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1st FEMaS Conference
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Overview on Irradiation Effects in Fusion Materials

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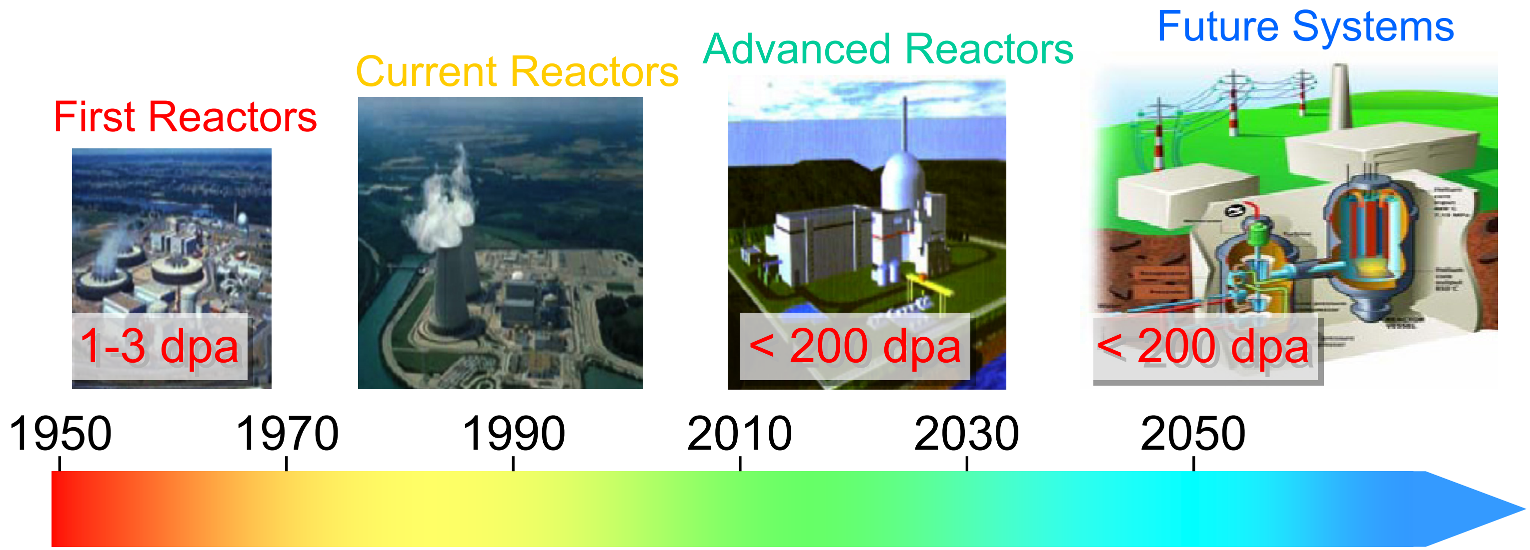
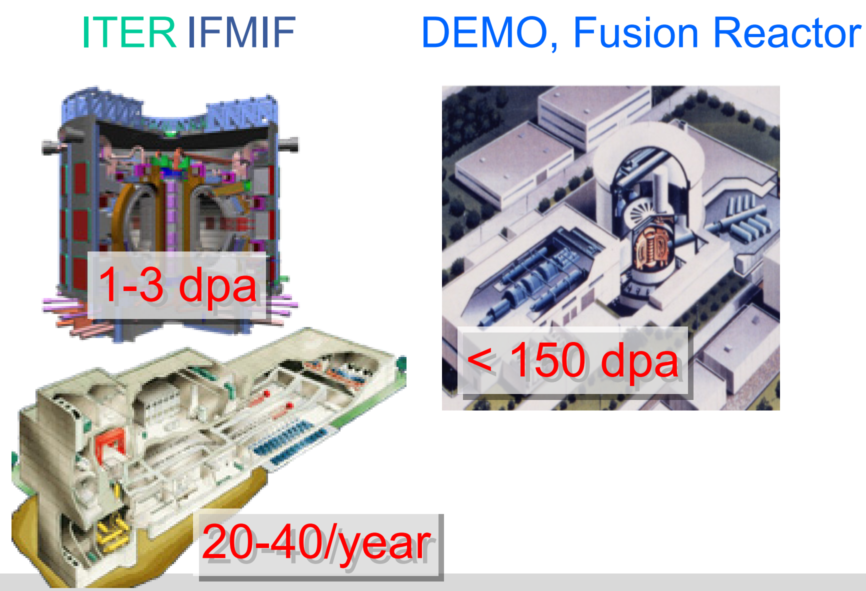
High Performance Materials for Energy





Strategic Missions:

- Electricity, Hydrogen, Heat
- Contribute to lower greenhouse gas emission

Specific challenges for fusion:

- Short development path
- More demanding loading conditions
- ~30 times more Helium/dpa in steels

Outline

- Comparison: Fusion, Fission, Spallation
  - Similarities and differences
  - Requirements and performance goals for structural materials

- Interaction of energetic particles (ions and neutrons) with condensed matter and related damage mechanisms
  - calculation of displacement damage („dpa“) in metals

- Irradiation damage effects in fusion materials
  - Mostly Steels and Oxide dispersion strengthened variants
  - Present status, critical issues and prospects

- Summary

FUSION:
Requirements for "in vessel components"

Karlsruhe Institute of Technology

Blanket: ≤30 dpa/yr, 2.5MW/m²

- Plasma Facing Materials
- Reduced Activation Structural Materials:
  - RAFM Steels, EUROFER 250-550 °C
  - EUROFER-ODS 250-650 °C
- Functional Materials
  - Neutron multiplier (Be)
  - Tritium Breeder (Li_4SiO_4,…)

Divertor: ≤10 dpa/yr, 10-15 MW/m²

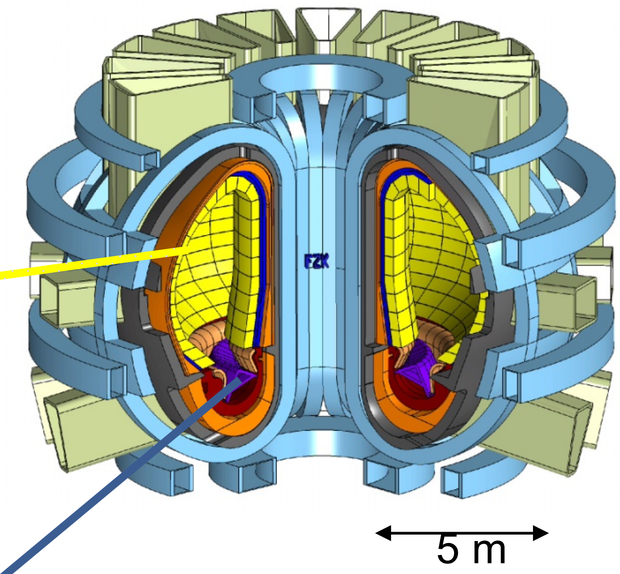
- Refractory alloys (e.g. W-ODS)

  850-1200 °C → ~600 - 1300 °C

- Nano-scaled RAF-ODS Steels

  300-650 °C → ~250 - 750 °C

DEMOnstration Reactor Concept



Power: 1.30 GW_e
Plant Efficiency: 37-45%

A. Möslang, ISFNT-8, Keynote Heidelberg, 2007

Requirements for “in vessel” structural materials

Fission – Fusion – Spallation: Three different irradiation loadings

	Fission (Gen. I)	Fission (Gen. IV)	Fusion (DEMO/PROTO)	Spallation (ADS)
Structural alloy T_{max}	<300˚C	500-1000˚C	550-1000˚C	400-600˚C
Max dose for core internal structures	**~1 dpa**	**~30-100 dpa**	**~150 dpa**	**≤60 dpa/fpy**
Max transmutation helium concentration	**~0.1 appm**	**~3-10 appm**	**~1500 appm (~10000 appm for SiC)**	**~2000 appm/fpy**
Particle Energy E_{max}	**<1-2 MeV**	**<1-3 MeV**	**<14 MeV**	**several hundred MeV**

Materials R&D towards:
- improved irradiation resistance
- enhanced temperature window
- convincing compatibility with coolants

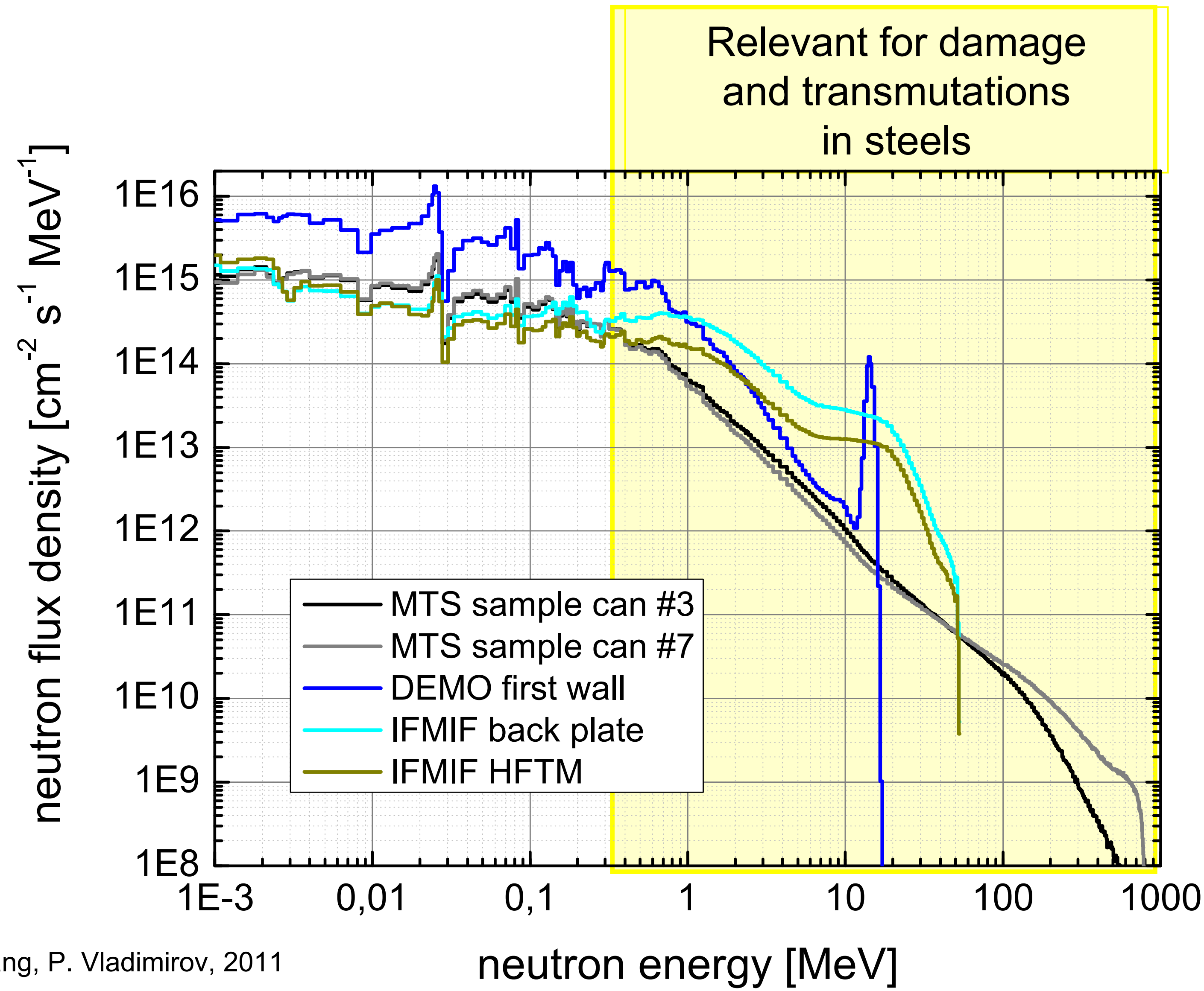
Typical Particle energies:

Particle energies

are usually measured in eV. 1 eV is the energy needed to accelerate one electron in an electric field of 1 Volt. 1eV = 1.6022×10^{-19} J

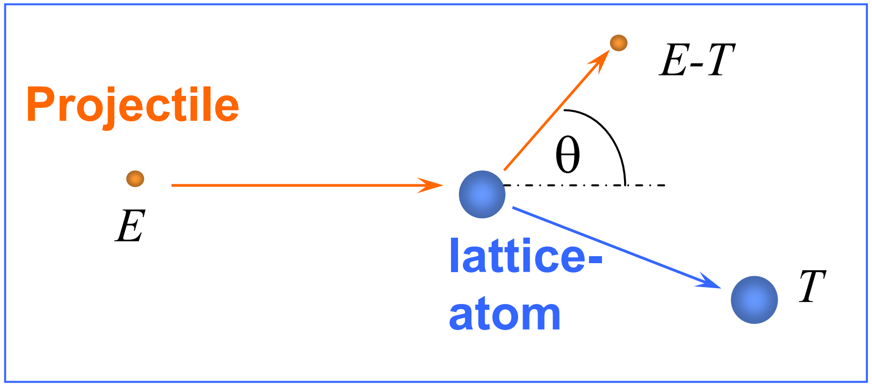
γ- irradiation	- from nuclear decay:		$\leq$ ~3 MeV
	- fission technology:		$\leq$ ~5 MeV
X-rays	- Tomography		$\leq$ ~450 keV
Neutrons	- fission reactors		$\leq$ ~5 MeV
	- fusion reactors		$\leq$ ~14 MeV
	- spallation sources		$\leq$ ~600 MeV
Charges particles	**- α-Particles**	nuclear decay	$\leq$ ~1-5 MeV
	- atoms	displacement damage	$\leq$ ~0.5 MeV
	- β decay		$\leq$ ~1 MeV

Irradiation effects depend seriously on neutron spectrum



A. Fischer, A. Möslang, P. Vladimirov, 2011

Ions and Neutrons: Interaction with matter
- energy loss by scattering -



Threshold energy E_d:
Min. energy to create a vacancy (V).
Ed depends on the lattice orientation
Crystal structure and material:

Fe:	$\langle E_d \rangle$ = 20-40 eV
W:	$\langle E_d \rangle$ = 193 eV

- **Primary damage:**
  Each projectile (e.g. Neutron, Electron, Ion) is scattered elastically, usually frequently at atoms in the solid state and creates thereby „PKA's" (primary knock-on atoms) in in different orientations and with different Energies T (PKA—energy spectrum)

