

# Overview of Radiation Damage Effects

Steve Roberts

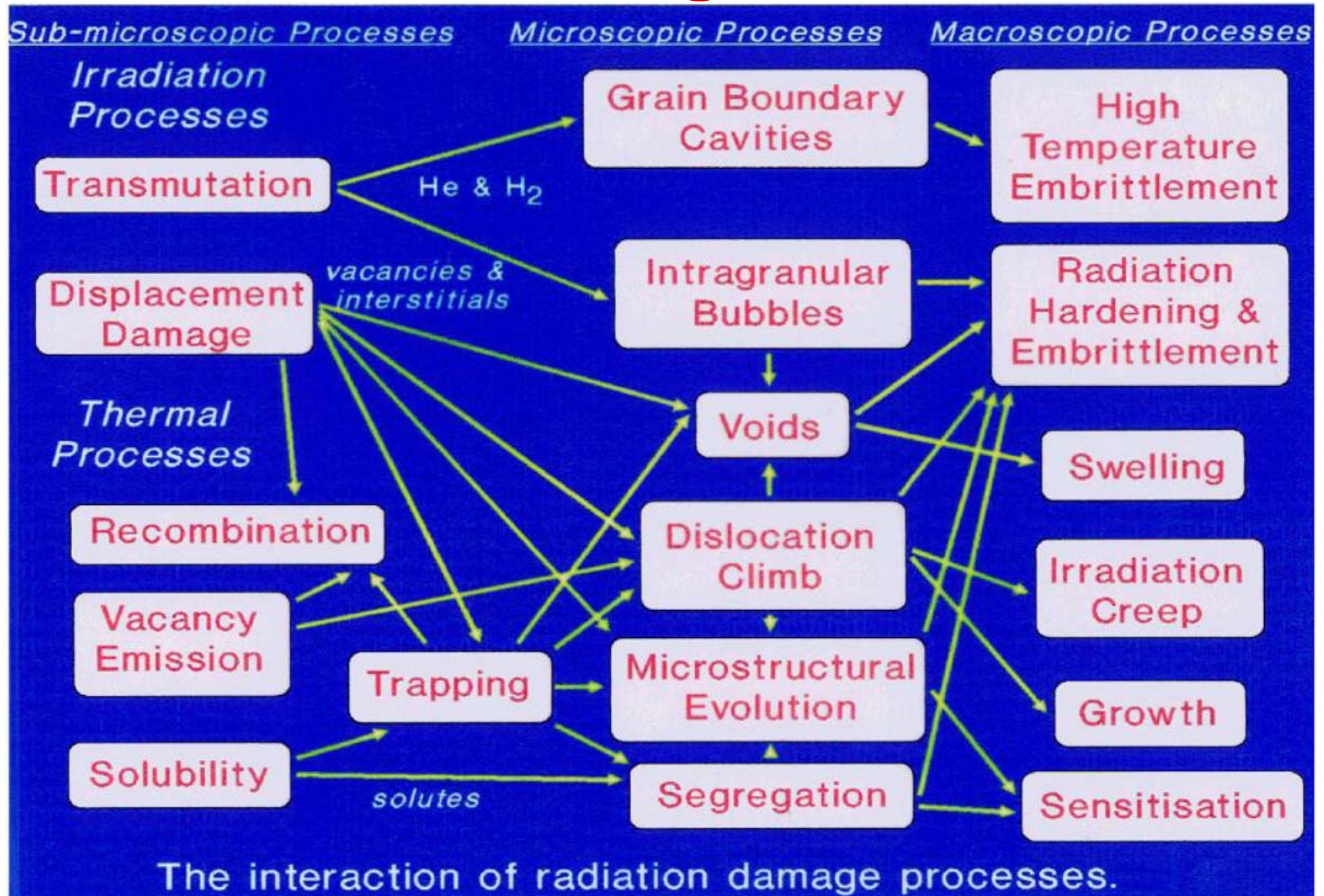
U. Oxford

May 19, 2015

2<sup>nd</sup> RaDIATE Collaboration Meeting

RAL

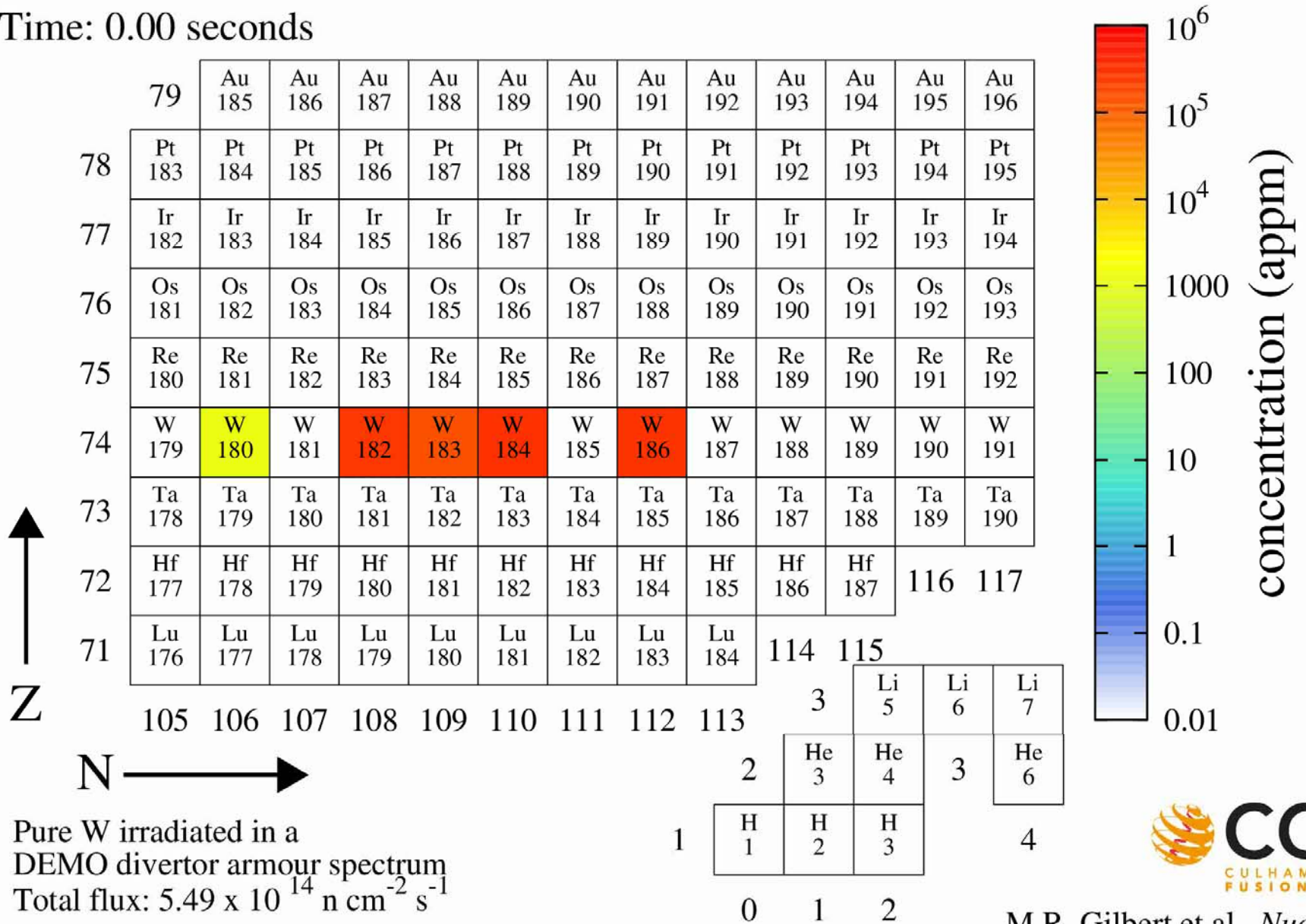
# Radiation damage in Materials



# Transmutation

# Tungsten Transmutations in Fusion Reactor

Time: 0.00 seconds



Pure W irradiated in a DEMO divertor armour spectrum  
 Total flux:  $5.49 \times 10^{14} \text{ n cm}^{-2} \text{ s}^{-1}$

m - concentration dominated by metastable nuclide(s)

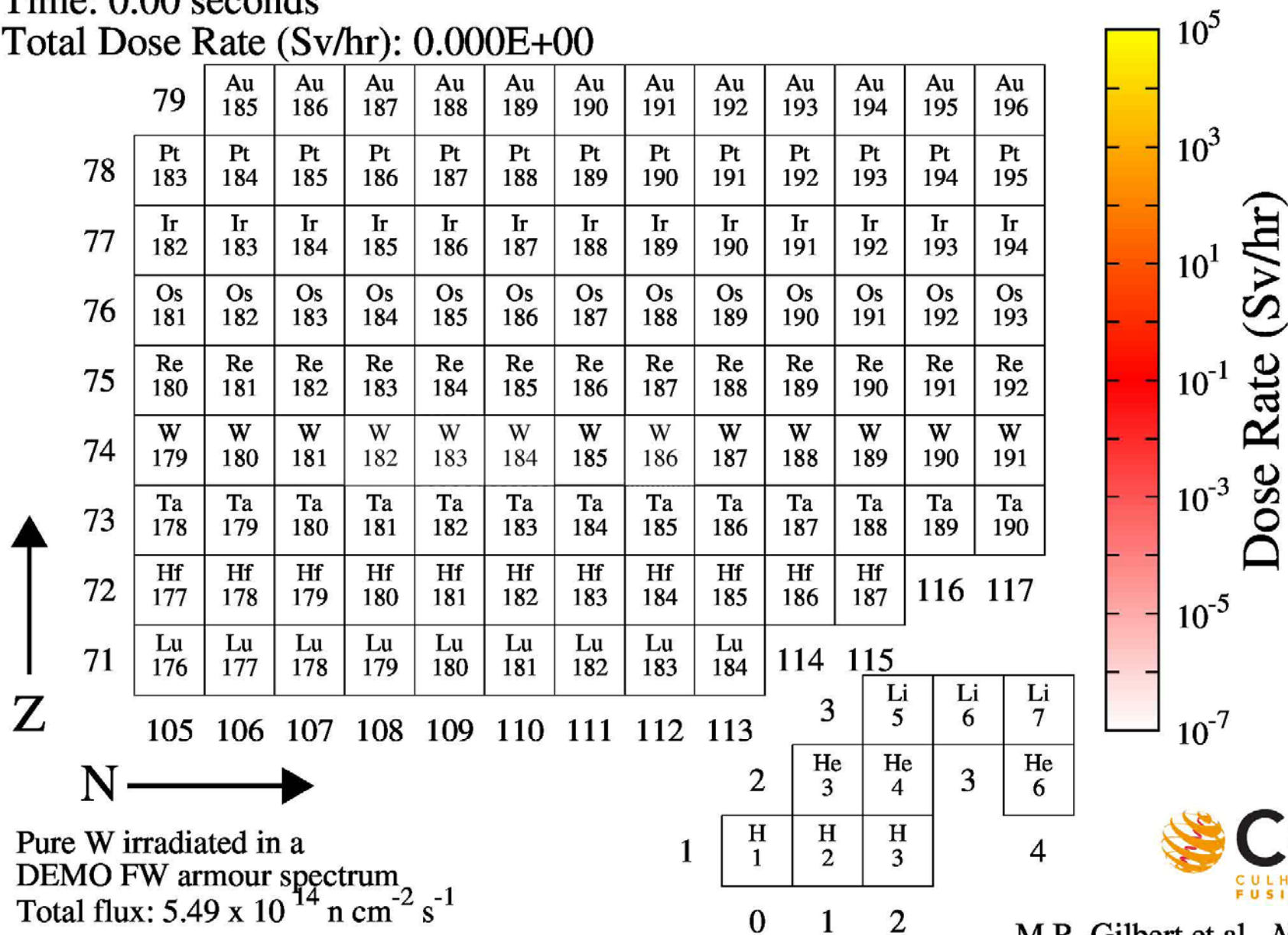




# Tungsten Transmutations - activity

Time: 0.00 seconds

Total Dose Rate (Sv/hr): 0.000E+00



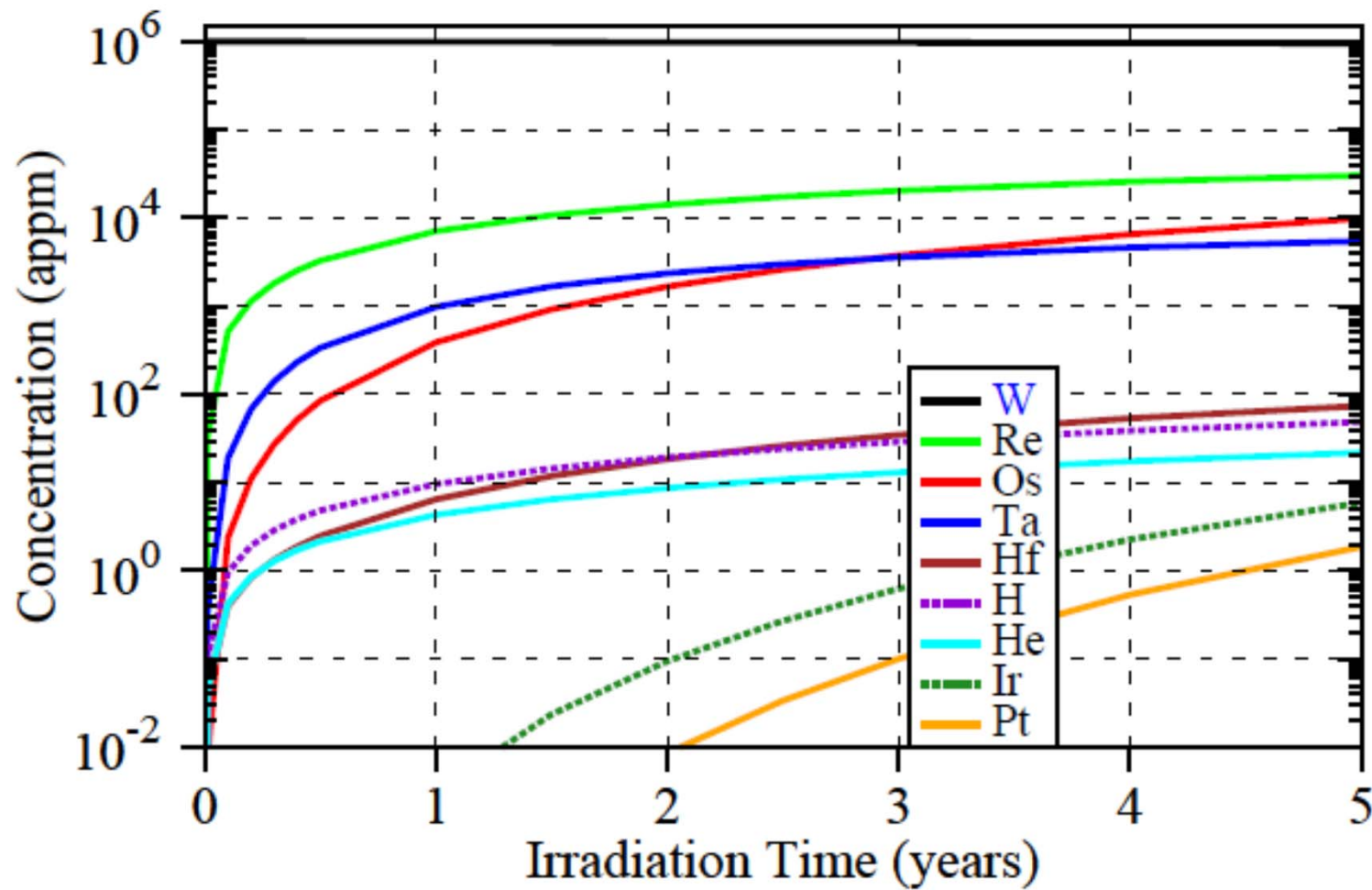
Pure W irradiated in a DEMO FW armour spectrum  
Total flux:  $5.49 \times 10^{14} \text{ n cm}^{-2} \text{ s}^{-1}$

m - Dose Rate dominated by metastable nuclide(s)



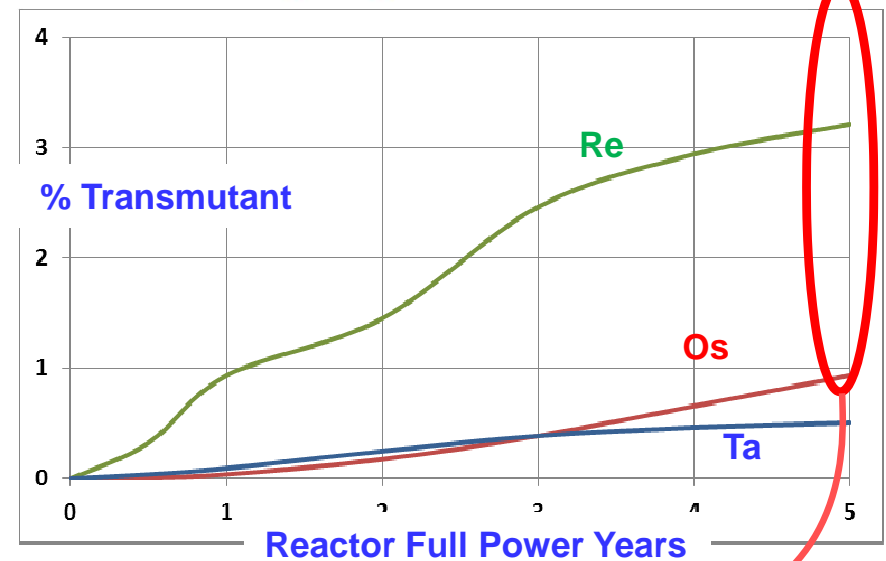
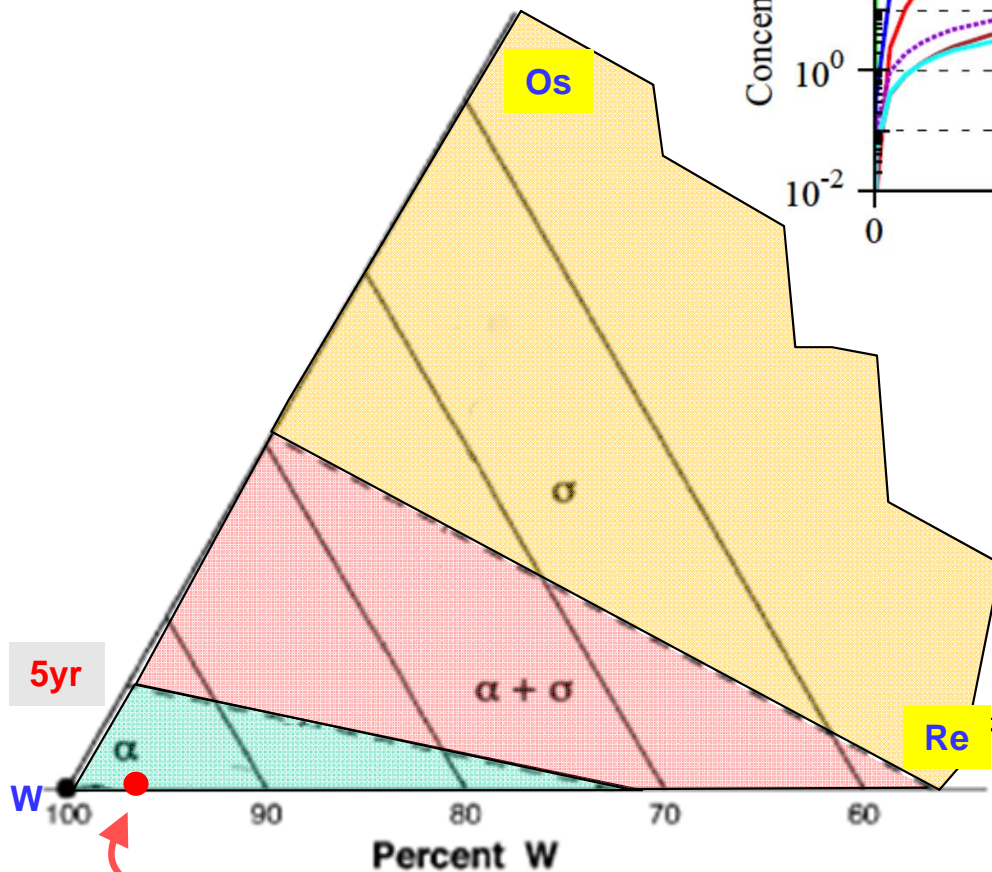
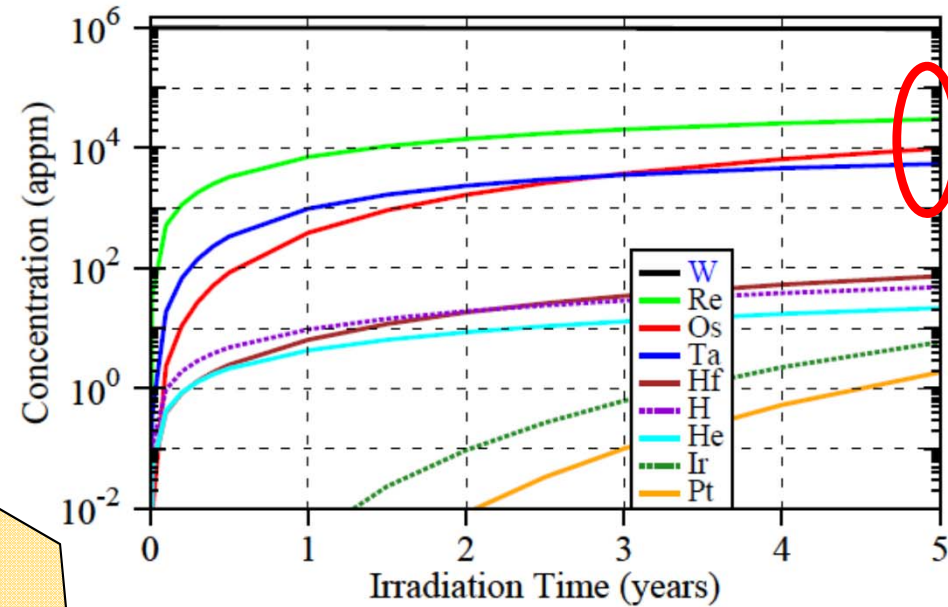
# Tungsten transmutation in fusion power reactor

- Pure W under outboard equatorial FW armour flux for 5 fpy



# Tungsten transmutation in fusion power reactor

- Pure W under outboard equatorial FW armour flux for 5 fpy



# Tungsten transmutation in fusion power reactor

Ion irradiation can't mimic transmutation effects

But we can MODEL what transmutations we expect

And can ion-irradiate pre-made W alloys

To see what effect displacement damage -

(and if we like, He, H )

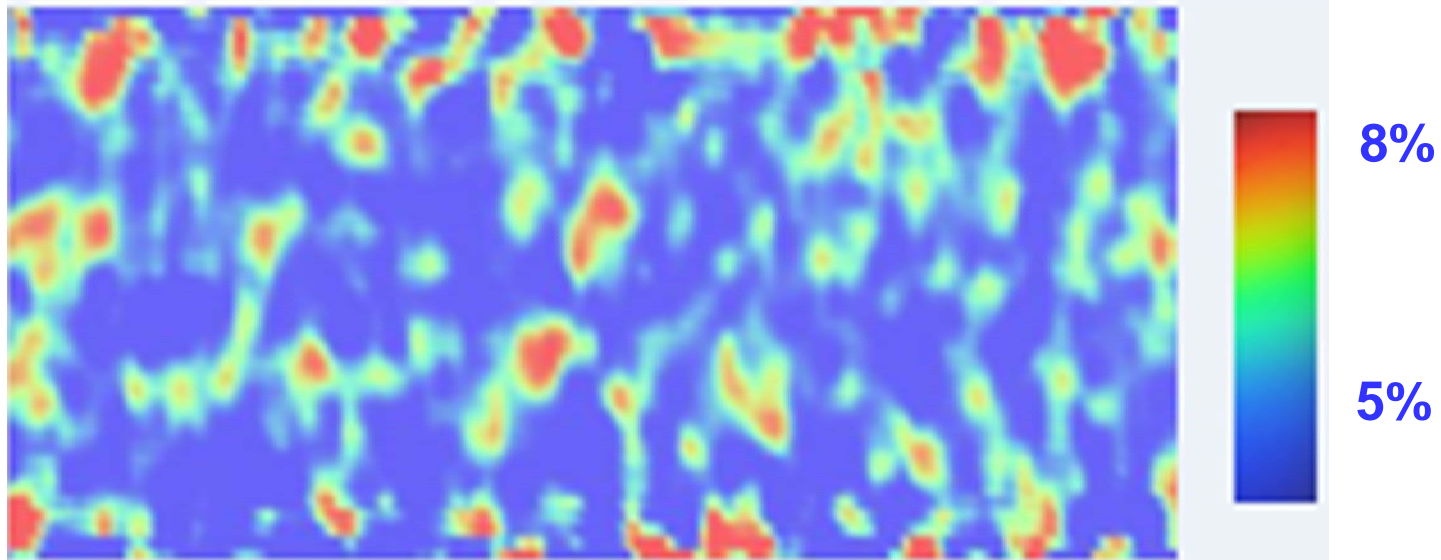
have on microstructures and properties.



