Damage accumulation in irradiated materials: influence on structural and functional properties

Some lessons learnt from fission studies

J. Jagielski

National Centre for Nuclear Research, Swierk/Otwock, Poland

NARODOWE CENTRUM
BADAŃ JĄDROWYCH
Świerk

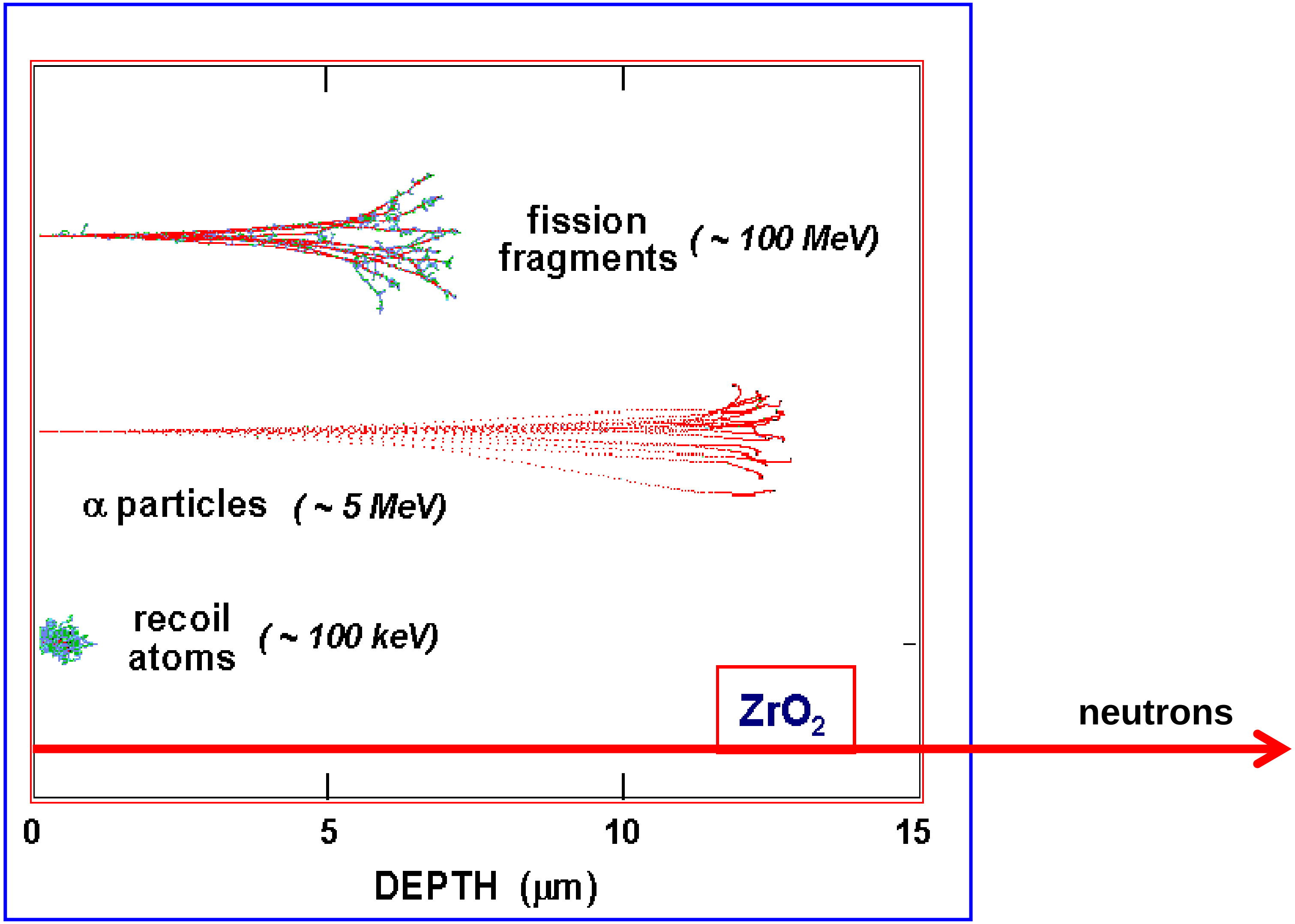
Strategy for material testing in nuclear environment

1. Selection based on classical material science
2. Analysis of radiation damage below Coulomb barrier
3. Testing in near-real environment
4. Analysis of samples from dismounted nuclear installations
5. Analysis of test samples from real nuclear installation

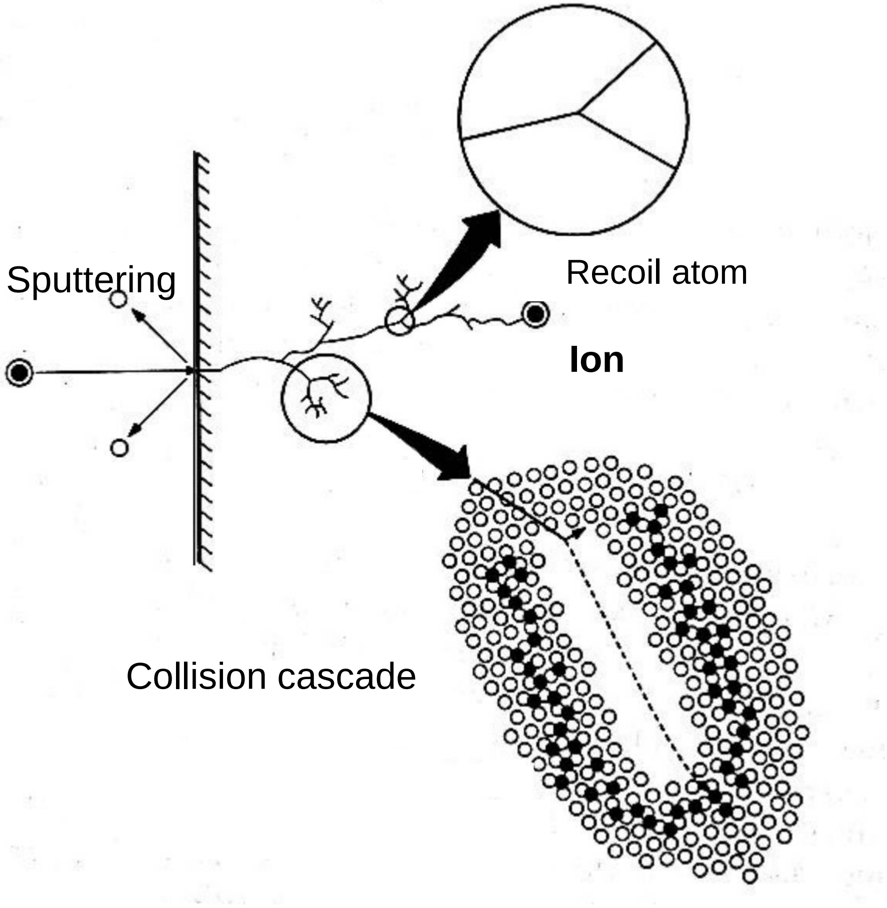
SAFETY ANALYSES (computer simulations) **vs EXPERIMENTAL VALIDATION**