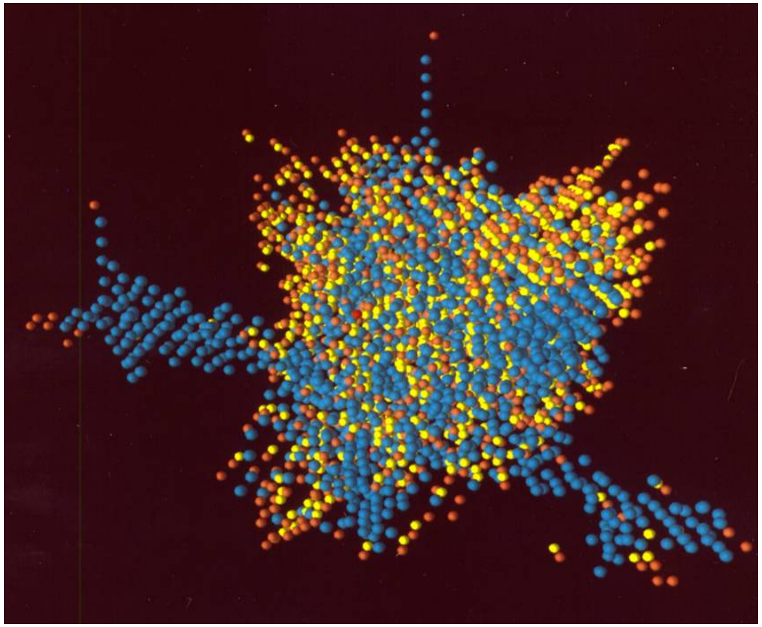
- **Secondary damage:**
  PKA's deposit their energy T as follows:
  - inelastic collisions with electrons (T_{elektr})
  - elastic nuclear reactions to create
    - Frenkel pairs (vacancy + interstitial atom)
    - cascade formation

Ions & Neutrons: Interaction with matter: displacement cascade ($T \gg E_d$)

If the energy T transferred to the lattice atom is very big, this energetic recoil atom (or primary knocked on atom PKA) will very effectively replace the surrounding atoms (equal masses, like in a billiard game):

Displacement cascade in Ni_3Al, T = 8 keV

Vacancies,
interstitial atoms
displaced atoms



(C. Lemaignan, M. Guttmann)

- High point defect density
- Chemical disorder
- topologic disorder

Interaction with matter: determination of the displacement damage

The displacement damage is usually measured in **„Displacements per atom (dpa)“.** 1 dpa means, that during irradiation each atom is displaced in average one time

Scattering events – like the scattering of ions on target atoms – is usually described via a **cross section:**

$$\sigma = \frac{\text{number of „reactions“ per scattering center/s}}{\text{current density of the incoming projectile}}$$

With the unity [$s^{-1}/(s^{-1}\ cm^{-2}) = cm^2$]
For better handling, often the unity „Barn“ [b] is used:

$$1b = 10^{-28}\ m^2$$

Light ion irradiation: In the energy range <30 MeV elastic nuclear reactions are dominating (that is, the sum of the kinetic energies = constant)

Ions: Interaction with matter: determination of irradiation damage

To determine the displacement damage, it is necessary, to handle the primary damage and the secondary damage differently:

A. Primry damage

For lighter ions with kinetic energies E from ~5 keV to ~30 MeV the differential Rutherford' cross section $d\sigma(E,T)$ is valid. It describes the „probability", that an ion (projectile) of mass M_1, der atomic number Z_1 und the energy E is scattered at a target atom of mass M_2 and the atomic number Z_2 , and thereby transfers the energy $T+dT$:

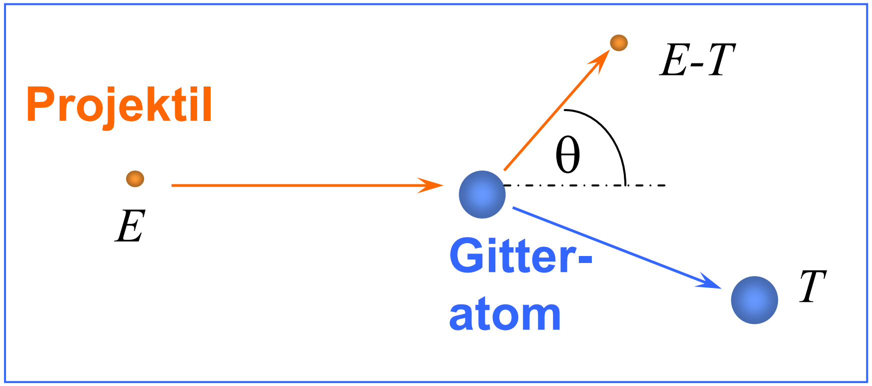
$$d\sigma(E,T) = 4\pi\, a_0^2\, Z_1^2\, Z_2^2\, \frac{M_1 E_R^2}{M_2 E T^2}\, dT \qquad (1)$$

„Bohr' radius" $a_0 = 0.053\ nm;\ E_R = e^2/a_0 = 13.6\ eV$

Ions: Interaction with matter: determination of irradiation damage

A. Primary damage

In the center of mass system
The following equation is valid
(θ≤180°):



$$T = \frac{4 M_1 M_2}{(M_1 M_2)^2} E \sin^2(\Theta/2) = T_{\max} \sin^2(\Theta/2) \qquad (2)$$

From eq Gl. (2) follows: Even at E = const. the PKAs have an energy spectrum
From eqs (1) u. (2) follows: With increasing E, the cross sections decline with $1/E^3$

Ions: Interaction with matter: determination of irradiation damage

B. Secondary damage

The PKA deposit the Energy T (often $T \gg E_d$) along a displacement cascade on the surrounding atoms, until it becomes thermalized.
The energy T splits into
- displacement energy T_{dam} (formation of FPs & sub cascades)
- Electronic excitation energy T_{electr}

The number of displaced atoms $\upsilon(T)$ is then (internat. recommendation):

$$
\begin{aligned}
\upsilon(T) &= 0 && for \quad T_{dam} < E_d \\
\upsilon(T) &= 1 && for \quad E_d \le T_{dam} \le 2E_d \\
\upsilon(T) &= \frac{k \cdot T_{dam}}{2E_d} && for \quad T_{dam} \ge 2E_d
\end{aligned}
\qquad (3)
$$

The displacement efficiency *k* is expected to be constant (NRT): *k =0.8; in Fe:* E_d *= 40 eV*
More detailed analysis by Molecular Dynamics calculations

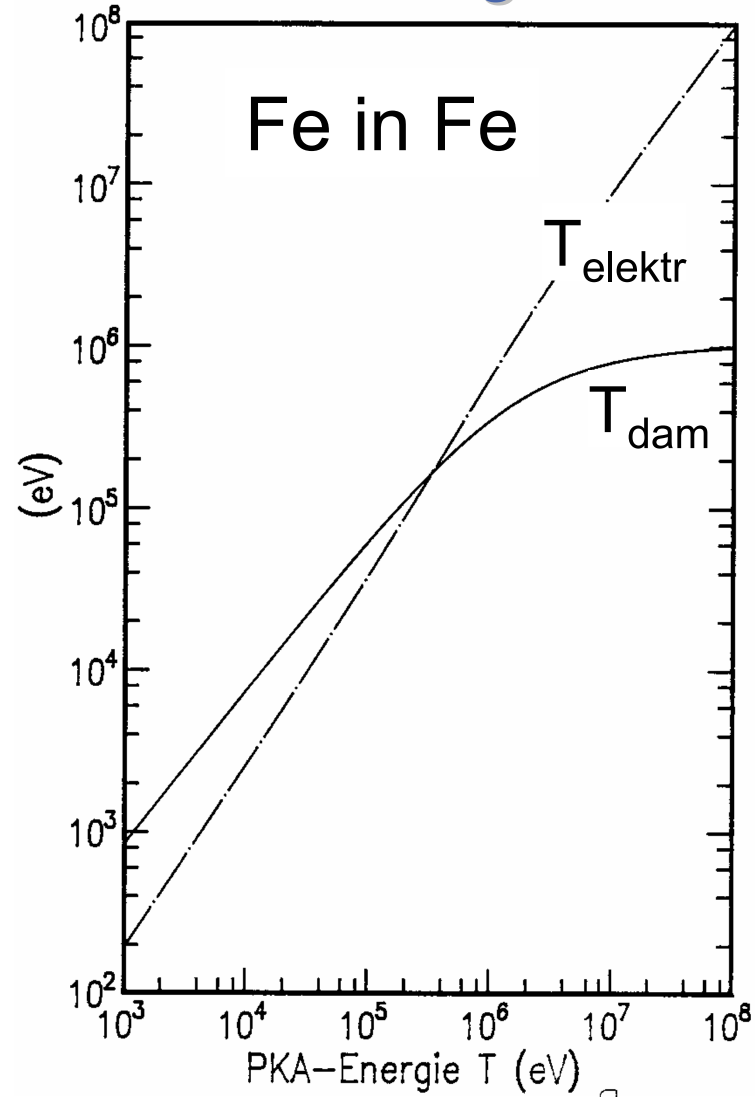
Ions: Interaction with matter: determination of irradiation damage

B. Secondary damage

- The damage energy T_{dam} has a maximum. PKA-Energies above 10^5 eV are, however, in praxis very seldom
- With increasing PKA-Energy T_{elektr} increases strongly and dominates above $3x10^5$ eV completely (heat production)
- **Example:** How much displacement damage we have in Fe for $T_{dam} = 2x10^5$ eV?

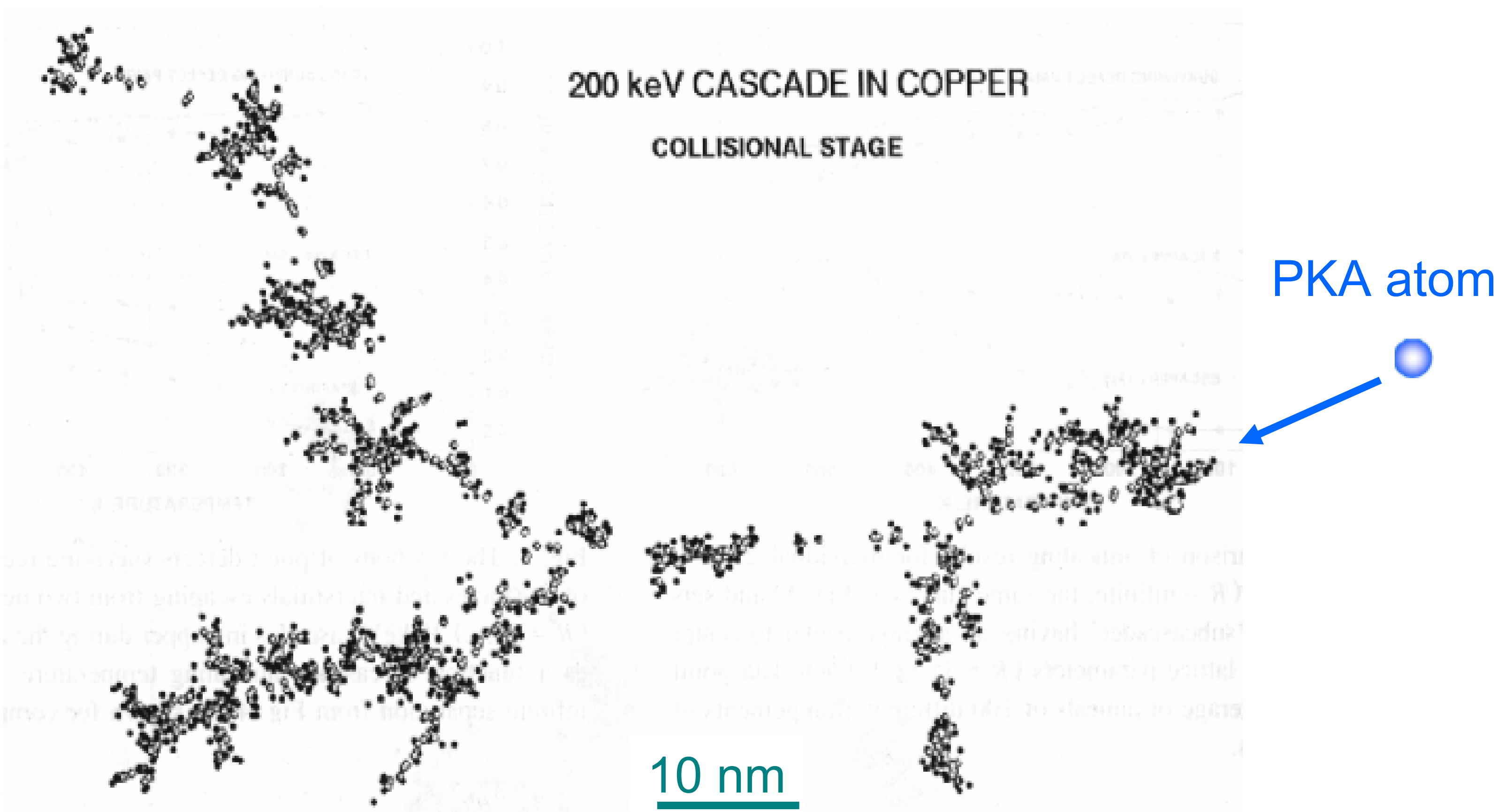
  From Eq. (3) follows:

  $\underline{\upsilon(T) = 2000}$ displacements !



Ions: Interaction with matter:
- visualizing the secondary damage -

The PKA-atom we have spoken about….



MARLOWE binary collision code

Ions: Interaction with matter: determination of the displacement damage

C. Combination of primary and secondary damage

To combine the primary damage (probability to create a PKA) with the secondary damage (number of displaced atoms per PKA), Eq. (1) is combined with eq. (3) and integrated over the entire enery range T.
Consequently the **total displacement cross section** for ions of energy E is:

$$\sigma_d(E) = \int_{E_d}^{T_{\max}} \left[\frac{d\sigma(E,T)}{dT} \right] \cdot \nu(T)\, dT \qquad (4)$$

That is, $\sigma_d(E)$ describes the average number of displacements per lattice atom and per ion/cm^2.

