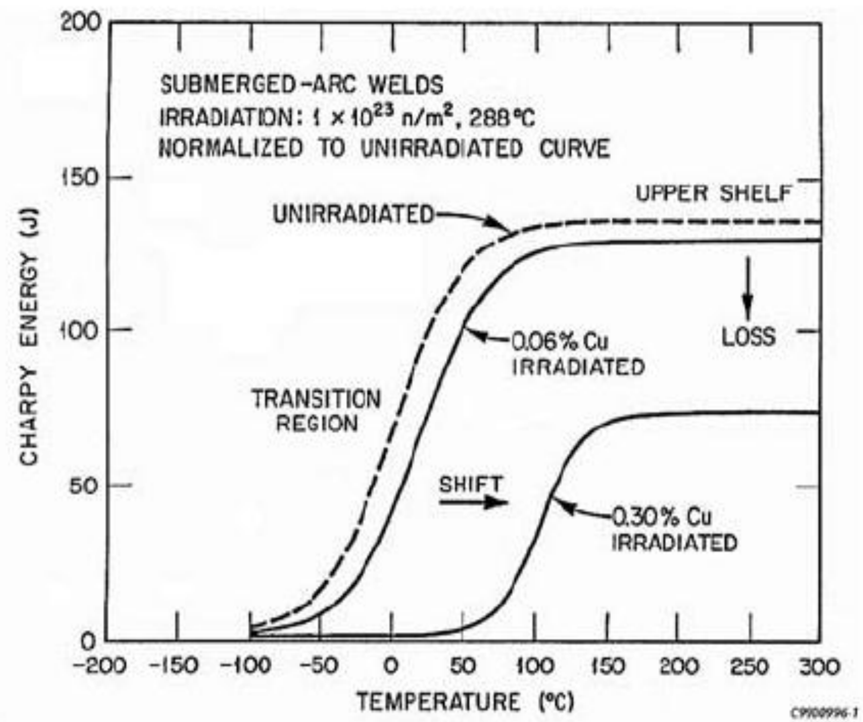
P	S	Cu	Co
< 80	< 80	< 800	< 300

Operating conditions: 150 bar, 300°C



Hardening and embrittlement



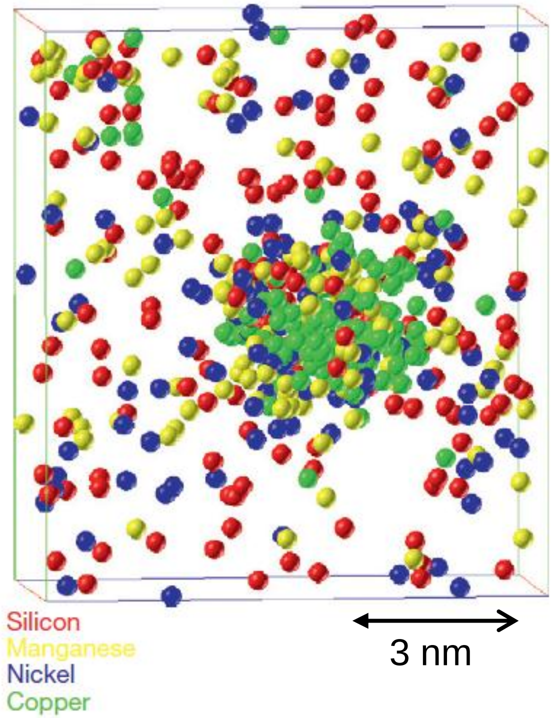


- **Irradiation hardening induces a shift in ductile to brittle transition temperature (DBTT)**
- **DBTT increases with Cu content**

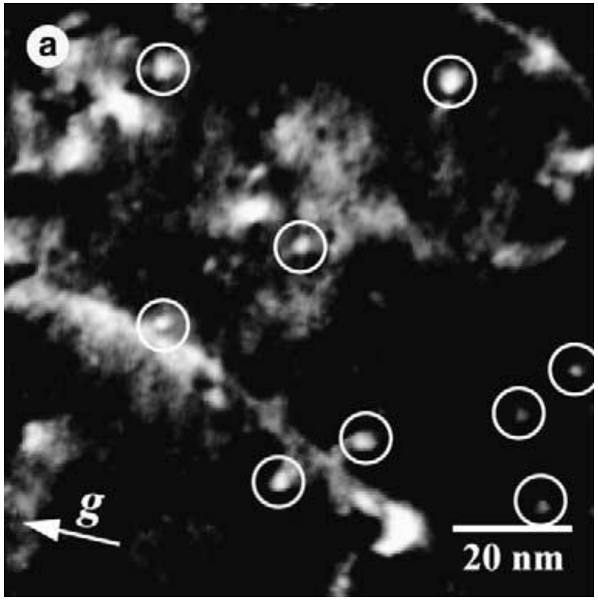
ORIGIN OF IRRADIATION HARDENING OF RPV STEELS