TECHNICAL PROBLEMS vs LEGAL ISSUES

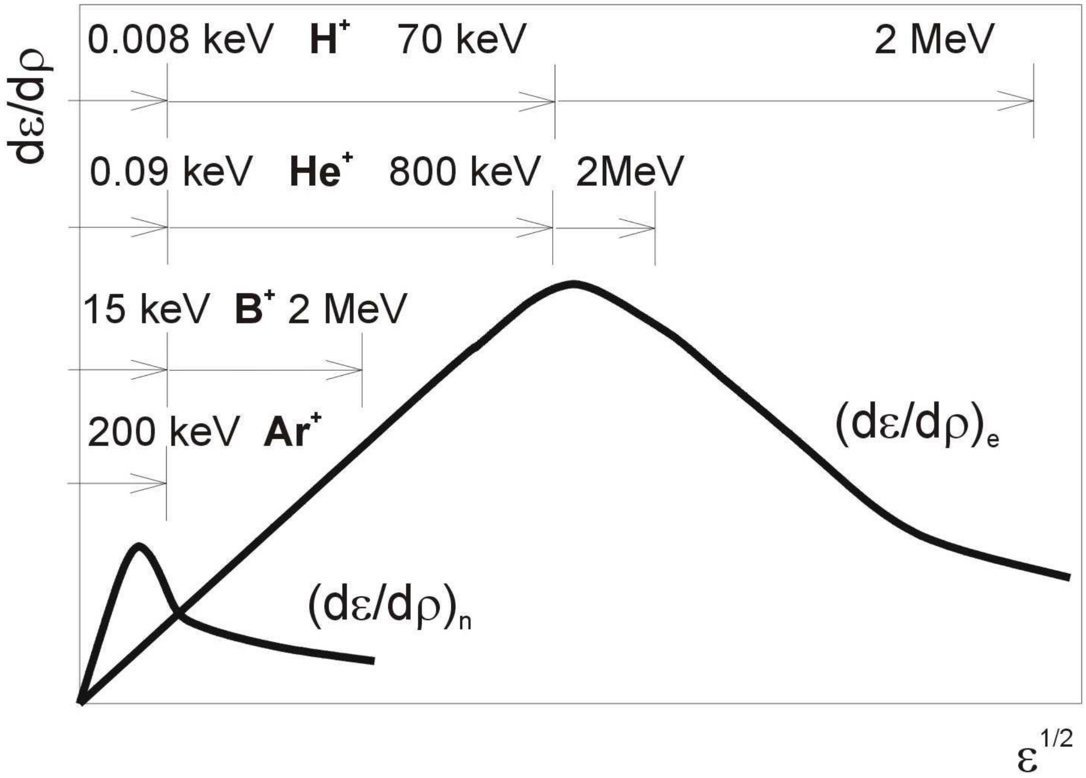
Defect production by fast particles



Defect production by fast particles



Defect production by fast particles



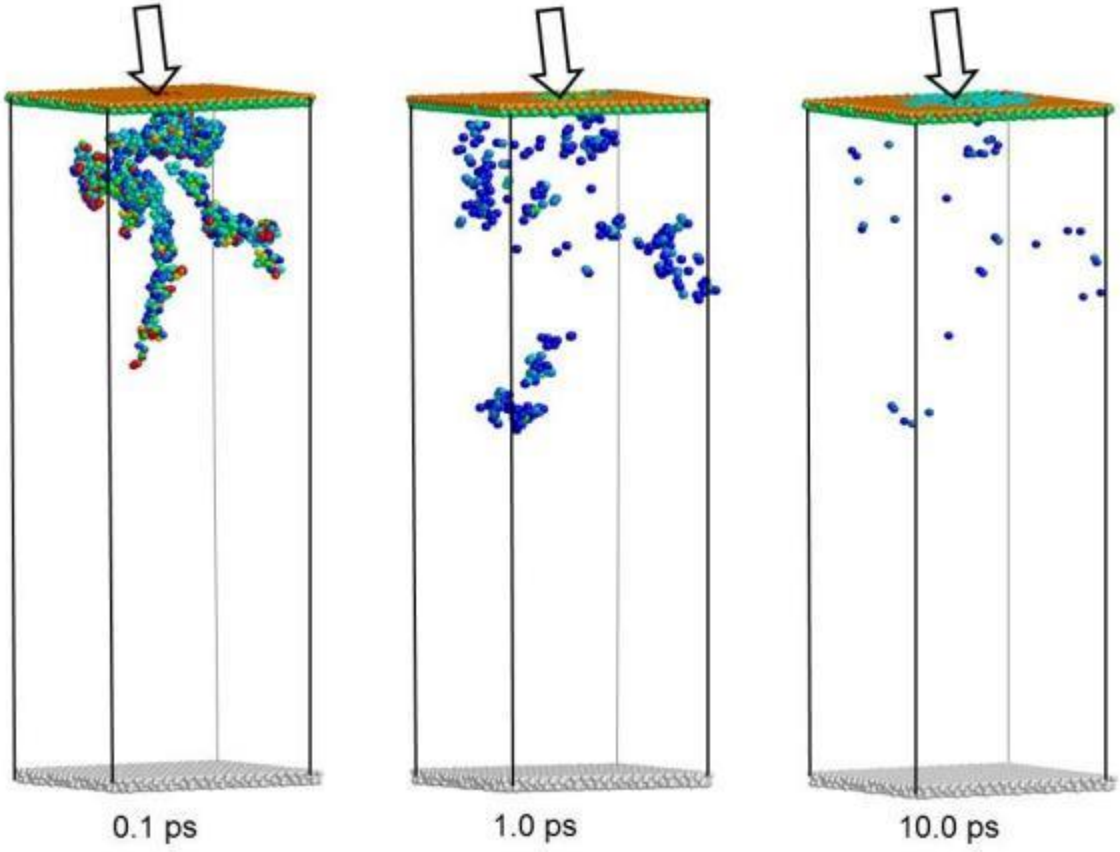
$$S = dE/dx = S_e + S_n$$

S_e: ionization
S_n: elastic collisions

S_e: keV/nm
S_n: d.p.a.

Defect production by fast particles

10 keV Si^+ in Si



Courtesy of Frank Posselt, HZDR

Defect production by fast particles

Short summary:

1. **Fast particles loose their energy in two independent processes: Se and Sn**
2. Inelastic collisions with electrons (Se) essentially produce no defects
3. Elastic collisions with target nuclei (Sn) displace atoms from lattice positions
4. Se dominates for light and swift particles (begining of the slowing down)
5. Sn dominates for slow and heavy particles (end of the trajectory)
6. **Most of the defects are produced by displaced target atoms**
7. **Most of the defects anneal out during evolution of displacement cascade (100 ps)**

Defect production by fast particles

Calculation of the damage level, Kinchin-Pease approach:

$$N_d = 0.8\ \Delta E_n/(2E_d)$$

ions

E_n – nuclear energy loss (elastic collisions)
E_d – displacement energy

$$N_d = E/(2E_d)\ (E<E_c)$$

neutrons

$$N_d = E_c/(2E_d)\ (E>E_c)$$

Defect production by fast particles

Calculation of the damage level:

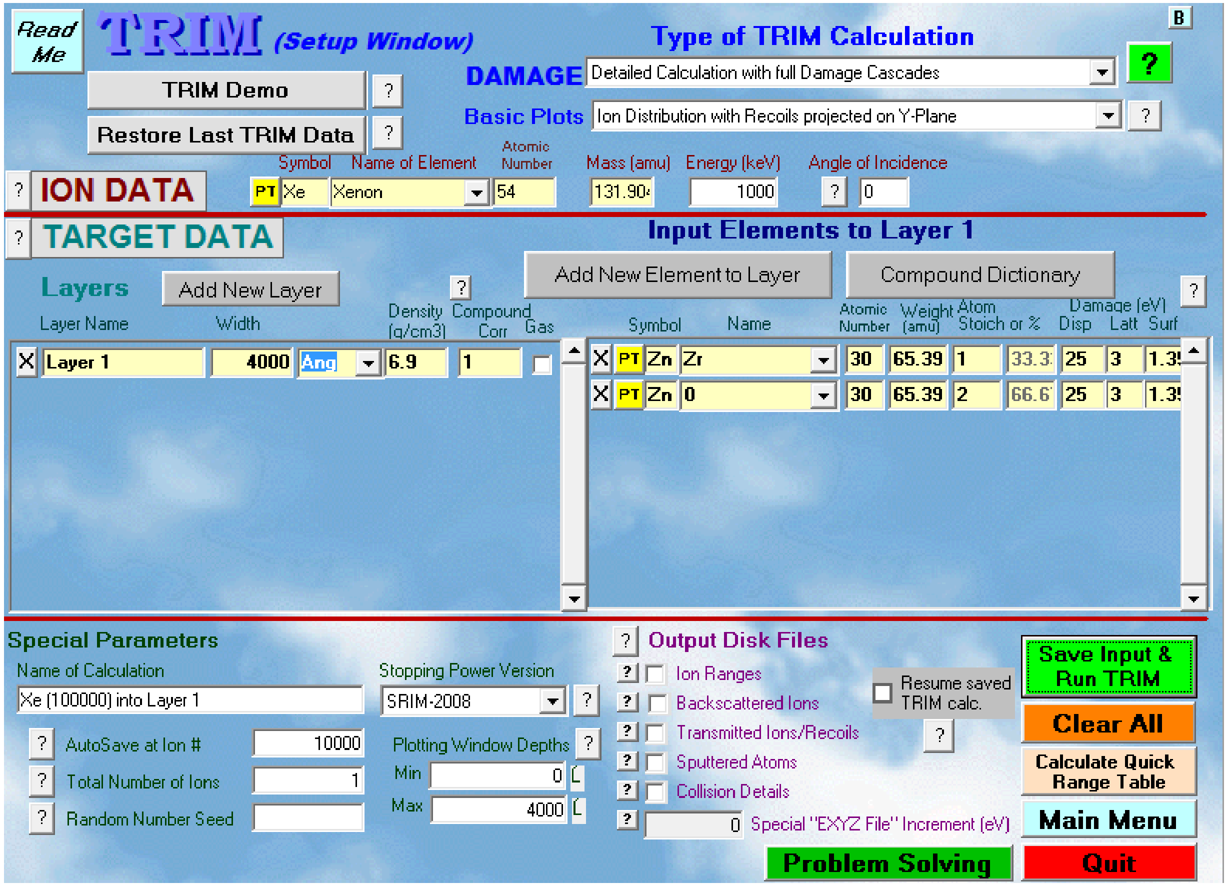
Example : 0.5 MeV neutrons interacting with iron [A=56] target.