The non-analytical Integral in Eq. (7) can be solved numerically (A. Möslang KfK Report 03.02.02P94B (1990))

Ions: Interaction with matter: determination of the displacement damage

C. Combination of primary and secondary damage

Die **total displacement cross section** follows then simply by multiplication with the Ion current Φ and the total irradiation time t:

$$Displacement\ \ damage\,[dpa] \;=\; \sigma_d(E)\cdot\Phi\cdot t \qquad (5)$$

Units: $\left[\frac{displ./\,Atom}{Ion\,/\,cm^2}\right]\cdot\left[\frac{Ions}{cm^2\cdot s}\right]\cdot[s]$

In this how for ion irradiations the displacement damage can be calculated

Neutrons: Interactions with matter: Determination of displacement damage

- As neutrons do not have an electric charge, they cannot transfer any energy to electrons. Neutrons can only “communicate” via the so called „Strong Interaction“ with *Protons* and *Neutrons* and consequently can transfer also energy via this interaction
- The range of neutrons in mater is therefore substantially longer as the range of ions, electrons or γ -radiation
- That is, neutrons can only scatter at the nuclei via
  - elastic interaction (sum of kinetic energy = const)
  - inelastic interaction (e.g. emission of γ-radiation)
  - non-elastic interaction (nuclear transformation via particle emission (n, p,α-particles,…)

  → Creation of long living radioactive isotopes
- In the vast majority, neutrons are not mono-energetic but have a broad energy spectrum

Neutrons: Interactions with matter: Determination of displacement damage

Therefore, to calculate the (average) **displacement cross-section for neutrons,** we have to integrate not only over all PKA-energies T, but in addition also over all neutron energies E.
From this it follows for neutrons from Eq. (7):

$$\sigma_d = \underbrace{\int_0^{E_{max}} \left(d\Phi / dE \right) dE}_{\text{Integration over all neutron energies}} \int_{E_d}^{T_{max}} \underbrace{\left[\frac{d\sigma(E,T)}{dT} \right]}_{\text{Probability of a PKA creation for a given Energy E}} \cdot \underbrace{\nu(T)}_{\text{Number of displacements per PKA}} dT \qquad (6)$$

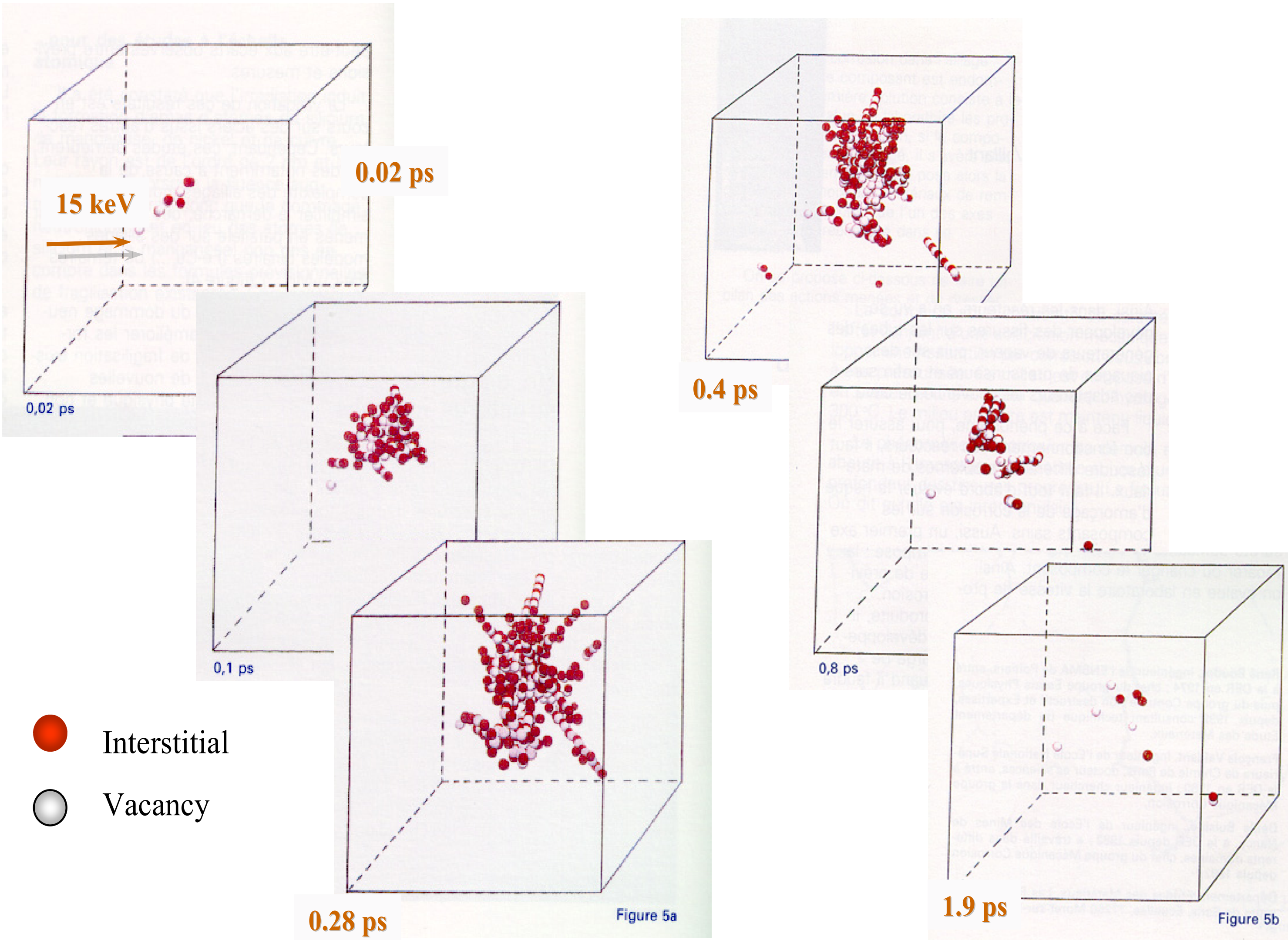
dΦ/dE shows, how much neutrons of a given energy *E*' we have in the intervall *(E'+dE)*

Neutrons: Interactions with matter: Determination of displacement damage

In analogy to Eq. (4), the **total displacement cross section** is then obviously given by multiplication of the integral neutron flux density Φ_{tot} and the total irradiation time t:

$$Displacement\ damage\,[dpa] = \sigma_d \cdot \Phi_{tot} \cdot t \qquad (7)$$

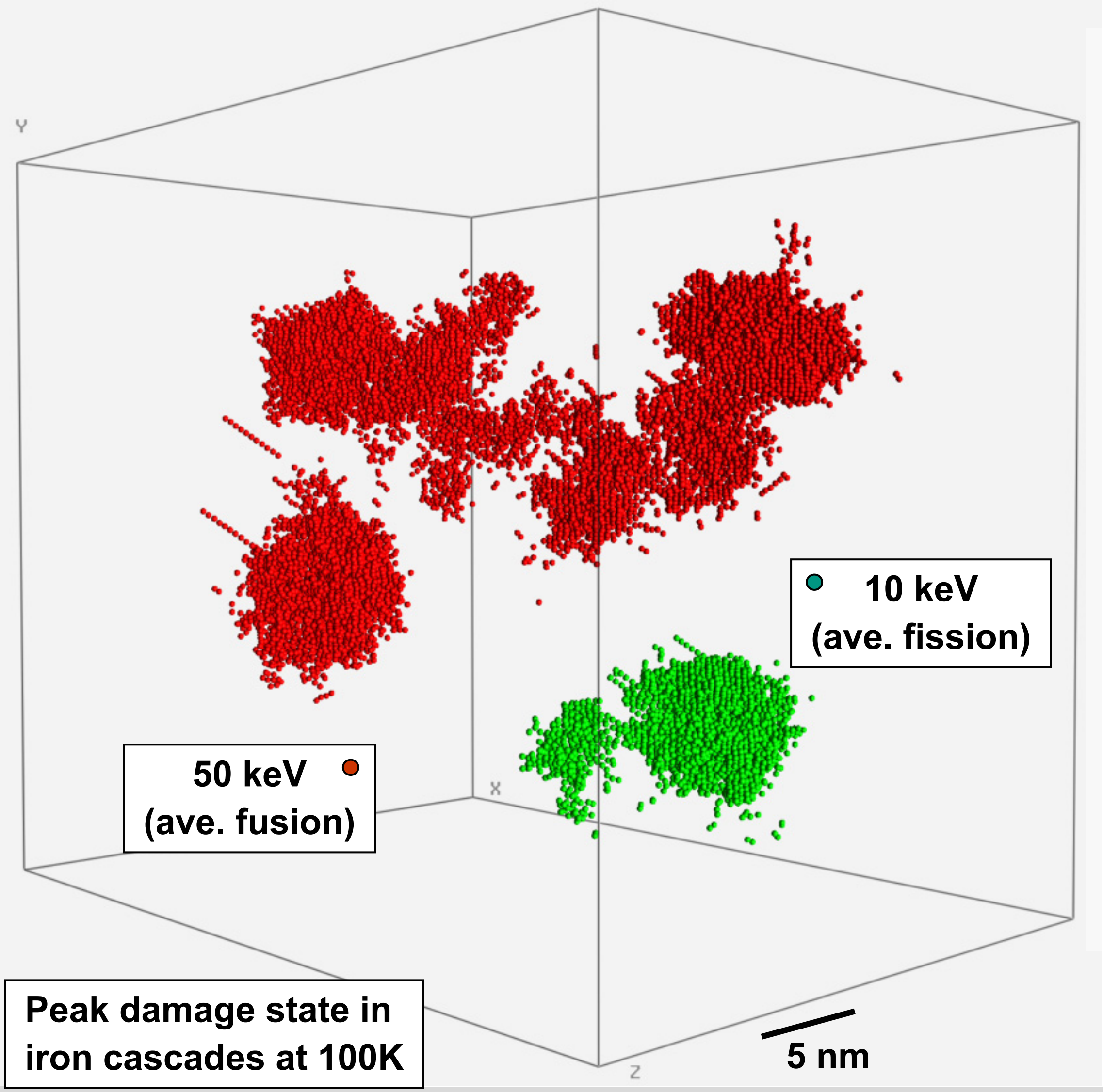
Development of cascades in time



Only very few defects survive!

(C. Lemaignan, M. Guttmann, EDF DER 1994)

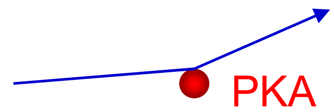
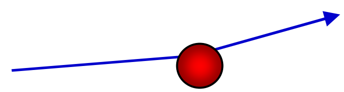
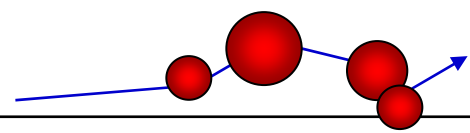
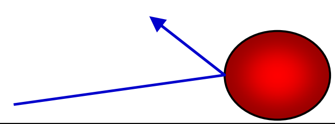
Displacement cascade simulations using molecular dynamics highlight similarities of fission and fusion irradiation environments



- DT fusion neutrons produce atomic recoils at much higher energies than fission neutrons
- Use of large-scale atomic simulations demonstrates that subcascade formation minimizes differences in defect production
- Average defect production per unit cascade energy is essentially the same for fission and fusion
- However, differences between fusion and fission irradiation are expected at high dose due to fusion's higher transmutant He and H production

Courtesy of R. Stoller, ORNL

Criteria for adequate materials irradiation: The «correct» PKA-Spectrum

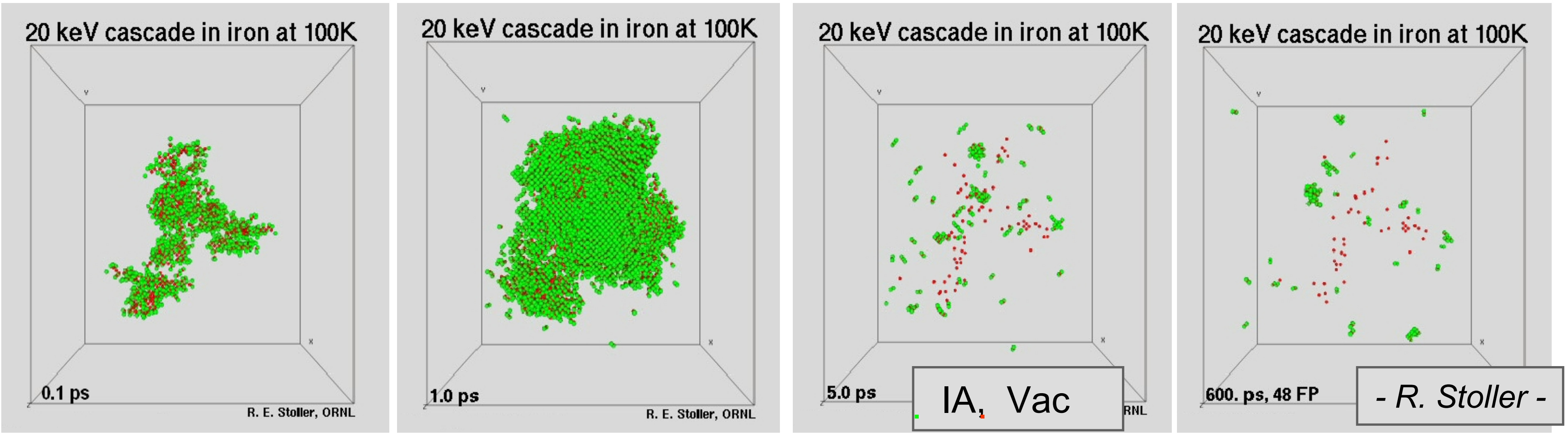
Particle type (E_{kin} = 1 MeV)	Typical recoil (or PKA) feature	Typical recoil energy T	Dominant defect type
Electron		25 eV	Frenkelpairs (FP: Vacancy-Insterstitial pair)
Proton		500 eV	
Fe-ion		24 000 eV	Cascades & sub-cascades
Neutron		45 000 eV	