# Radiation-induced clustering in alloys

**W- 5%Re should be a stable solid solution  
... but it's not when it is irradiated**

**Under Fusion Power Reactor conditions,  
pure W transmutes to give 5%Re in ~ 7 years.**

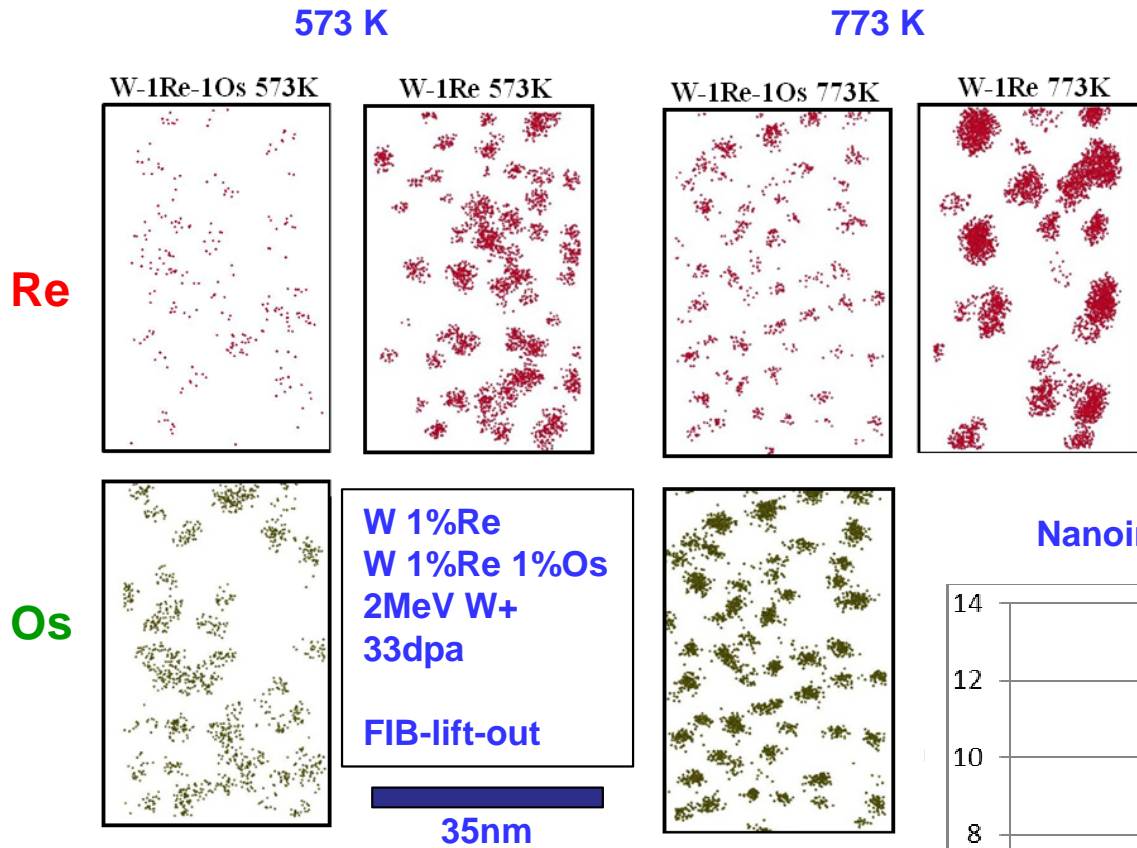


**Ion irradiation to  $2.64 \times 10^{15}$  W<sup>+</sup>/cm<sup>2</sup> (33dpa)**

**Dose rate:  $3.57 \times 10^{-4}$  dpa / s**

**Temperature: 300°C**

# Clustering and Hardening in “Transmuted” W



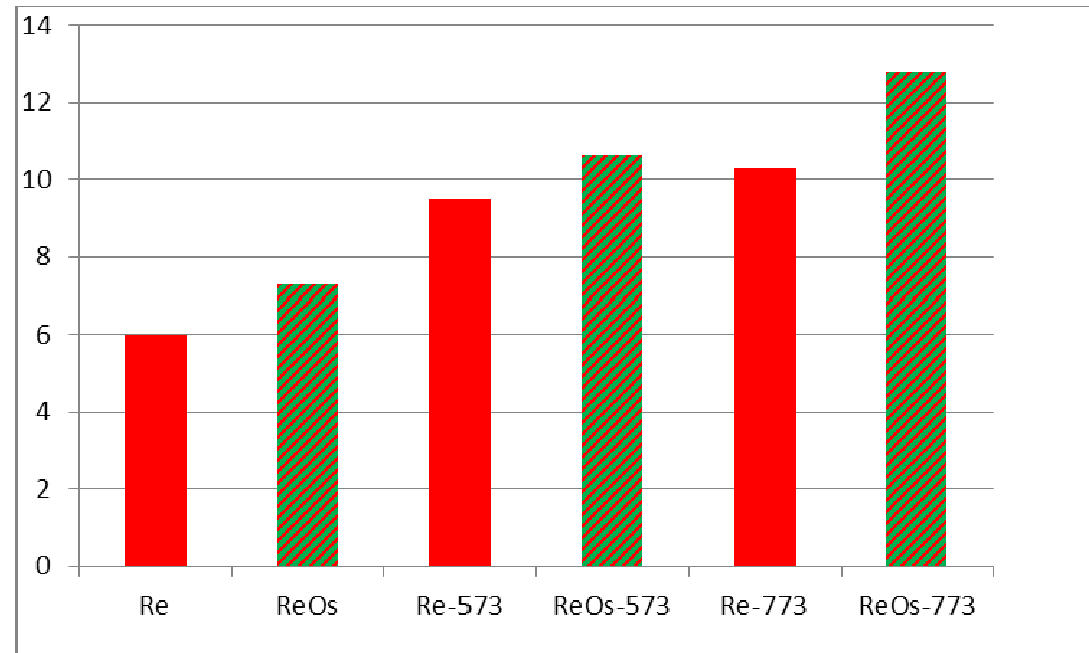
Preliminary analysis indicates that the clusters are very **weak** obstacles:

$$\Phi_c \approx 85^\circ$$

But there are lots of them, very closely spaced - especially in W-Re-Os

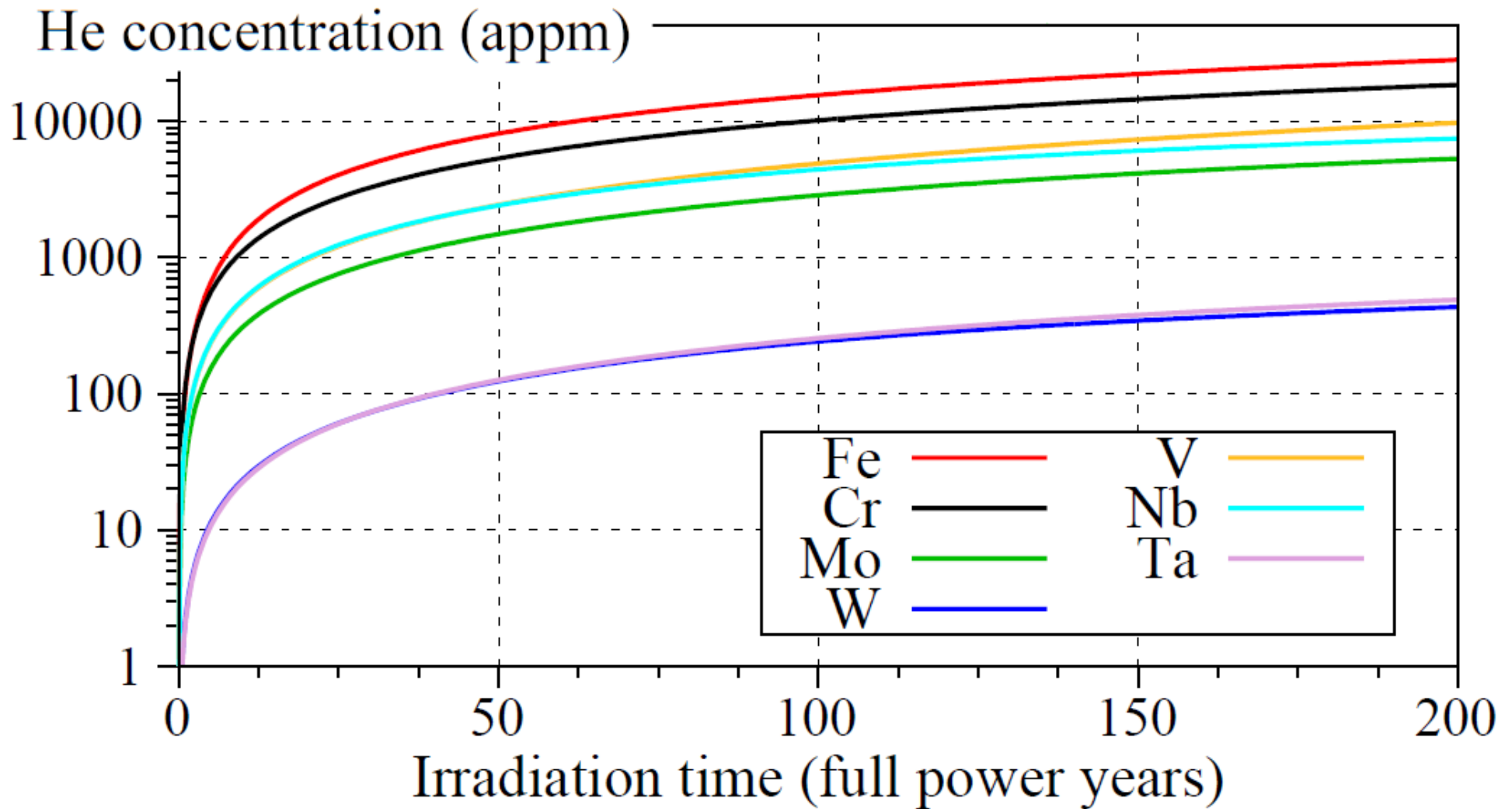
Same would apply to neutron irradiation ???

Nanoindentation hardness (GPa) (100nm depth)



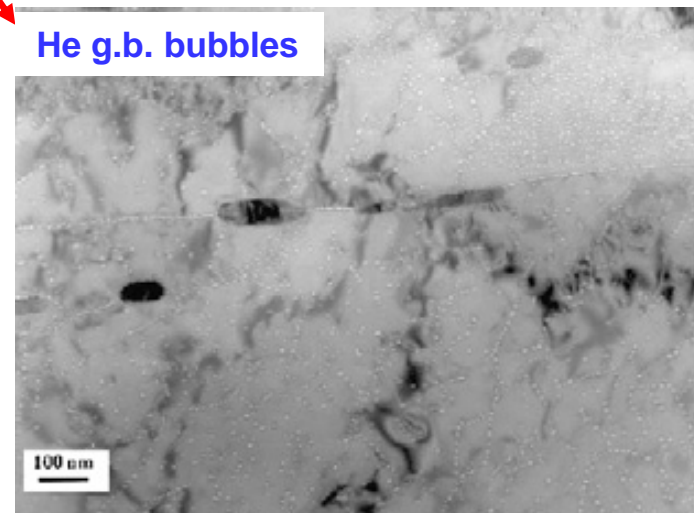
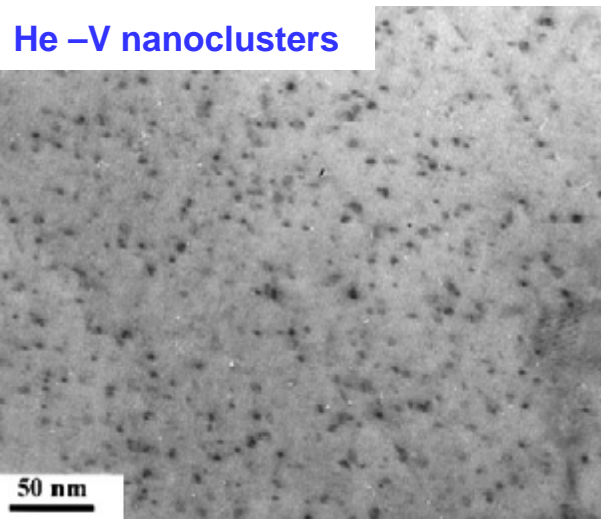
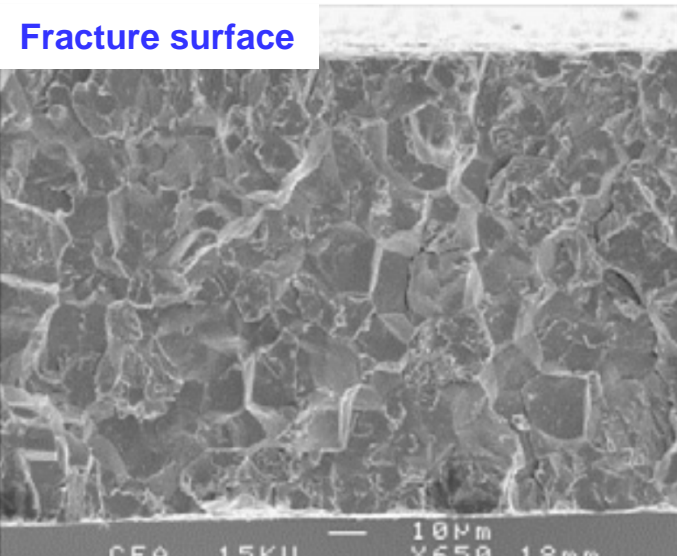
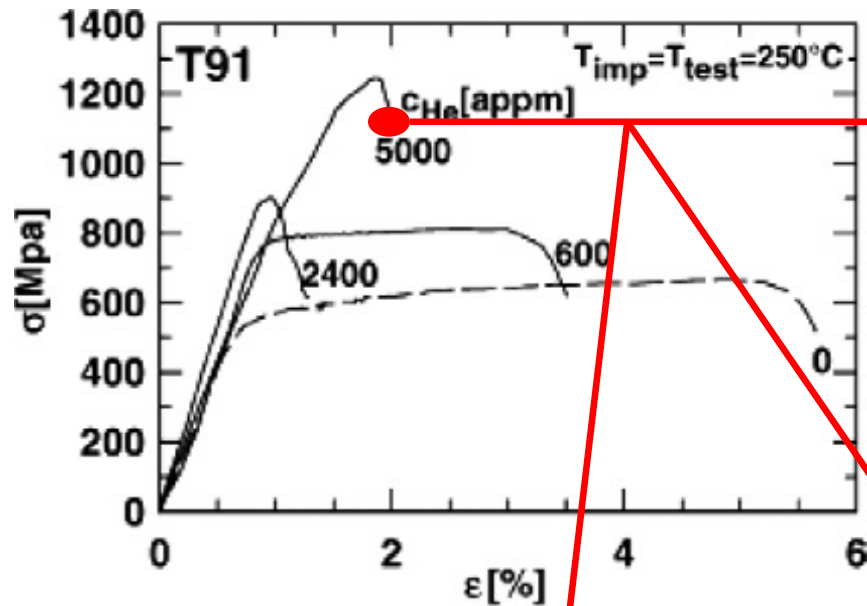
# **Transmutation gases**

# Transmutations producing He in fusion power reactor



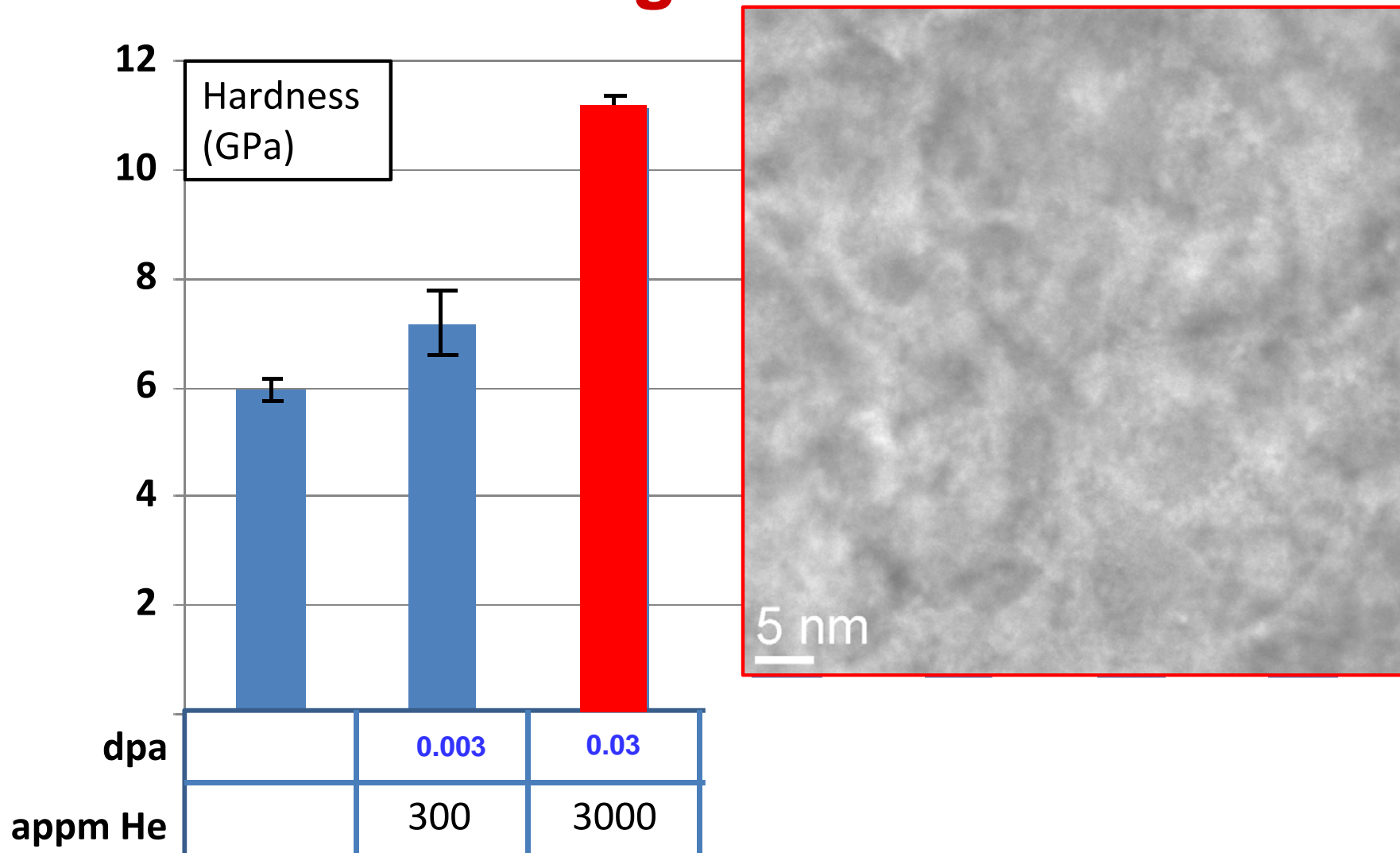


# Effects of Implanted He on T91 steel



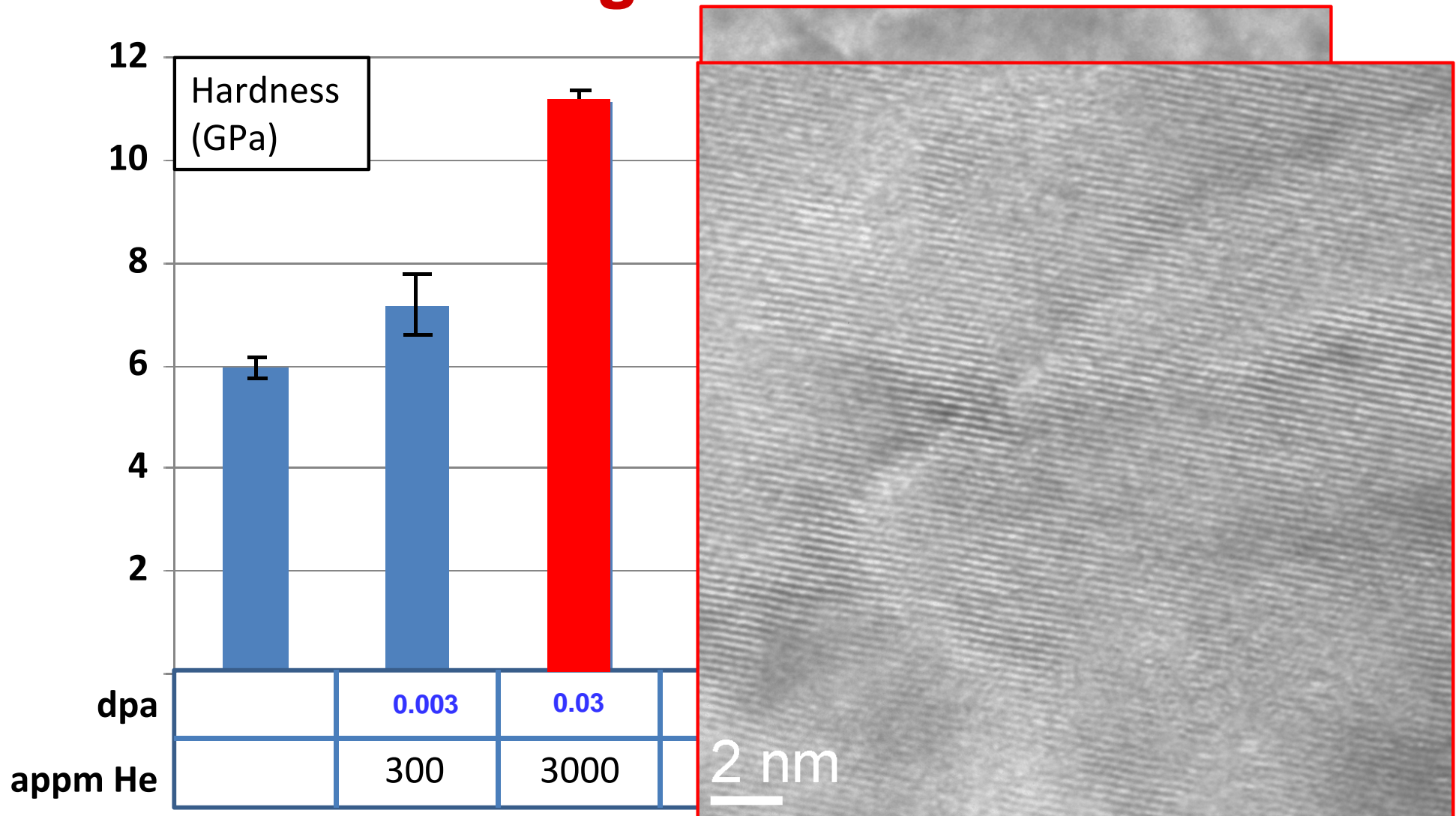
“Uniform implantation of 23 MeV  $\alpha$ -particles up to 5000 appm at 250°C carried out at the compact cyclotron of Forschungszentrum Jülich (FZJ)”

# Tungsten – Hardening by Displacement Damage and Helium



Polycrystalline W 99.99% pure, sequentially ion-implanted with W<sup>+</sup> and He<sup>+</sup> at 300°C  
W implantation depth 0 - 200nm; He implantation depth range 0 - 2500 nm  
Hardness data at 100 nm indenter depth .

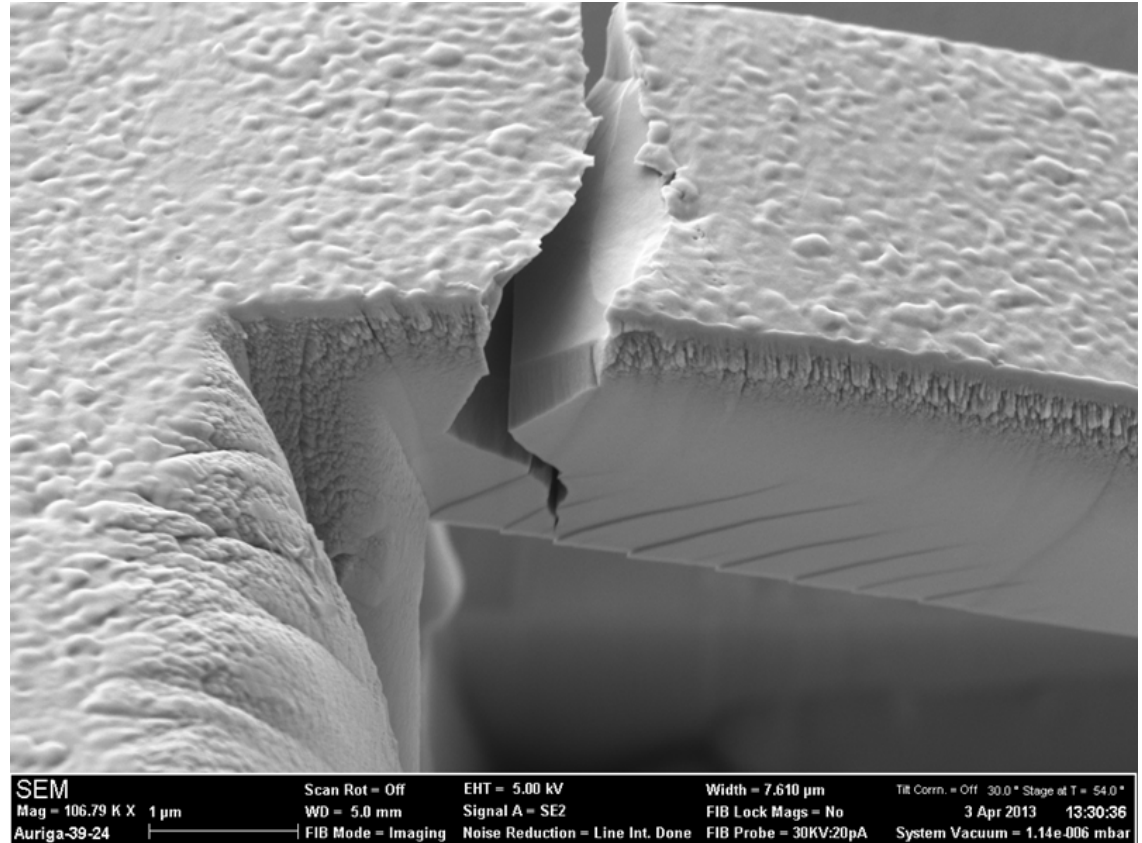
# Tungsten – Hardening by Displacement Damage and Helium



Polycrystalline W 99.99% pure, sequentially ion-implanted with W<sup>+</sup> and He<sup>+</sup> at 300°C  
W implantation depth 0 - 200nm; He implantation depth range 0 - 2500 nm  
Hardness data at 100 nm indenter depth .

# Tungsten – Embrittlement by Displacement Damage and Helium

Irradiation	Fracture ?
none	0 / 7
1.7 dpa W <sup>12+</sup>	1 / 16
600 appm He	0 / 13
1.7 dpa W <sup>12+</sup> + 600 appm He	7 / 10



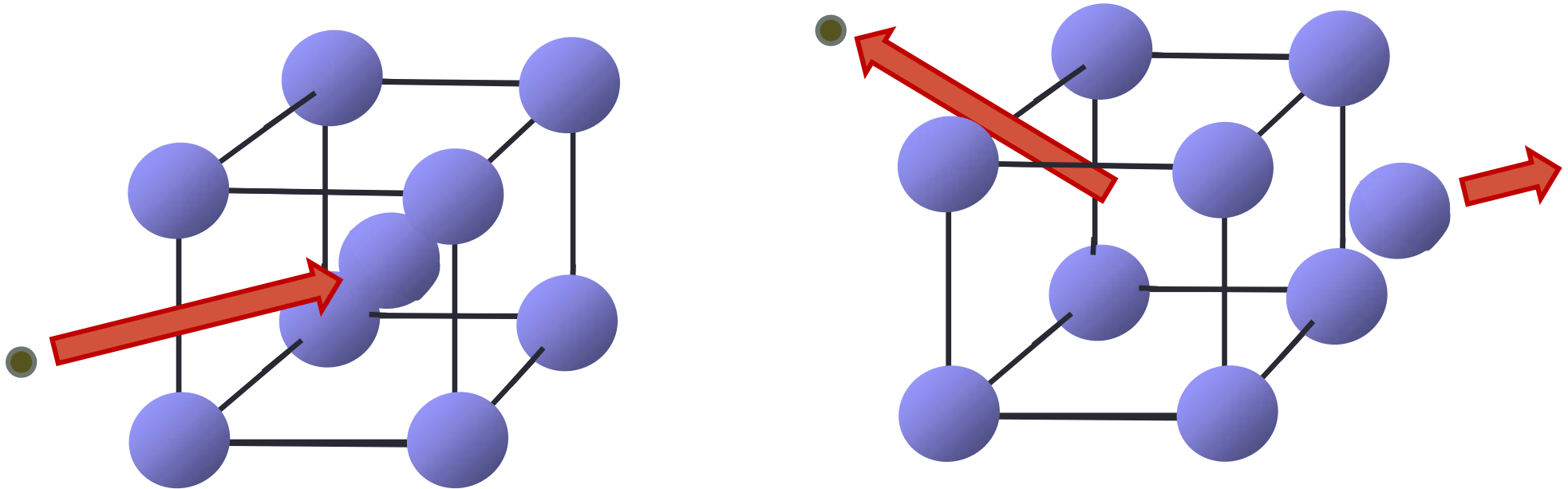
Polycrystalline W 99.99% pure, ion-implanted with W<sup>12+</sup> (36MeV) and He<sup>+</sup> at 800°C  
W + He simultaneously implanted  
W implantation depth ~2.5 µm; He depth range ~ 2.8 µm  
Fracture data from microbeams 3 µm deep .