E_n = 0.5 MeV N = 0.85 x 10^{23} atoms/cm^3 σ_{el} = 3 b, E_d = 24 eV
Φ = 10^{15} n/cm^{2}s Λ = 4A $(1+A)^2$ = 0.069 and N_d = 350 dpa per neutron collision and R_d = 9 x 10^{16} displacements/cm^{3}s = 10^{-6} dpa/s

DONES: <10-30 dpa per year, ion accelerator: 150 dpa per day

Defect production by fast particles

Calculation of the damage level:



Type of TRIM Calculation

DAMAGE: Detailed Calculation with full Damage Cascades

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

ION DATA

Symbol	Name of Element	Atomic Number	Mass (amu)	Energy (keV)	Angle of Incidence
PT Xe	Xenon	54	131.904	1000	0

TARGET DATA

Layers

	Layer Name	Width		Density (g/cm3)	Compound Corr	Gas
X	Layer 1	4000	Ang	6.9	1	☐

Input Elements to Layer 1

		Symbol	Name	Atomic Number	Weight (amu)	Atom Stoich	or %	Damage (eV) Disp	Latt	Surf
X	PT	Zn	Zr	30	65.39	1	33.3	25	3	1.3
X	PT	Zn	0	30	65.39	2	66.6	25	3	1.3

Special Parameters

Name of Calculation: Xe (100000) into Layer 1

Stopping Power Version: SRIM-2008

AutoSave at Ion #: 10000

Total Number of Ions: 1

Random Number Seed:

Plotting Window Depths: Min 0, Max 4000

Output Disk Files

- ☐ Ion Ranges
- ☐ Backscattered Ions
- ☐ Transmitted Ions/Recoils
- ☐ Sputtered Atoms
- ☐ Collision Details

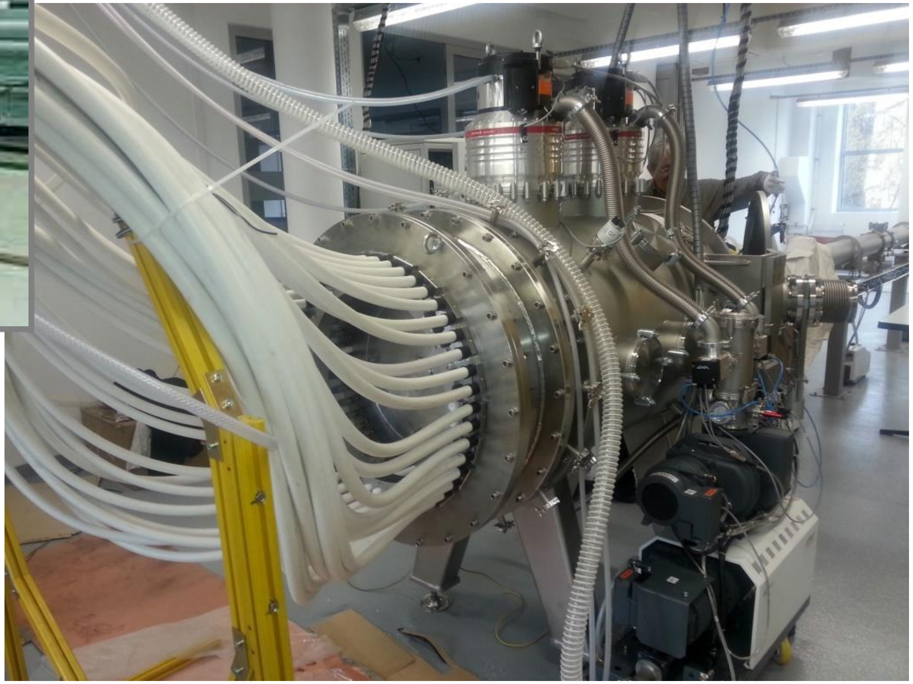
0 Special "EXYZ File" Increment (eV)

☐ Resume saved TRIM calc.