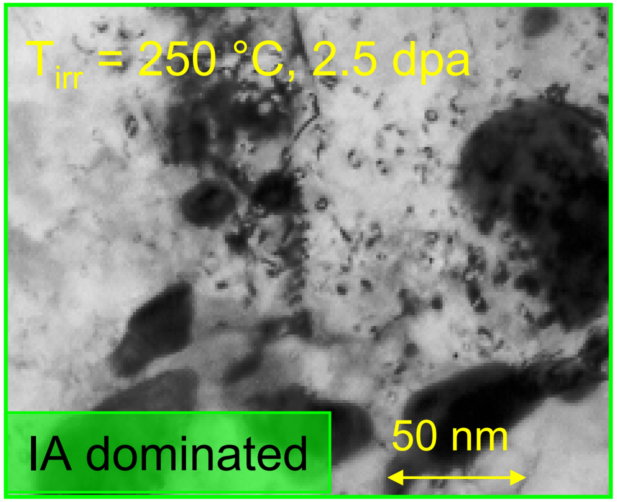
Typical impact on materials properties:

- FPs as "freely migrating defects": Alloy dissolution, segregation, irradiation creep
- Cascades & sub-cascades: Irradiation hardening, ductility reduction

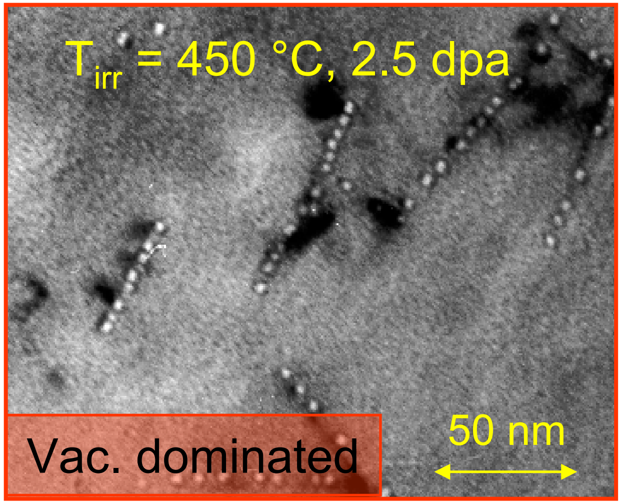
MD Simulation und comparison with TEM

- Interaction of energetic projectiles with condensed matter -



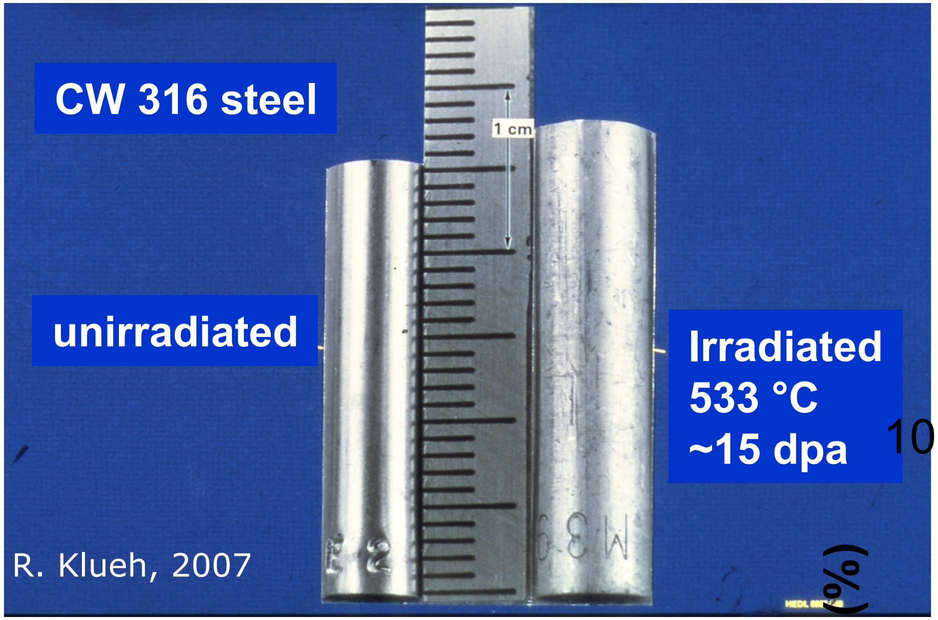


E. Materna-Morris, IMF I

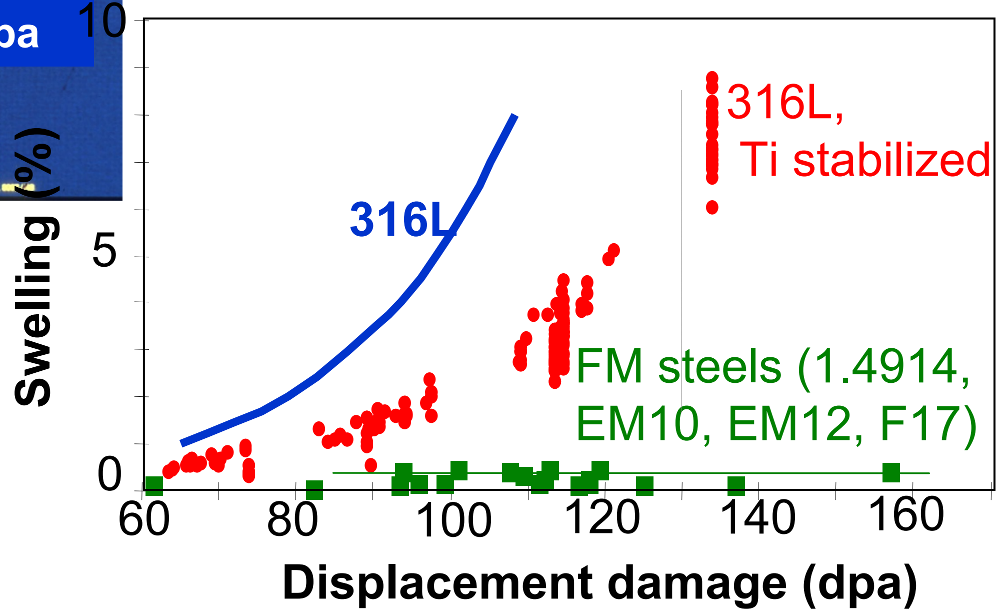


Ferritic/Martensitic Steels vs. Austenitic Steels

Irradiation-induced swelling

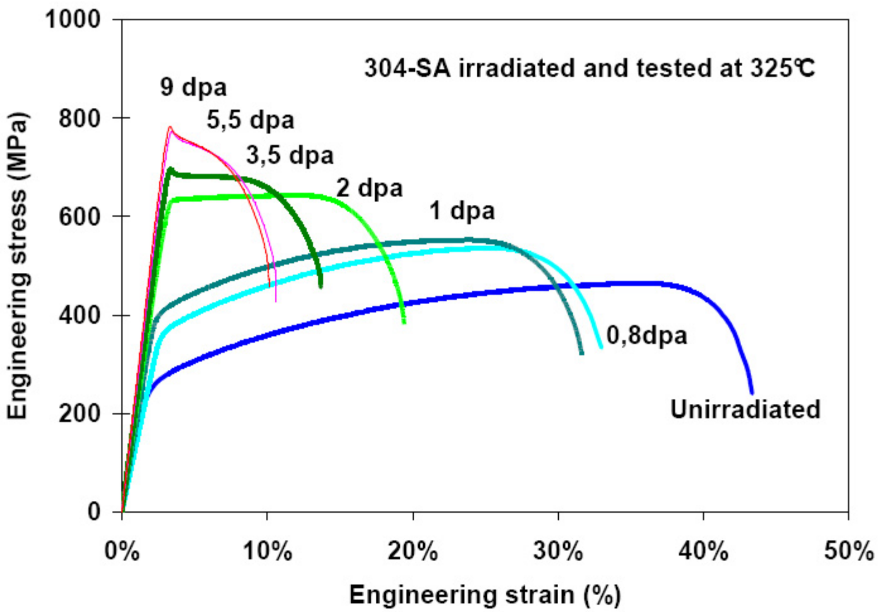


Phénix :
Fuel Element Cladding irradiation



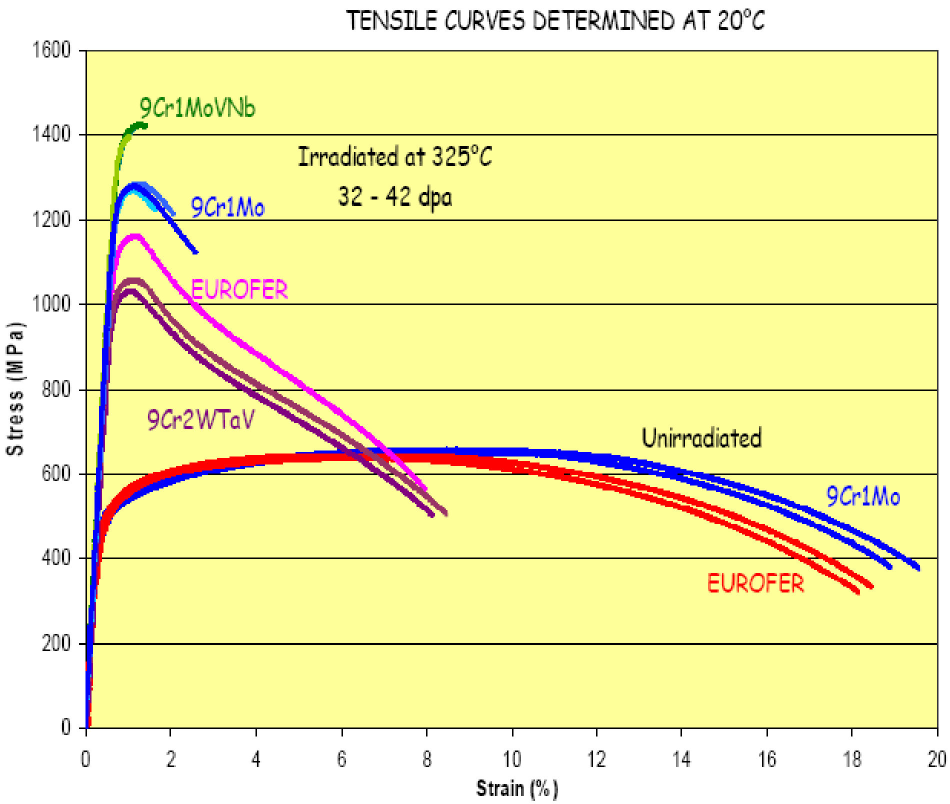
Steels after Neutron irradiation

Austenitic steel 304



Y. De Carlan et al, ASTM STP, 2004

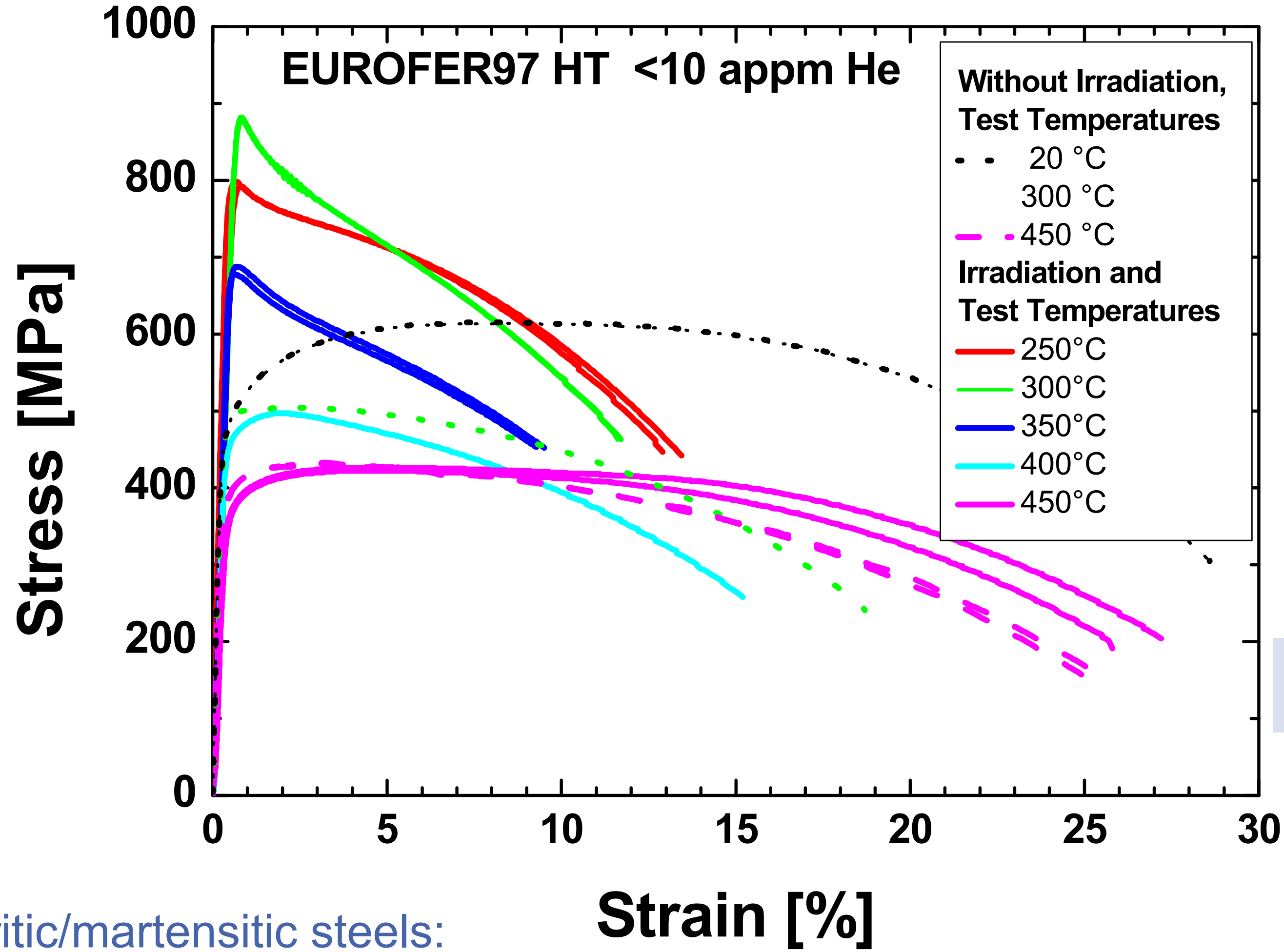
Ferritic-Martensitic steels



A. Alamo et al, EFDA-report 2006

Neutron irradiation below ~400°C: Increase strength, decrease ductility

Tensile properties after neutron irradiation (~15 dpa)