Interaction of dislocations with:

- Solute rich clusters



- « matrix » dammage (vacancy and interstitial clusters)



- Probably combination of both
- Open question: « visible » defects cannot account quantitatively for observed hardening

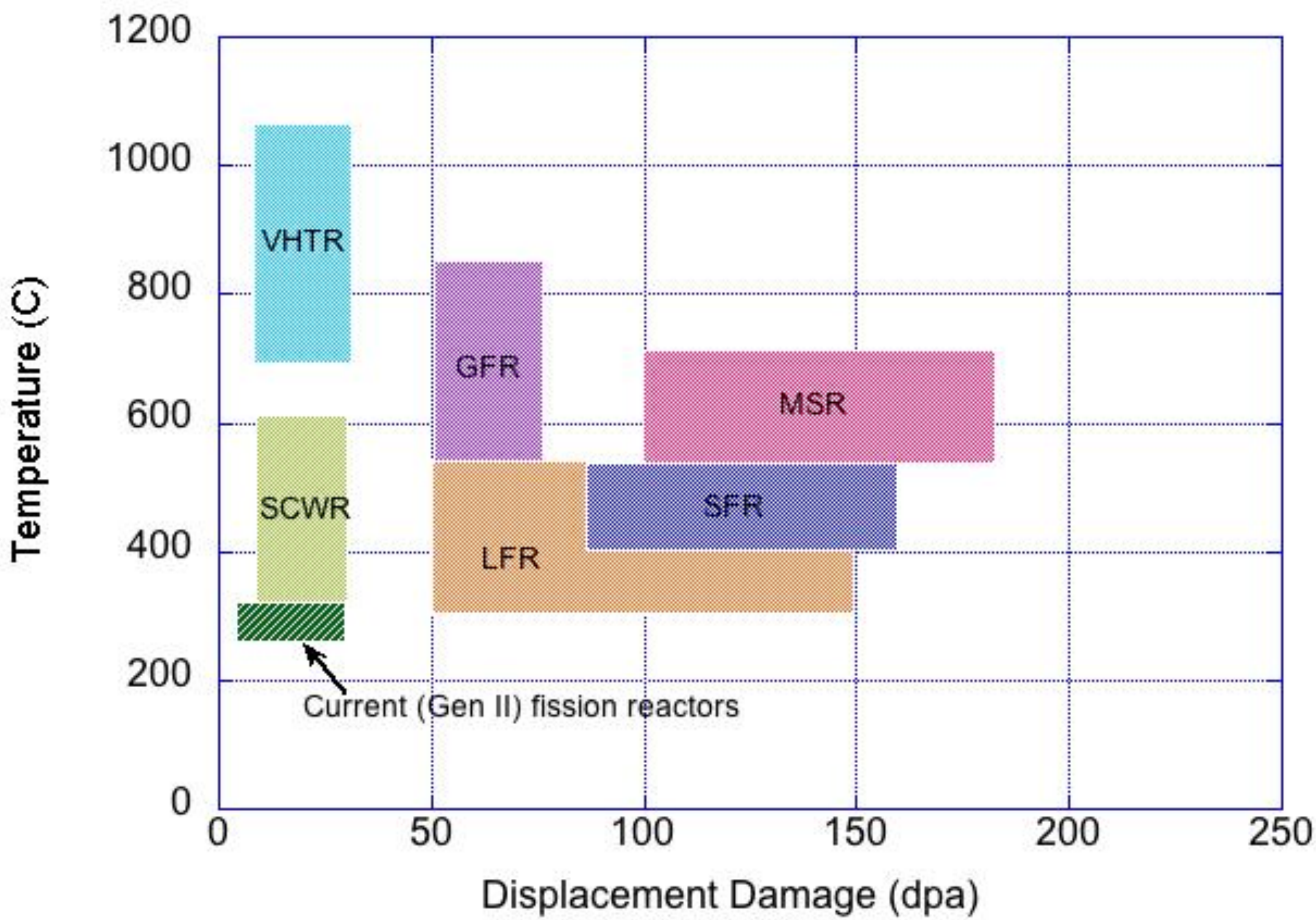
MATERIALS ISSUES IN
FUTURE REACTORS
(FISSION GEN IV AND FUSION)

Materials Environment Comparaison with classical PWR

	Fission (Gen. I/II) PWR…	Fission (Gen. IV)	Fusion (Demo)
temperature max	<300˚C	500-1000˚C	550-1000˚C
Irradiation dose max	~50 dpa	~30-200 dpa	~150 dpa
transmutation concentration He	~0.1 appm	~3-10 appm	~1500 appm (~10000 appm for SiC)
Heat extracting fluids	H_2O (PWR: pression 155 bars)	He, H_2O, Pb-Bi, Na	He, Pb-Li, Li