www.srim.org

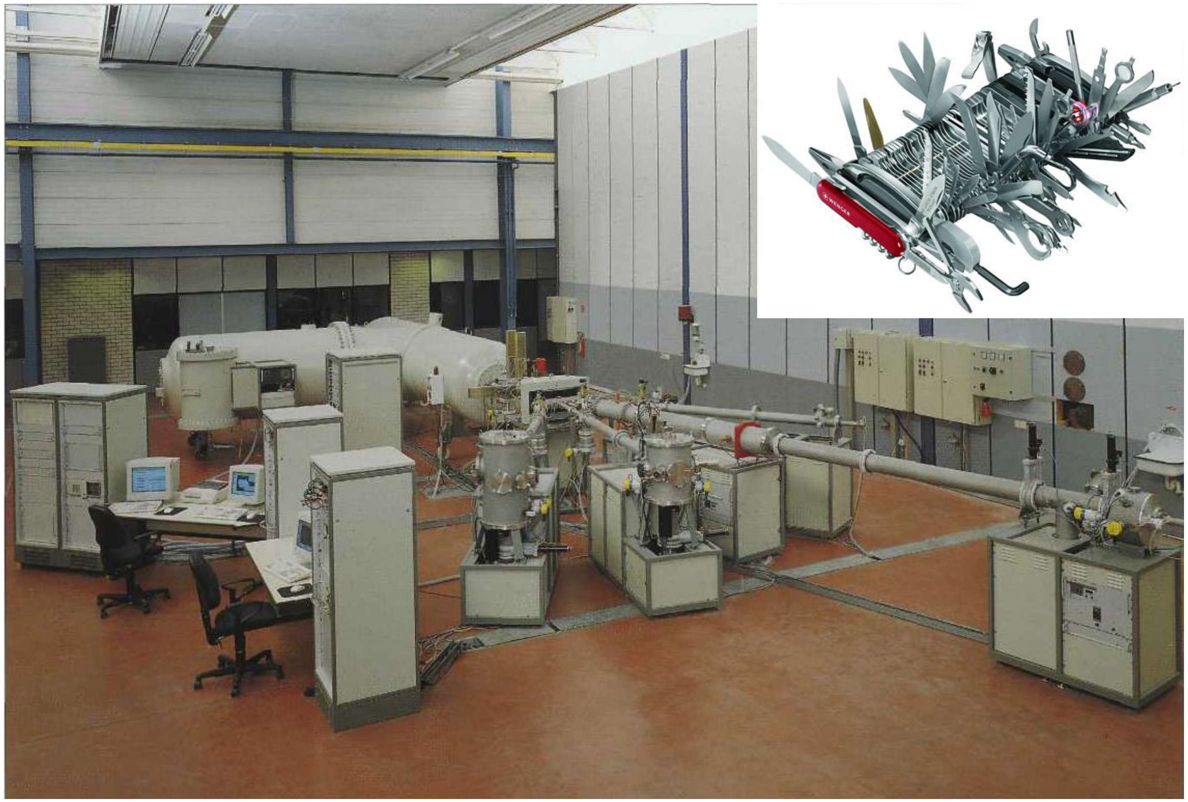
Damage creation

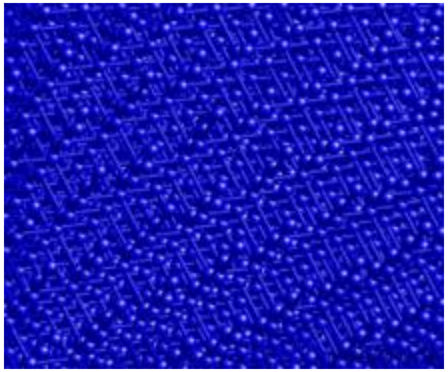
Ion Irradiation / Plasma pulses

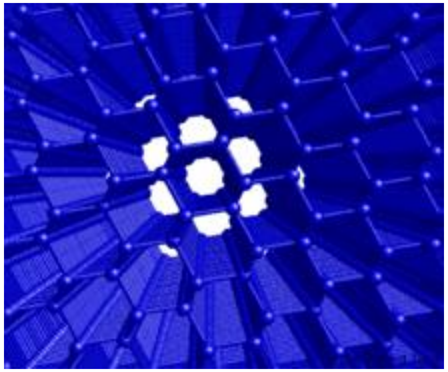


Damage analysis

RBS/C: Chanelling

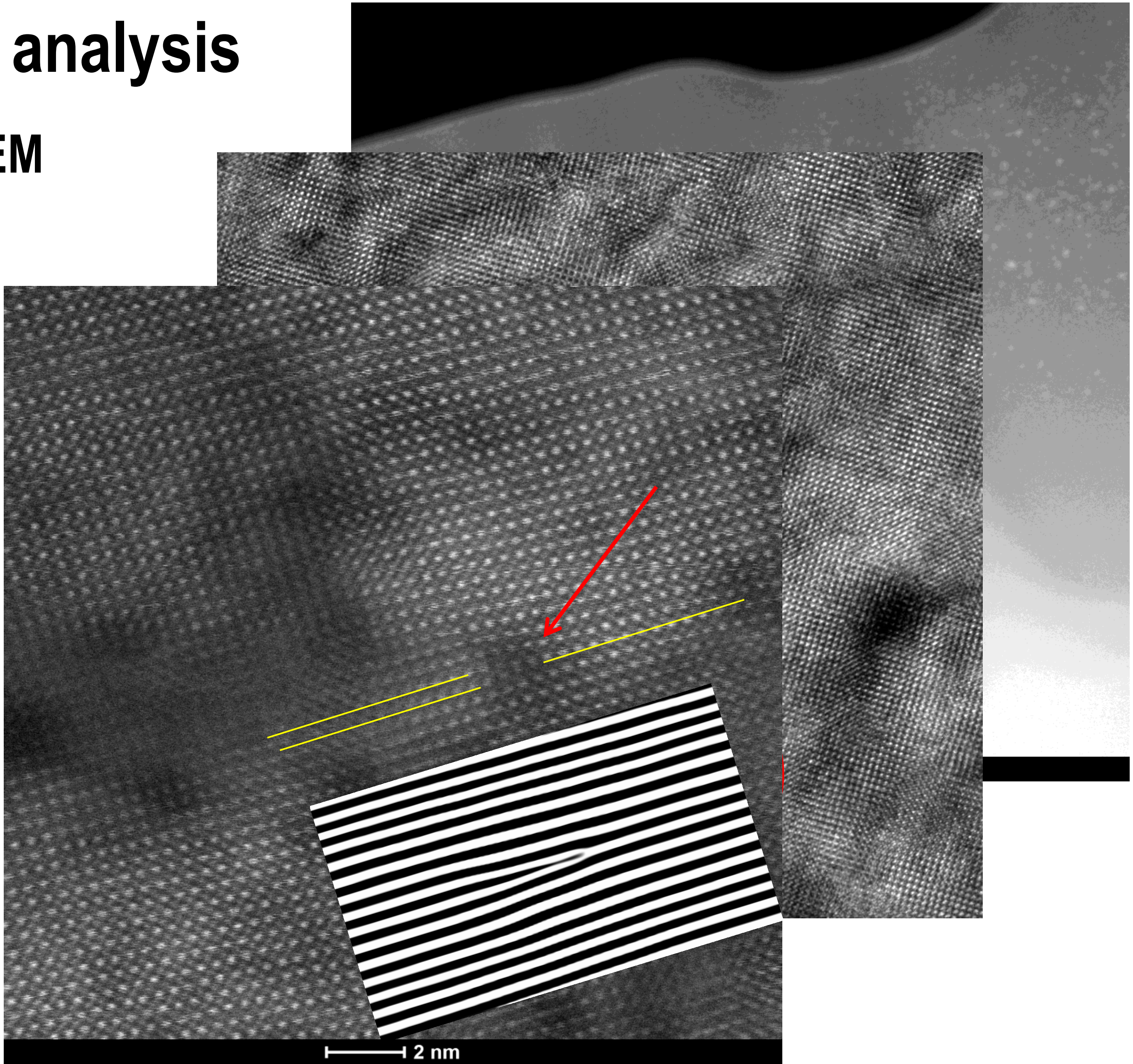






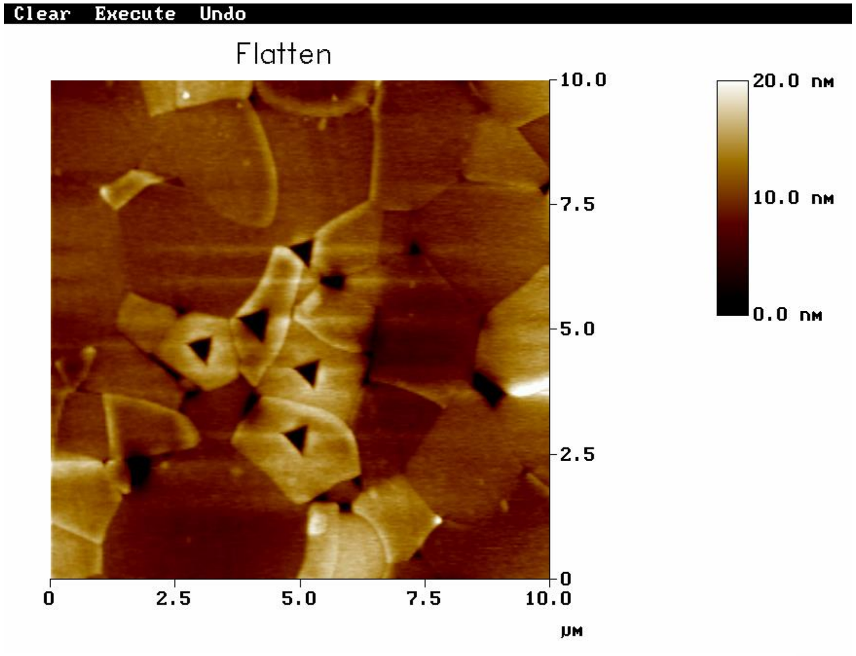
Damage analysis

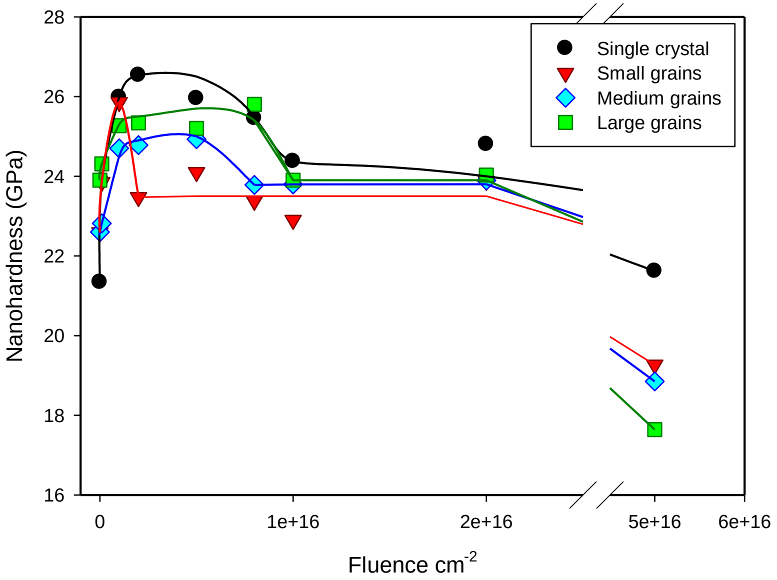
TEM/HRTEM



Damage analysis

Nanoindentation





Damage analysis

Other techniques

1. Scanning microscopy: SEM/EDS/EBSD/FIB
2. X-Ray diffraction: XRD/GXRD/HRXRD
3. Raman
4. Positrons: SPIS
5. Luminescence: CL, PL, IL
6. ……