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

Ferritic/martensitic steels:

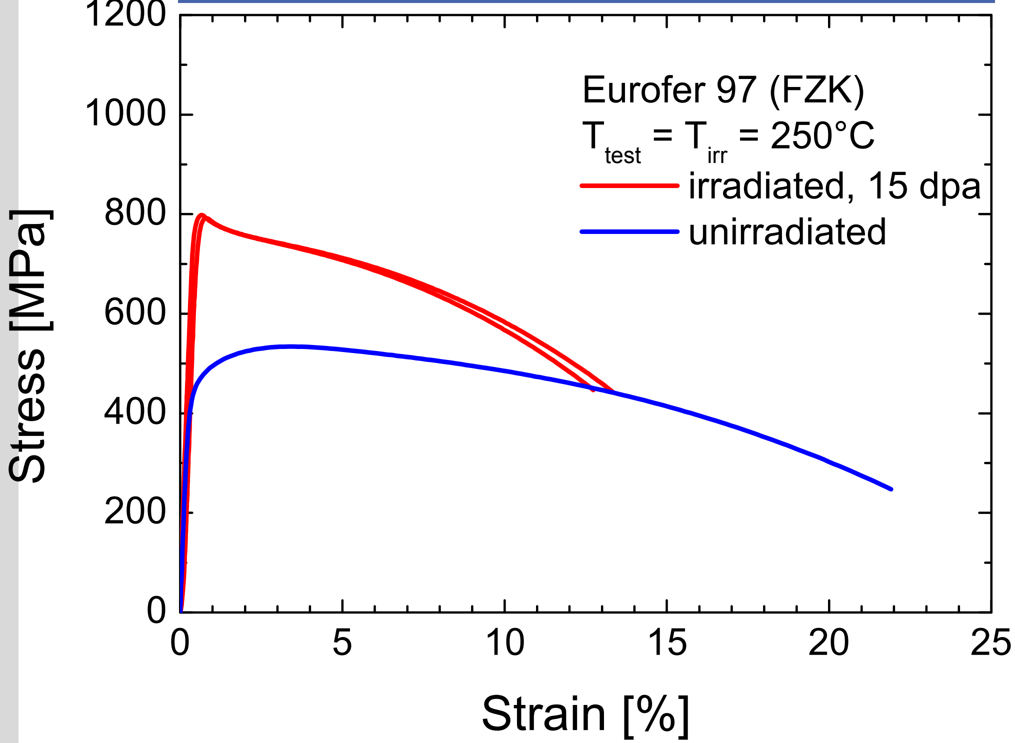
– Significant strength increase (irradiation hardening) for T_{irrad} < 400 °C

– This irrad. hardening comes mostly from interstitial type loops and α'-precipitates. These loops and precipitates do not form above about 400-420 °C

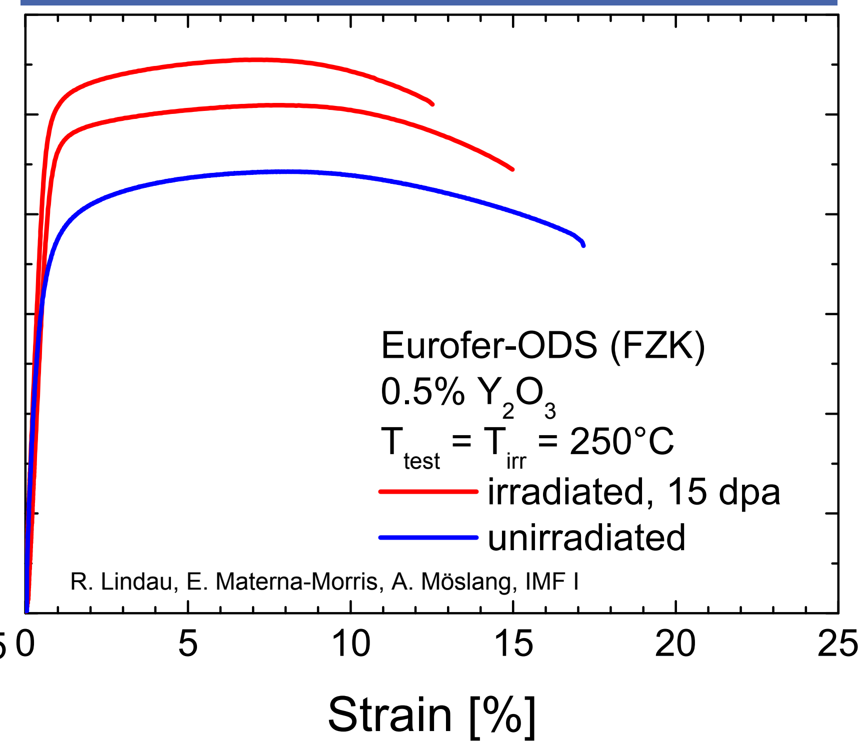
ODS EUROFER after Neutron irradiation:
Substantial Improvement of tensile properties

R. Lindau, et al, KIT

RAFM Steel



RAFM-ODS Steel

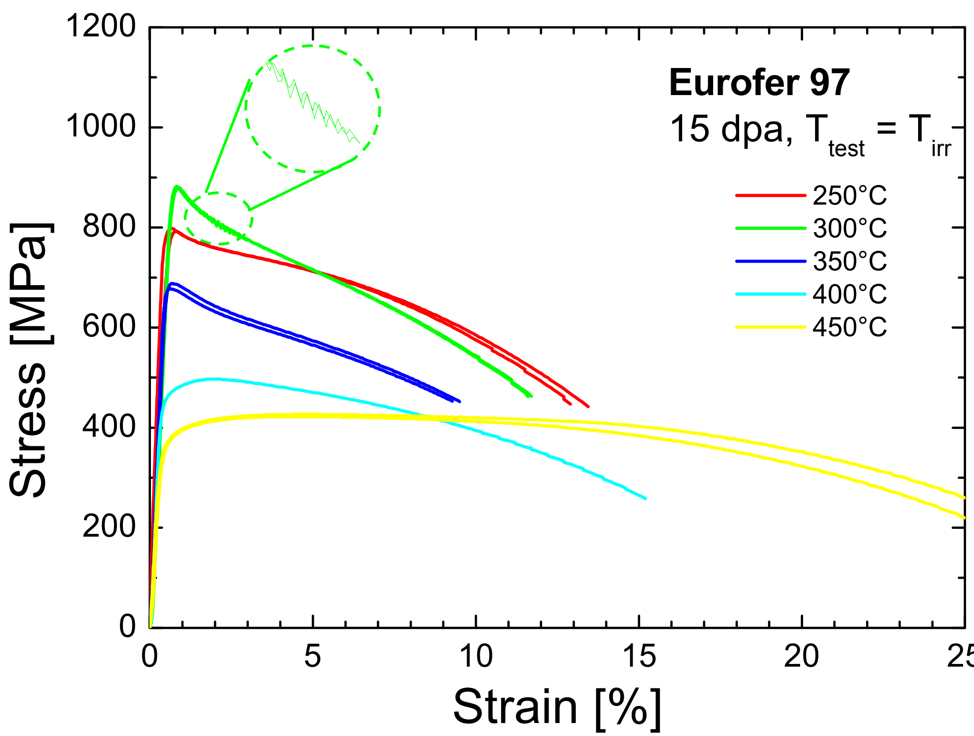


☹ Substantial irradiation hardening
☹ Early strain localization due to dislocation channeling → A_u ~0.3%

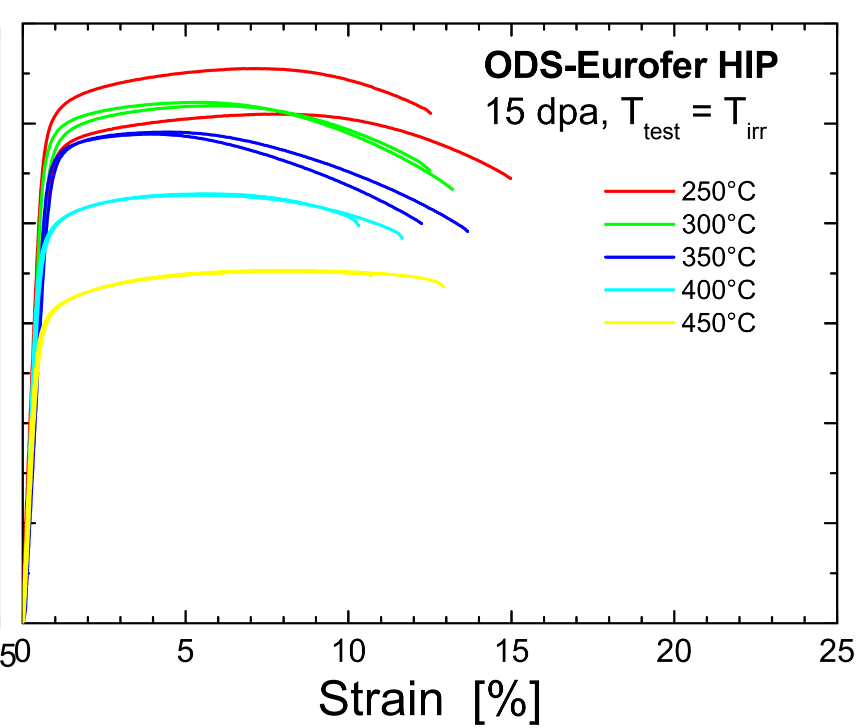
☺ Somewhat less irrad. hardening
☺ Still work hardening → almost no loss of uniform elongation (A_u ~7%)

ODS EUROFER after Neutron irradiation:
Substantial Improvement of tensile properties in a wide temperature window

RAFM Steel



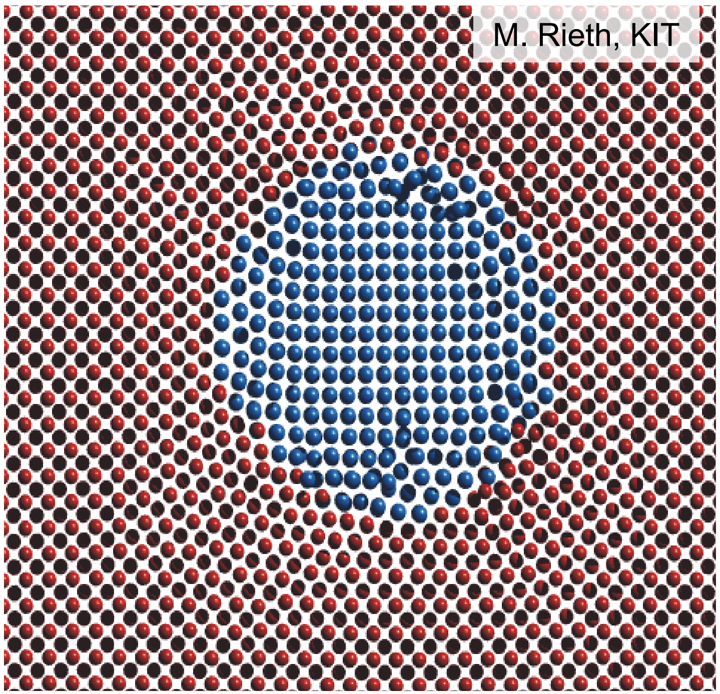
RAFM-ODS Steel



R. Lindau, et al , KIT

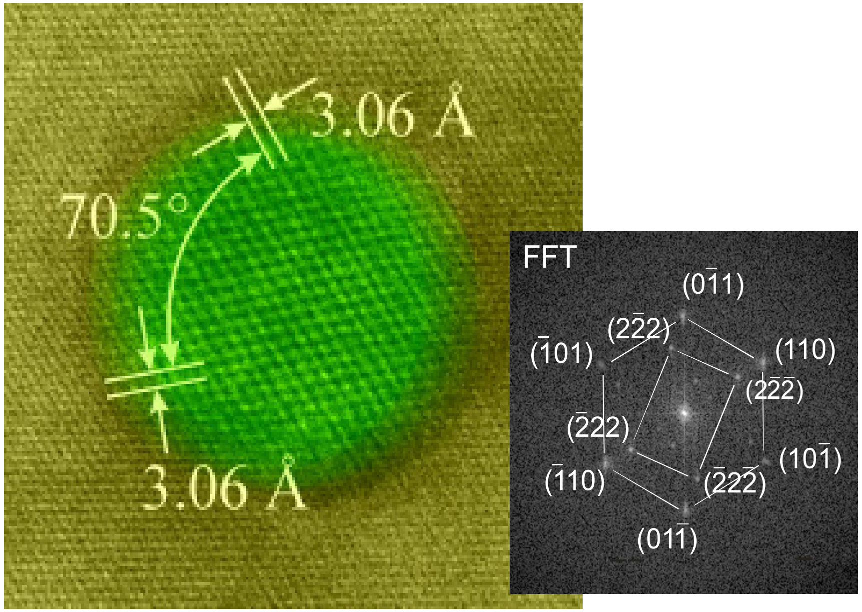
Coherency properties of nano-dispersoides in steel matrix

Molecular Dynamics Simulation



Experimental validation via HRTEM

M. Klimenkov, KIT

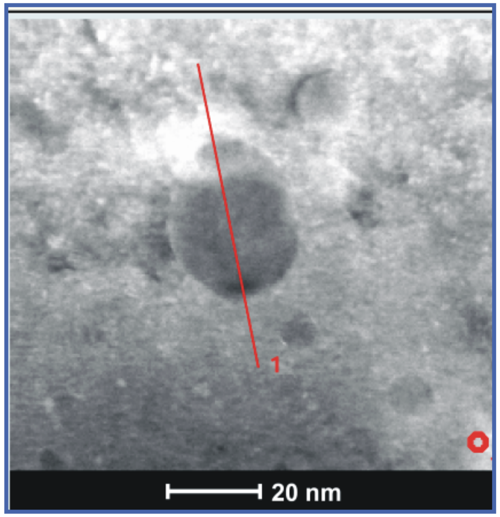


- $(111)Y_2O_3$ || $(110)FeCr$ - orientation of atomic planes, misfit only 0.5 %
- Coherence despite of the high melting temperature (~2500 °C) of Y_2O_3