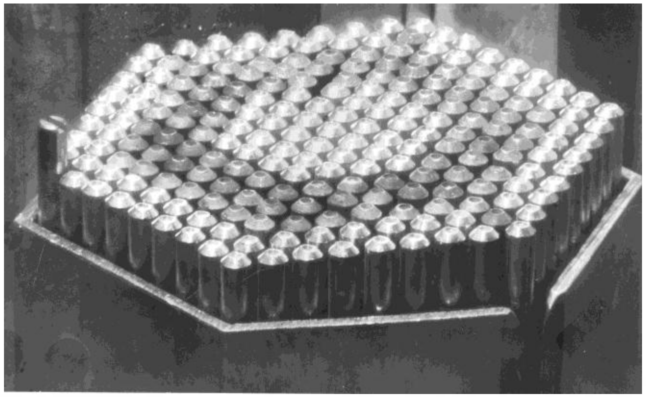
No requirement on pressure

New reactors : Gen IV et Fusion
Comparison with classical PWR

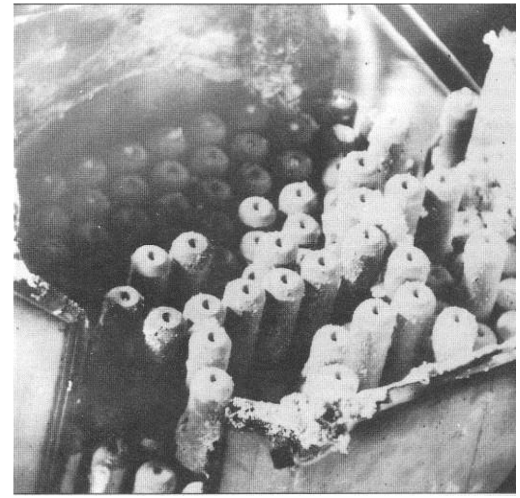