**“Damage”**

# Elastic scattering of neutrons

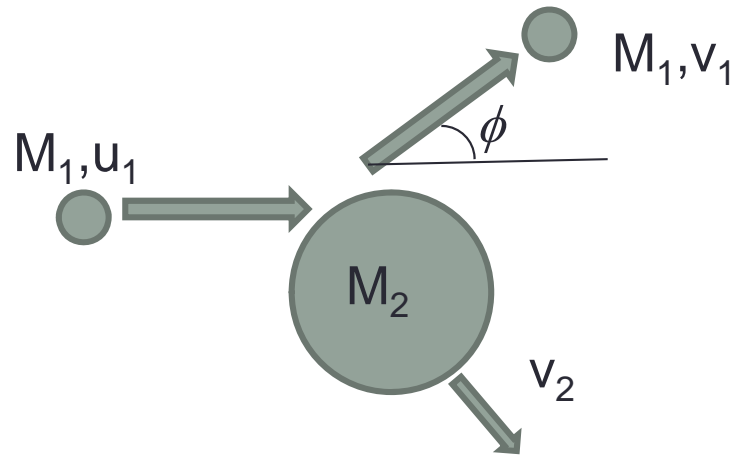
.... What about the “target” atoms?



	$E_d$		$E_d$		$E_d$
Al	~32eV	Fe	~24eV	Si	~13eV
Cu	~25eV	W	~40eV	C (graphite)	~25-60eV

Fusion neutrons are ~14MeV !

# Elastic scattering of neutrons



$$v_1^2 = 2(1 - \cos \phi) \frac{u_1^2 M_1^2}{(M_1 + M_2)^2}$$

$$E_2 = \Lambda E_1 \sin^2(\phi/2)$$

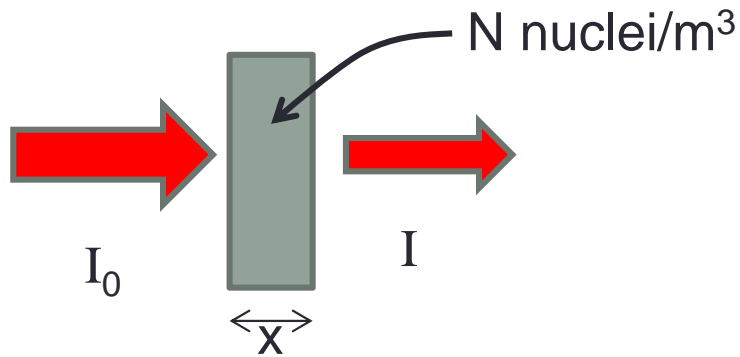
$$\Lambda = \frac{4M_1 M_2}{(M_1 + M_2)^2}$$

$$\bar{E}_2 = \Lambda E_1 / 2$$

For 14 MeV neutrons into iron,  $M_1 = 1$ ,  $M_2 = 56$ , so  $\Lambda = 0.069$

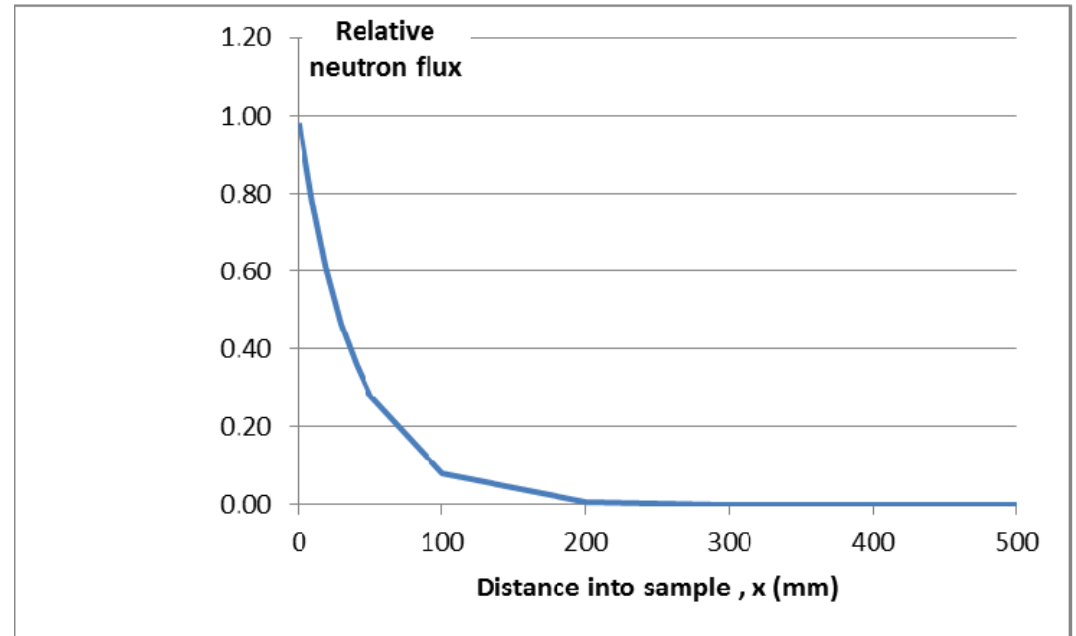
So  $\bar{E}_2 = 482$  keV .... about 34 collisions per neutron

# Elastic scattering of neutrons



$$I = I_0 \exp(-N\sigma x)$$

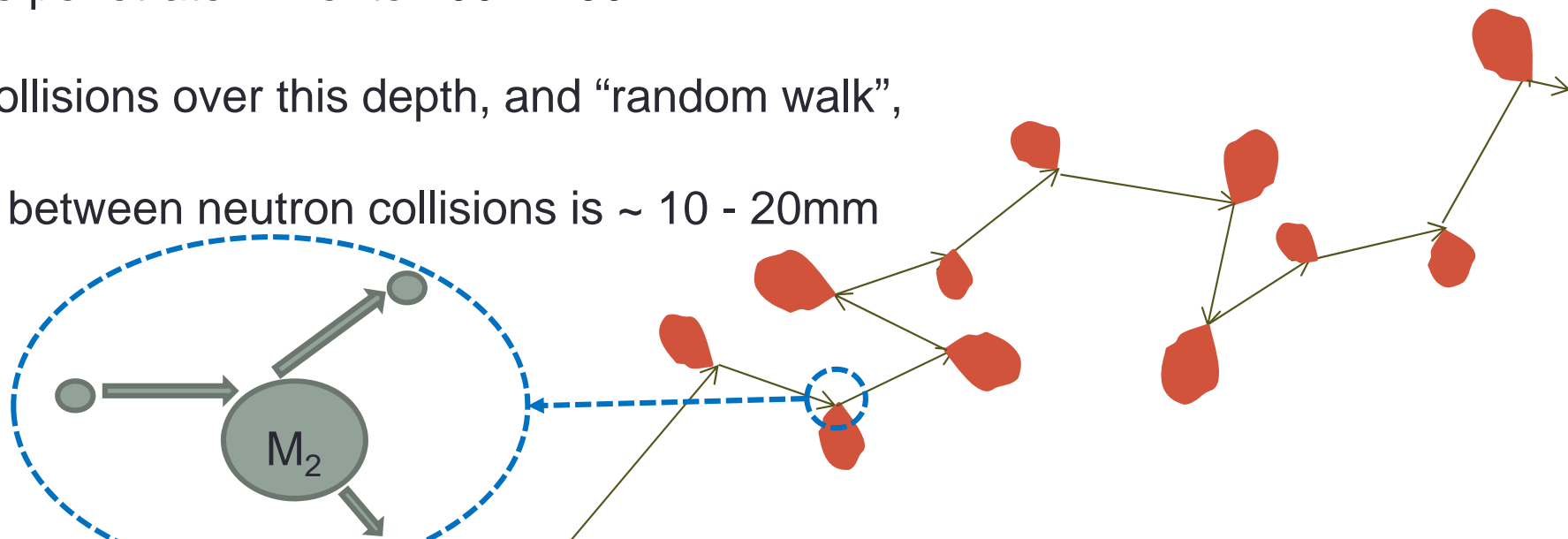
For  $\sigma = 3.2$  barns,  
 $N = 8 \times 10^{28} \text{ m}^{-3}$



Neutrons penetrate in Fe to 100 – 200 mm

If ~ 30 collisions over this depth, and “random walk”,

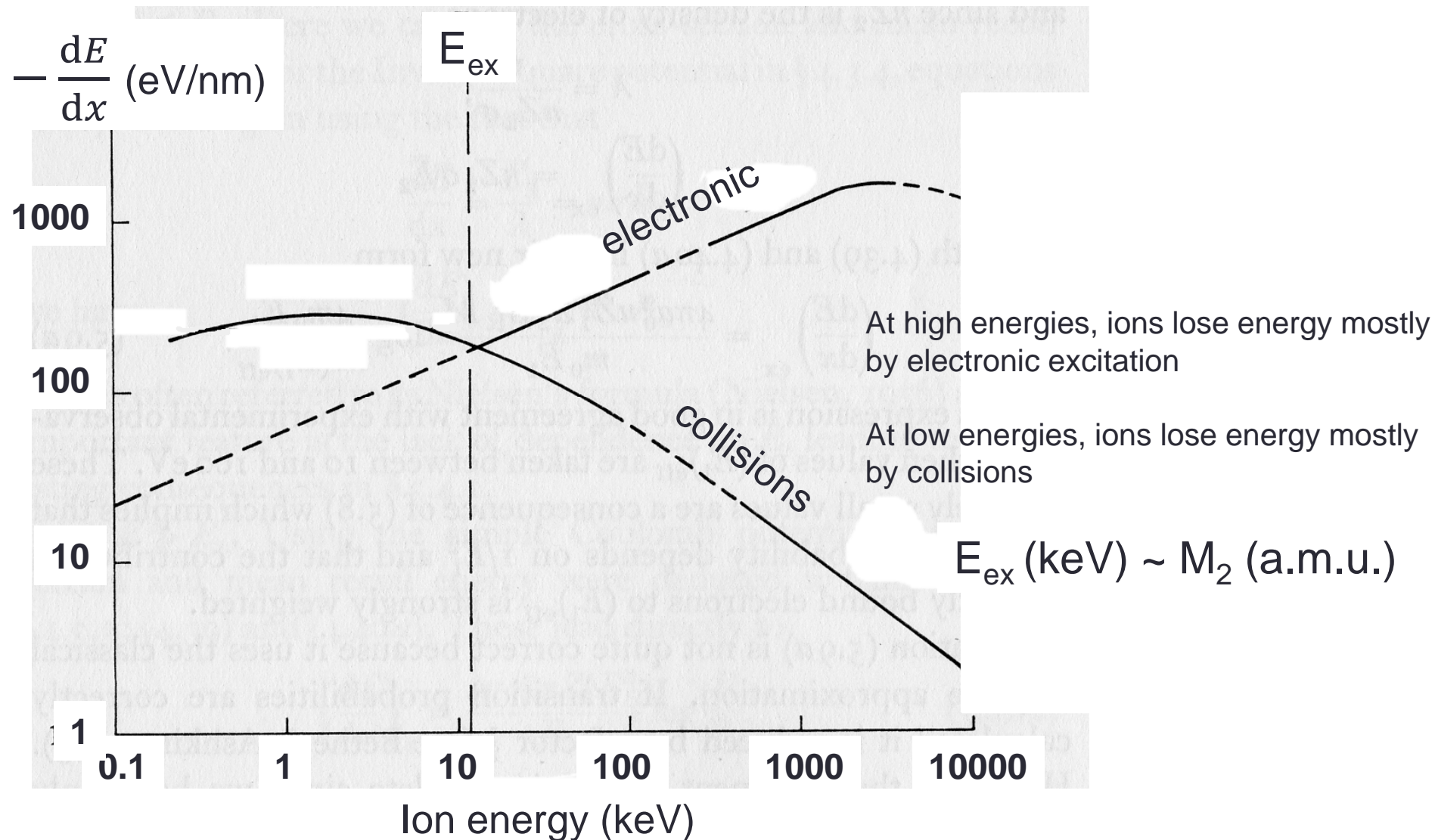
Spacing between neutron collisions is ~ 10 - 20mm





# The collision cascade

Energy loss from C ions in graphite



# SRIM / TRIM

The image displays the SRIM/TRIM software interface, which is used for simulating ion beam interactions with materials. The main window, titled "SRIM-2012.03", shows the simulation parameters and results for a He ion beam incident on a Tungsten target.

**TRIM Setup Window:**

- Type of TRIM Calculation:** DAMAGE (Detailed Calculation with full Damage Cascades)
- Basic Plots:** Ion Distribution with Recoils projected on Y-Plane
- ION DATA:** He, 4.003 amu, 500 keV, 0 degrees
- TARGET DATA:** Tungsten, 74, 193.8, 1, 100, 25, 3, 8.6
- Special Parameters:** Stopping Power Version: SRIM-2008, Max Target Depth: 20000

**Simulation Results:**

- ION:** He (10) into Layer 1 (1 layers, 1 atoms)
- Calculation Parameters:** Backscattered ions: 2, Transmitted ions: 0, Vacancies/ion: 219.7
- ION STATS:** Longitudinal Range: 762 Å, 1467 Å; Lateral Proj.: 1617 Å, 2117 Å; Radial: 2634 Å, 1511 Å
- ENERGY LOSS:** Ionization: 97.87, 0.51; Vacancies: 0.03, 0.11; Phonons: 0.23, 1.25
- SPUTTERING YIELD:** TOTAL: 0.000000, 0.00

**Depth vs. Y-Axis Plot:**

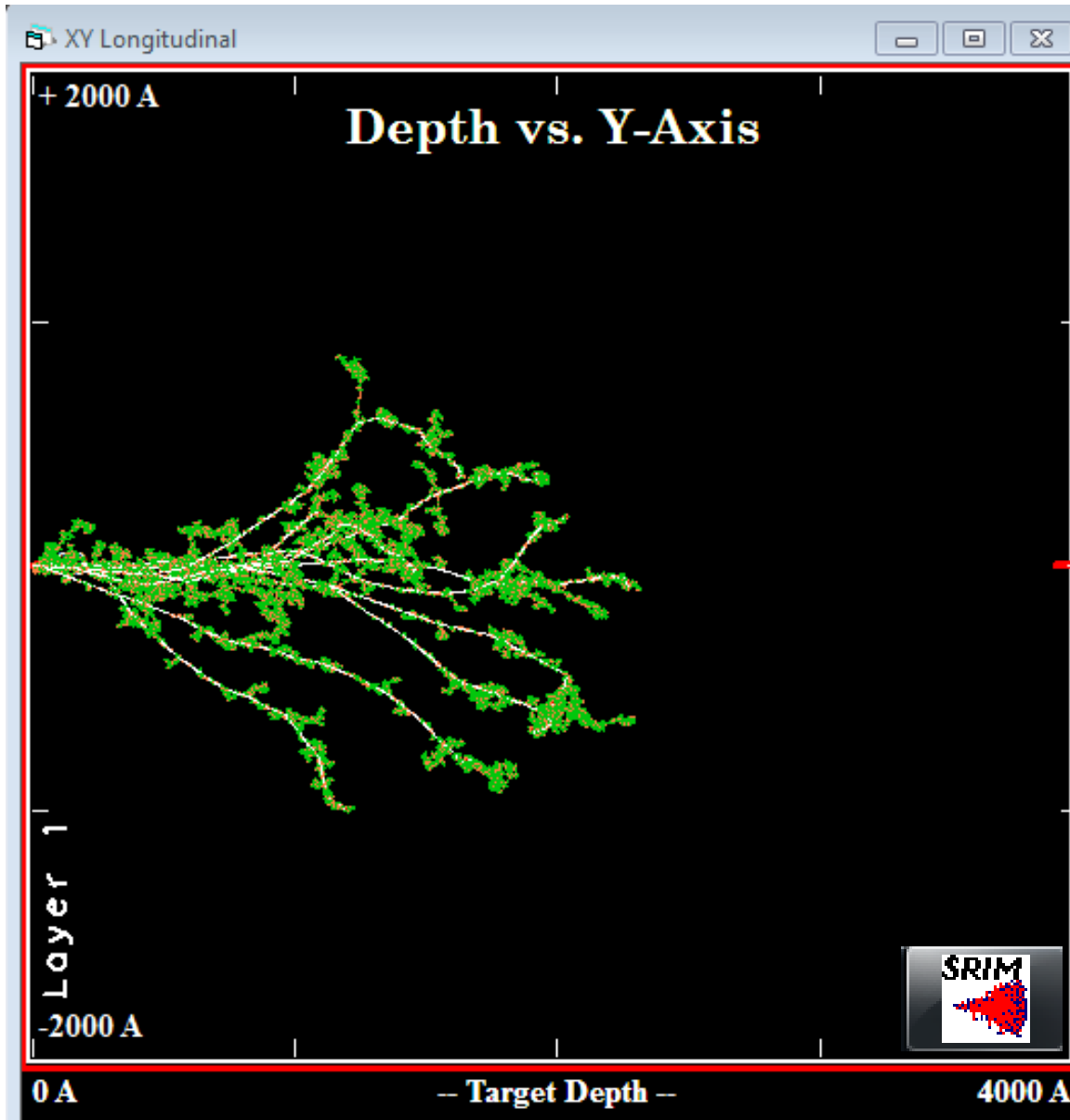
The plot shows the distribution of ions and recoils as they travel through the target. The Y-axis represents the depth (from -1 nm to +1 nm), and the X-axis represents the Y-axis (from 0 Å to 2 nm). The plot shows a dense cluster of ions and recoils near the surface, with a tail extending into the target.

**DISTRIBUTIONS:**

- Ion Distribution
- Ion/Recoil Distribution
- Lateral Range
- Ionization
- Phonons
- Energy to Recoils
- Damage Events
- Integral Sputtered Differential ions
- Backscattered ions
- Transmitted ions
- Collision Details
- 3-D Plots: Ion Distribution 3D, Recoil Dist. 3D, Ionization 3D, Phonons 3D, Target Damage 3D

<http://www.srim.org/>

# The collision cascade

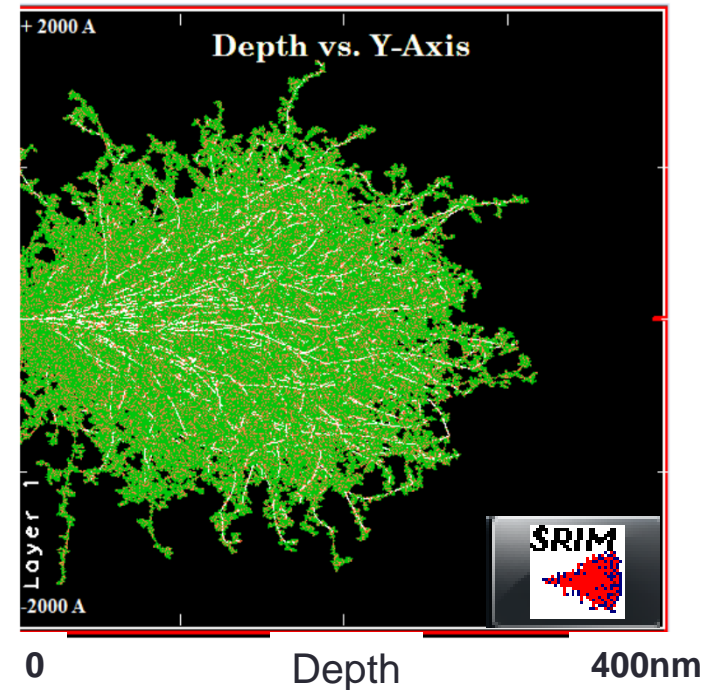
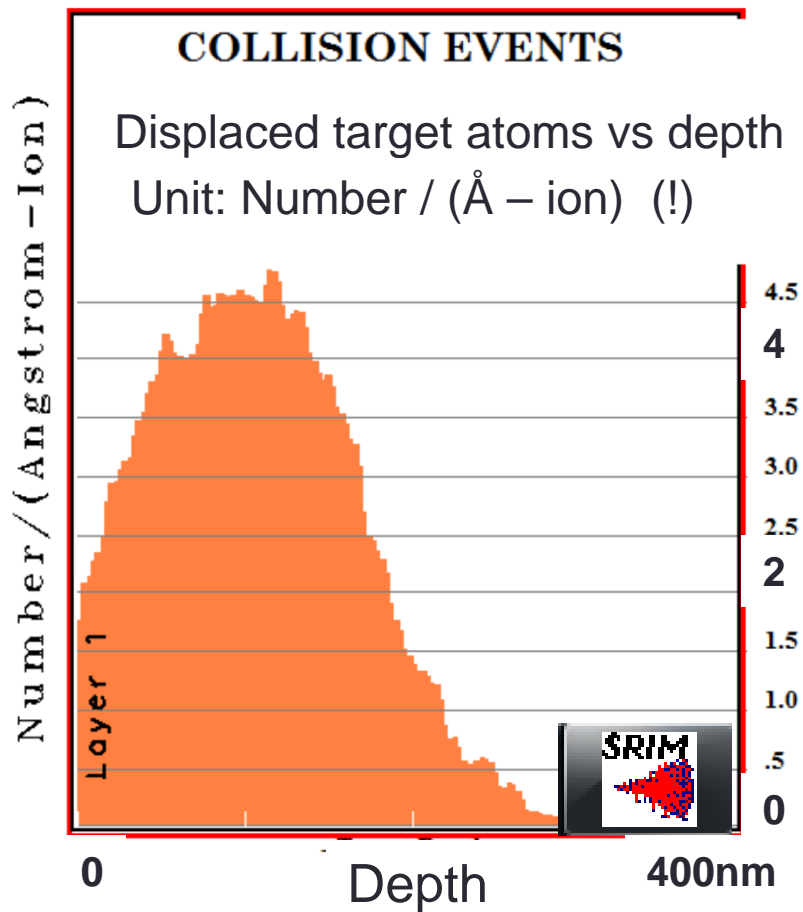


Tracks of ten 482keV Fe ions in Fe target.

“Consequent events” show in red and green.

Note long gaps between sub-cascades, and randomness of process.

# Ion irradiation: dpa



750 ion tracks:  
482keV Fe ion in Fe target

Here: Fe ions into Fe

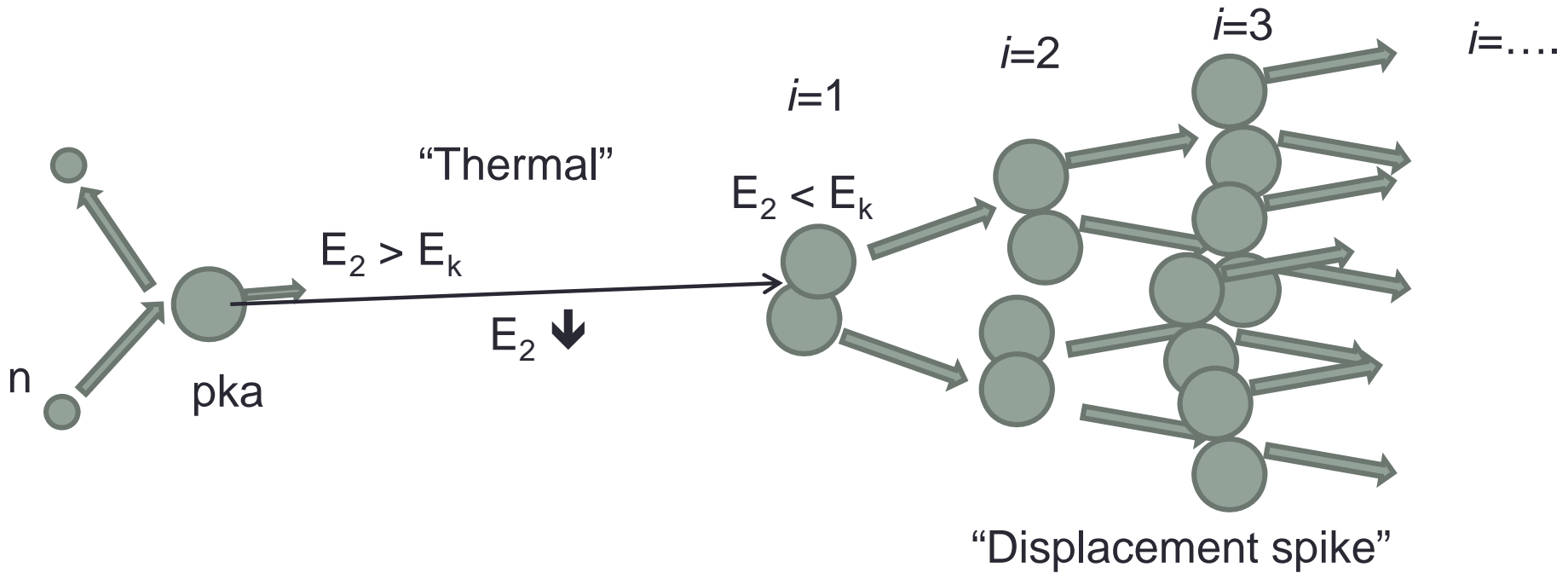
D: ~ 4.5 at peak  
 $\rho$ :  $8 \times 10^{28} \text{m}^{-3}$

$\phi$ : typically  $10^{18} \text{m}^{-2}$  ( $10^{14} \text{cm}^{-2}$ )  
= 0.56 dpa

dpa = displacements per (target) atom  

$$= \frac{D\phi}{\rho}$$
 D: displacements / (m – ion)  
 $\phi$ : irradiating particles /  $\text{m}^2$   
 $\rho$ : atoms /  $\text{m}^3$  in target

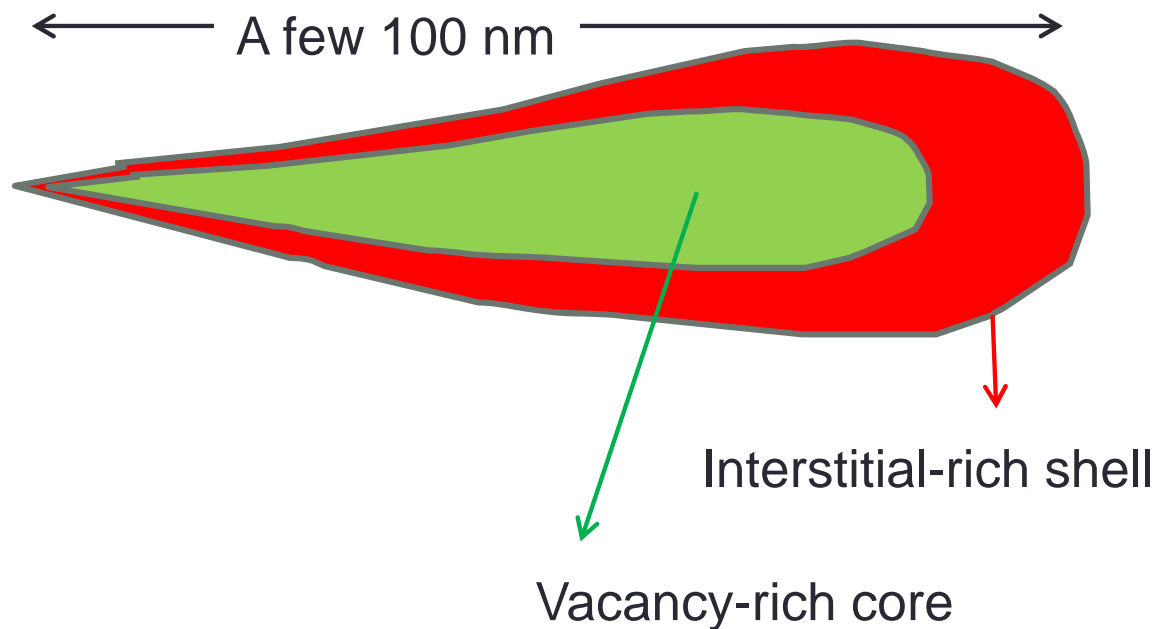
# The collision cascade: evolution after initiation