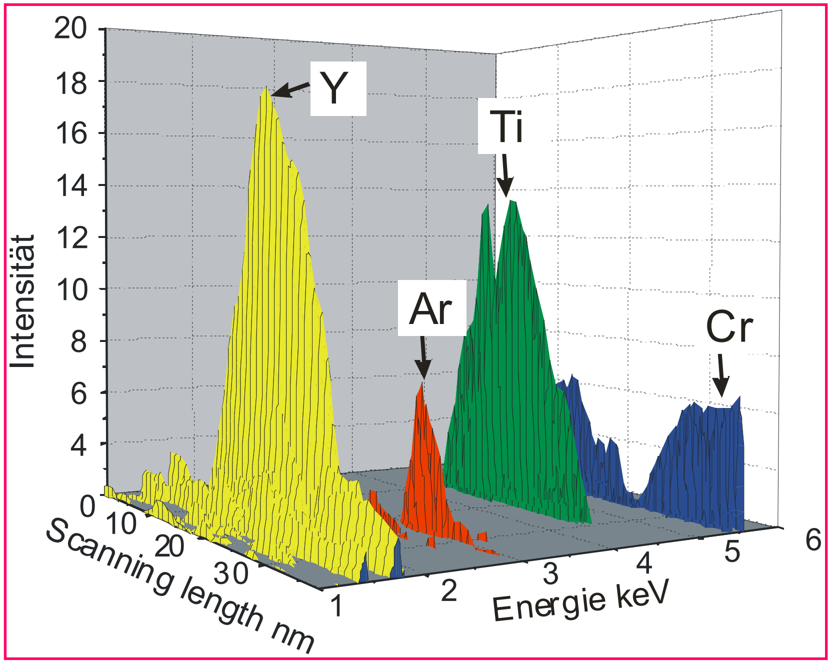
ODS RAFM Steels TEM Element Analysis

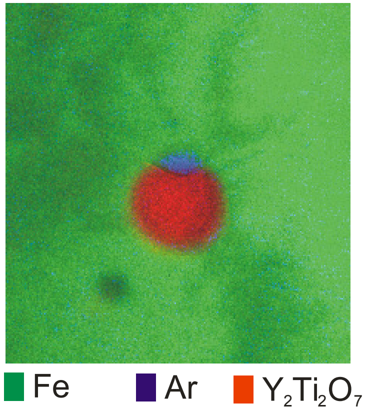
- Imaging of Ar in Nano-Bubbles -

TEM Bright field



EFTEM with HAADF Detector

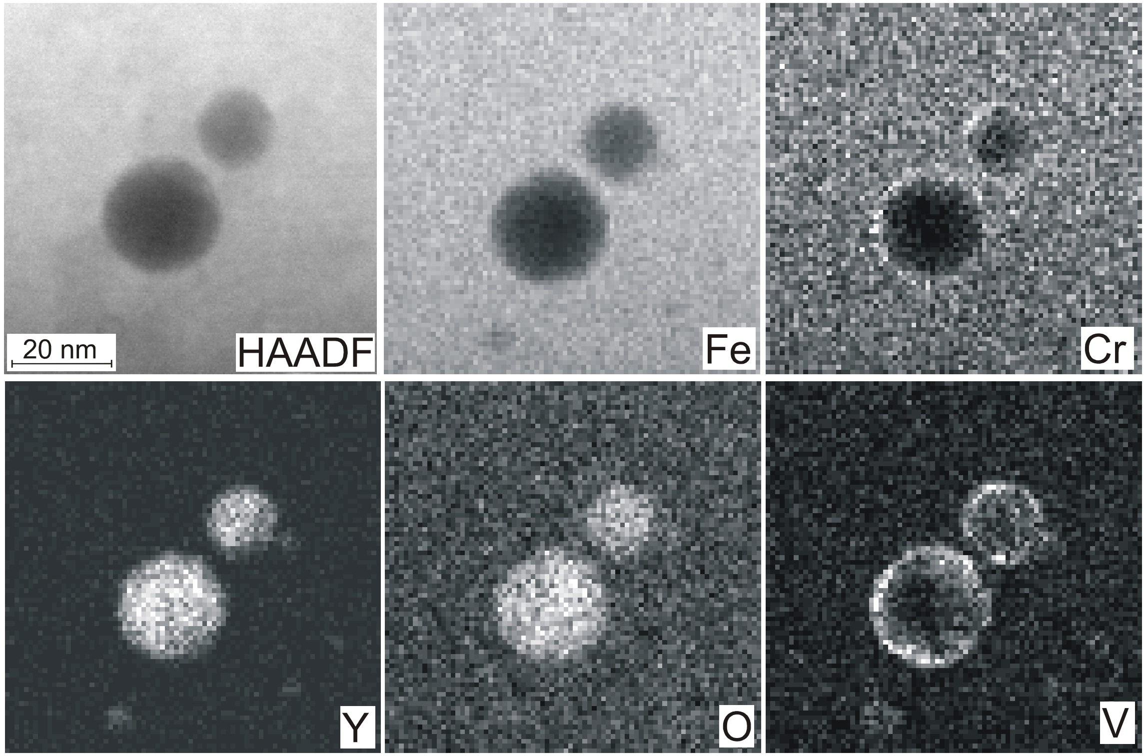


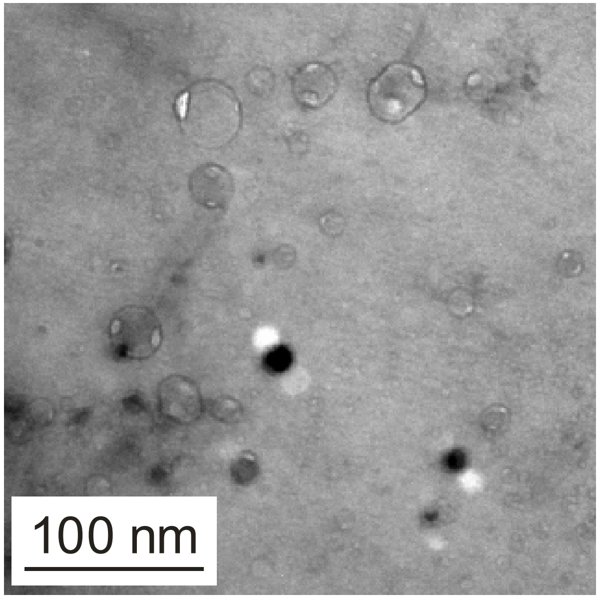


M. Klimiankou et al, IAM, KIT

+ Usually (not in EUROFER-ODS) Ar gas is used during mechanical alloying
+ Nano-dispersoides (Y_2O_3, $Y_2Ti_2O_3$) are very effective trapping centers for noble gases (→ suppression of He embrittlement)

Analytical TEM: nanoscaled iron based ODS-alloys

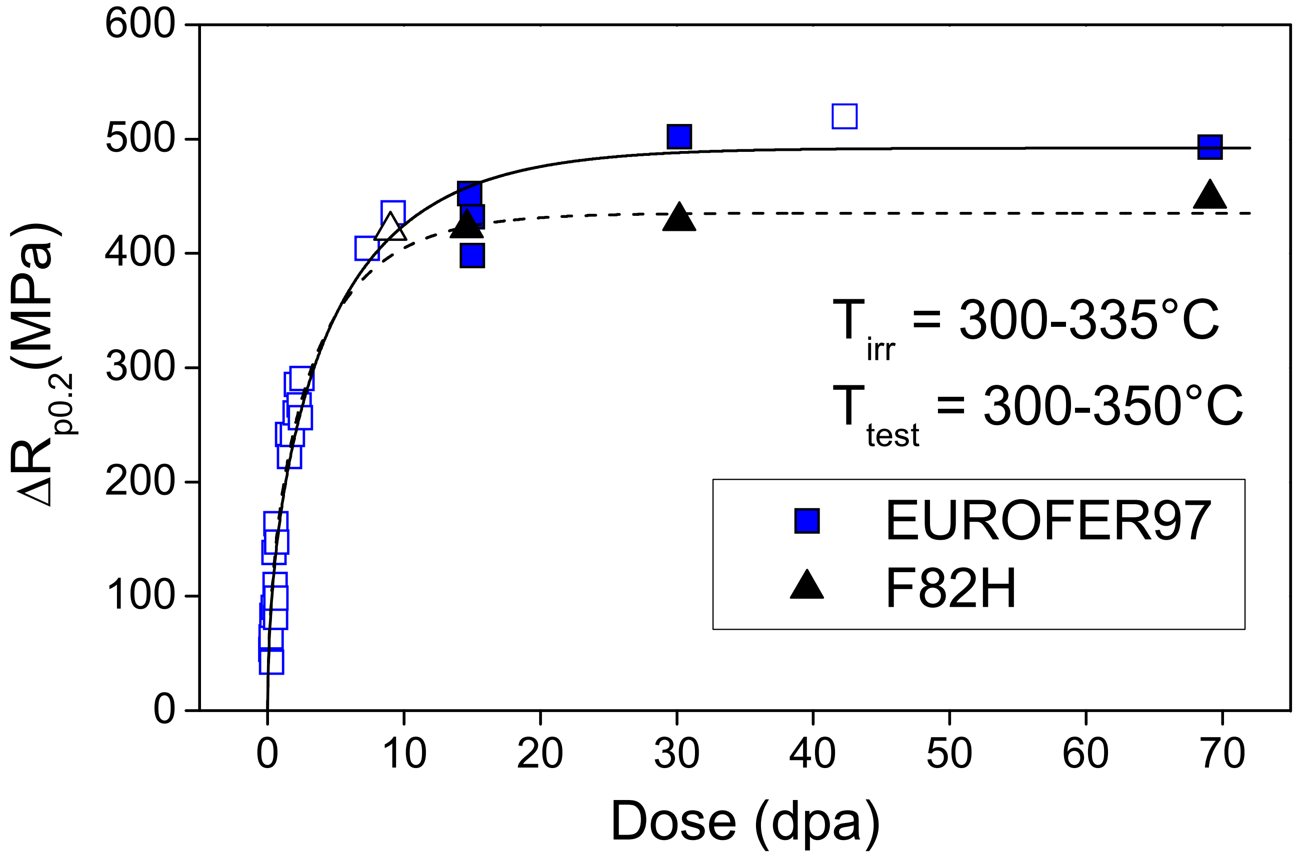




M. Klimenkov, IAM, KIT

„Interface-Engineering“:
Nanoscaled ODS particles like Y_2O_3 or $Y_2Ti_2O_7$ are indispensable “Marketplaces” for defect recombination & trapping of diffusing alloy elements

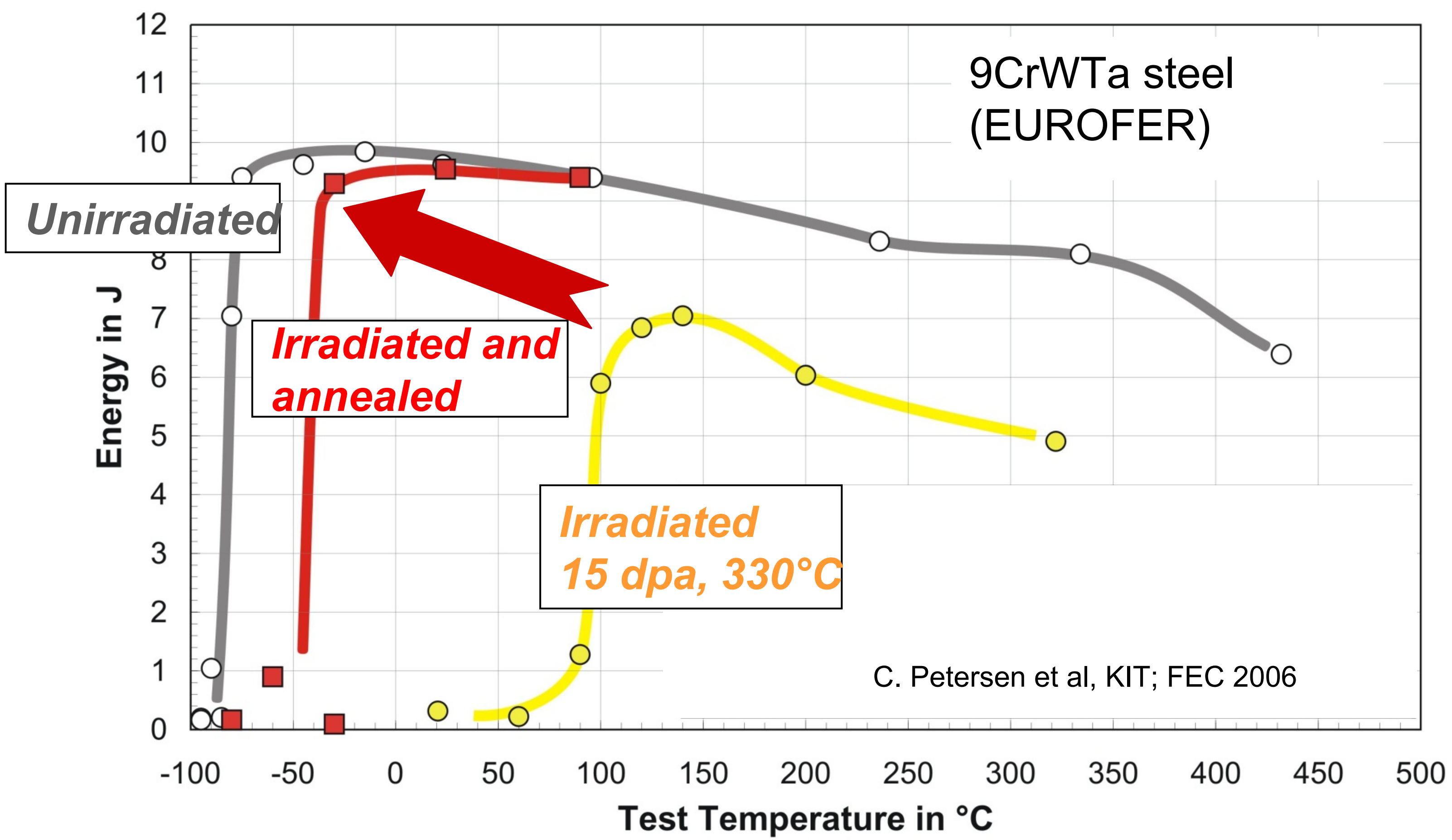
Neutron irradiation, “no” helium: Irradiation induced yield strength seems to saturate