Functional properties

Inactive laboratory

1. **Structural analysis, sample preparation**
2. **Nanomechanical Lab:** *nanoindentation, RT, HT, SPM*
3. **Mechanical Lab:** *hardness, strength, fracture, brittleness*
4. **Corrosion Lab:** *HT corrosion, stress corrosion, reaction with gases*
5. **Validation of safety analyses**

Hot cell laboratory

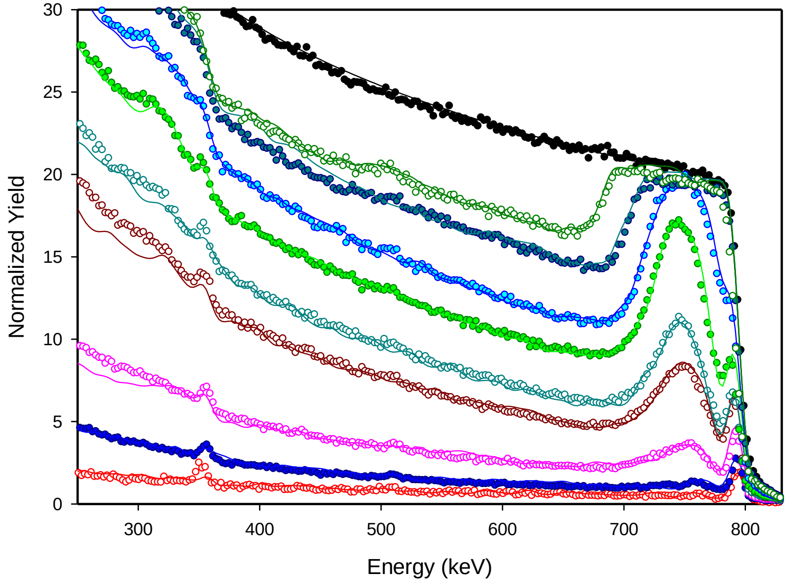
1. **Structural analysis, sample preparation**
2. **Nanomechanical Lab:** *nanoindentation, RT, HT, SPM*
3. **Mechanical Lab:** *hardness, strength, fracture, brittleness*
4. **Corrosion Lab:** *HT corrosion, stress corrosion, reaction with gases*

Damage accumulation kinetics

1. Quantitative measurement of damage level
2. Dependency of damage level vs. irradiation measure (fluence, d.p.a.)
3. Method of choice: RBS/C combined with MC simulations

Advantages of RBS/C + MC simulations:

- Possibility to analyze multielemental targets
- Ability to determine defect distribution in thick layers
- Potential to reproduce RBS/C spectra recorded on samples containing simple (amorphous) and complex (dislocations) defects



RBS/C spectra recorded on SiC crystal fitted with amorphous defects

Existing models

Gibbons (Single Impact and Damage Accumulation)

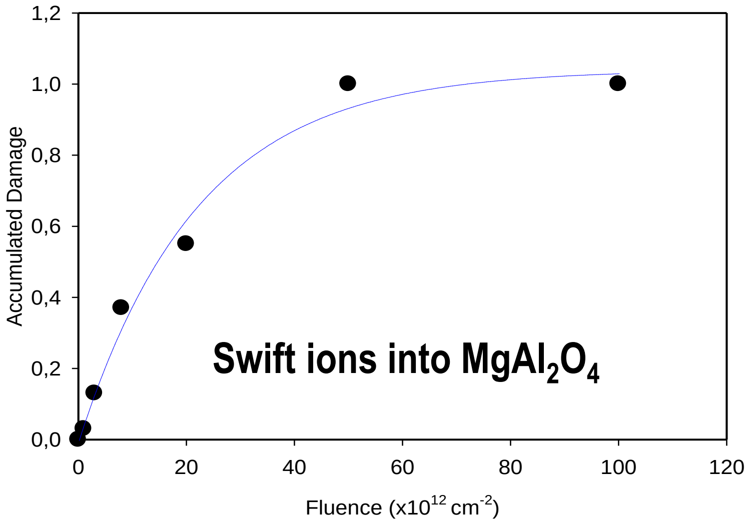
Direct Impact / Cascade Overlap

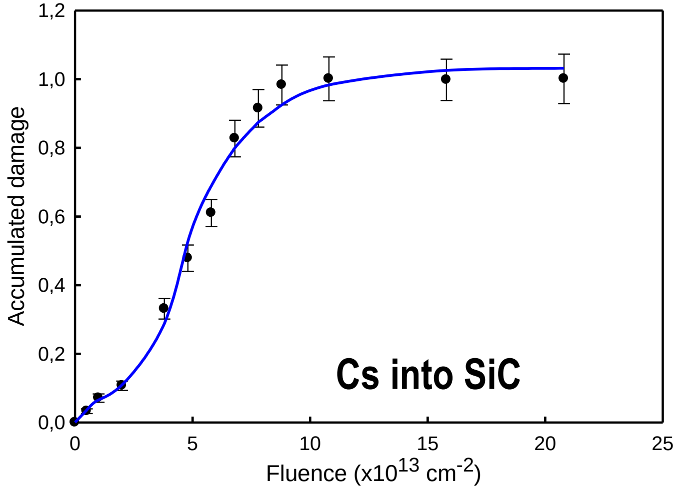
Nucleation and Growth

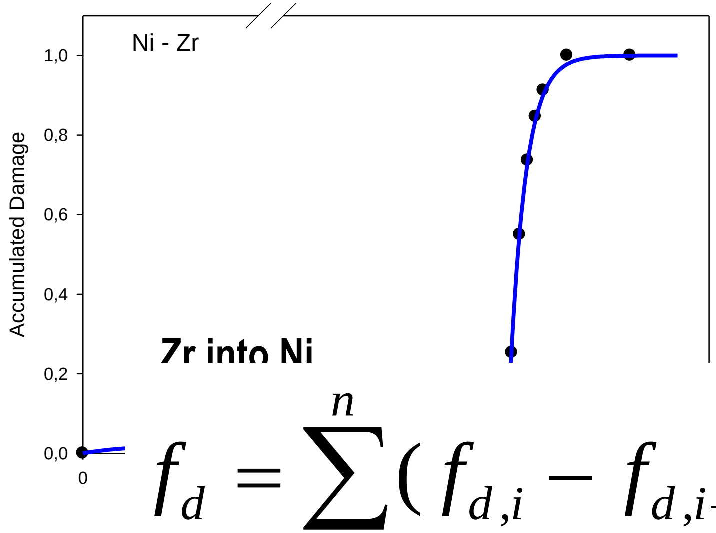
DI/DS (Direct Impact / Defect Stimulated)

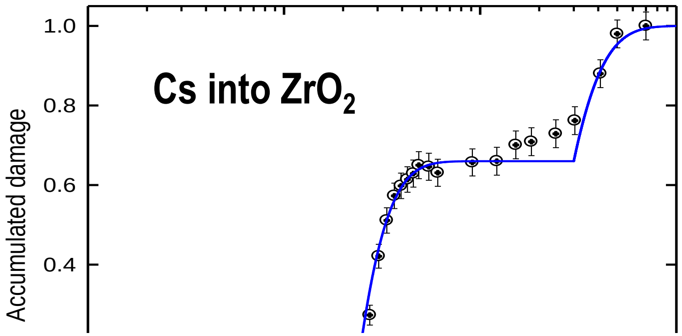
MSDA (Multi Step Damage Accumulation)

Multi-stage damage accumulation









$$f_d = \sum_{i=1}^{n} (f_{d,i} - f_{d,i-1}) G[1-\exp(-\sigma_i(\Phi-\Phi_i))]$$

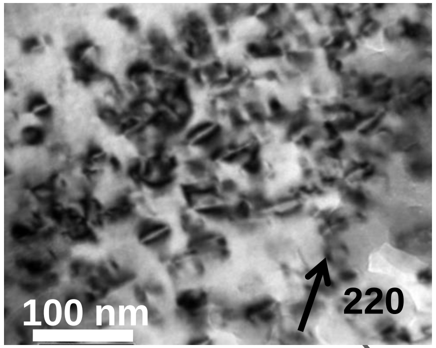
Case:
radiation damage in ZrO_2 crystal

Low-energy irradiation:

In-situ experiment at RT; 4 MeV Au^+, fluence increasing up to $2x10^{16}$ cm^{-2},
Analysis: RBS/C with 1.6 MeV He^+