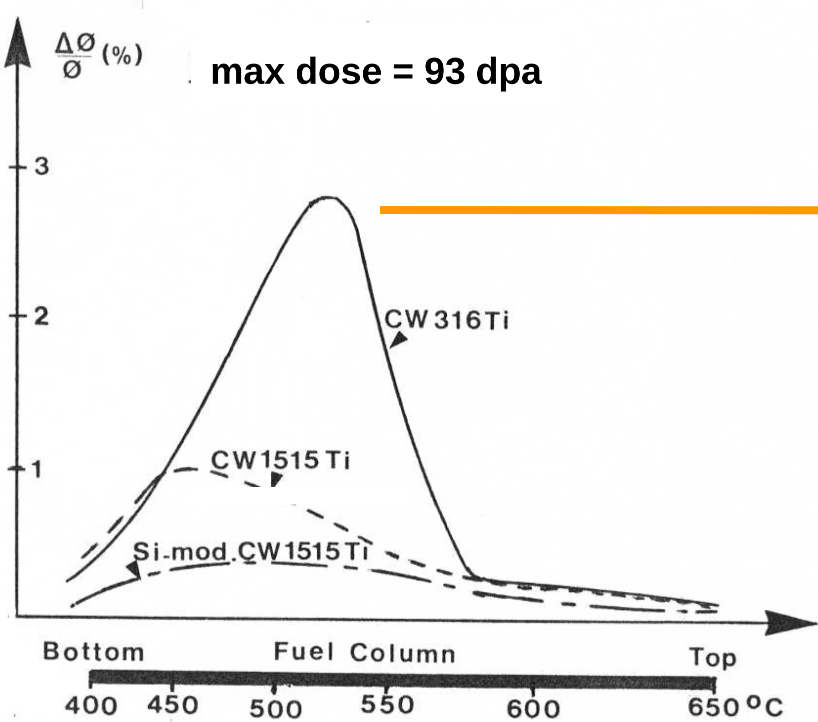
INNOVATIVE
FUEL CLADDING FOR SFR

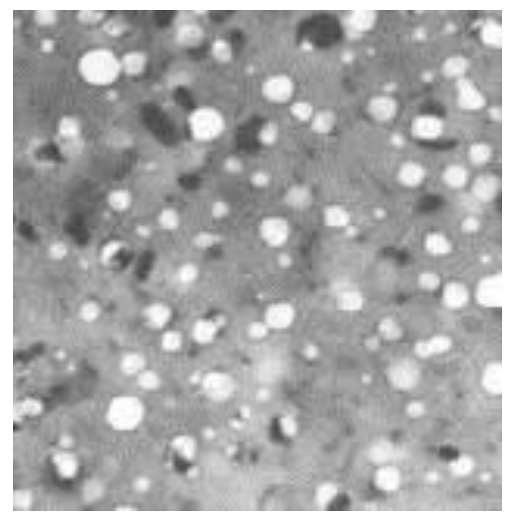
SWELLING OF SFR FUEL CLADDING



Irradiation