E. Gaganidze et al, KIT
submitted to JNM

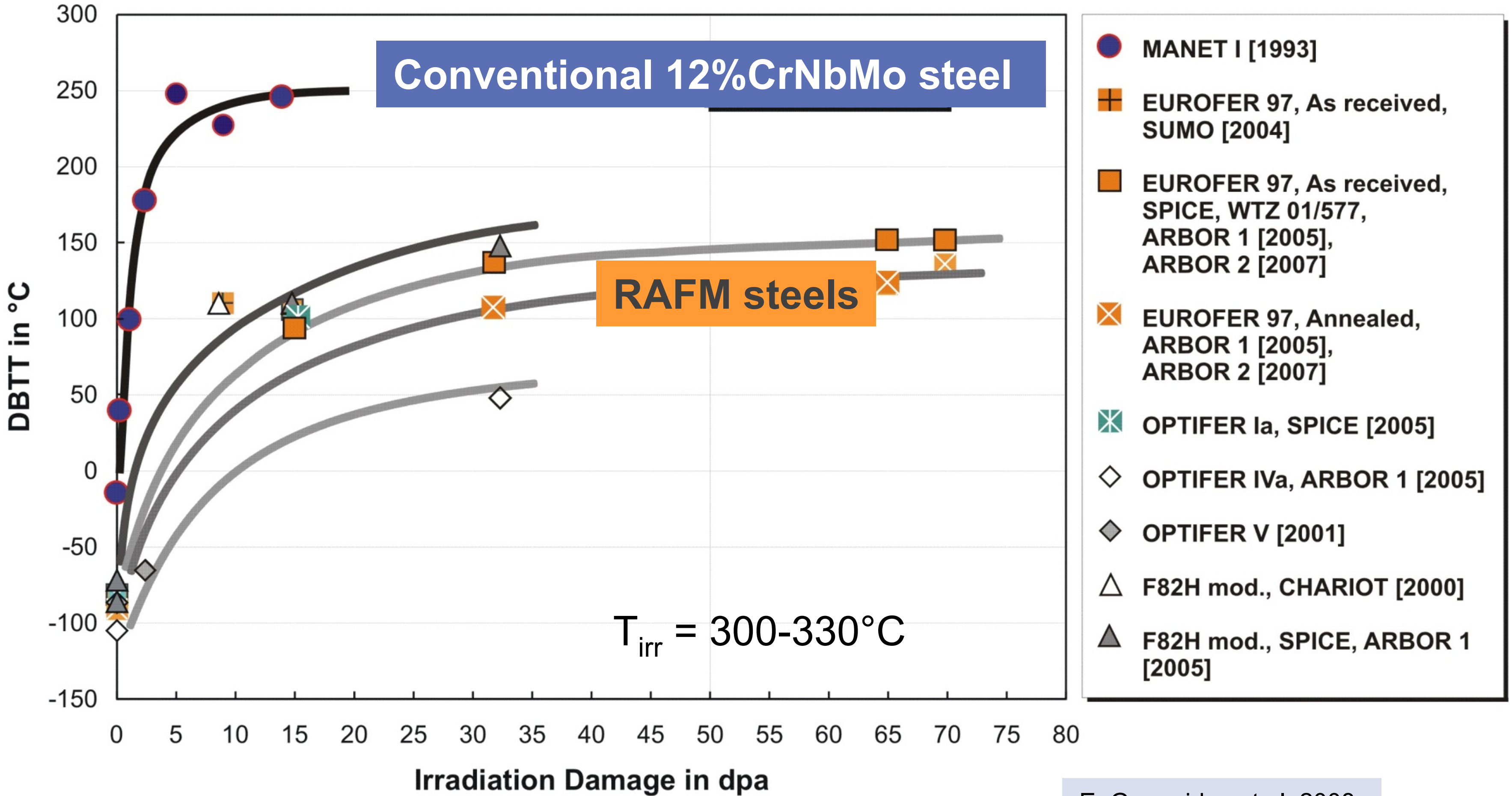
“Orowan-type” fit (solid line): $\Delta\sigma_{irr} = M\alpha\mu b\sqrt{Nd} \approx \Delta\sigma_{sat}\sqrt{\left[1-\exp(-\Theta/\Theta_0\right]}$

Is it possible to anneal irradiation embrittlement?



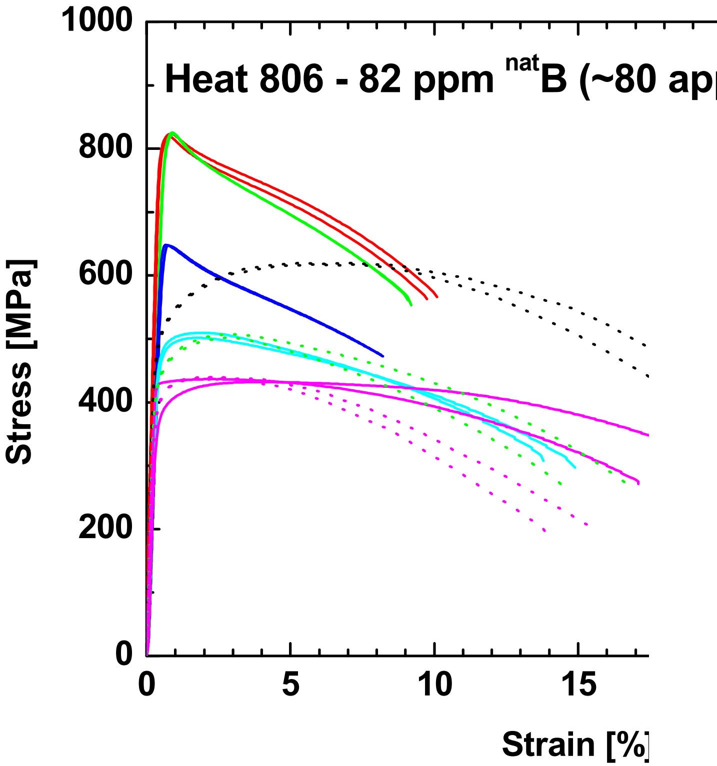
- How often can this recovery be repeated?
- What happens if large concentrations of He are present?

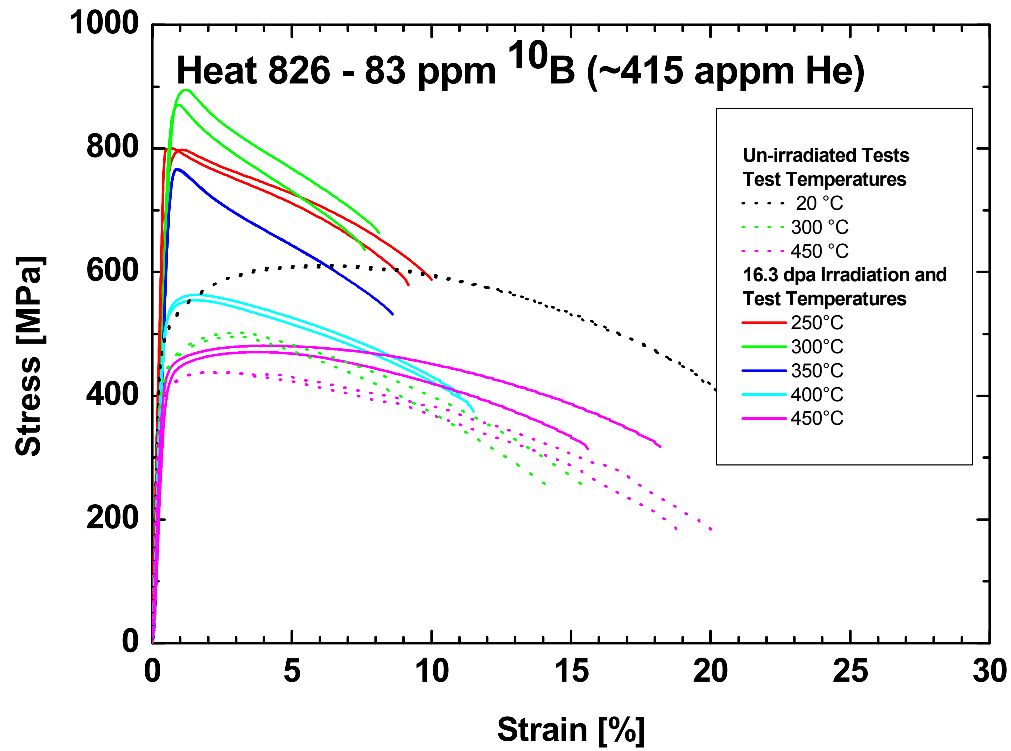
Irradiation induced Ductile Brittle Transition Temperature shows quasi-saturation



E. Gaganidze et al, 2008

16 dpa Neutron irradiation, Helium effects after B-doping



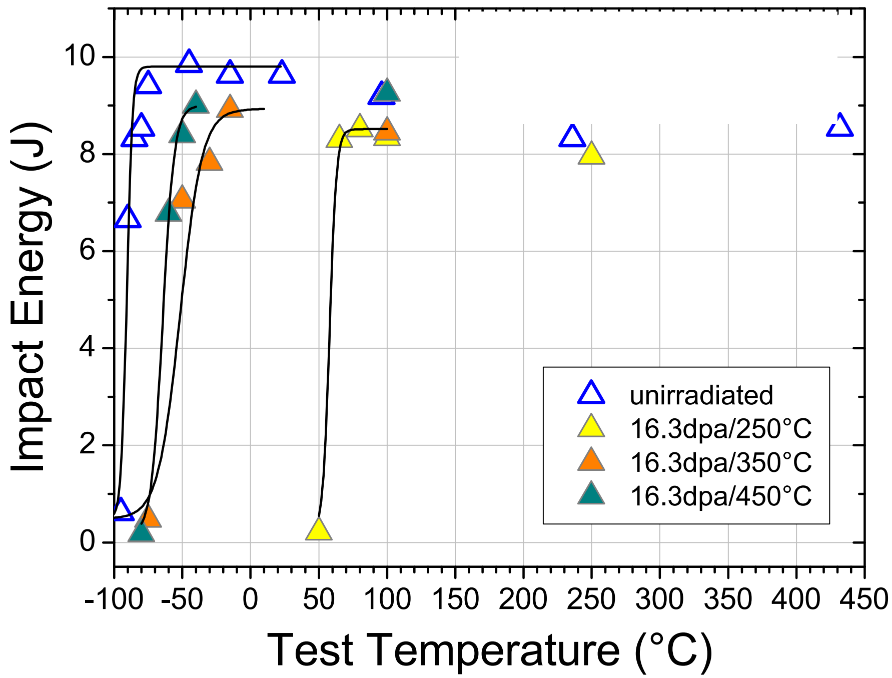


E. Materna-Morris, et al.
JNM 386(2009)422

≤415 appm: He shows strength increase but no reduction of rupture strain

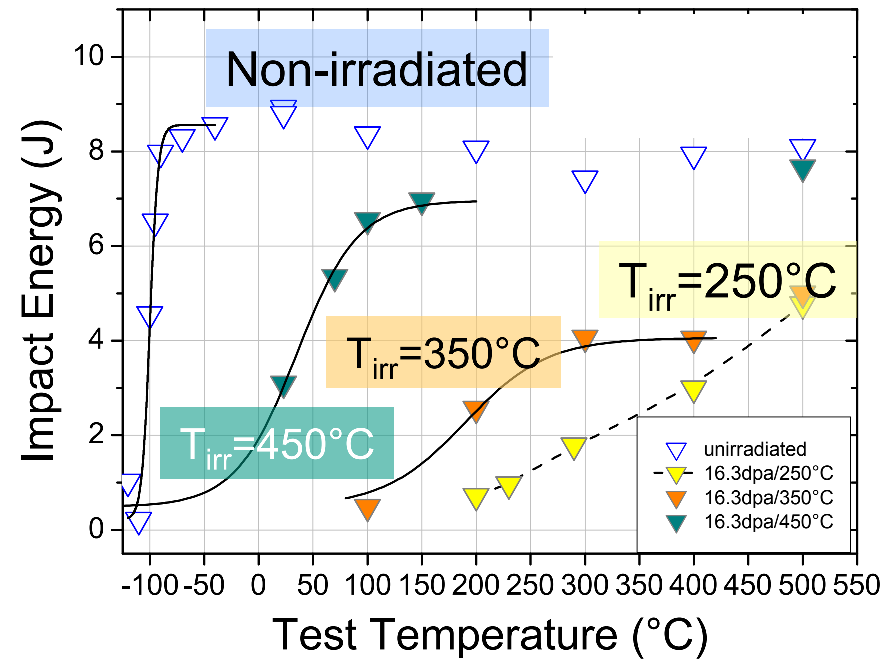
Irradiation induced DBTT after 16 dpa HFR irradiation:
Effect of irradiation temperature and He concentration

EUROFER97 HT, <10 appm He



T_{irr}=250 °C: ΔDBTT = 149 °C

EUROFER-type, ~415 appm He



T_{irr}=250 °C: ΔDBTT = 370 °C

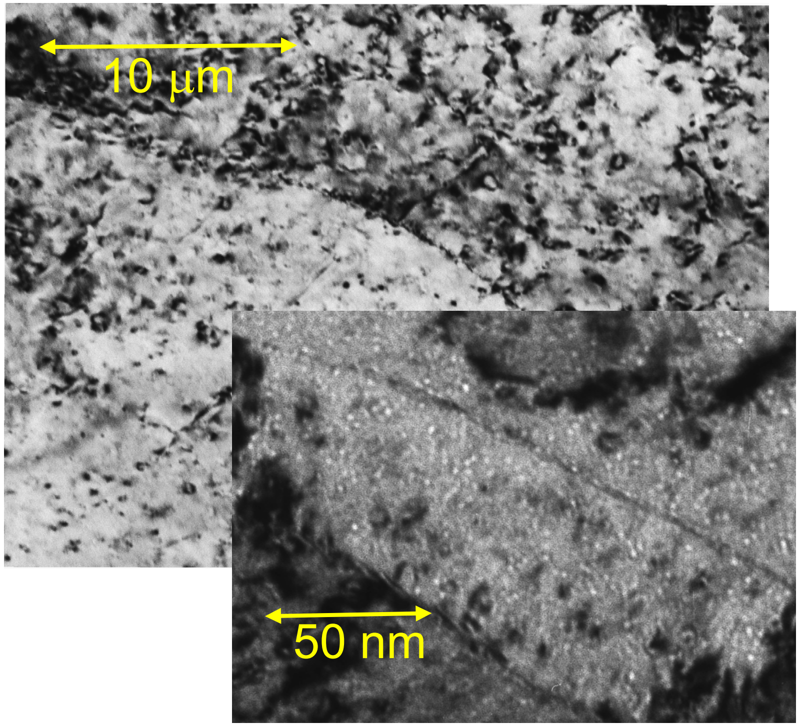
E. Materna-Morris et al, SOFE-2009

Microstructure after neutron irradiation (~15 dpa)