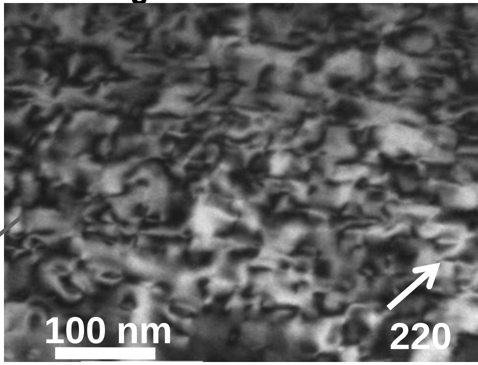
Case study: irradiated zirconia

Dislocation loops

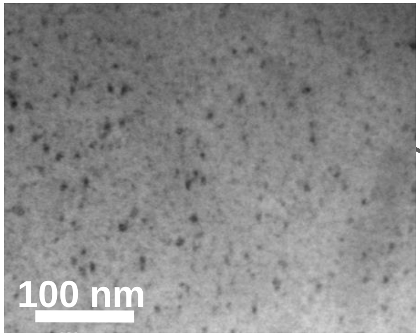


Relaxation of the elastic strain

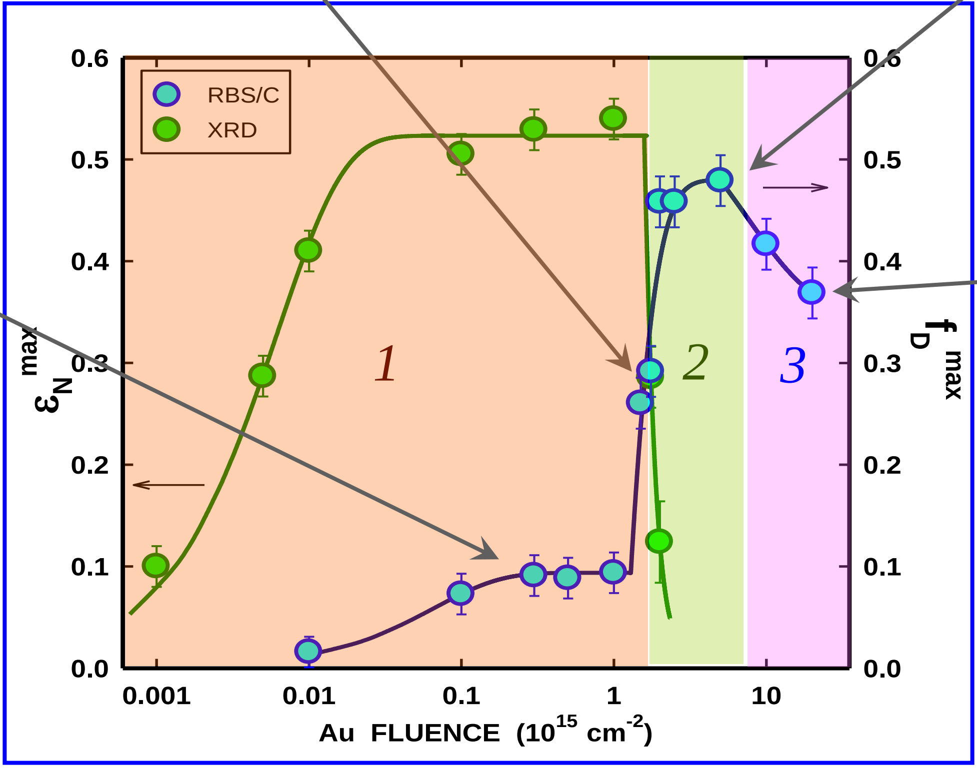
Network of tangled dislocations



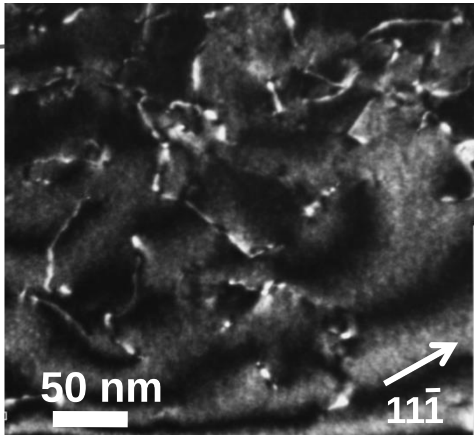
Small defect clusters



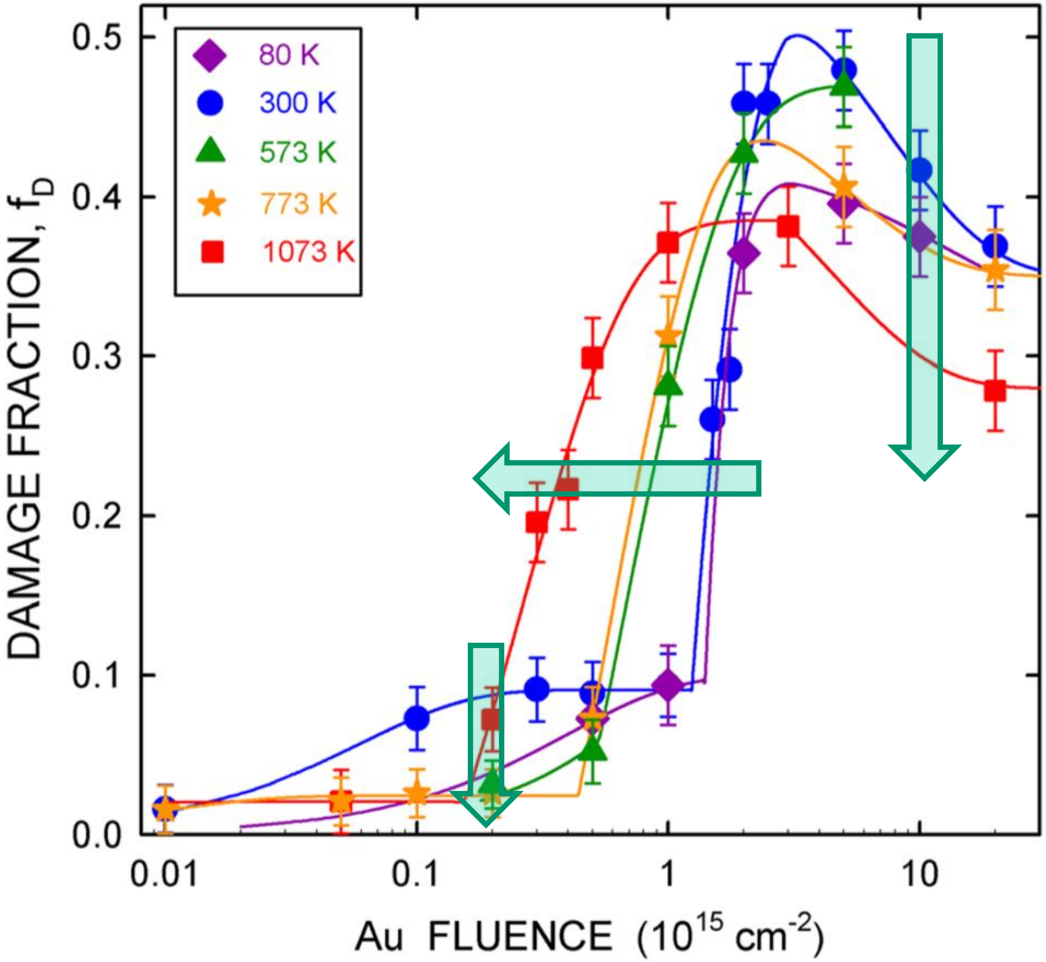
Increase of the elastic strain



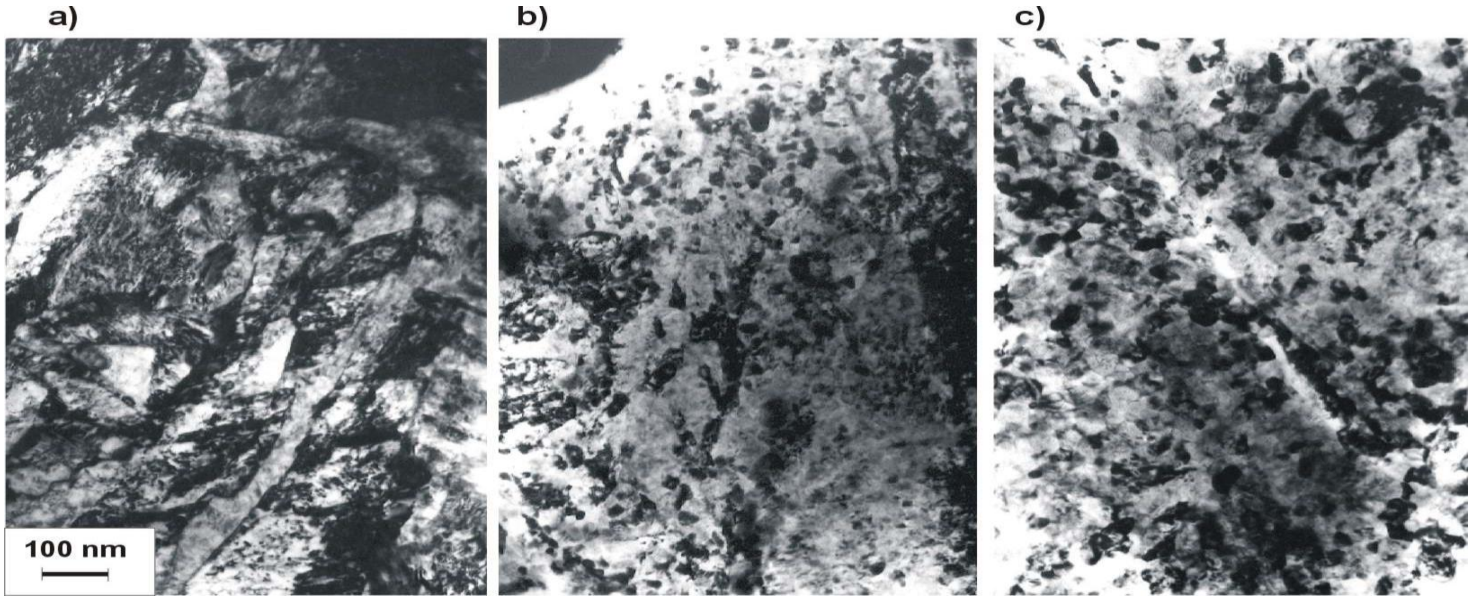
Long dislocations



Role of the temperature

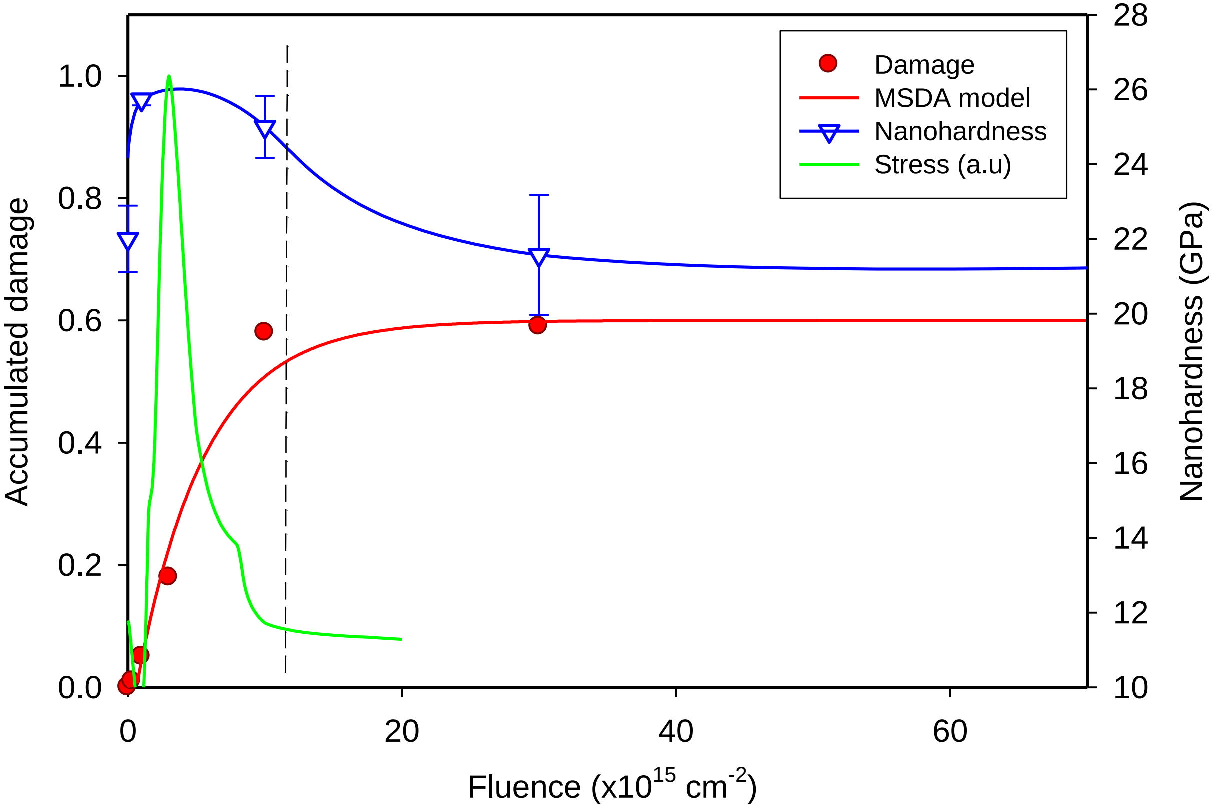


Ferritic steel

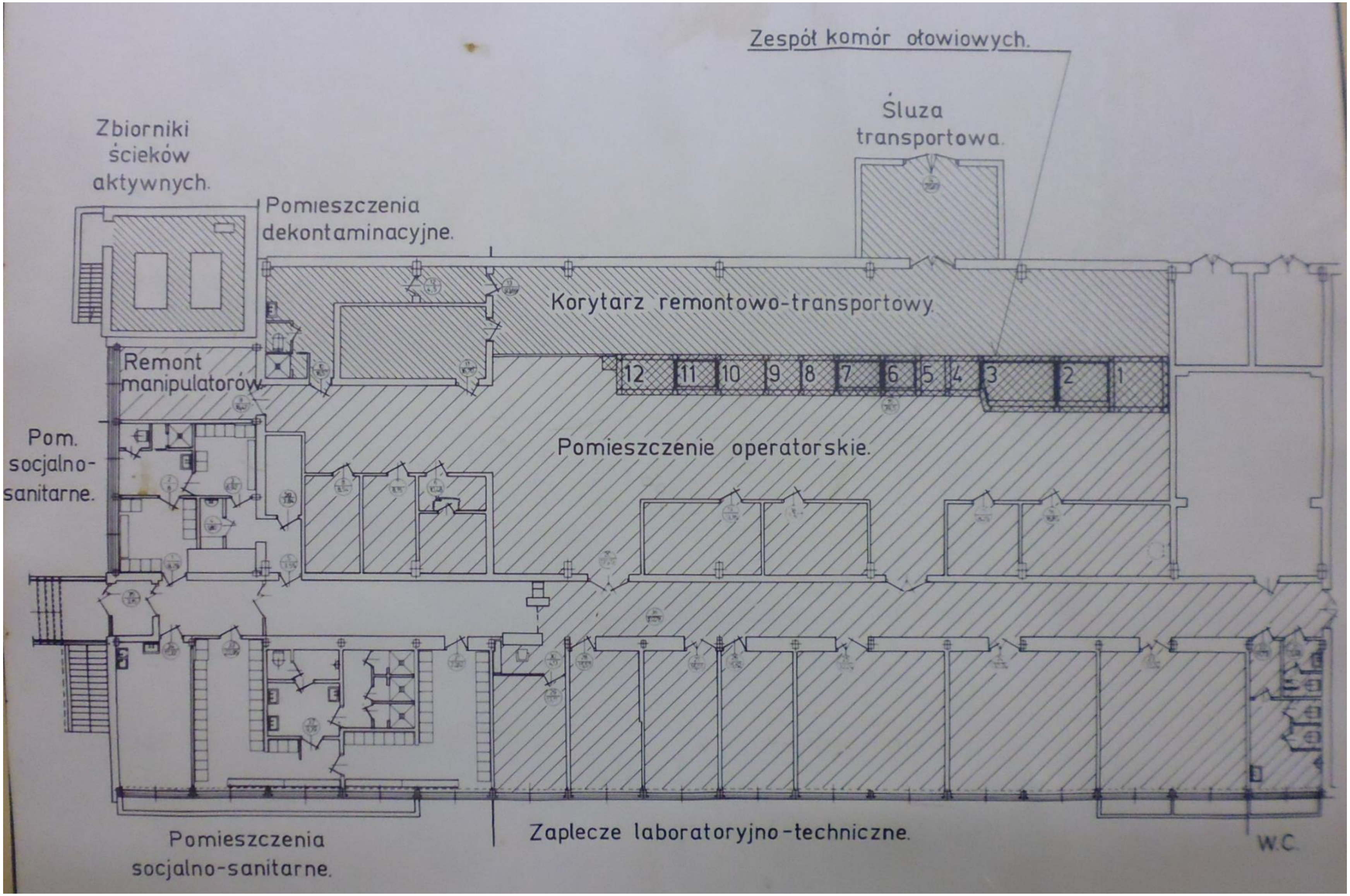


nieimplantowane **1×10^{17} at.N/cm^2, 100keV** **2×10^{17} at.N/cm^2, 100keV**

Mechanical properties of irradiated spinel