After  $i^{\text{th}}$  stage,  
We have  $2^i$  displaced atoms:

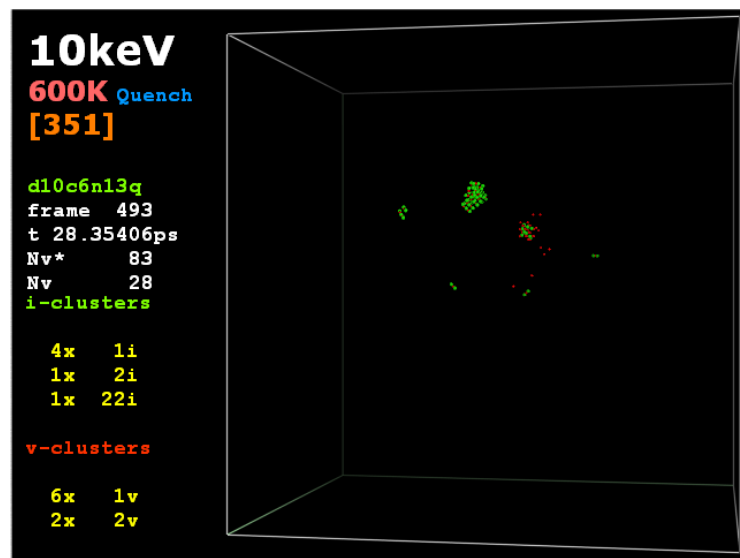
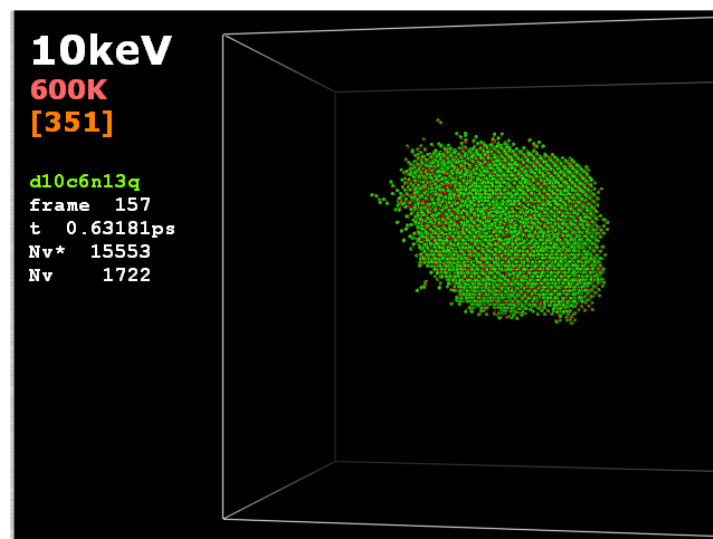
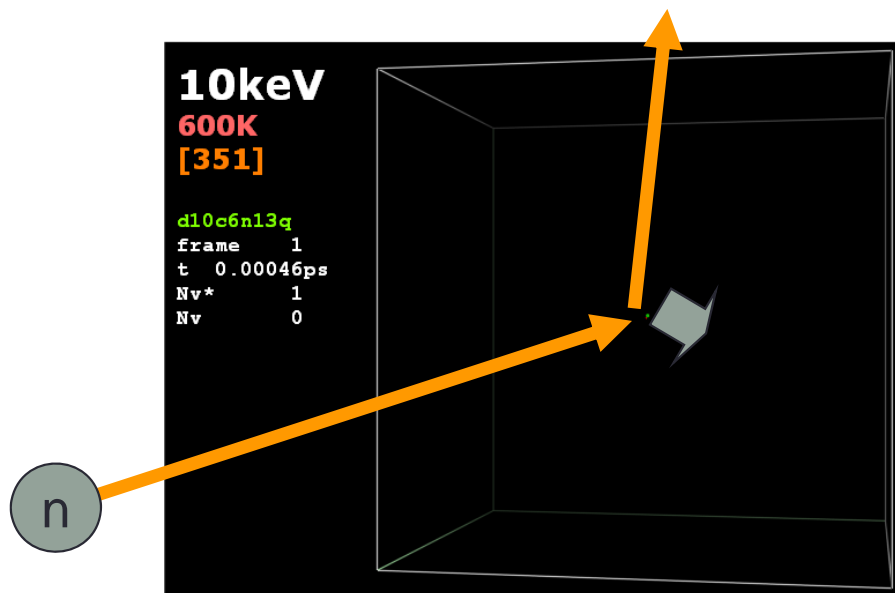
$$\text{Stops when: } \frac{E_k}{2^i} < 2E_d$$

$$\text{So } N_{\text{displacements}} = 2^i = E_k / 2E_d$$





# The collision cascade: evolution after initiation



“Molecular dynamics” simulation: up to 30 ps.

Only the out-of-place atoms are shown –  
vacancies in green; self interstitials in red.

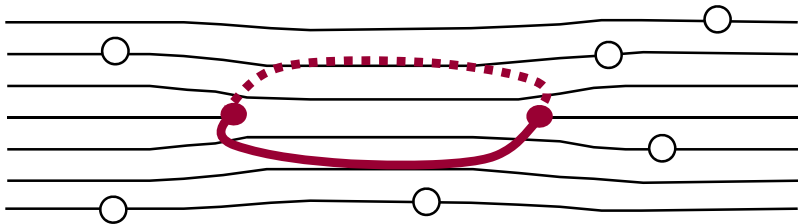
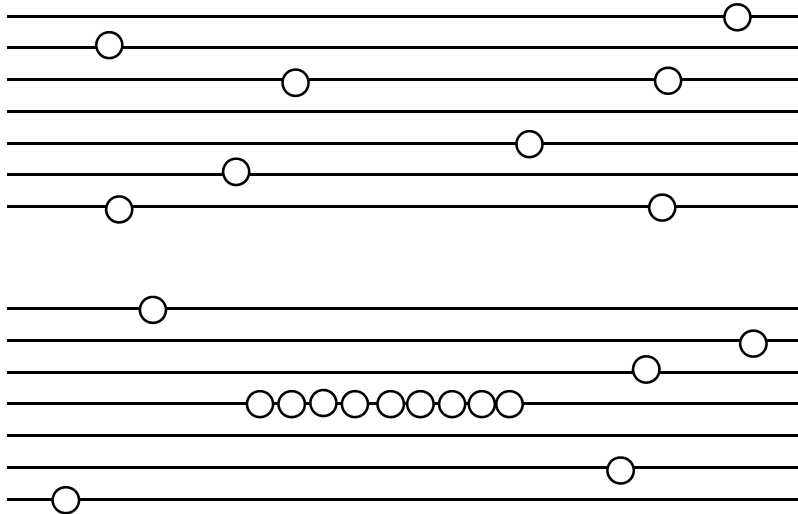
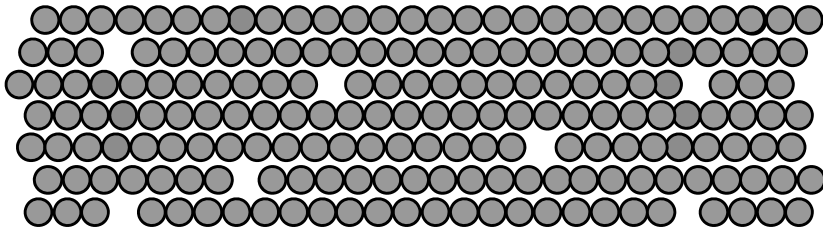
Started by a low-energy collision (10keV ion):  
end of cascade branch.

$$10 \text{ keV} < E_{\text{ex}}$$

$$\text{so } N_{\text{displacement}} \sim 10000/25 = 400$$



# Radiation → dislocation loops

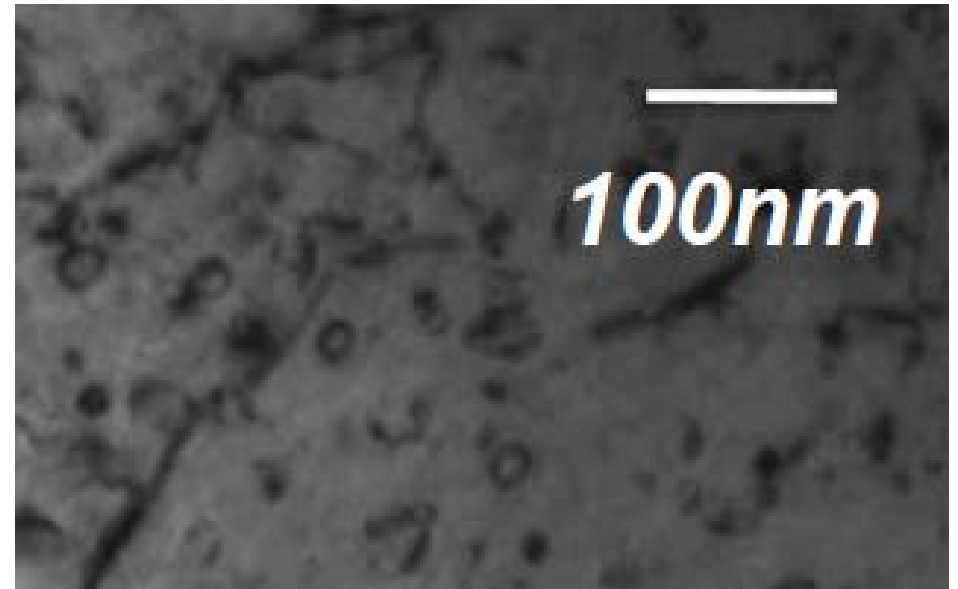
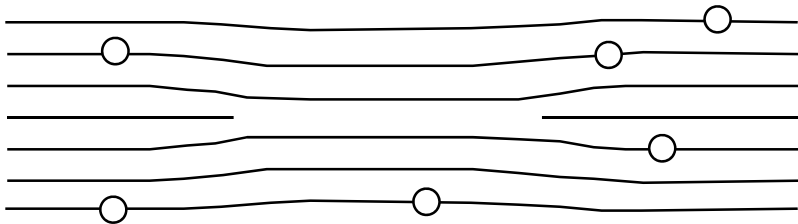
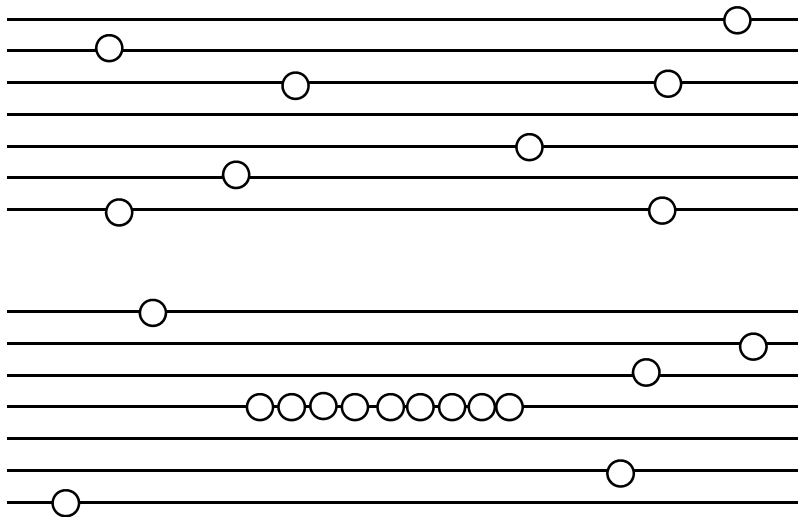
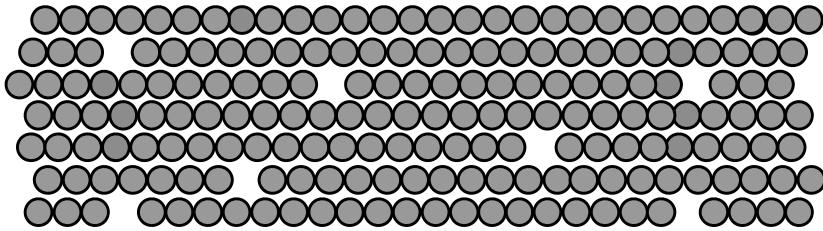


Missing sheet of atoms



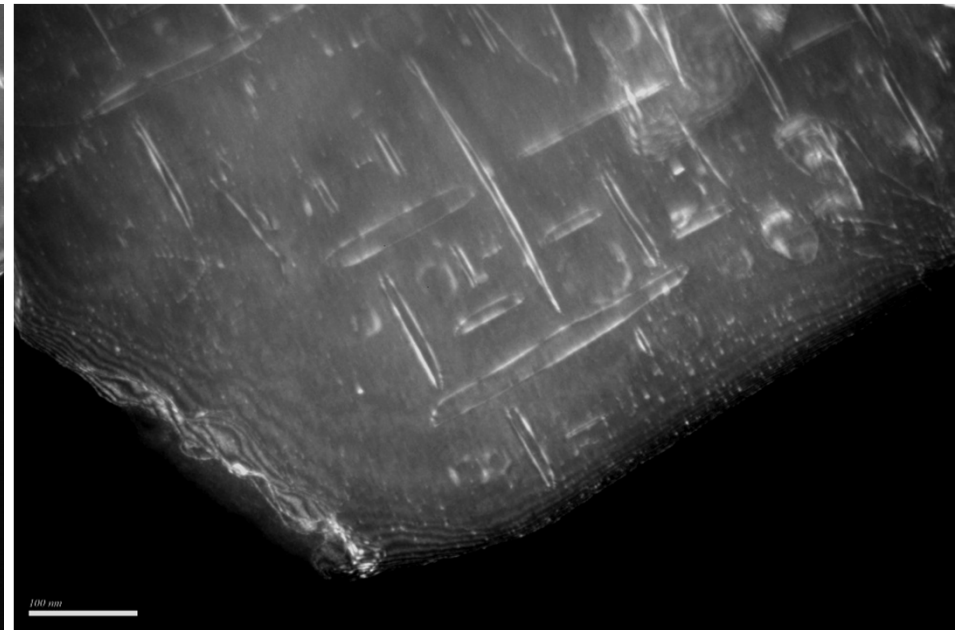
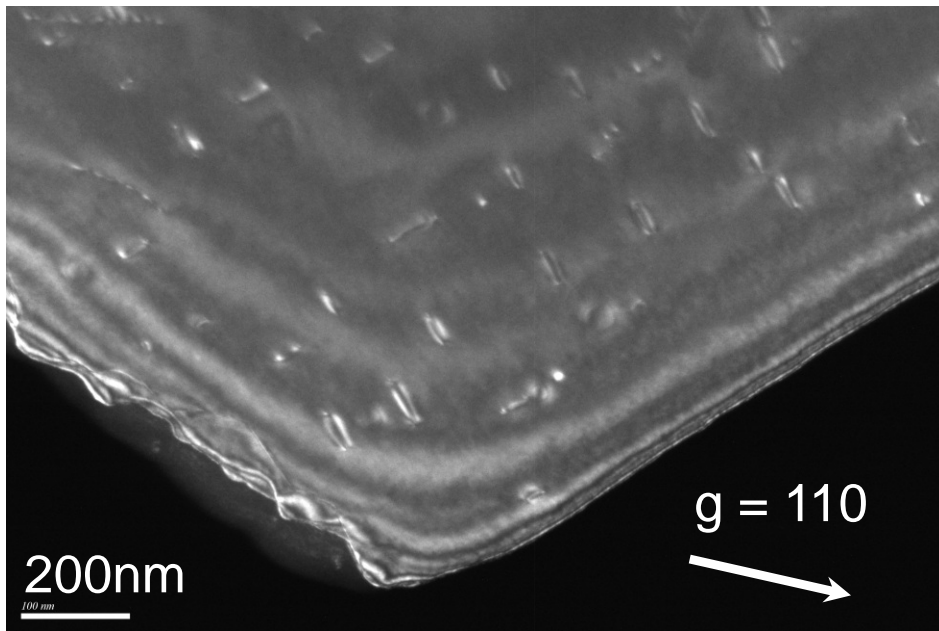
Dislocation loop

# Radiation → dislocation loops



Iron, ion-irradiated to 2.5 dpa at 300°C

## Dislocation loops in Fe irradiated at 500°C



Dose:  $3 \times 10^{18}$  ions  $\text{m}^{-2}$ ,

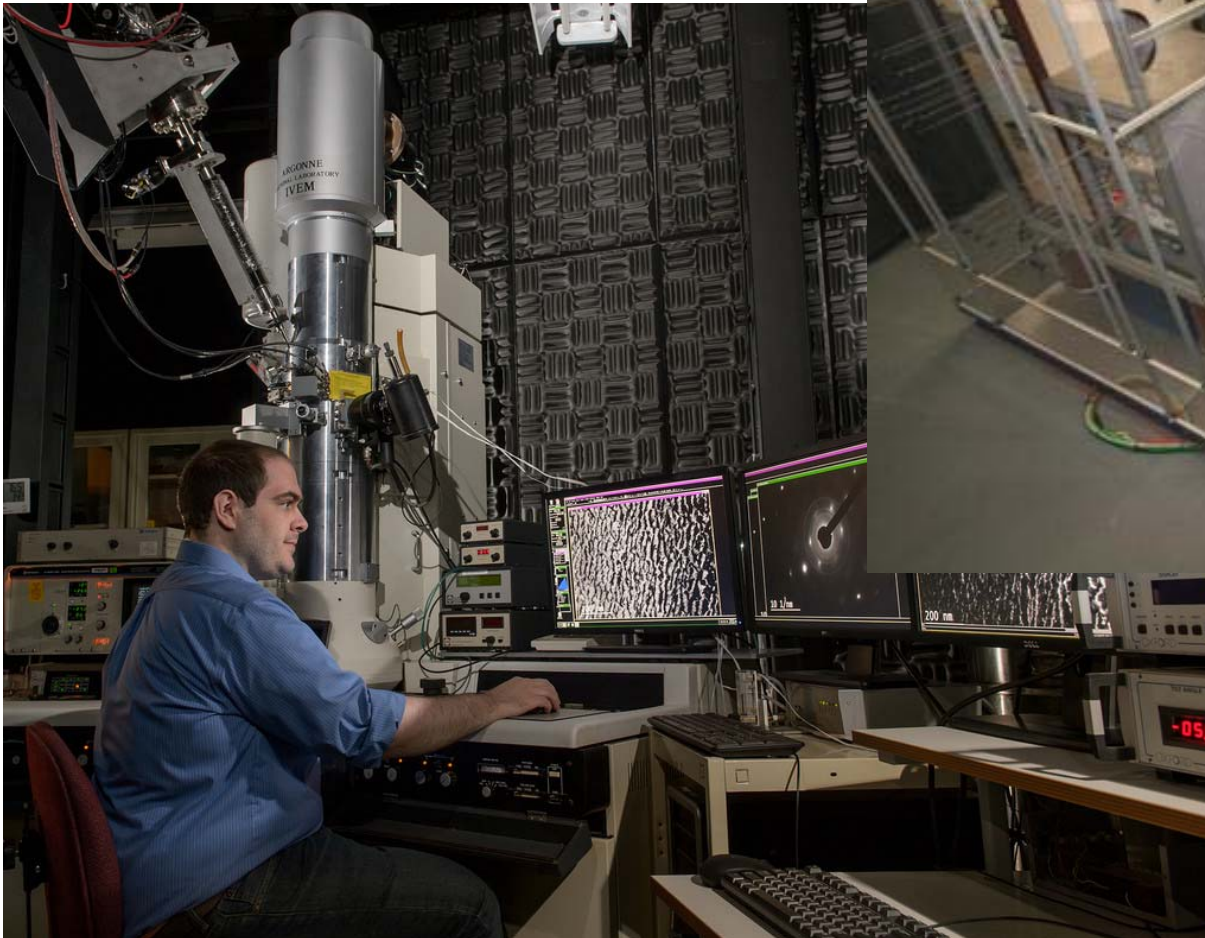
Dose:  $1 \times 10^{19}$  ions  $\text{m}^{-2}$

UHP-Fe irradiated at 500°C with 150 keV  $\text{Fe}^+$  ions

- loops are of  $\langle 100 \rangle$  type.
- loops are of *interstitial* type

# Radiation Damage as it happens...

IVEM – Argonne NL



MIAMI – U. Huddersfield



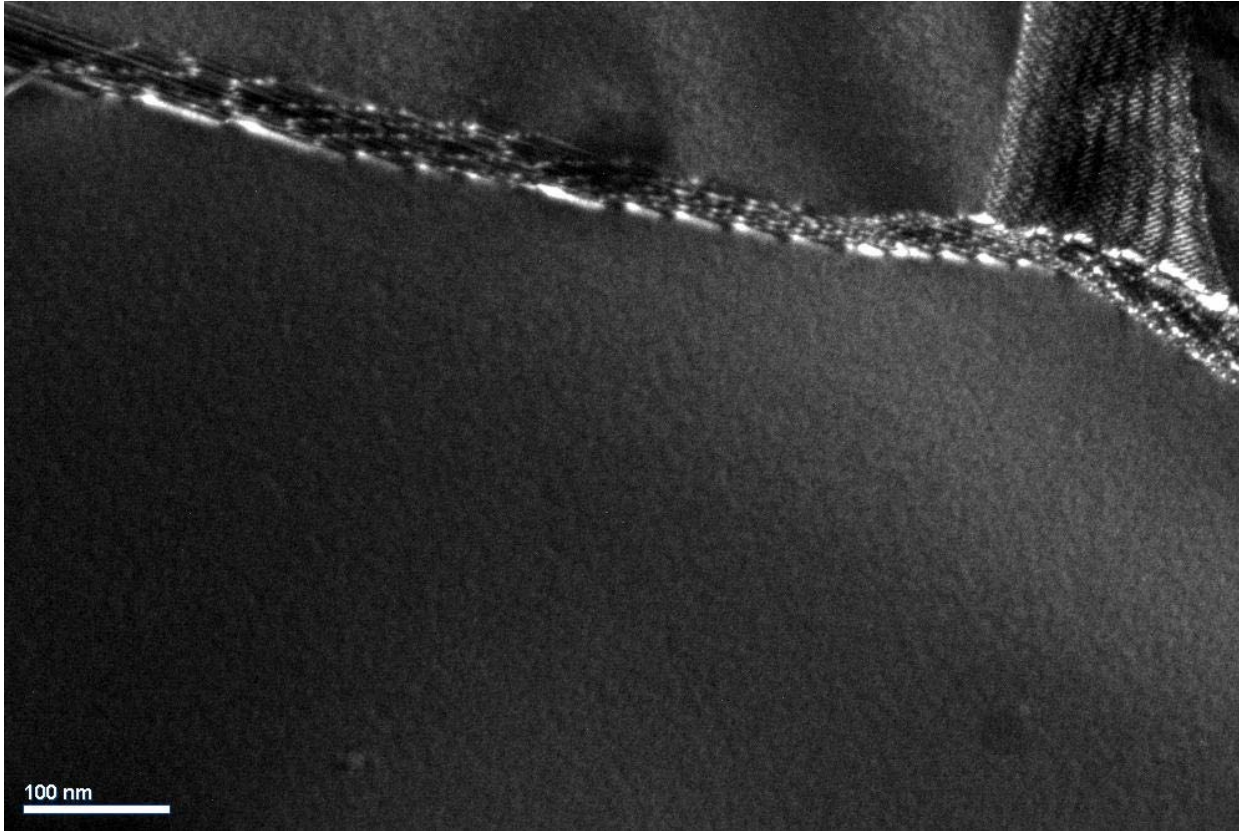
# Damage accumulation; Fe, 300°C , high dose