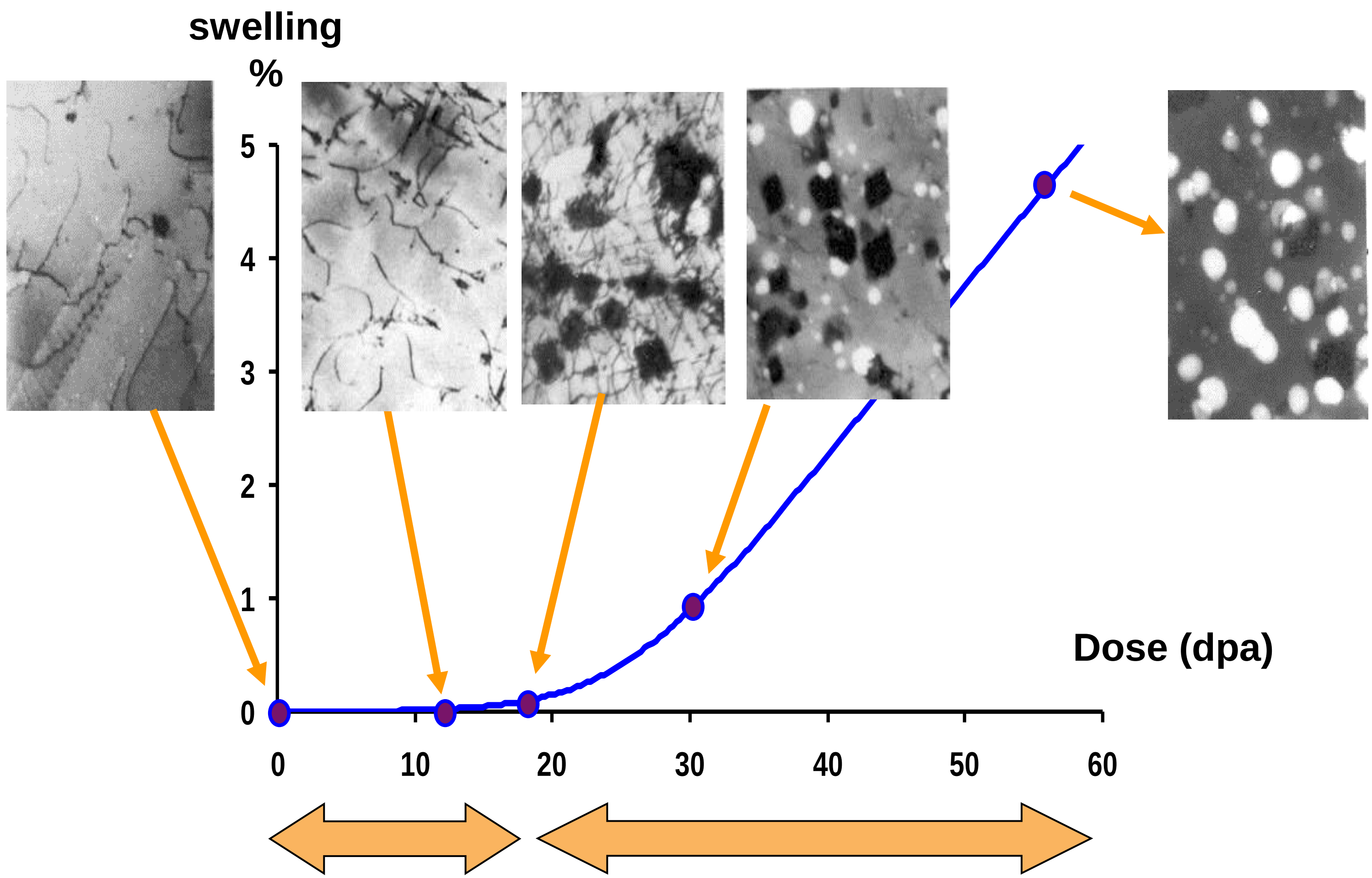




cavities

SWELLING OF AUSTENITIC STEELS

SA 316 Phénix 600°C

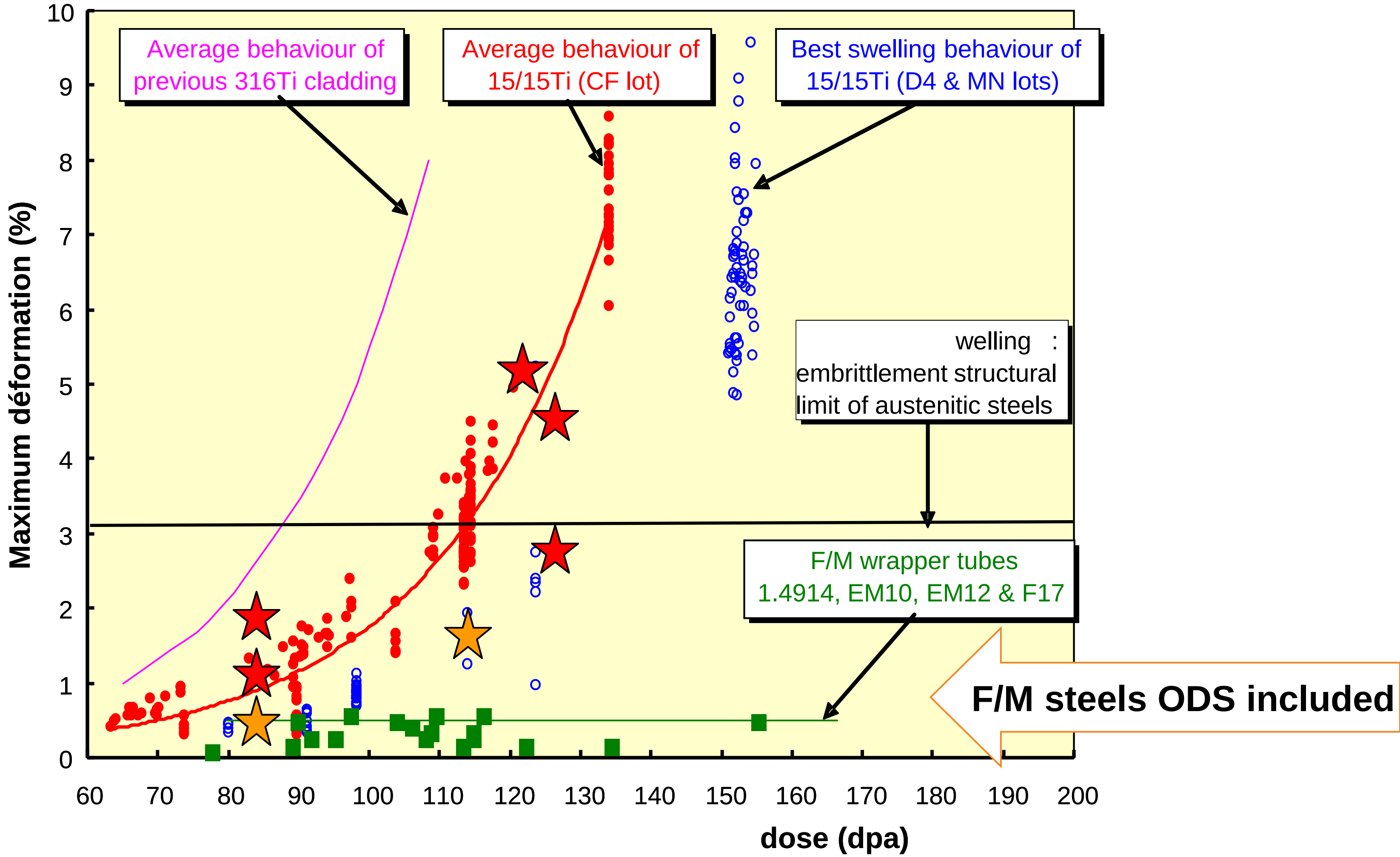


Incubation period (nucleation of cavities)