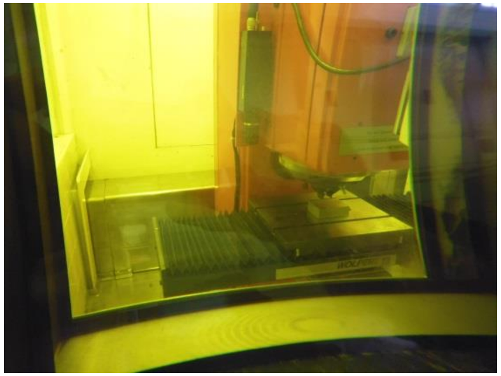


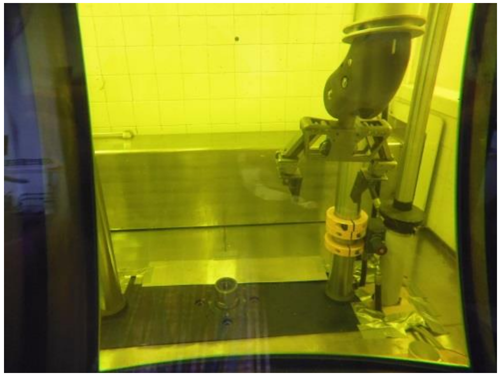
Hot cell Lab

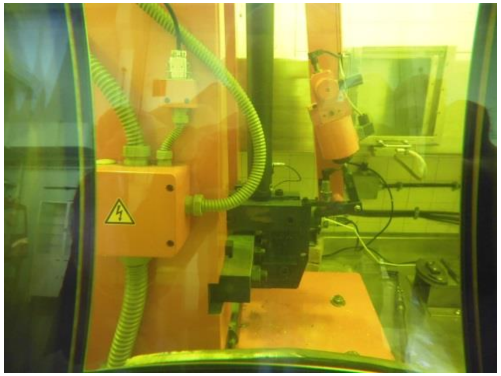

Zespół komór ołowiowych.
Śluza transportowa.
Zbiorniki ścieków aktywnych.
Pomieszczenia dekontaminacyjne.
Korytarz remontowo-transportowy.
Remont manipulatorów
12
11
10
9
8
7
6
5
4
3
2
1
Pom. socjalno-sanitarne.
Pomieszczenie operatorskie.
Pomieszczenia socjalno-sanitarne.
Zaplecze laboratoryjno-techniczne.
W.C.

Hot cell Lab: main equipment

Hot cell Lab: main equipment



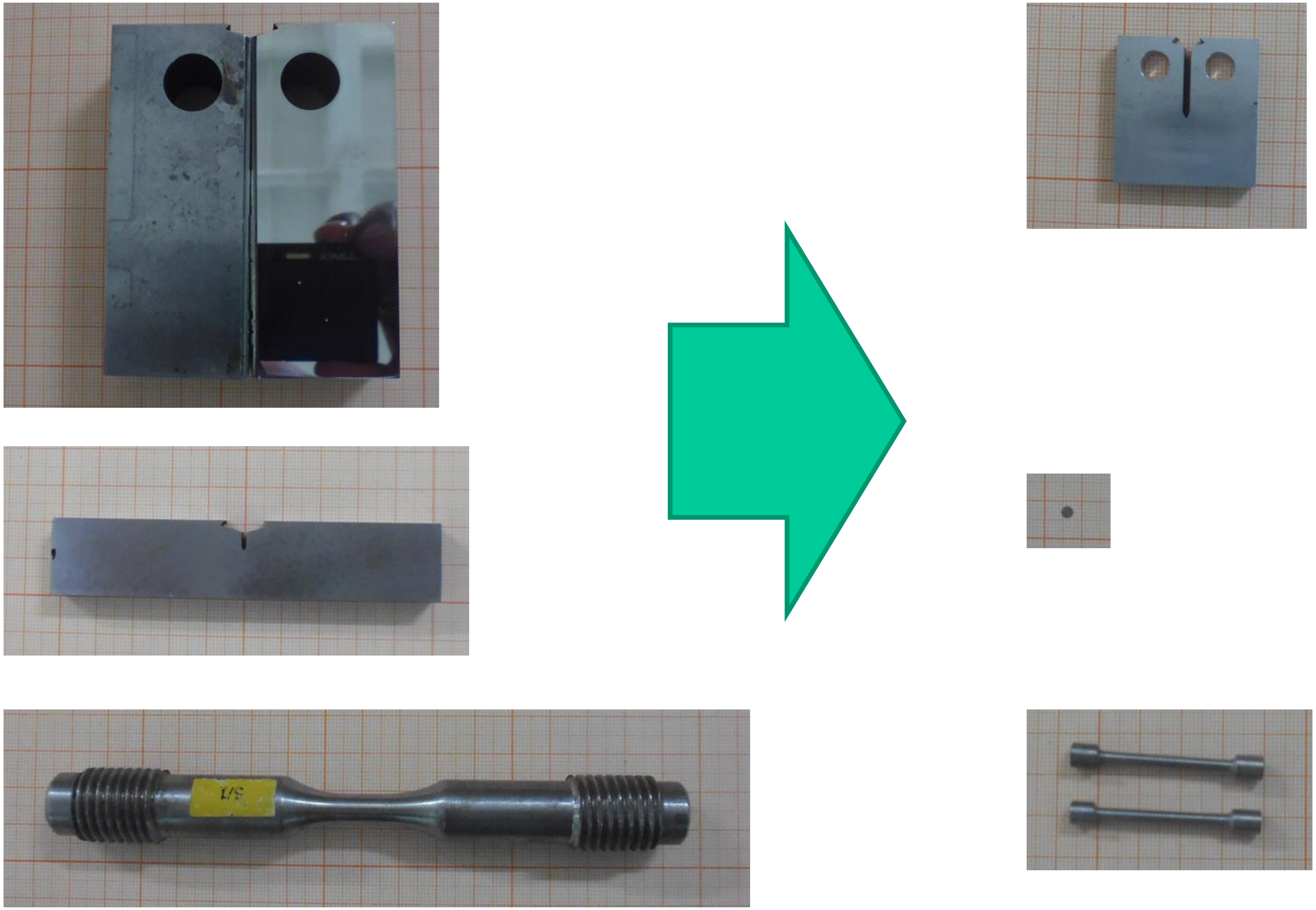




Hot cell Lab: mandatory conditions

1. Safety
2. Security
3. Access control
4. Dosimetry
5. Waste collection
6. Certificates
7. Accreditation

Hot cell Lab: Samples



Conclusions

Analysis of irradiation effects in materials should include **ion irradiation**.

Research infrastructure needed is similar to that used in **research on fission**: close cooperation is thus reasonable.

Urgent need to develop protocols of mechanical measurements on **miniaturized samples**.

Validation experiments for safety analyses should be included in the research program.

Topic to be discussed with regulatory bodies: **licensing requirements** for fusion devices.

Acknowledgement

Andrzej Turos, Lech Nowicki, Lionel Thomé, Frédérico Garrido, Pascal Aubert, Bruce Arey, Libor Kovarik, Yanwen Zhang, Łukasz Kurpaska, Iwona Jóźwik, etc, etc…

Thank you for your attention