Example: 9CrWTa steel, effect of dpa and 415 appm He

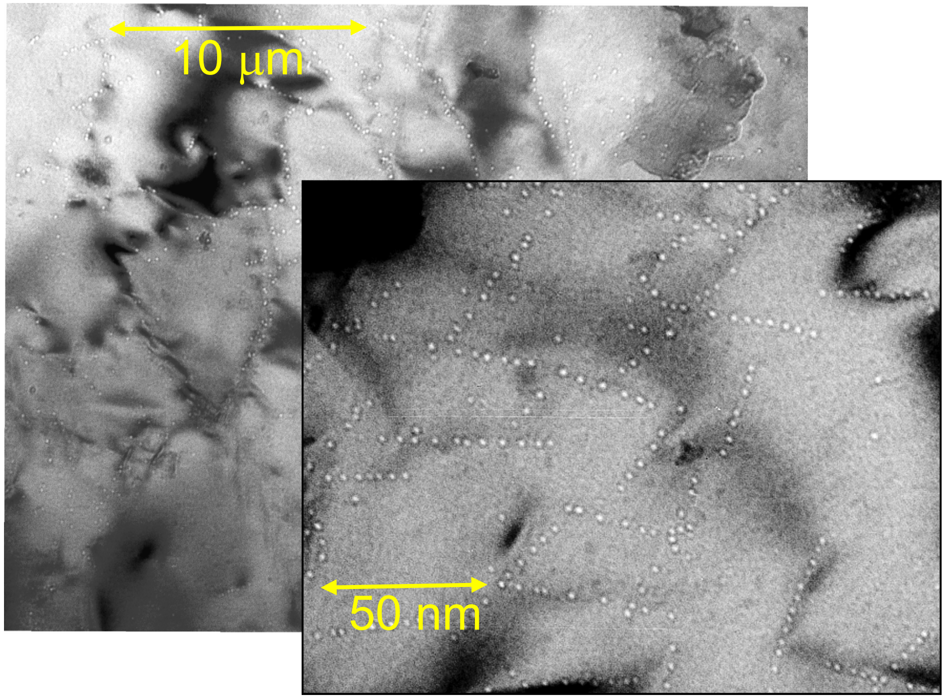
E. Materna-Morris et al, 2008

$T_{test} = T_{irr} = 300$ °C



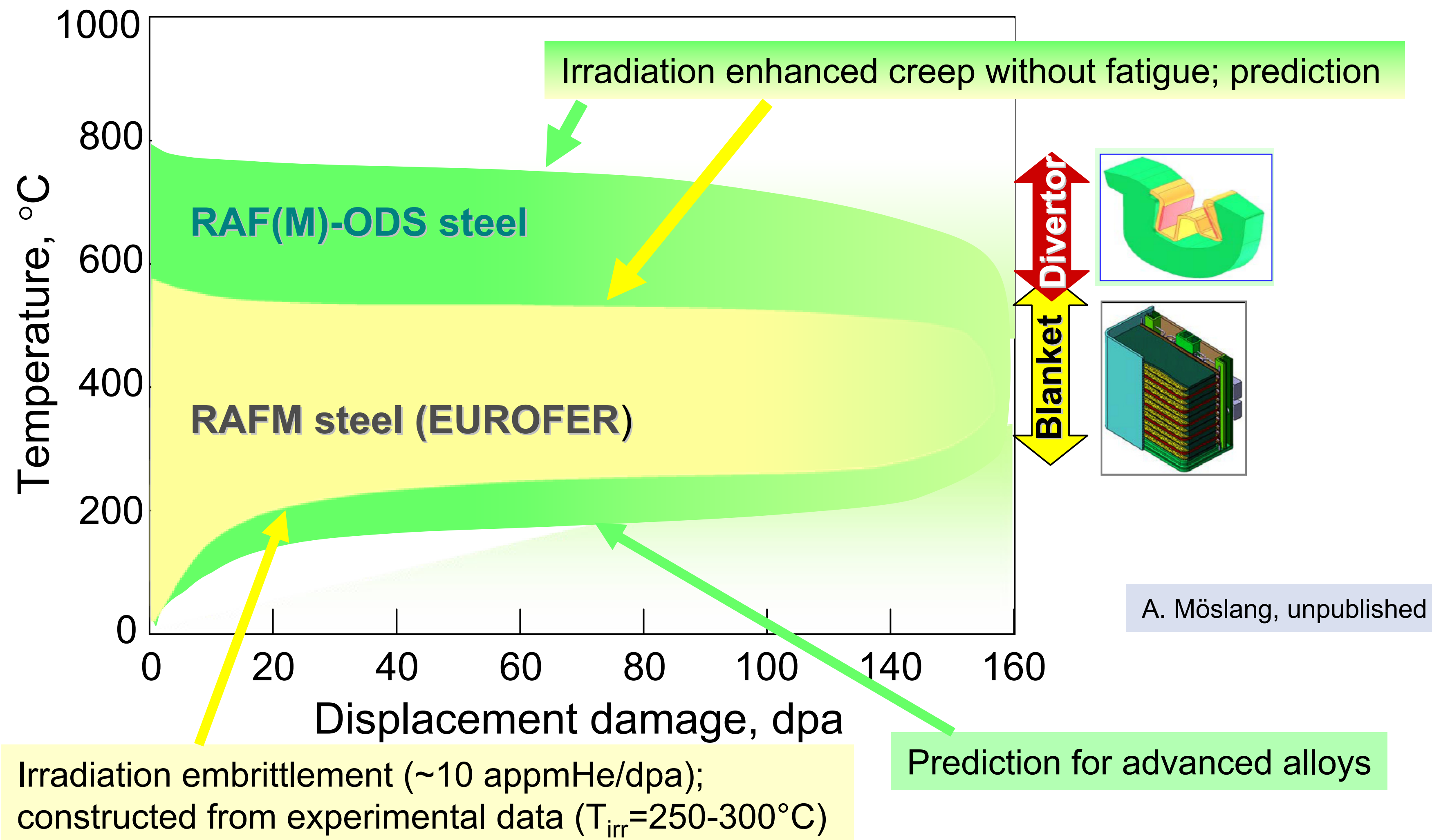
- Small loops & precipit. (dark dots)
- Small He bubbles (white dots)

$T_{test} = T_{irr} = 450$ °C

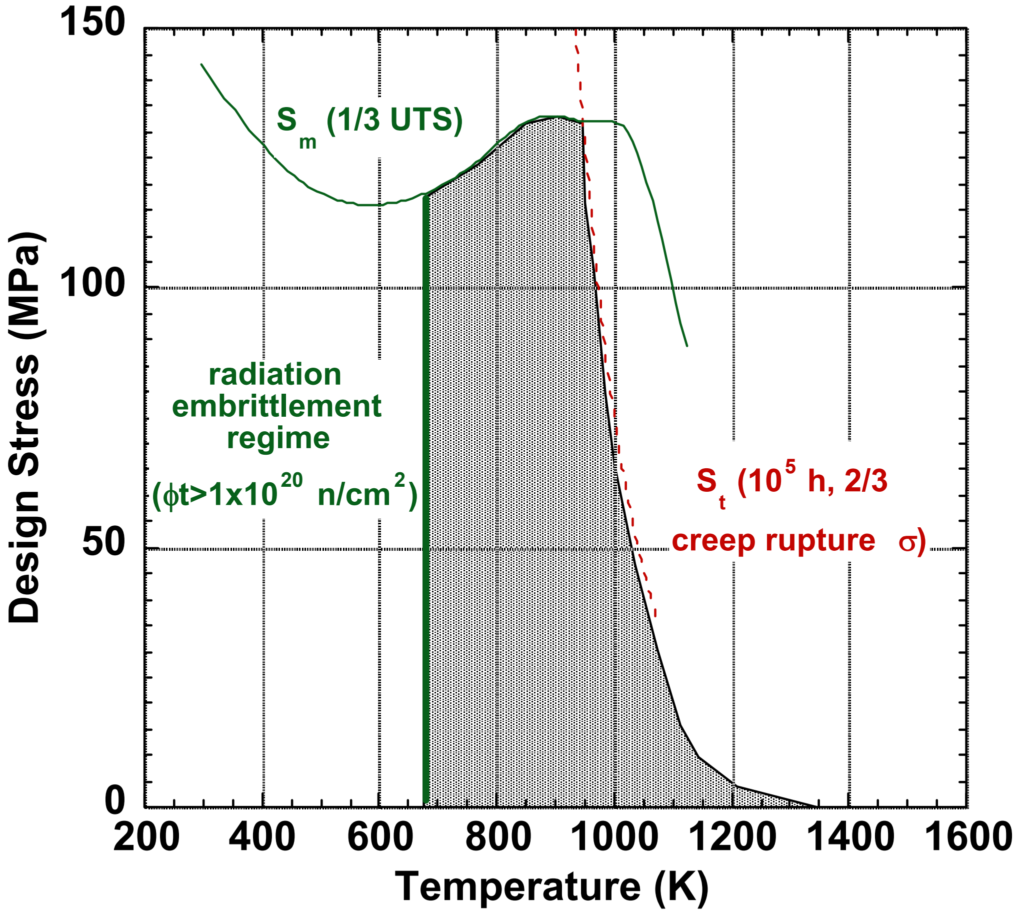


- Small loops & precipitates not formed
- He bubbles along dislocation lines

Application window of RAF(M)-ODS-Steels
- schematic -



V alloys Reference: V-4Cr-4Ti Design Window



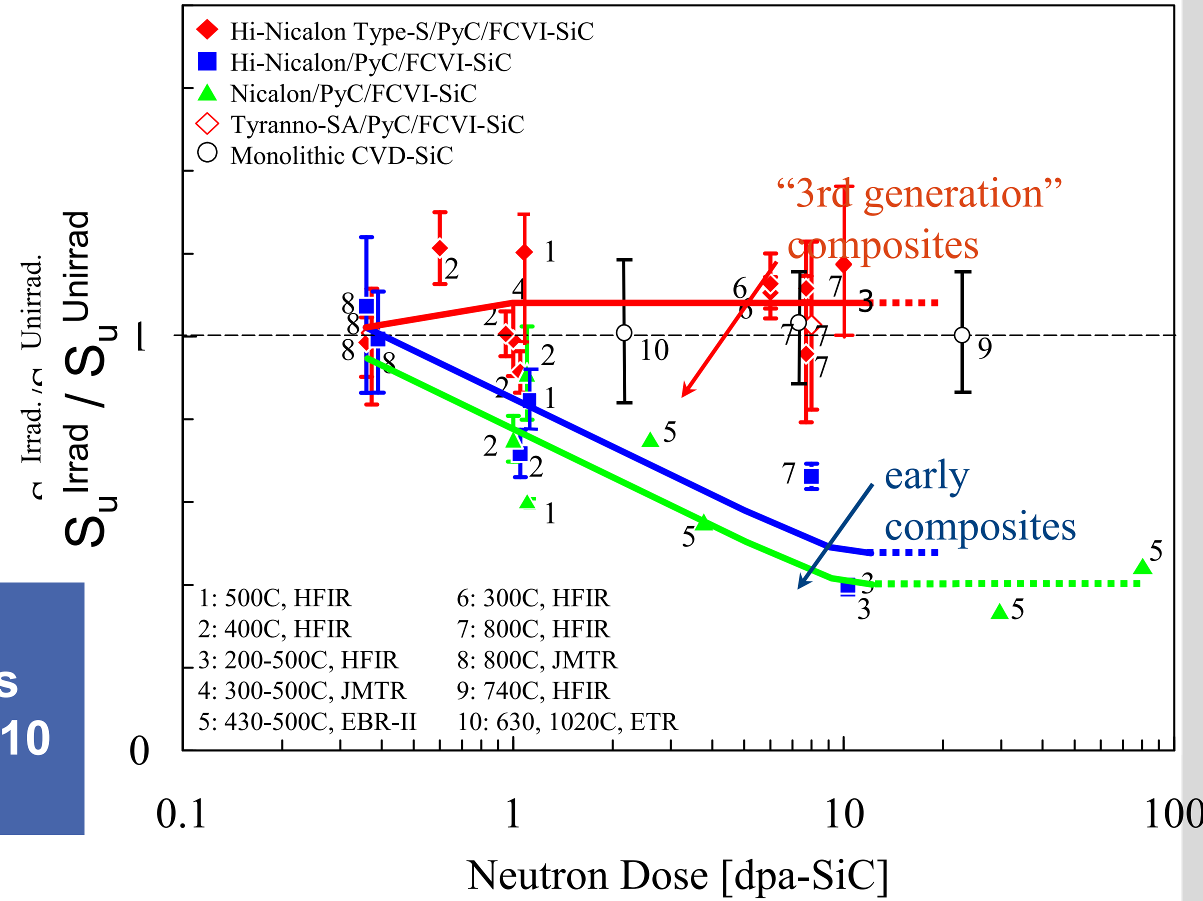
S. Zinkle et al, ORNL

+ Irradiation embrittlement below 400-420 °C
+ Creep rupture strength comparable to state-of-the-art RAFM ODS steels
+ Coatings (like CaO, AlN) to prevent from MHD and embrittlement not yet available

SiC_f/SiC Composites for Irradiation Studies

S. Zinkle, L. Snead et al.

Reference in US/JAPAN collaboration: Chemical Vapor Infiltrated (CVI) SiC composites



Bend strengths of irradiated "3rd generation" composites show no degradation up to 10 dpa

Future work:
Advanced matrix infiltration R&D; joining; hermetic coatings; SiC/graphite composites

Summary
Application window of today's materials (~10 dpa)