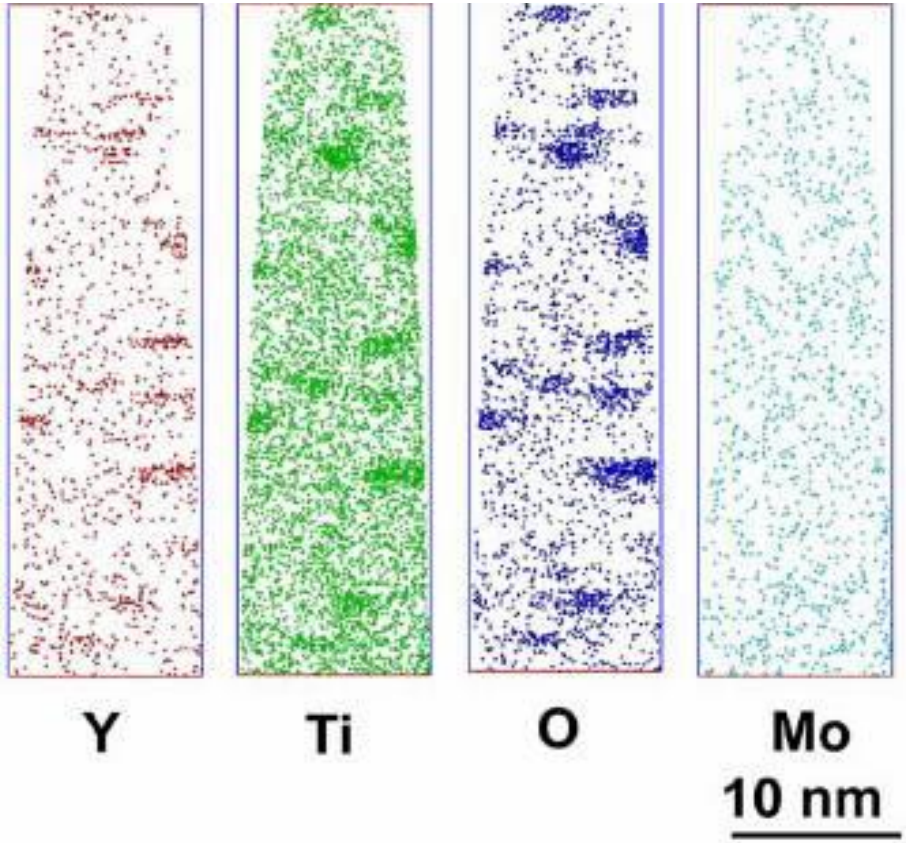
Growth of cavities

SWELLING OF AUSTENITIC AND FERRITIC/MARTENSITIC STEELS

Global behaviour of 15/15Ti cladding & F/M wrapper tubes :
max clad diametral deformation & max cross flat increase of W/T

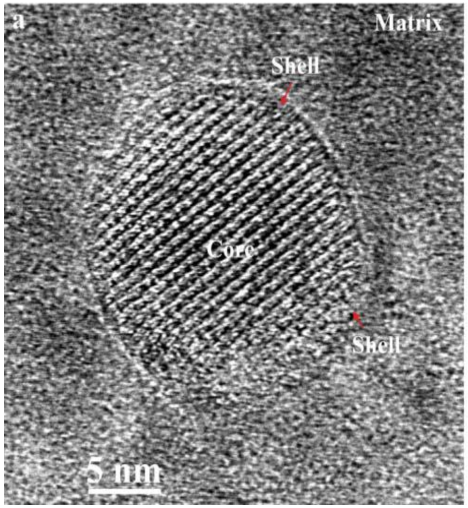


OXIDE DISPERSION STRENGHENED (ODS) STEELS



Tomographic Atom Probe,

Miller (2004)