# Loop density vs dose: W-5%Re

g=200  
0

Unit:  $10^{13}W^+/cm^2$





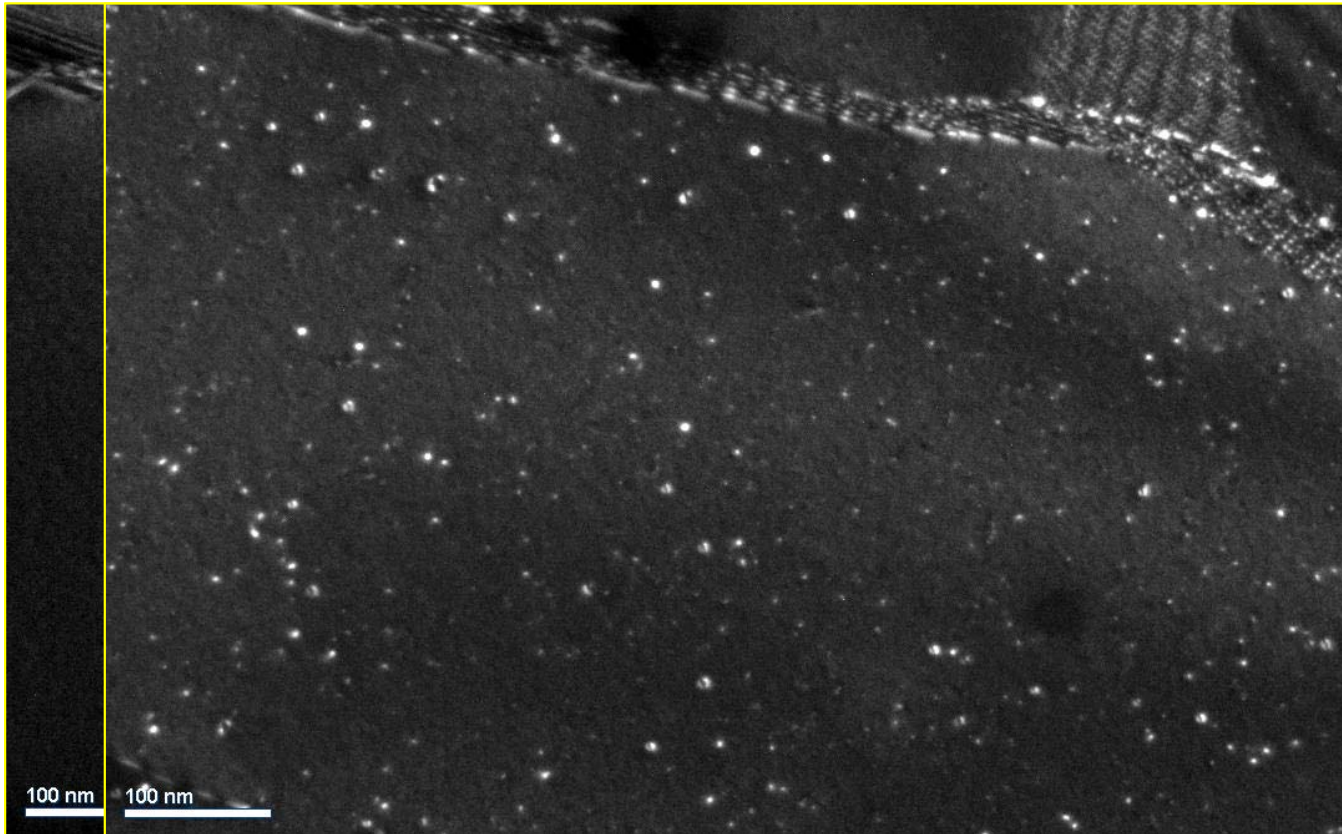
# Loop density vs dose: W-5%Re

$g=200$

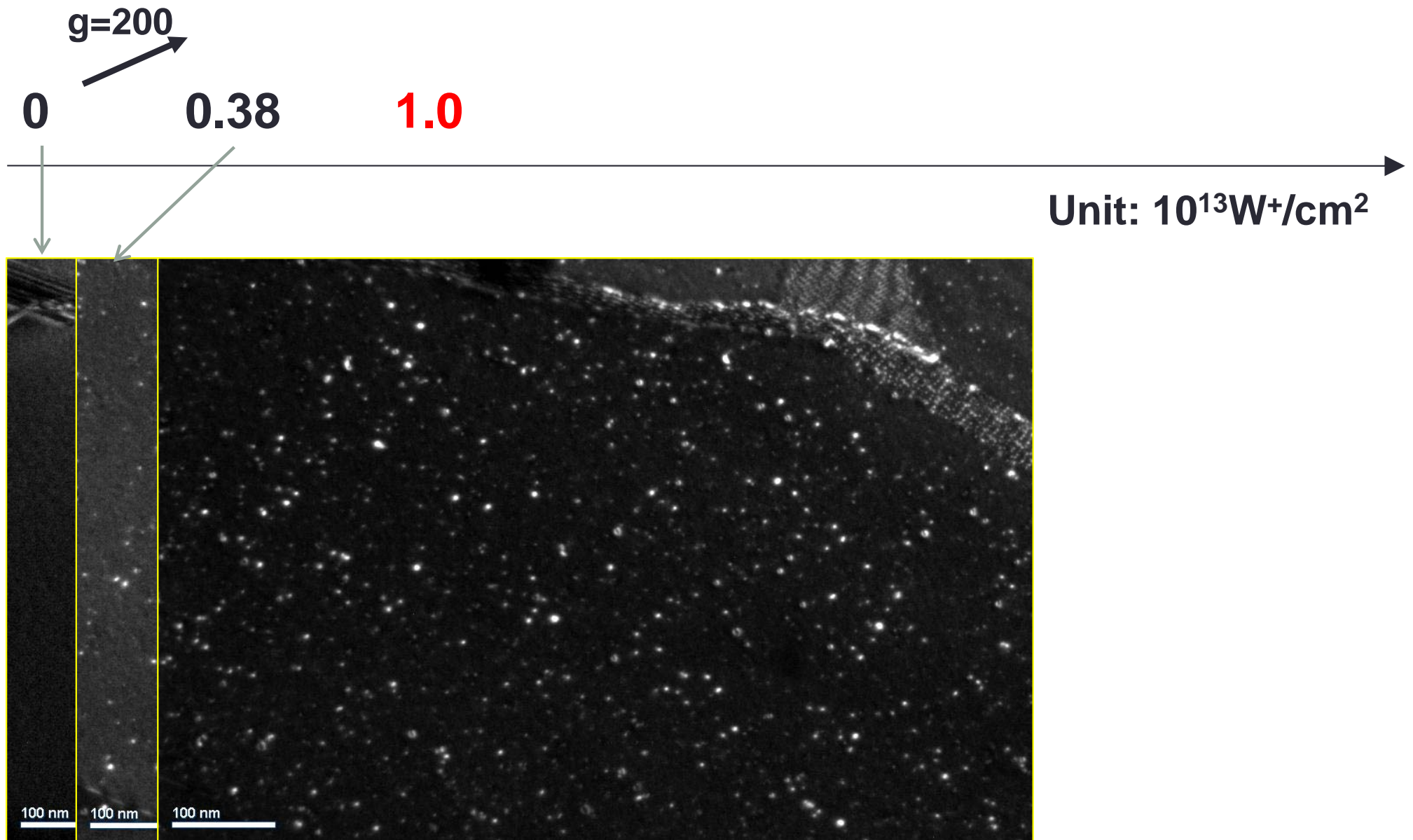
0

0.38

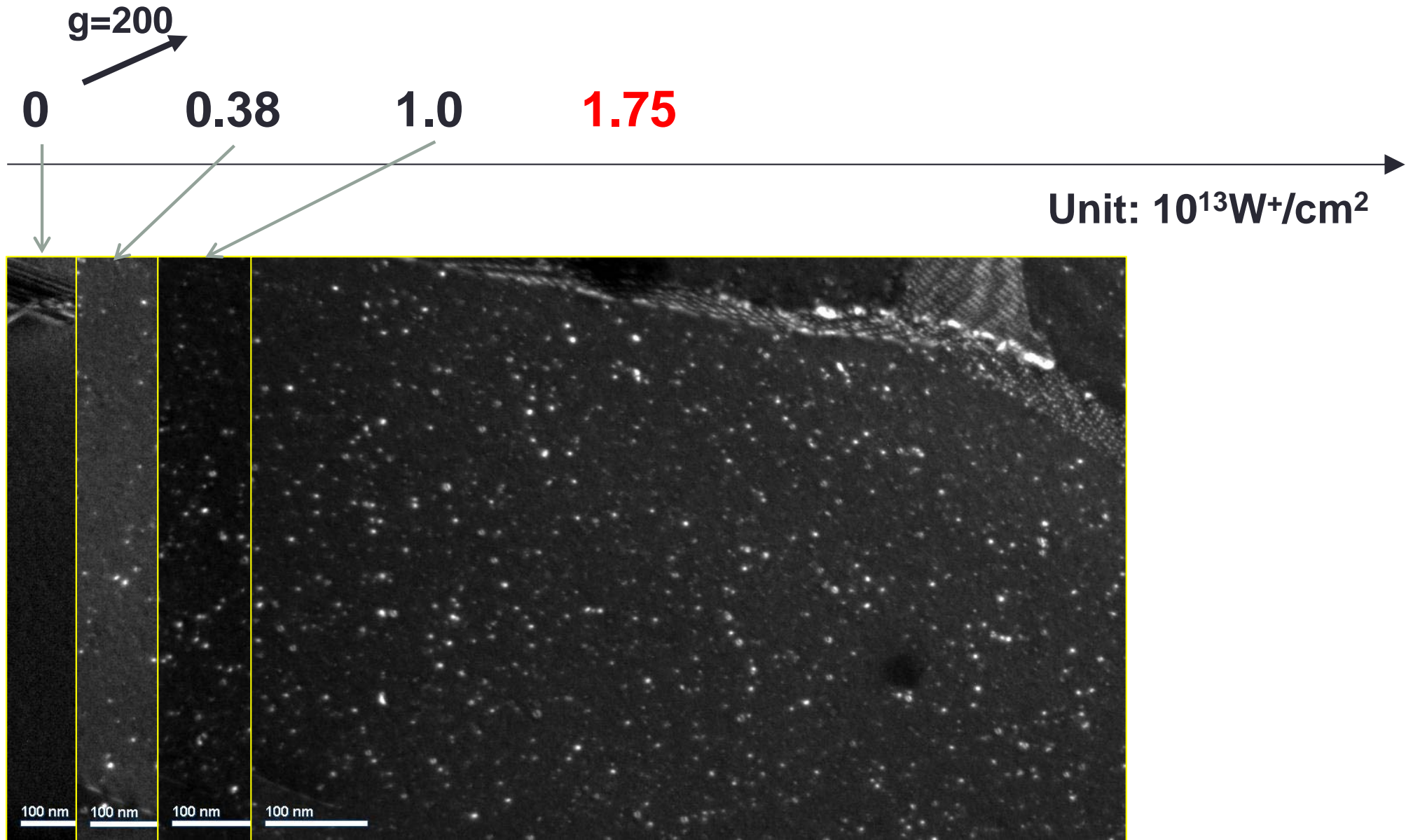
Unit:  $10^{13}W^+/cm^2$



# Loop density vs dose: W-5%Re

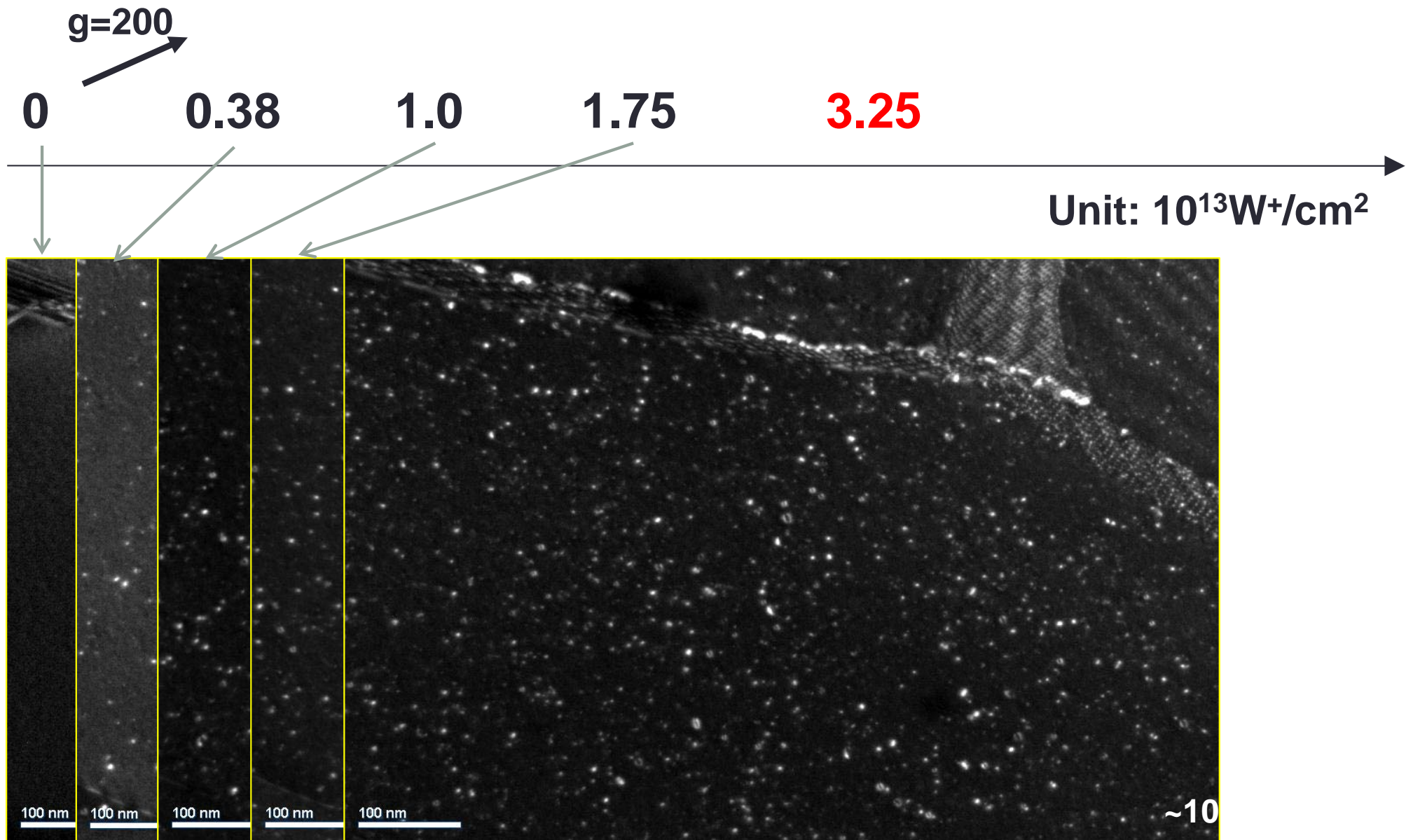


# Loop density vs dose: W-5%Re

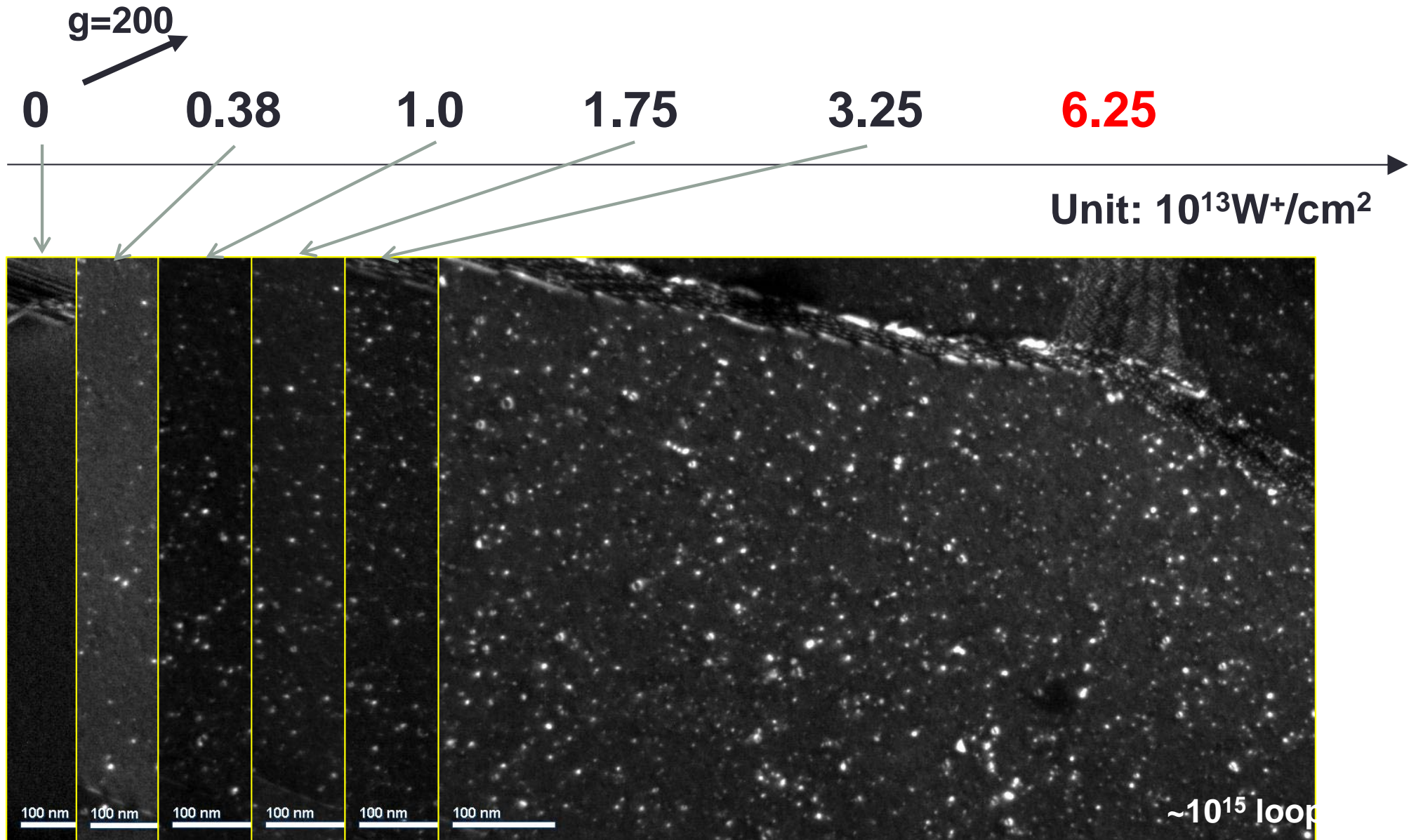




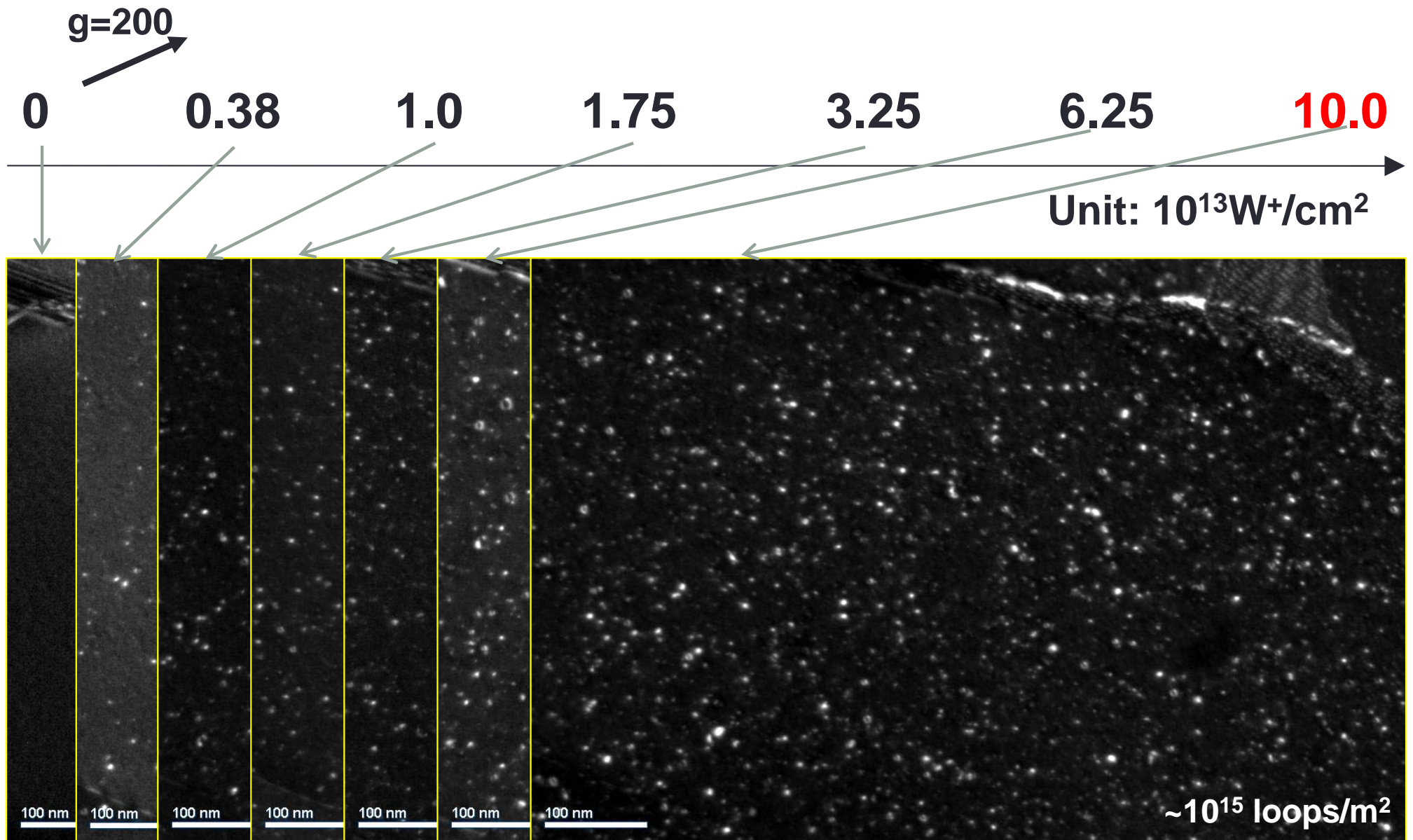
# Loop density vs dose: W-5%Re



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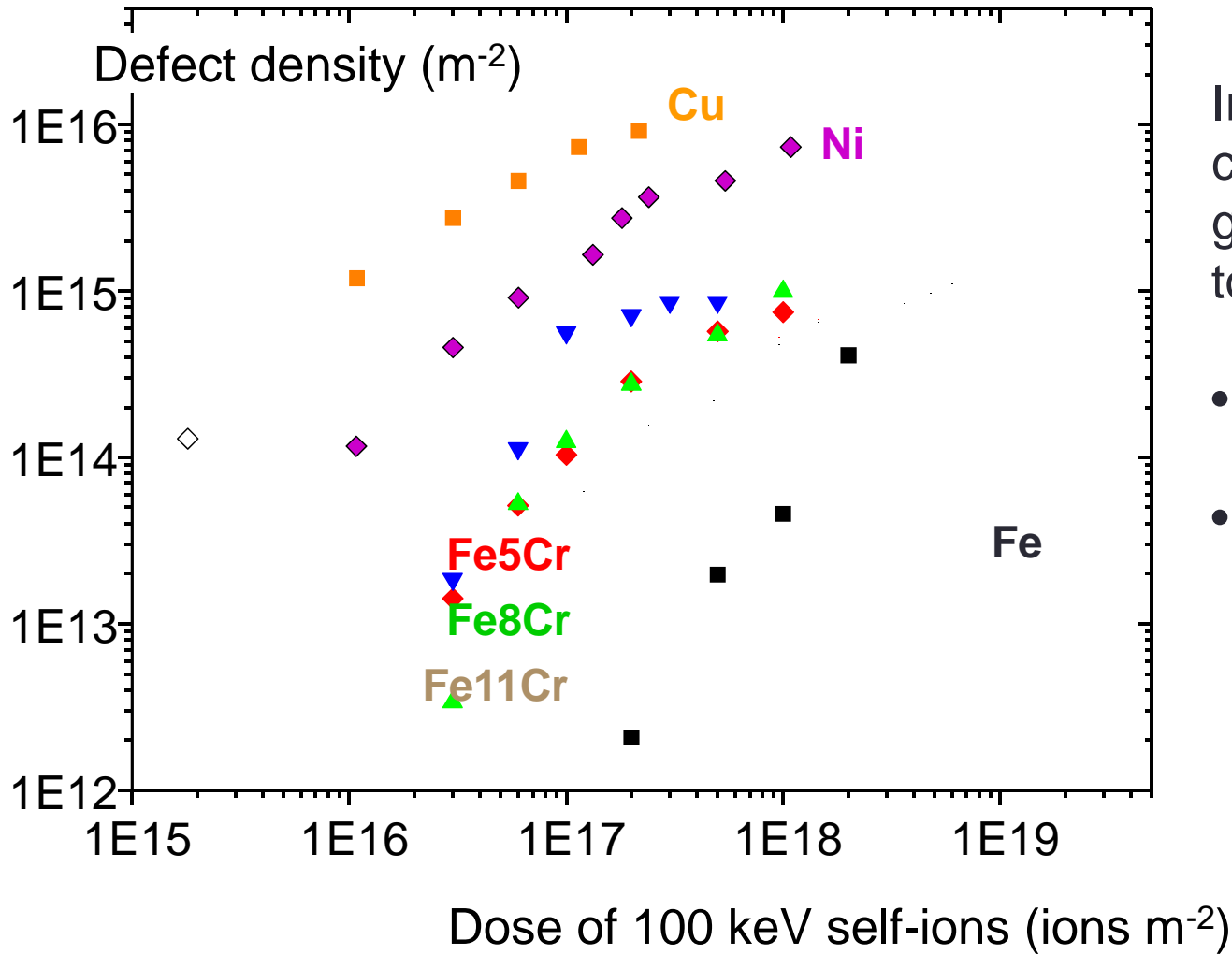
# Loop density vs dose: W-5%Re





# Self-ion irradiations of pure materials and FeCr alloys

## - 100keV room temperature irradiations



Iron-based metals (Body centred cubic metals in general?) are more resistant to radiation damage.

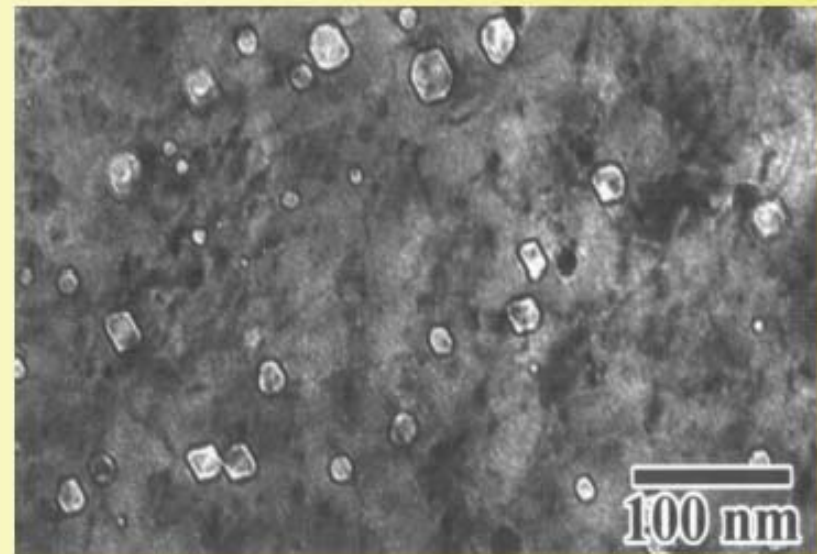
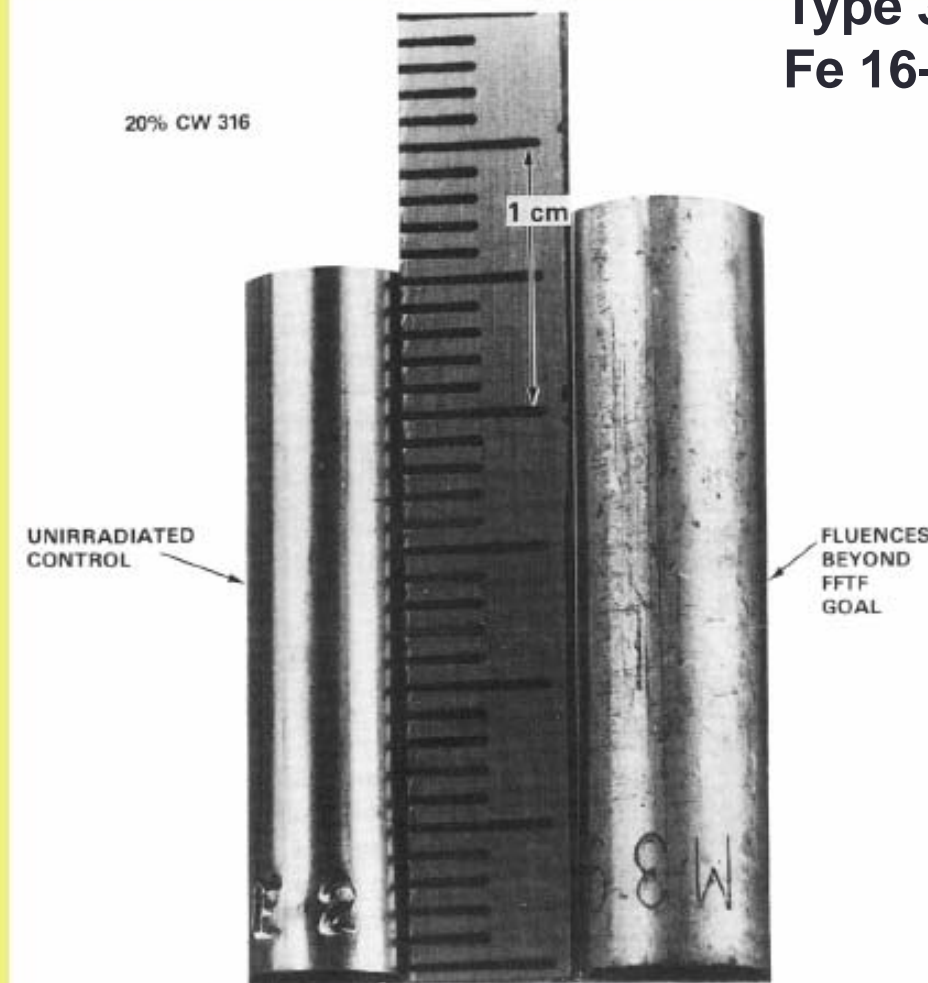
- Fewer defects
- Threshold dose

# Effects of radiation damage on materials

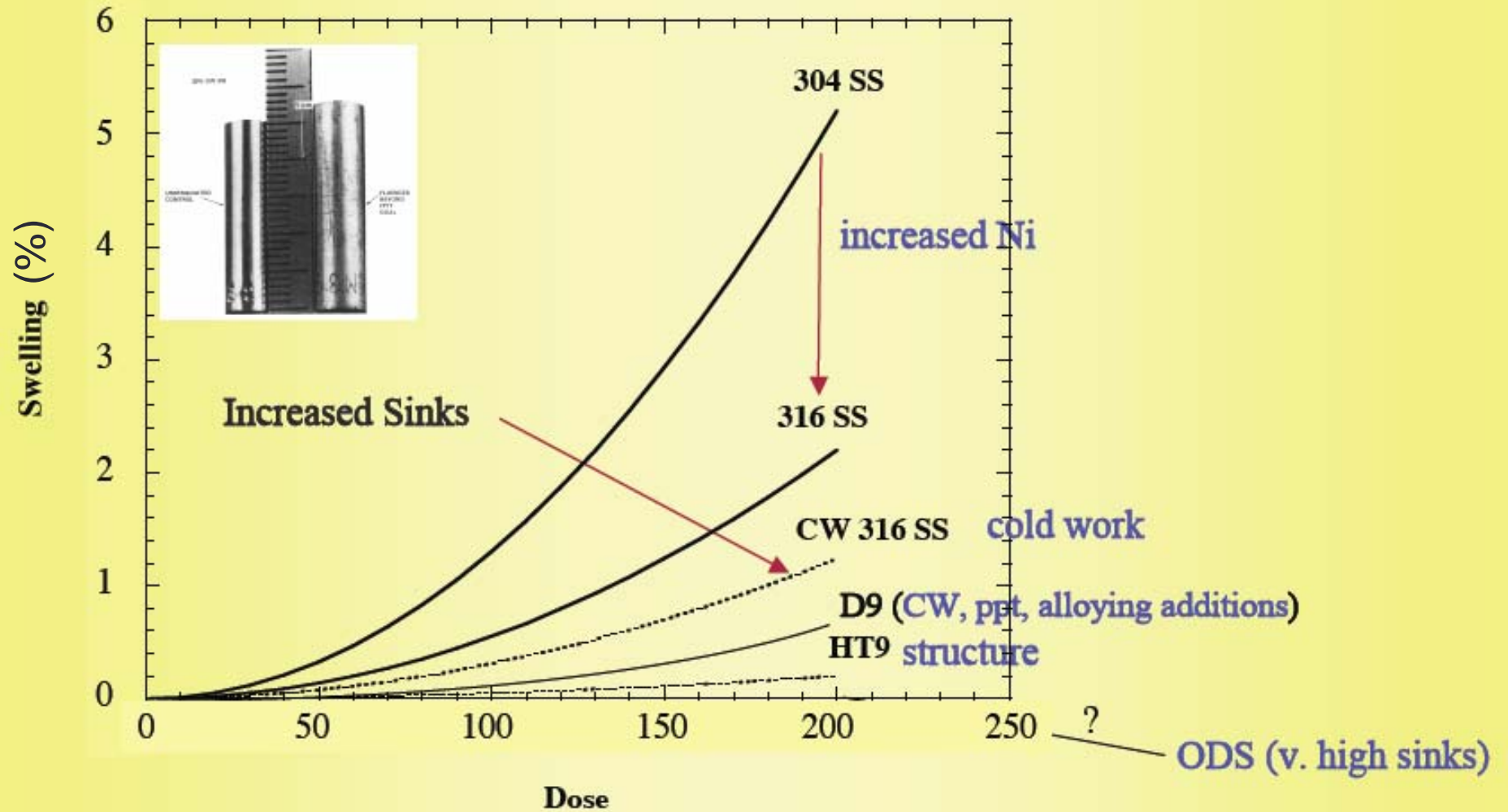
1. **Sputtering**
2. **Stored energy**
  - a) “Wigner energy” release
3. **Point defect accumulation**
  - a) Swelling, dislocation loops, nano-voids
  - b) Changes in thermal & electrical conductivity
4. **Enhanced diffusion**
  - a) Radiation-enhanced creep
  - b) Faster kinetics of phase transitions
  - c) Radiation-enhanced grain-boundary segregation
5. **Gas from transmutation**
  - a) Bubbles, swelling (with 2)
6. **Soluble and insoluble transmutation products**
  - a) Hardening, precipitation
7. **Knock-on randomisation of structure**
8. **Non-equilibrium microstructures?** (related to 3, 6)
9. **Hardening** (from 2, 4, 5)
10. **Embrittlement** (from 7, 3c, 4)
11. **Radiation-enhanced corrosion** (related to 3a, maybe 5)

# Radiation-induced swelling

Type 316 stainless steel:  
Fe 16-18%Cr, 10-14%Ni, 2%Mo, <0.08%C

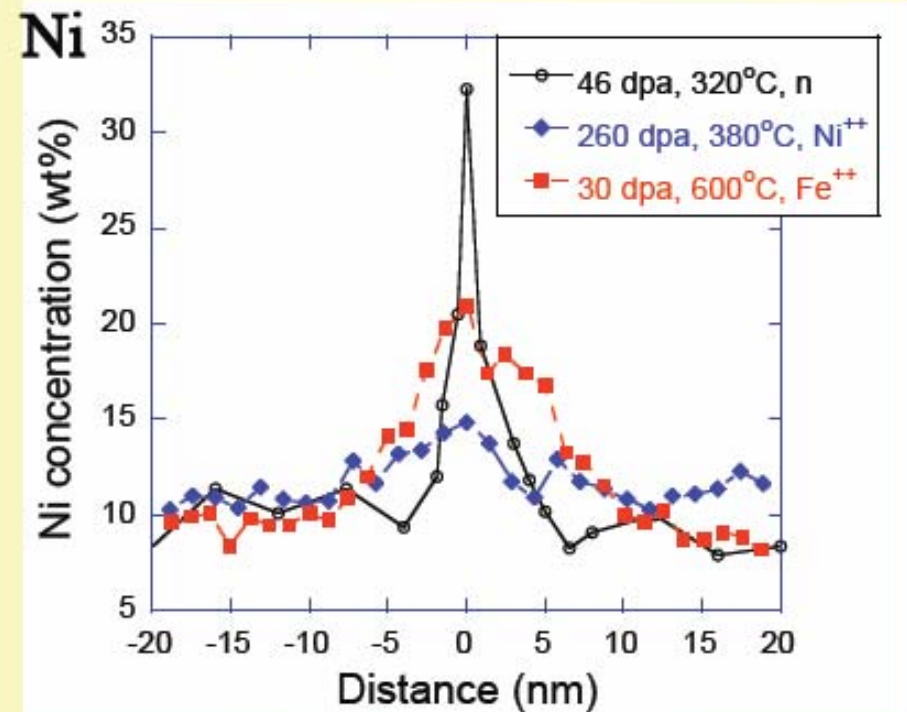
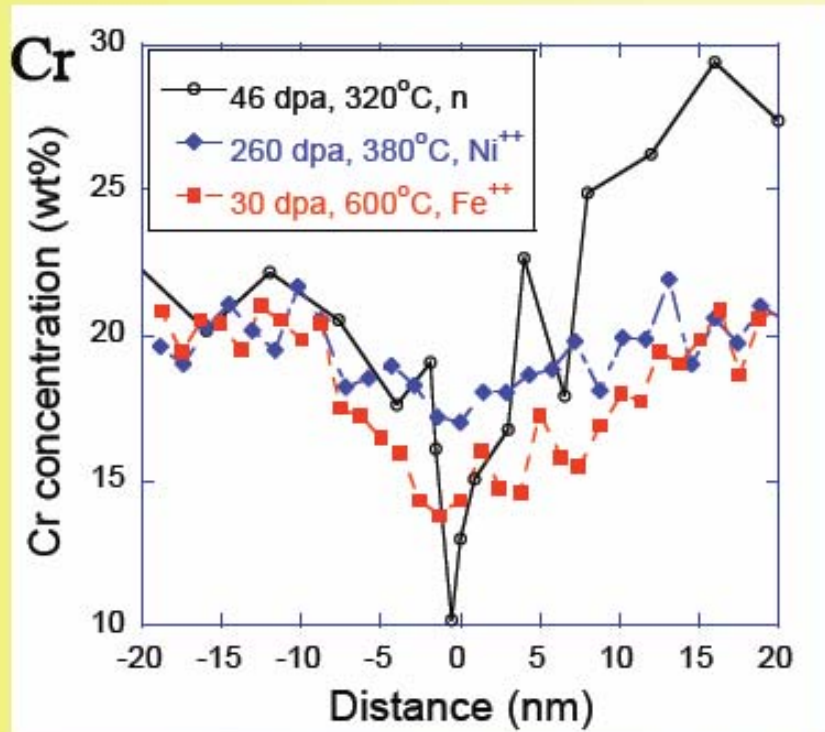


# Radiation-induced swelling



# Radiation-induced grain boundary segregation

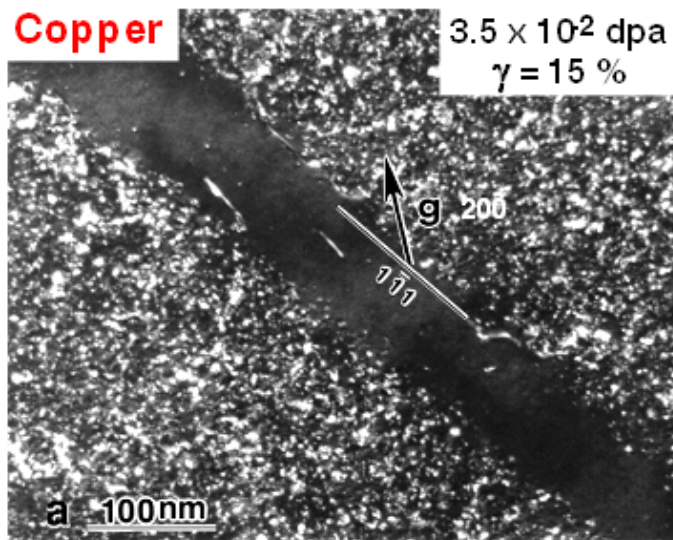
Type 304L stainless steel: Fe 18-20%Cr, 8-12%Ni, <0.03%C



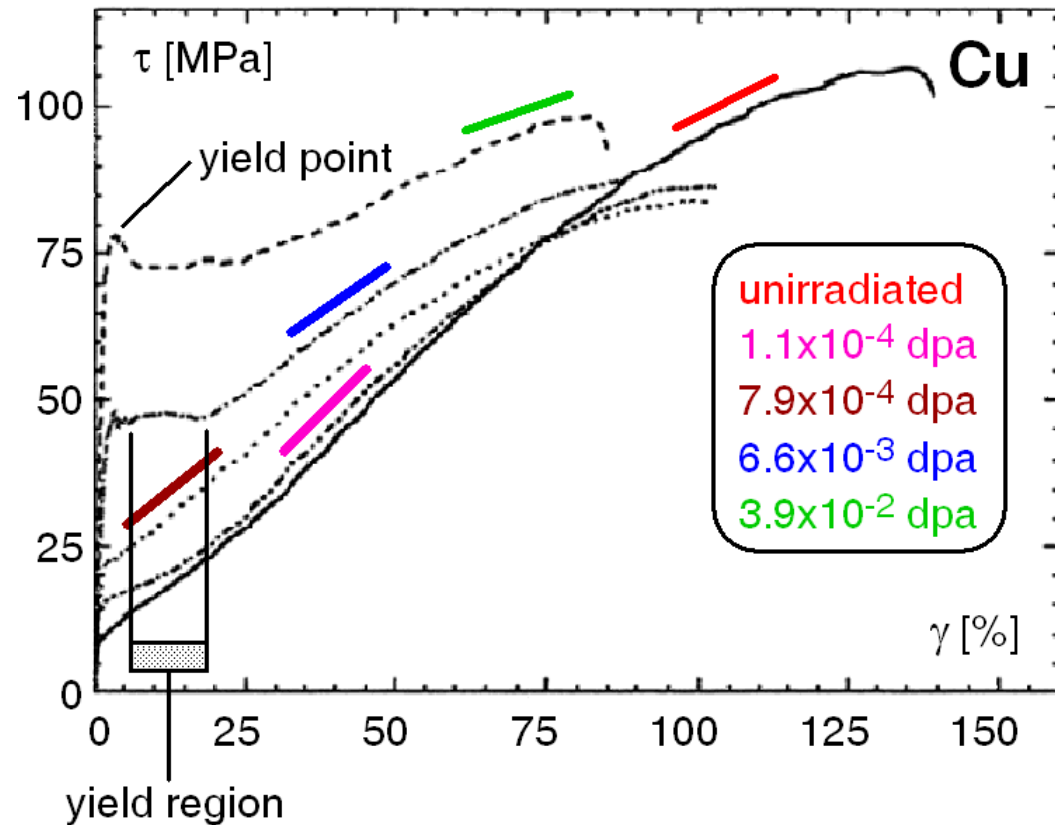
- Depletion of Cr and enrichment of Ni are consistent among all the irradiations.
- Self-ion irradiations produced wider and shallower segregation profiles compared to those by neutron irradiations



# Radiation-induced dislocation loops: effects on mechanical properties

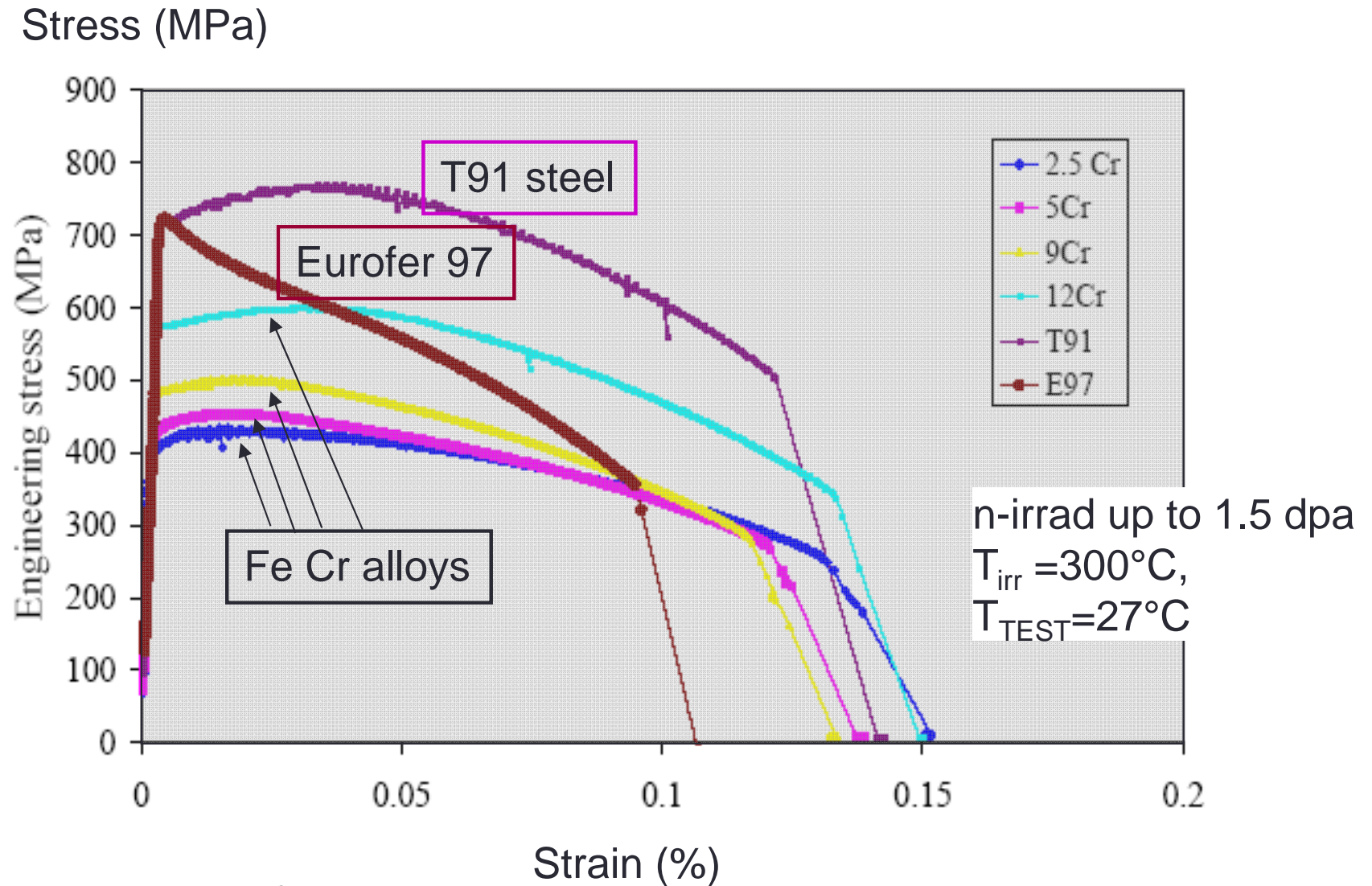


“Strain localisation”





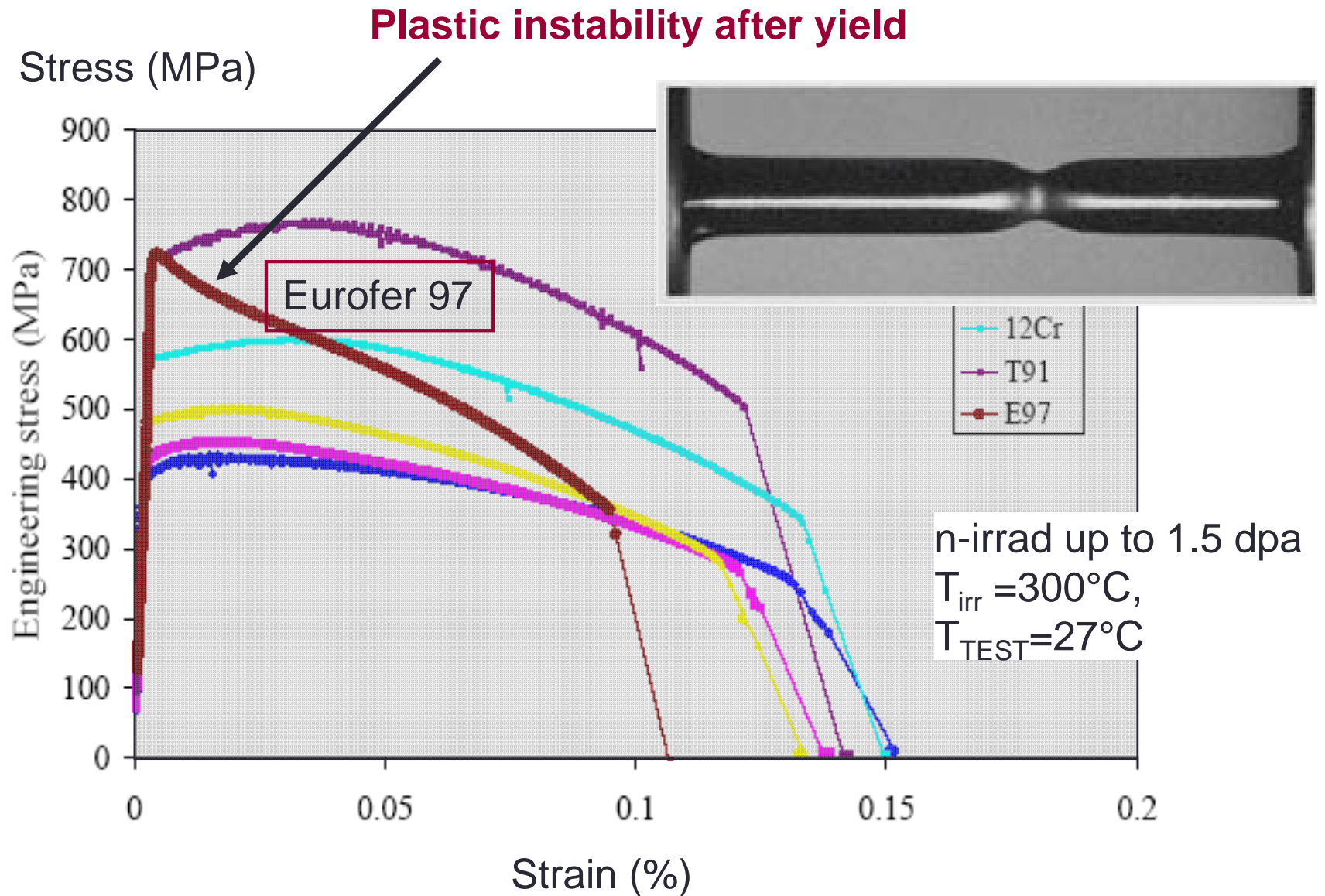
# Stress-strain curves: Iron alloys



Eurofer 97: Fe - 8.9%Cr - 1%W - 0.2%V - 0.14%Ta - 0.12%C

T91: Fe - 8.3%Cr - 0.4%Mn - 1%Mo - 0.2%V - 0.08% Nb - 0.1%C

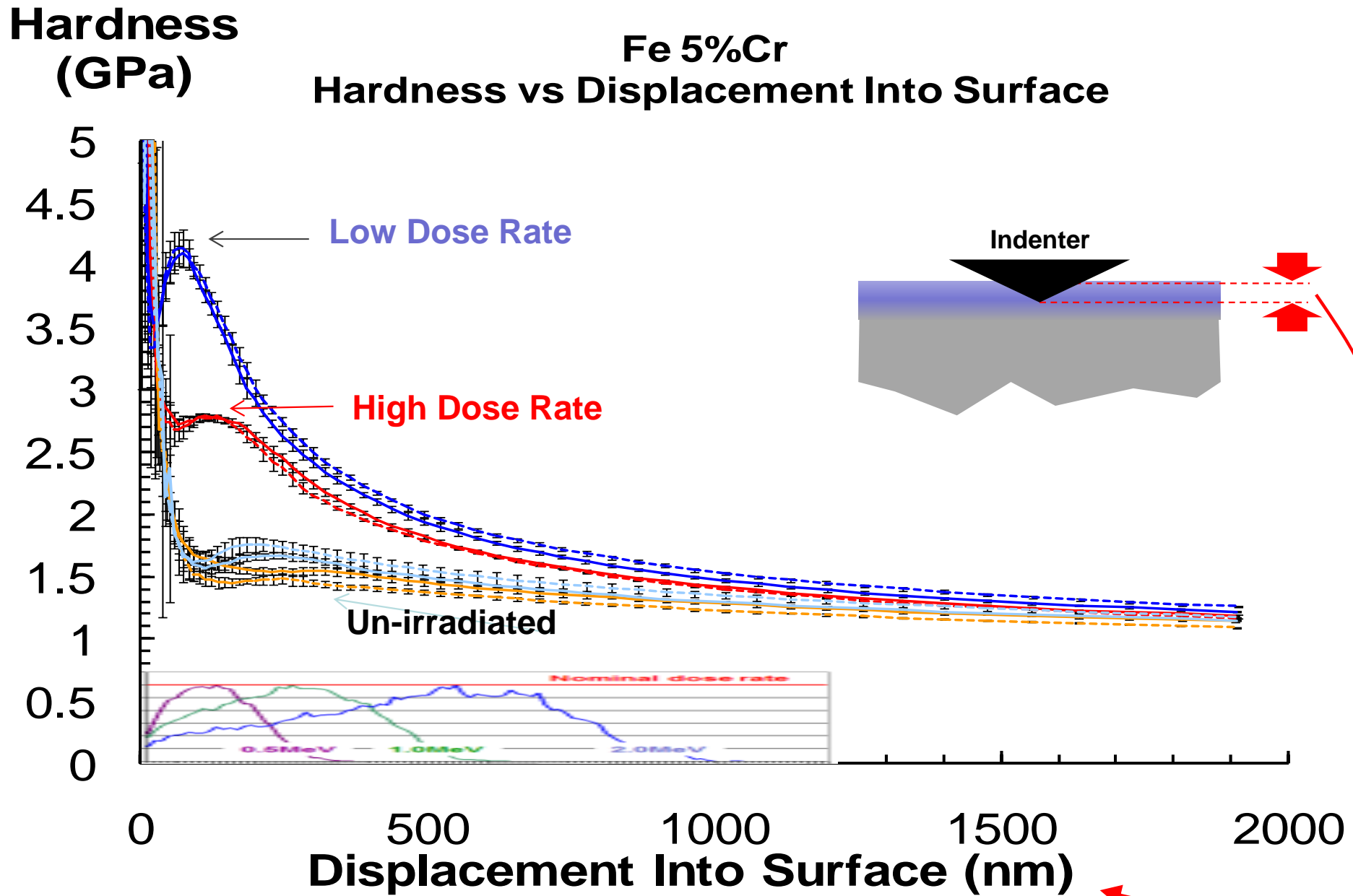
# Stress-strain curves: Iron alloys



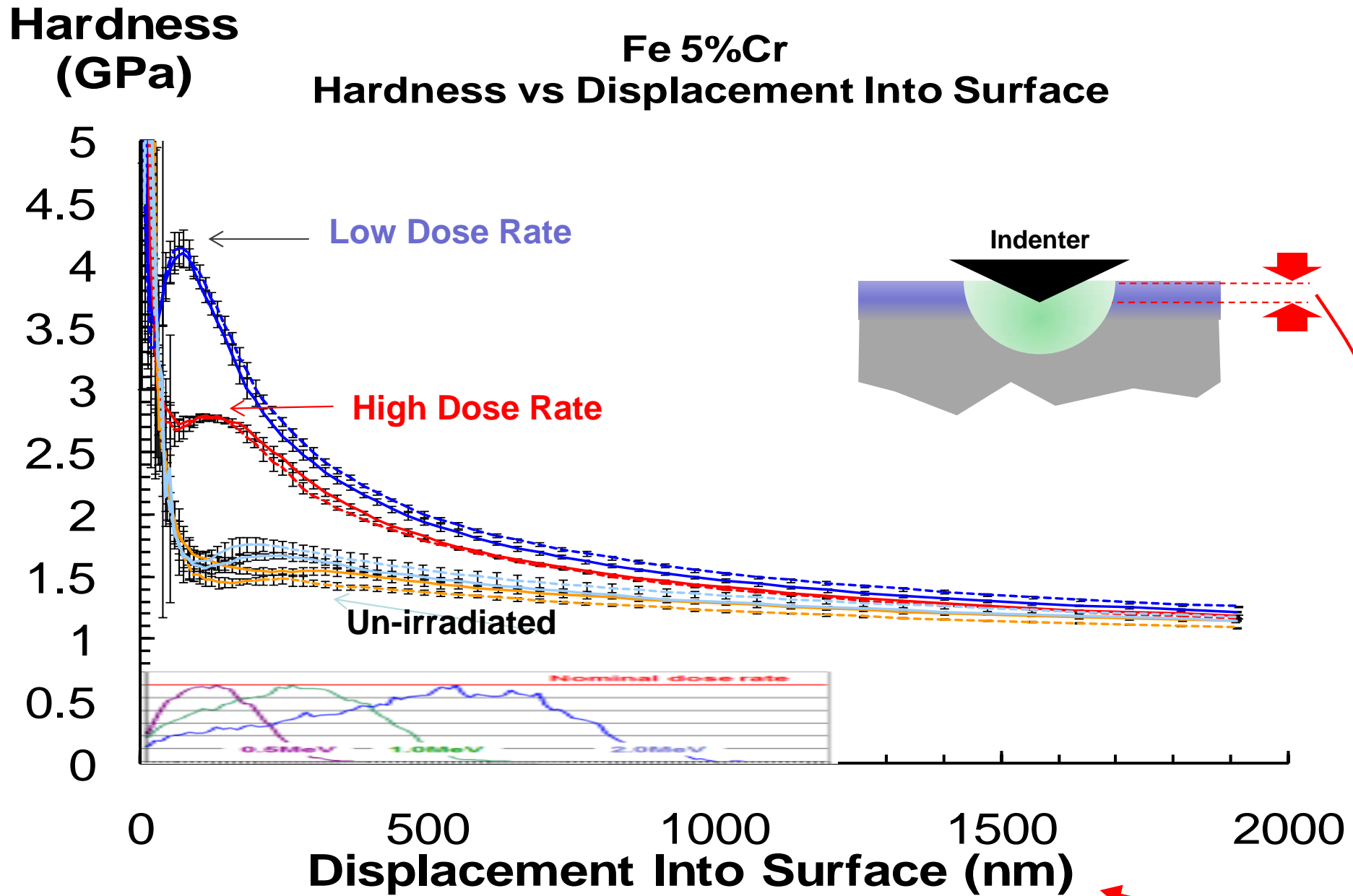
# Dose Rates

Radiation Source	Dose Rate (dpa / s) in Iron-based Alloys
Fission Reactor Pressure Vessels (RPV)	$\sim 10^{-12} - 10^{-11}$
Rotating Target Neutron Source (RNTS-II)	$\sim 10^{-10}$
Fast Flux Test Facility (FFTF)/DEMO Fusion Reactor	$\sim 10^{-8} - 10^{-6}$
Ion Implantation – Low Dose Rate	$3 \times 10^{-5}$
Ion Implantation – High Dose Rate	$6 \times 10^{-4}$
HVEM Irradiation	$\sim 10^{-3}$