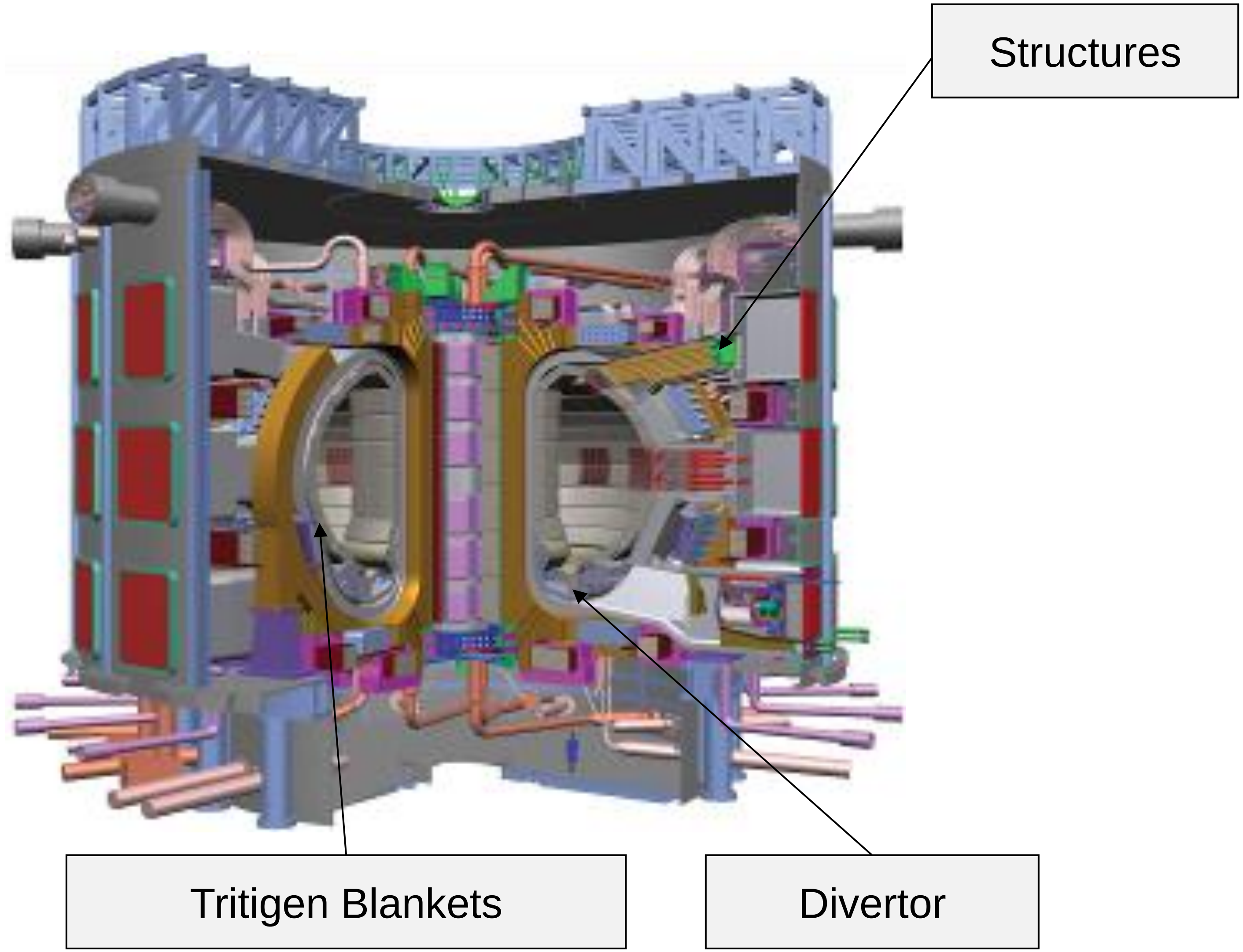


TEM,
Hsiung (2009)

FUSION

Innovative fuel cladding

ITER: A MATERIALS PROBLEM…



FUSION: A MATERIALS PROBLEM…

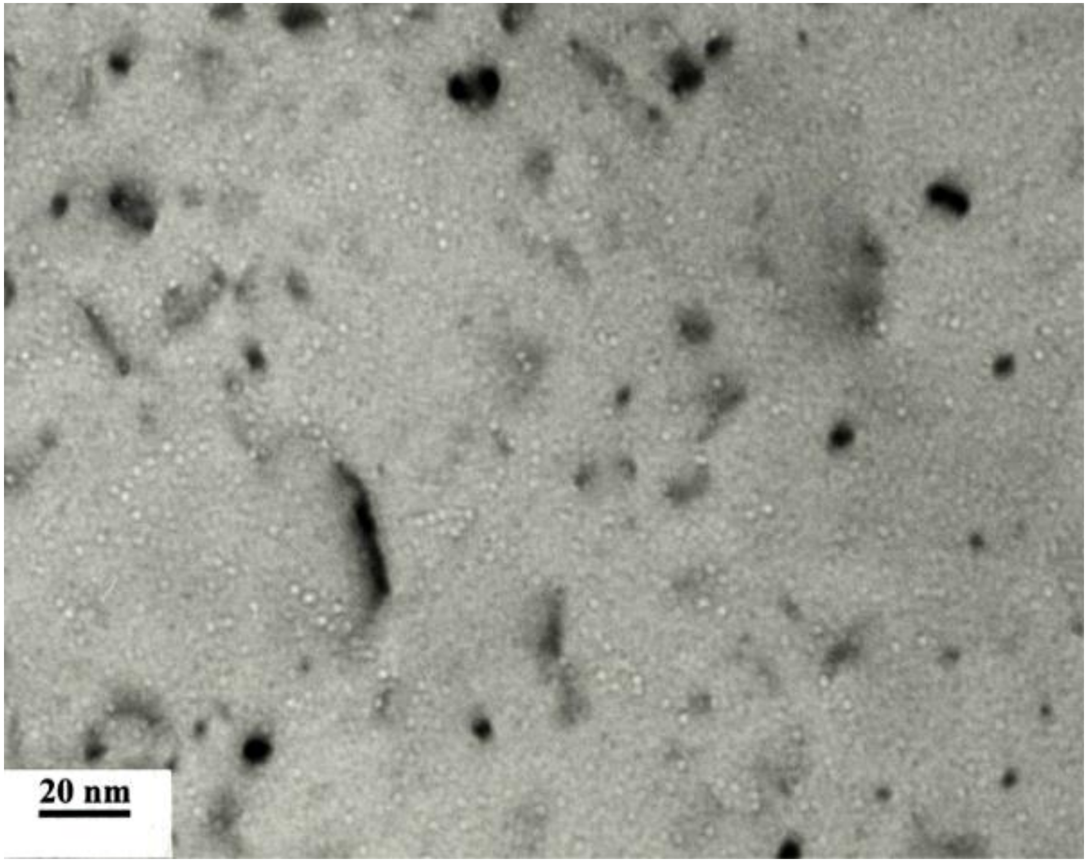
« It’s a wonderful idea to put the sun in a box…except we don’t know how to make the box ! » (Sébastien Balibar)

- Plasma facing materials: high temperature, highly reactive
- Materials for the divertor: high erosion
- Structural Materials: high irradiation doses (embrittlement, swelling…)