# Nanoindentation hardness: Fe 5%Cr 0.6dpa

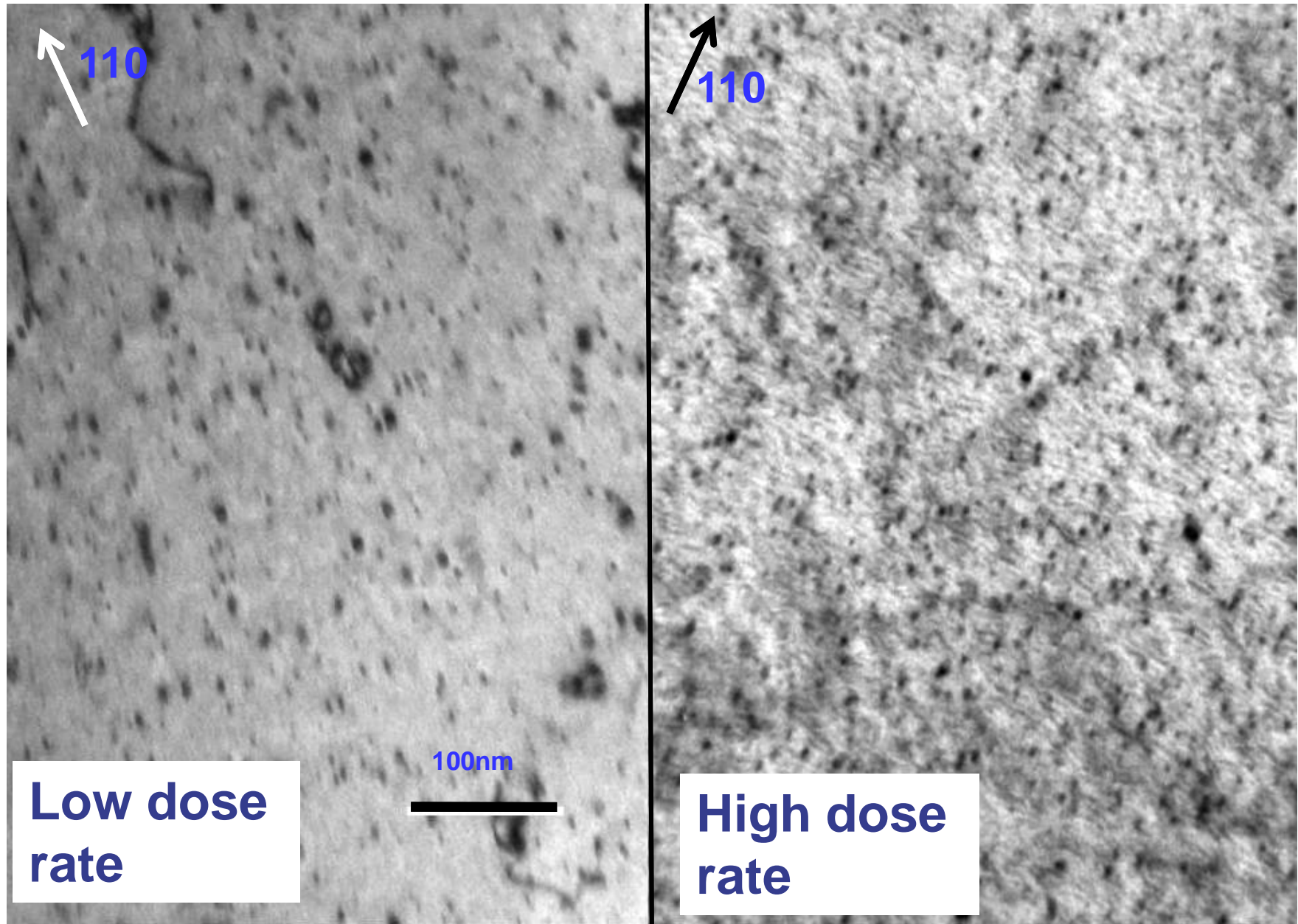


# Nanoindentation hardness: Fe 5%Cr 0.6dpa

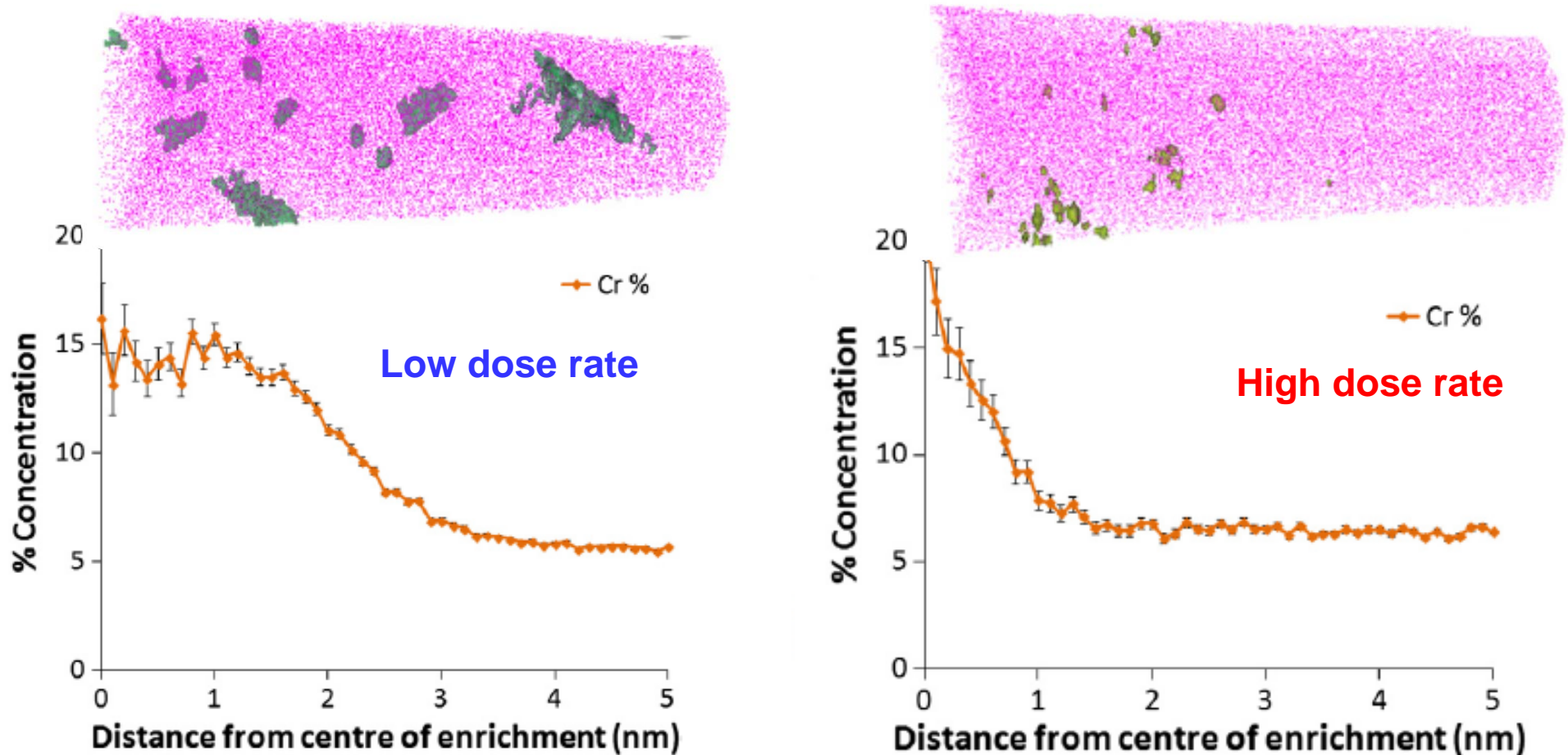




# TEM of ion irradiation damage Fe 5%Cr 300°C

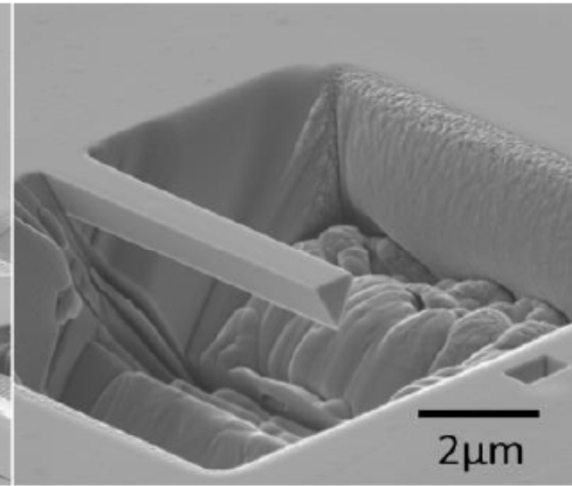
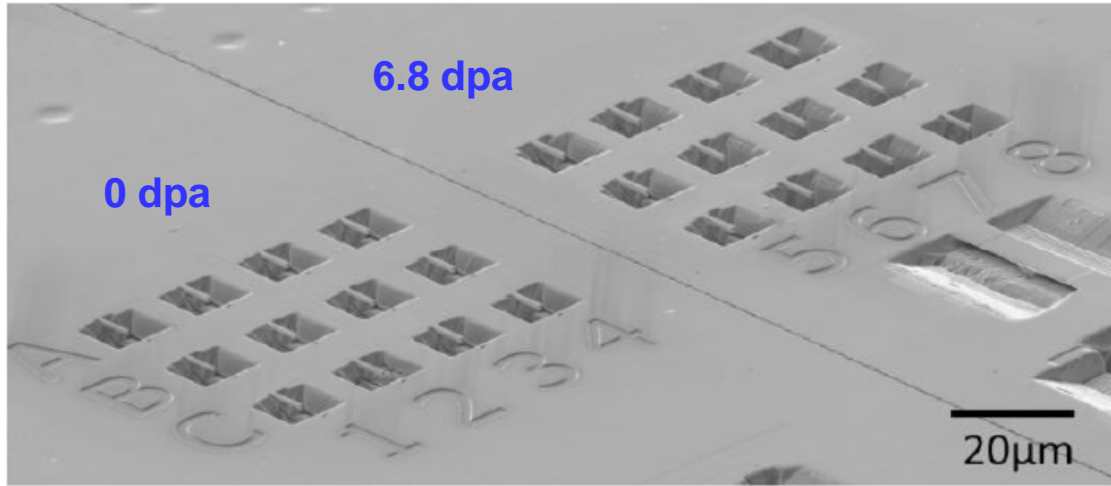


# APT of ion irradiation damage Fe 5%Cr 400°C



APT data for the Fe 5%Cr alloy irradiated at 400 °C with the low dose rate (a) and high dose rate (b). The figure includes an atom map showing Fe atoms and a 0.5 at.% Cr N isoconcentration surface (i) and proximity histograms showing the variation in composition from the centre of enrichment outwards into the matrix (ii). Centre of enrichment is defined as the region of highest Cr N concentration.

# Micro-mechanical Testing

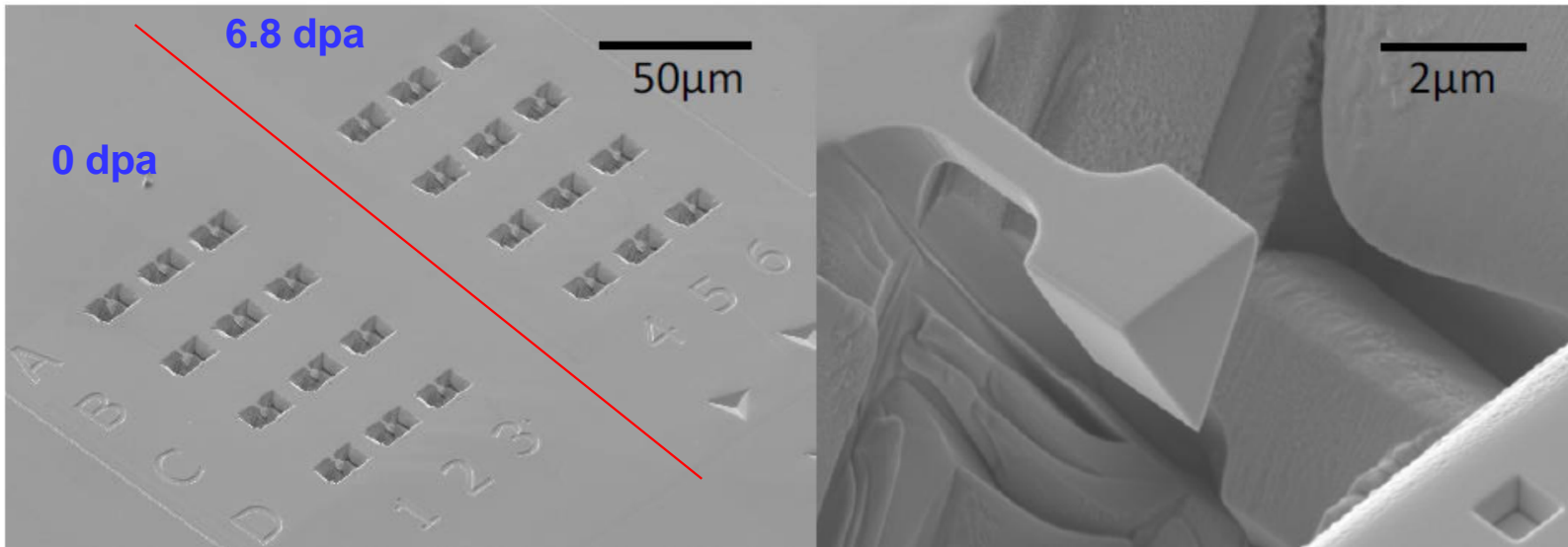


Fe-12%Cr

Ion – irradiated  
Fe<sup>+</sup>  
0.5MeV & 2MeV  
320°C

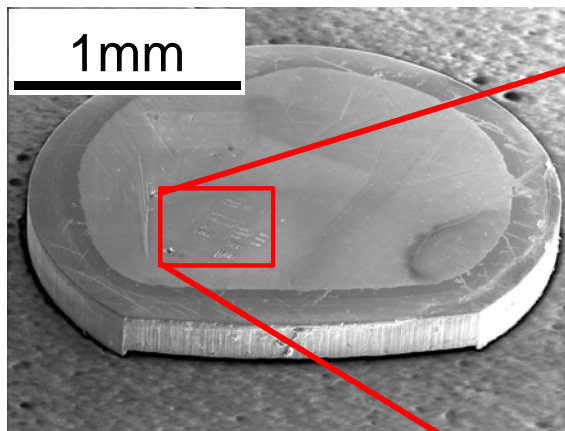


# Micro-mechanical Testing



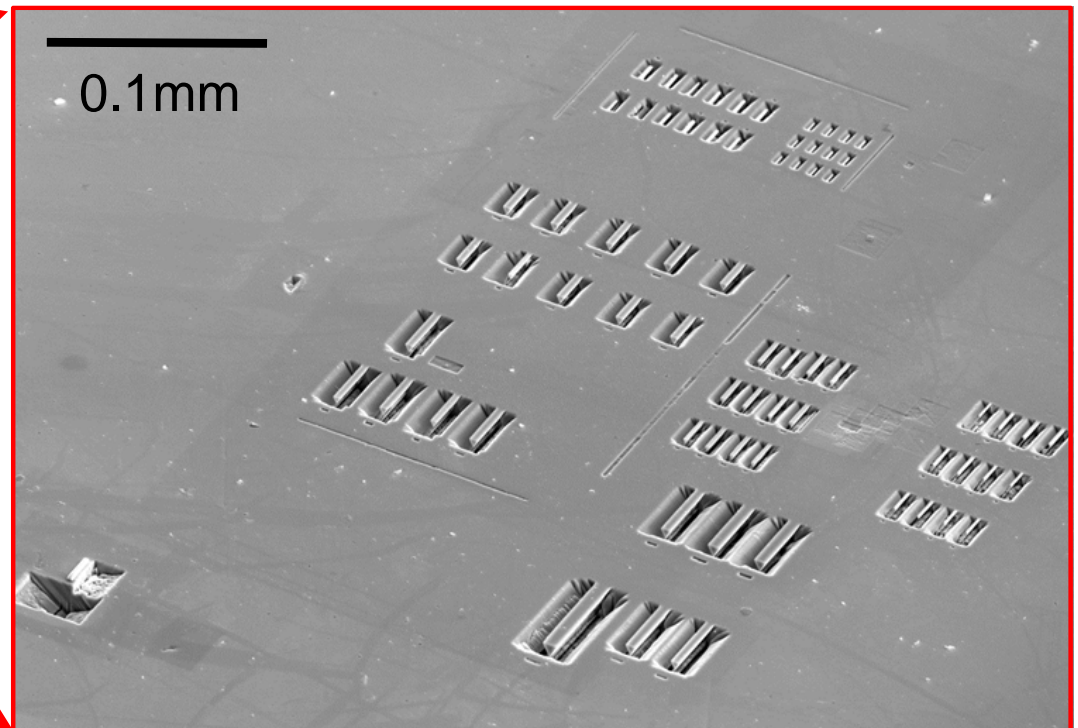
Fe-12%Cr

Ion – irradiated  
Fe<sup>+</sup>  
0.5MeV & 2MeV  
320°C

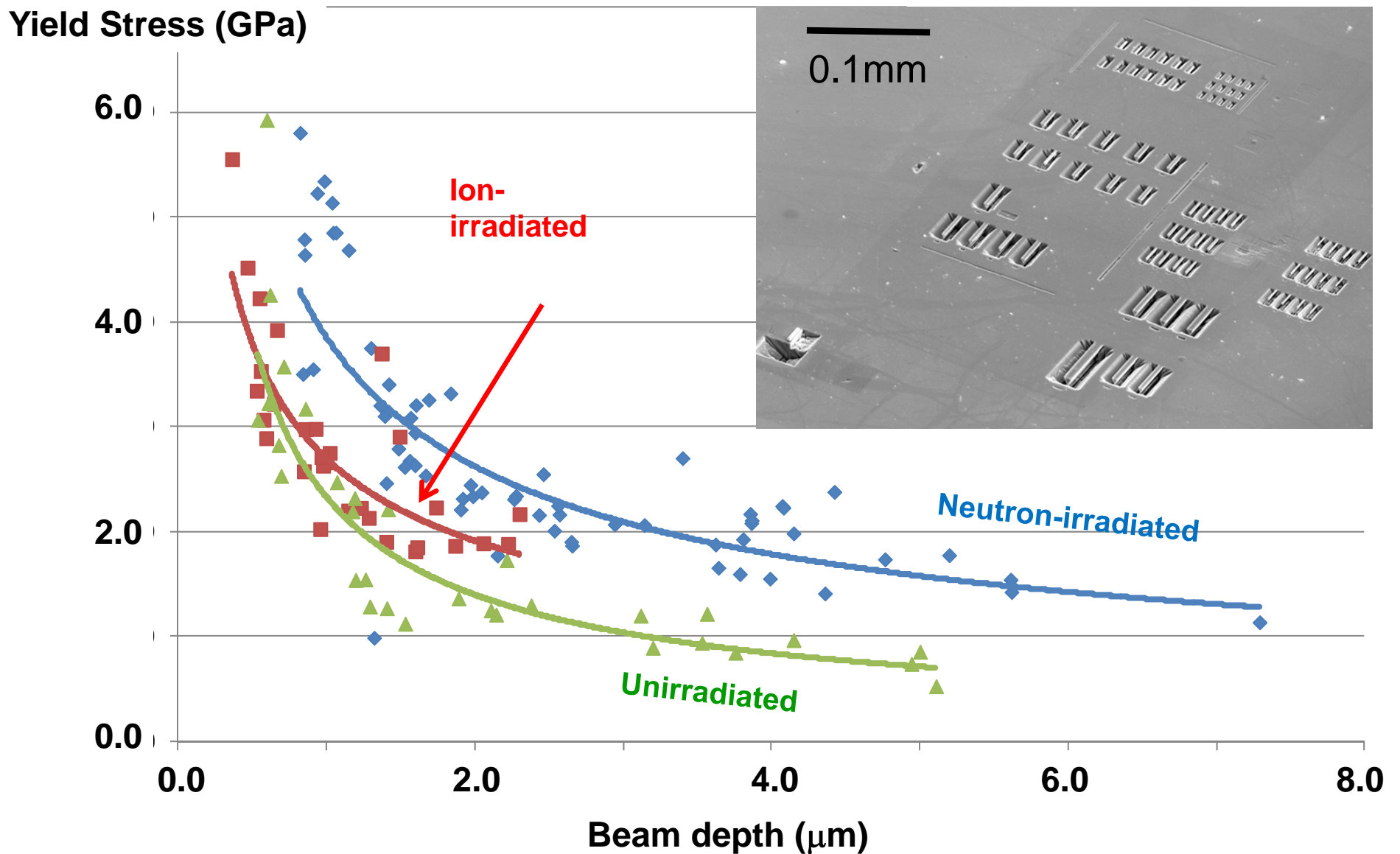


Fe-6%Cr

neutron –  
irradiated  
288°C  
1.7 dpa

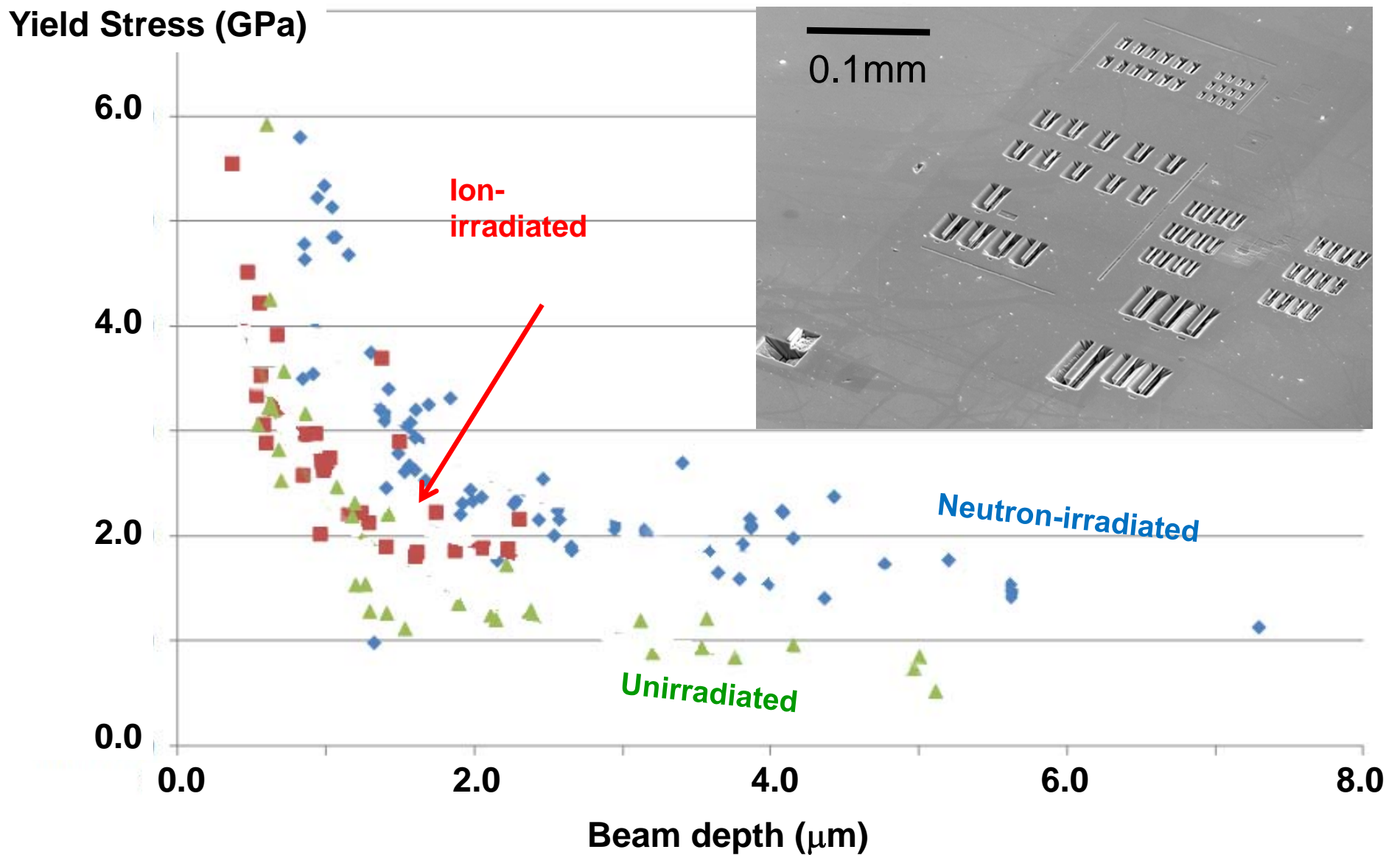


# Micromechanical testing Fe-6%Cr – Size effects

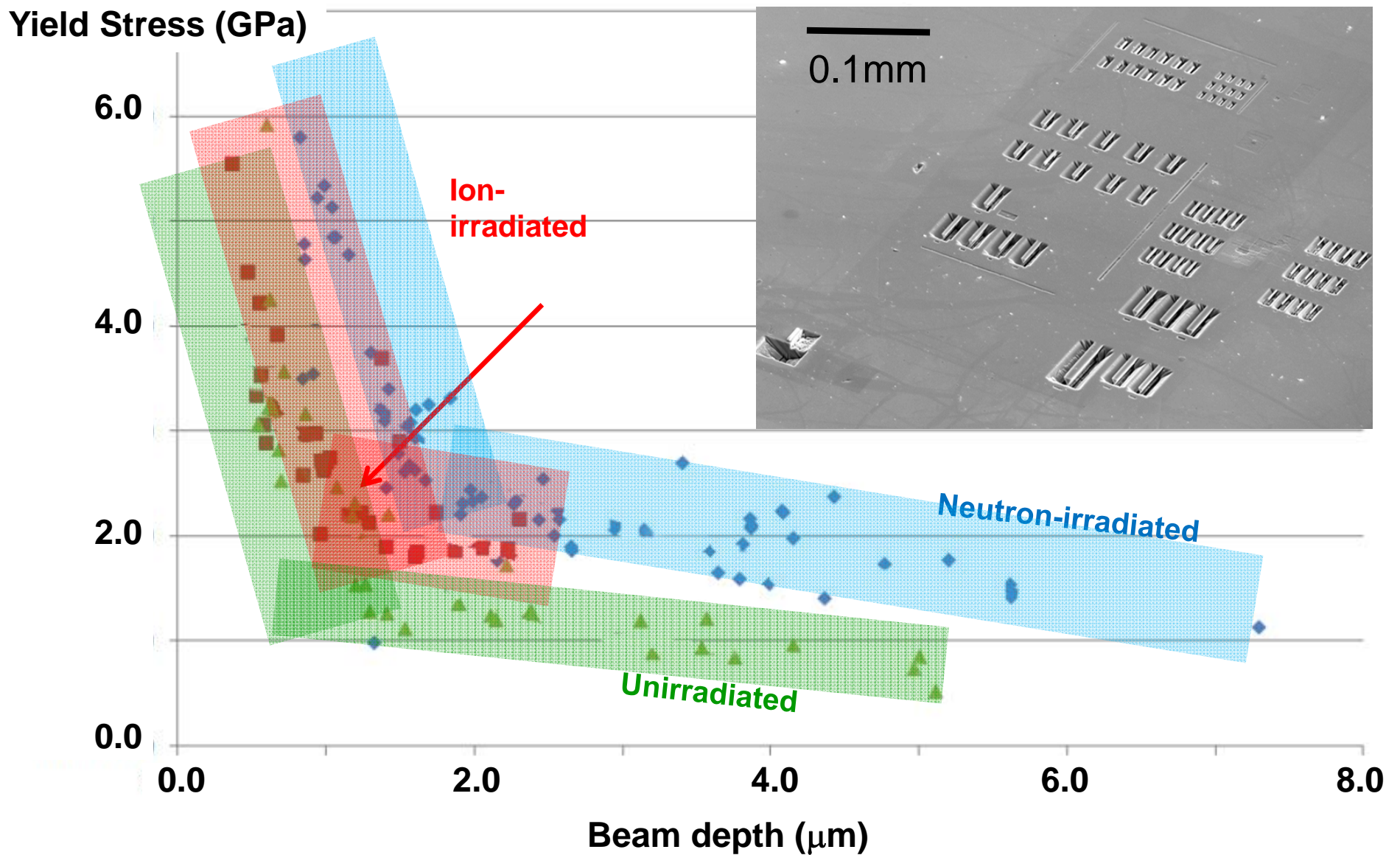




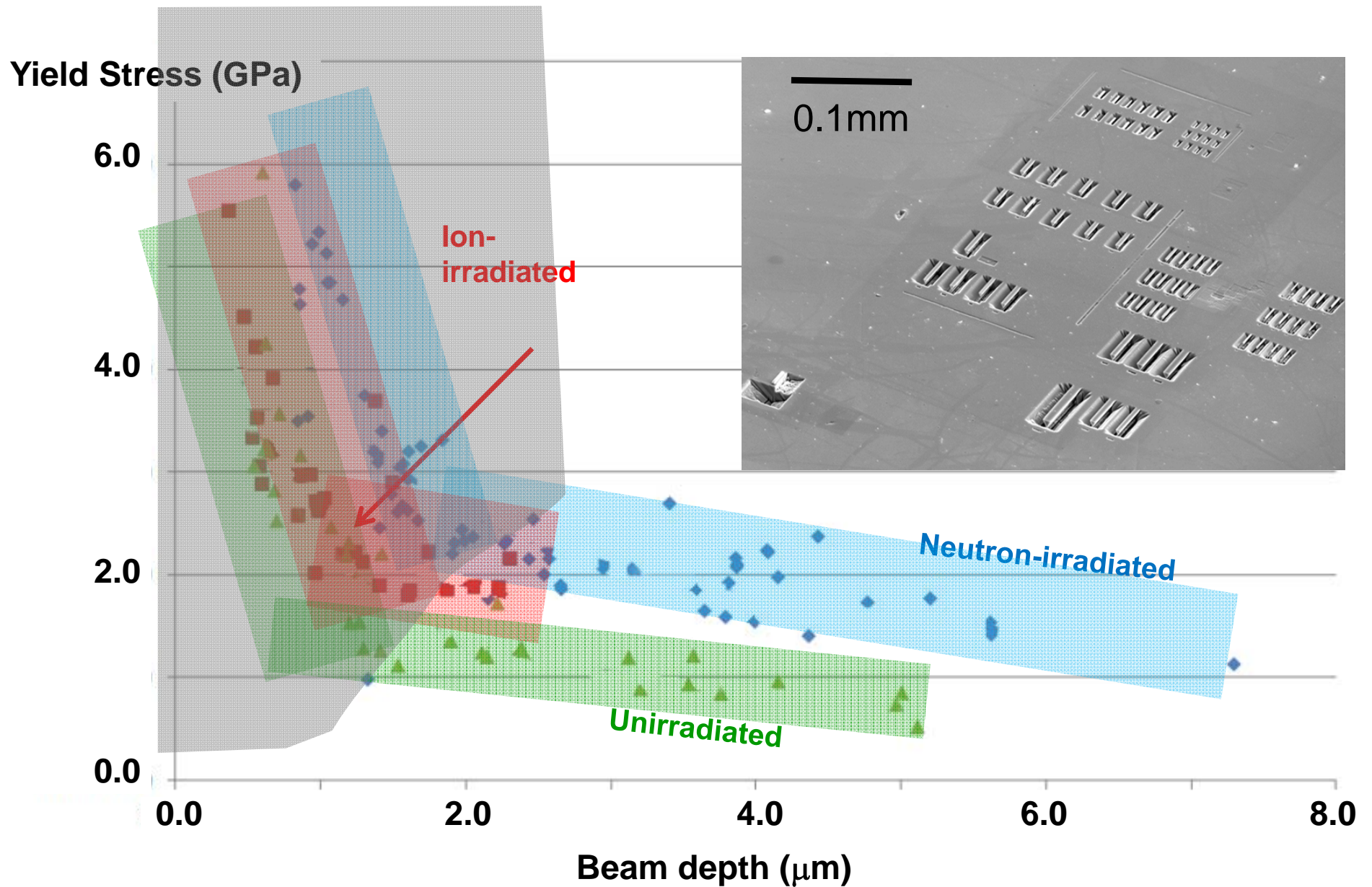
# Micromechanical testing Fe-6%Cr – Size effects



# Micromechanical testing Fe-6%Cr – Size effects



# Micromechanical testing Fe-6%Cr – Size effects



**Protons ?**



ION

Ion Type **H** 1.008 amu  
 Ion Energy **2** MeV  
 Ion Angle **0** degrees

Completed **99999** of **99999**

SHOW LIVE DATA HELP

TARGET DATA

? H (10) into Layer 1 (1 layers, 1 atoms)

Layer Name	Width (A)	Density	Fe (55.84)	Solid/Gas	Stop Corr.
1 Layer 1	250000	7.866	1.00000	Solid	1

Plots

PLOT Window

0 A - 250000 A

Max Target Depth 250000

COLLISION PLOTS

Ion/Recoils (XY) All  
 Ion/Recoils (XZ) None  
 Ions (no recoils) Tile  
 Lateral View (YZ) Clear

Background color White/Black

DISTRIBUTIONS

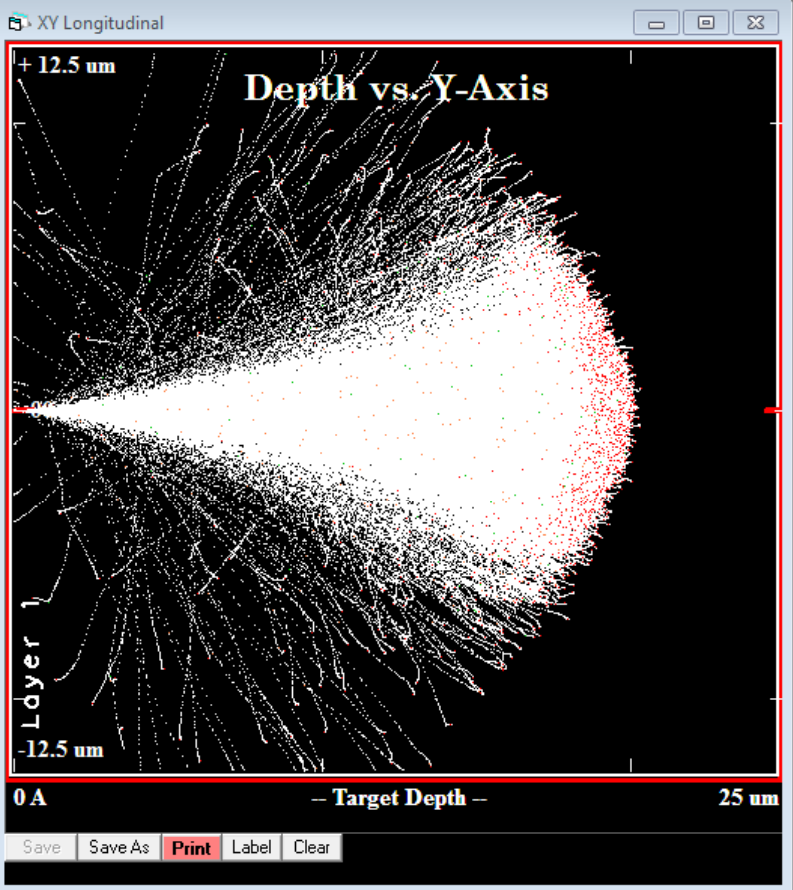
File Plot

Ion Distribution  
 Ion/Recoil Distribution  
 Lateral Range  
 Ionization  
 Phonons  
 Energy to Recoils  
 Damage Events  
 Integral Sputtered  
 Differential Ions  
 Backscattered Ions  
 Transmitted Ions  
 Collision Details

3-D Plots 3D Help

Ion Distribution 3D  
 Recoil-Dist. 3D  
 Ionization 3D  
 Phonons 3D  
 Target Damage 3D

HELP



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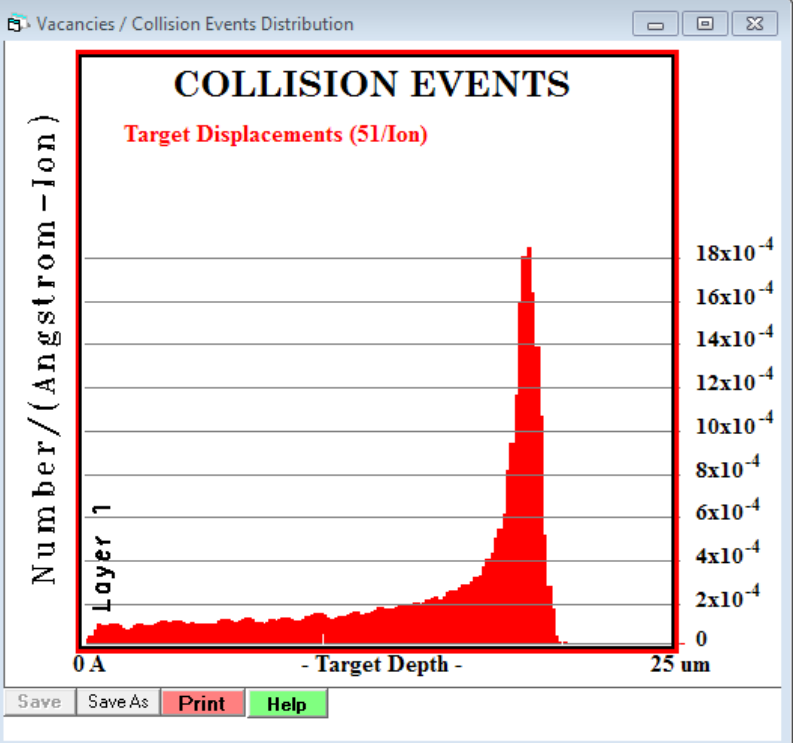
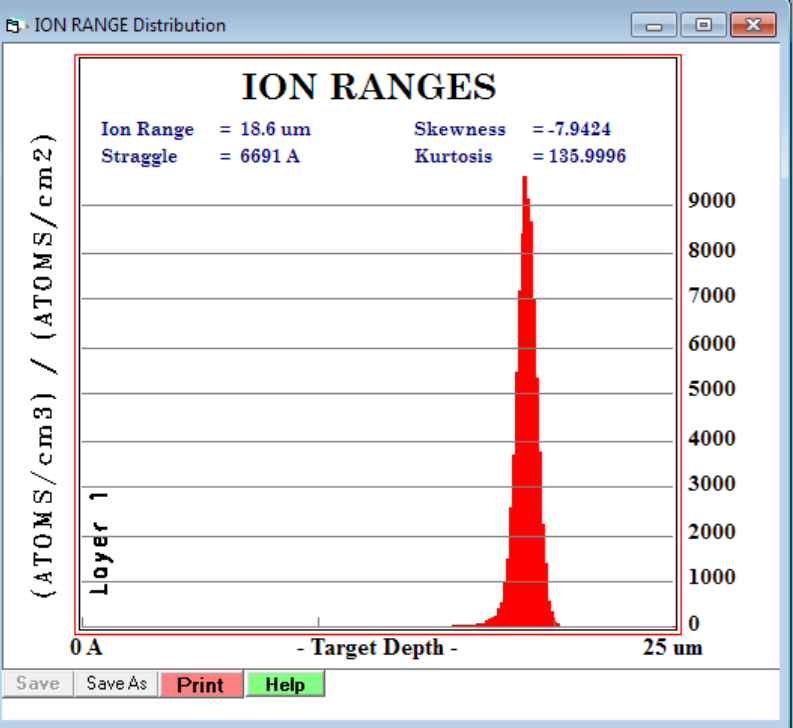
Fe

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Number

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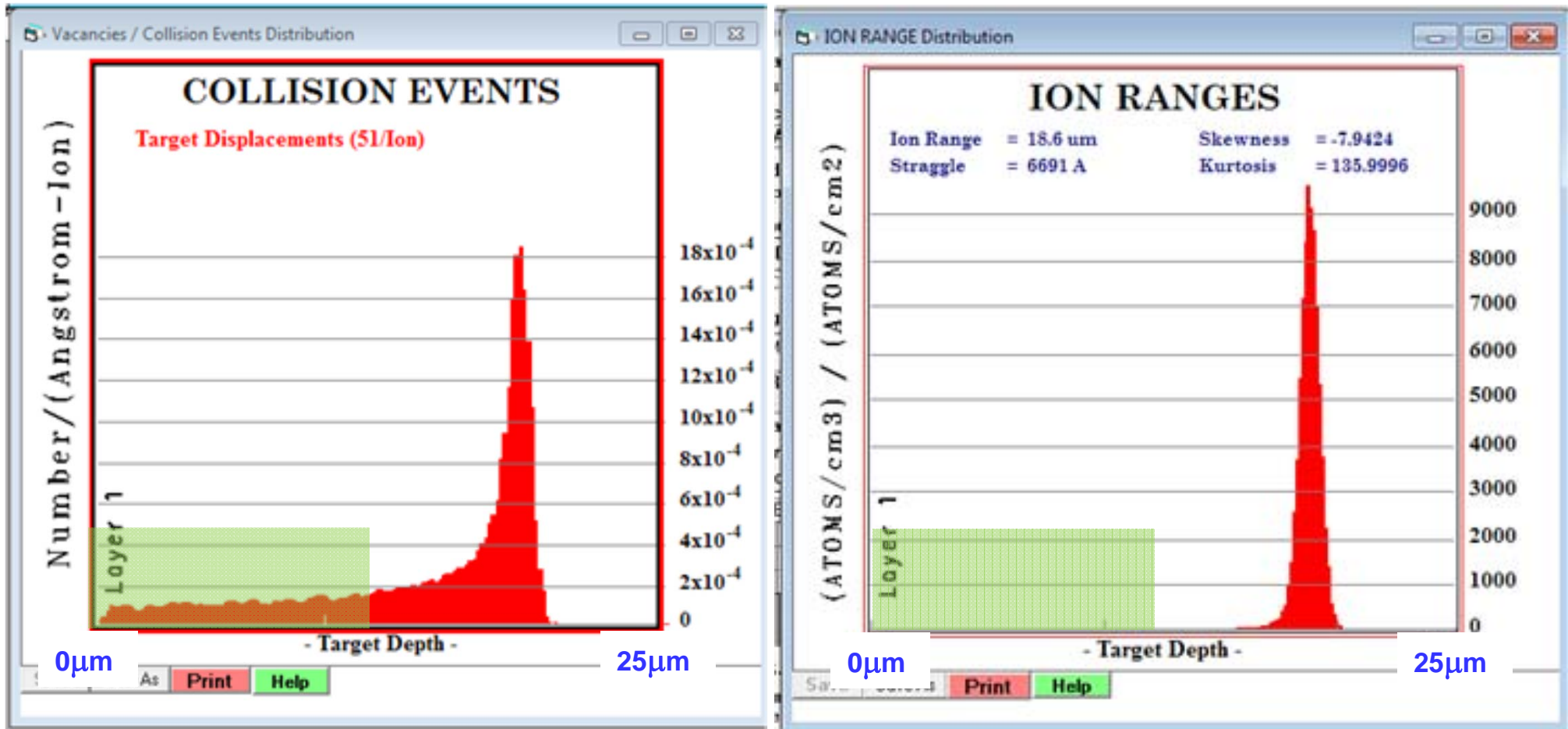


SRIM : 2 MeV protons into Fe



# Proton irradiation for (micro) mechanics?

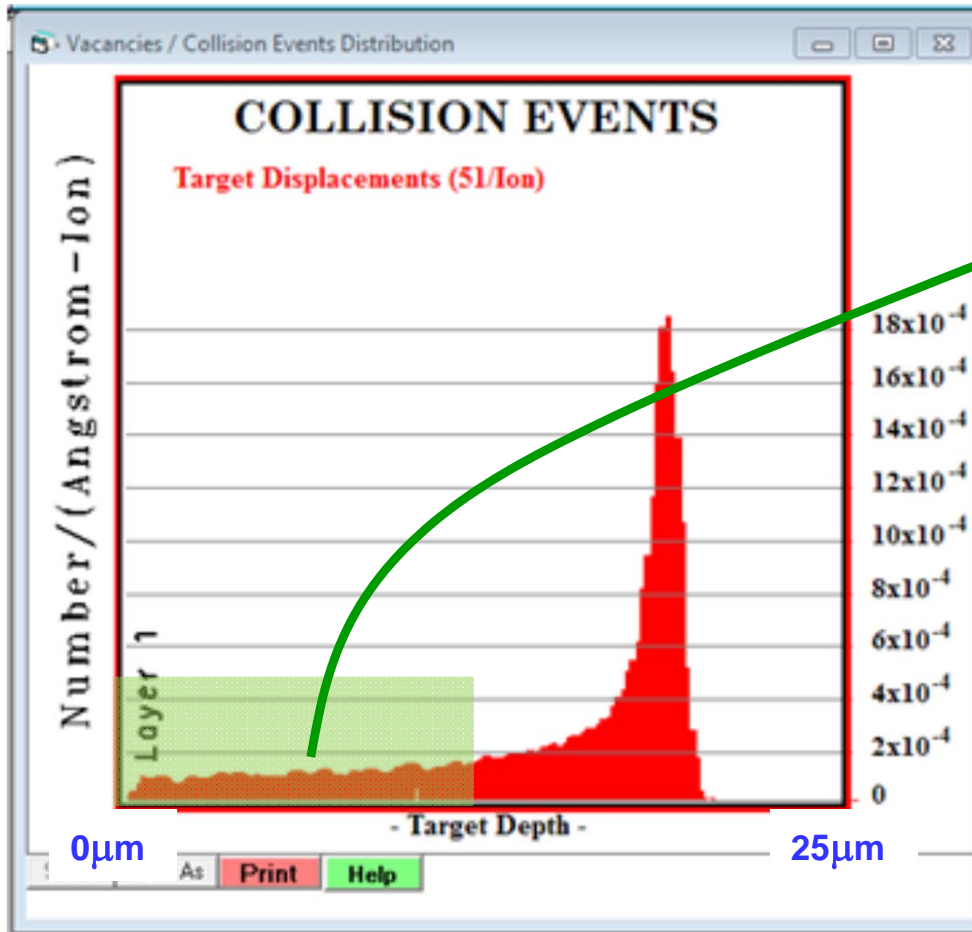
SRIM : 2 MeV protons into Fe



Could use specimens 10 – 12  $\mu\text{m}$  thick – well beyond the size-dependent mechanics regime

# Proton irradiation for (micro) mechanics?

SRIM : 2 MeV protons into Fe



For 2MeV  $\text{H}^+$  into Fe:

Total damage:

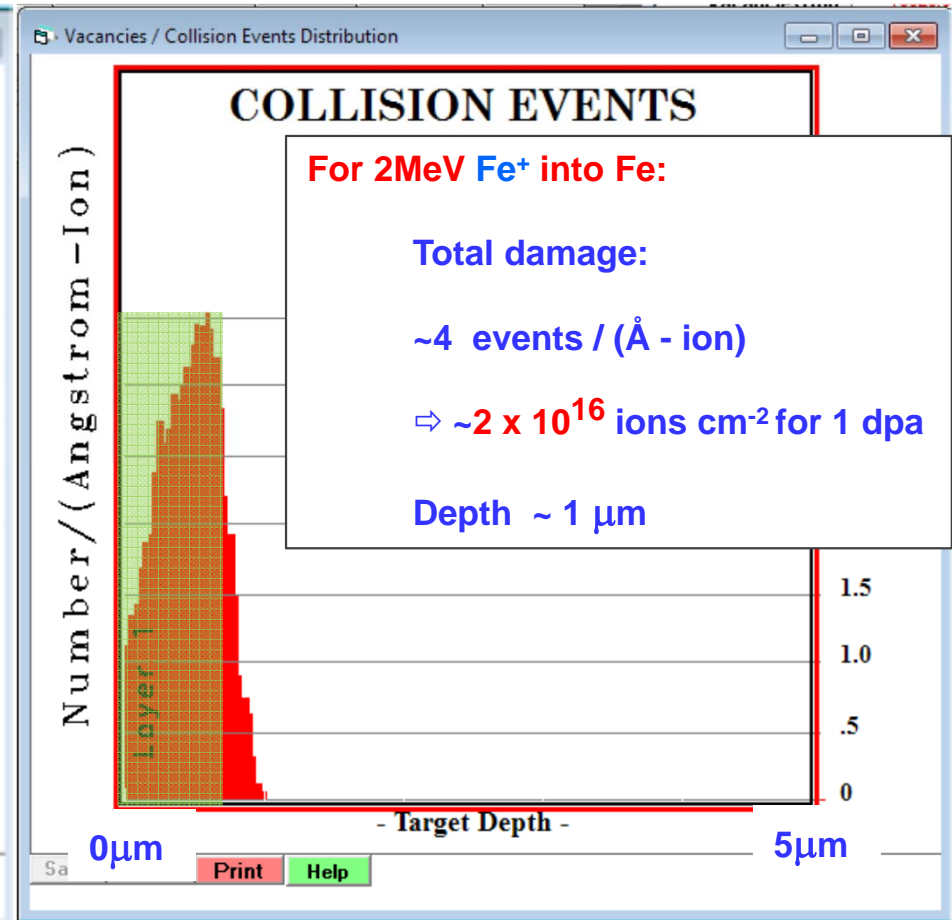
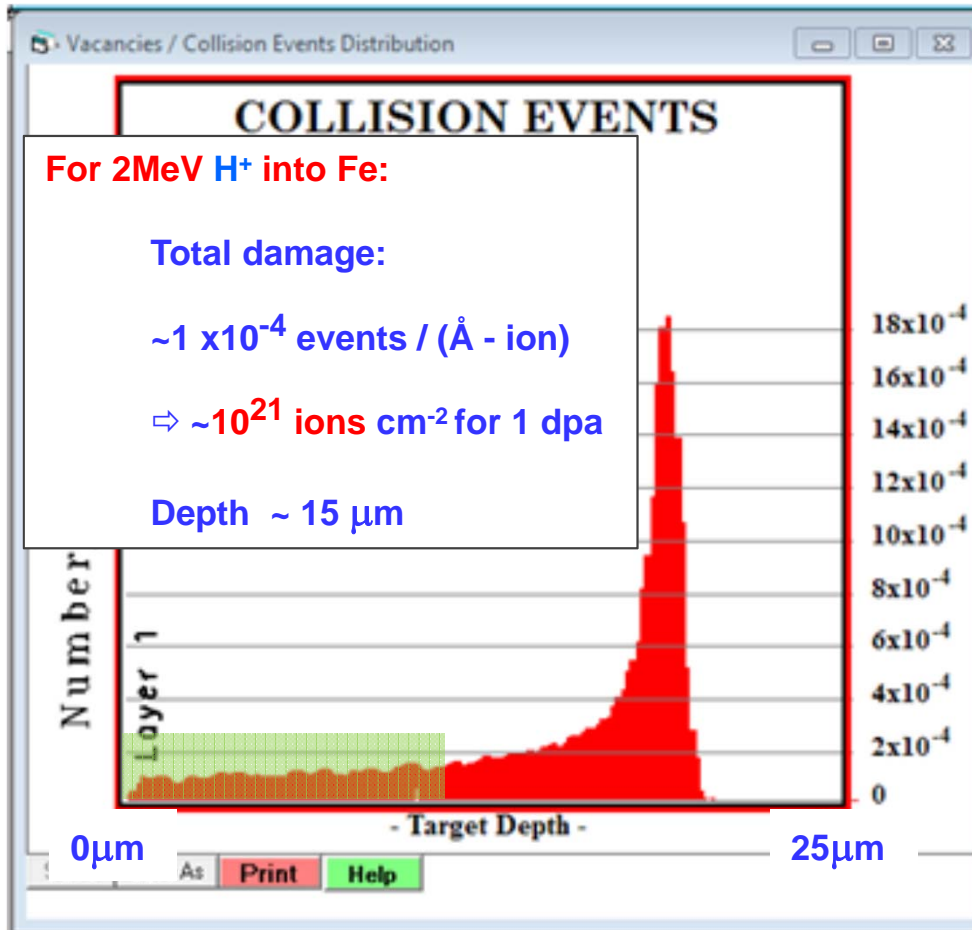
$\sim 1 \times 10^{-4}$  events / ( $\text{\AA}$  - ion)

$\Rightarrow \sim 10^{21}$  ions  $\text{cm}^{-2}$  for 1 dpa

Depth  $\sim 15 \mu\text{m}$

# Proton irradiation for (micro) mechanics?

SRIM : 2 MeV protons into Fe





# Radiation damage in Materials