A real challenge for scientists and engineers

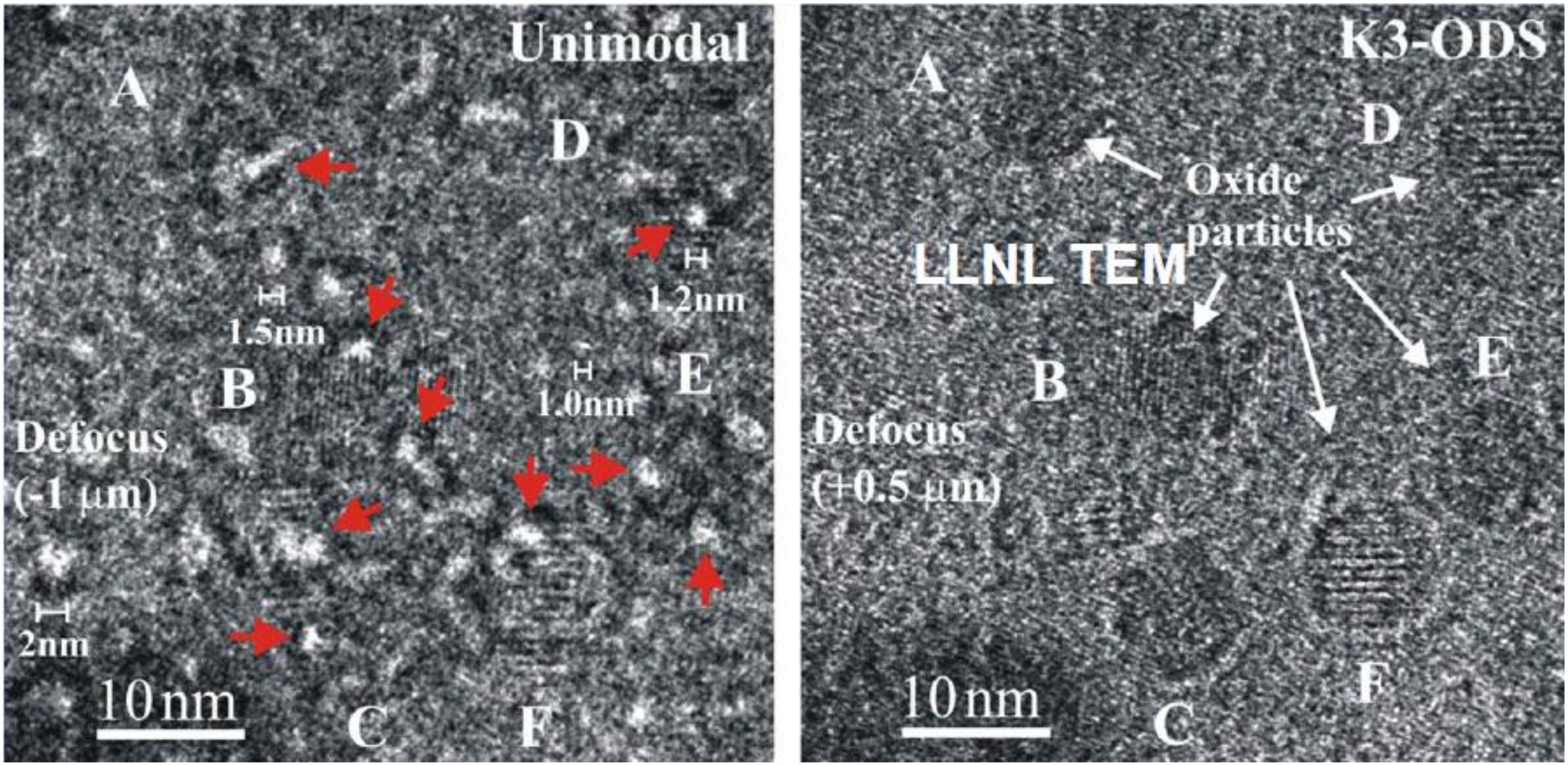
SPECIFICITY OF FUSION NEUTRONS

- D + T => ^{4}He + n (14,1 MeV)



- Helium embrittlement

Dual Beam irradiation/implantation(Jannus) – 425°C, 40 dpa, 80 appm He/dpa
K3-ODS 16Cr-4.5 Al-0.3 Ti-2W-0.37 Y_2O_3



Hsiung et al., J. Nucl. Mater. 409 (2011) 72 ;

CONCLUSIONS

Materials for nuclear energy:

- A requirement to built safe and sustainable devices, today and tomorrow
- Limiting factor for innovative options and to make dreams come true
- A scientific and technological challenge: multiscale modelling is at the heart of the problem

Caveats:

- Multiscale modelling platform <u>should not hide the missing fundamental blocks</u>
- Understanding the missing blocks requires <u>studies on model materials</u>
- Only if we admit that, we can hope to go beyond qualification toward real materials development, in a realistic manner, combining experiments and modelling