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Joint ICTP-IAEA Workshop on Physics of Radiation Effect and its Simulation for Non-Metallic Condensed Matter

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Combination of experimental tools and computer modelling for investigation of radiation damage - fusion applications

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OUTLINE

- Introduction: modelling + validation
- Material Performance, Modelling and Simulation Tools
- Damage in a Fusion machine: validation experiments
- Conclusions

Introduction: modelling + validation

- Modelling tools based on existing and new mathematical algorithms and computer facilities have been developed over the last decades.

- *Ab-initio* computation of electronic structures allows the basic properties (structure, formation, migration) of point defects to be arrived at. This has made possible the full modeling of *self-diffusion*, as of the crucial effects of impurities.
  - **For insulators the *ab-initio* approach, i.e. an approach based on rigorously taking into account the quantum character exhibited by physics at the atomic scale, is indispensable if electronic effects are to be taken on board, in particular the damage due to particles other than high-energy neutrons, electrons, and photons.**

Introduction: modelling + validation

- Molecular dynamics is the basic tool for the investigation of ballistic damage processes, however its effectiveness is dependent on the quality of the interatomic potentials used.

- Predictions of long-term microstructural evolution kinetics, rely on already highly developed models, that have shown good performance with respect to metals, application of **which to ceramics, however, is only just beginning.**

Introduction: modelling + validation

- The understanding, and modeling of mechanical behavior are far more advanced for metals than for ceramics, however the multiscale approach, starting from the atomic scale, is still barely at an initial stage.

- Modeling must be closely coupled with experiment.
  - it is indispensable to conduct a targeted experiment drive, aimed at ascertaining basic physical properties, and behaviors, and at the parametrization, and validation of the models.Thus, charged-particle irradiation – involving ions, and electrons – affords the possibility of mimicking, and analyzing, in detailed fashion, damage mechanisms in small, inactivated samples, which are thus amenable to a whole range of measurements, and observation, from the atomic scale up, both *in situ*, and *ex situ*.

Material Performance, Modelling and Simulation Tools

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Some Objectives of Modelling of n-Radiation

- To understand fundamental mechanics governing the behaviour of a physical system
- To model the behaviour (description in equations)
- To predict (changes in) material performance

Material performance includes

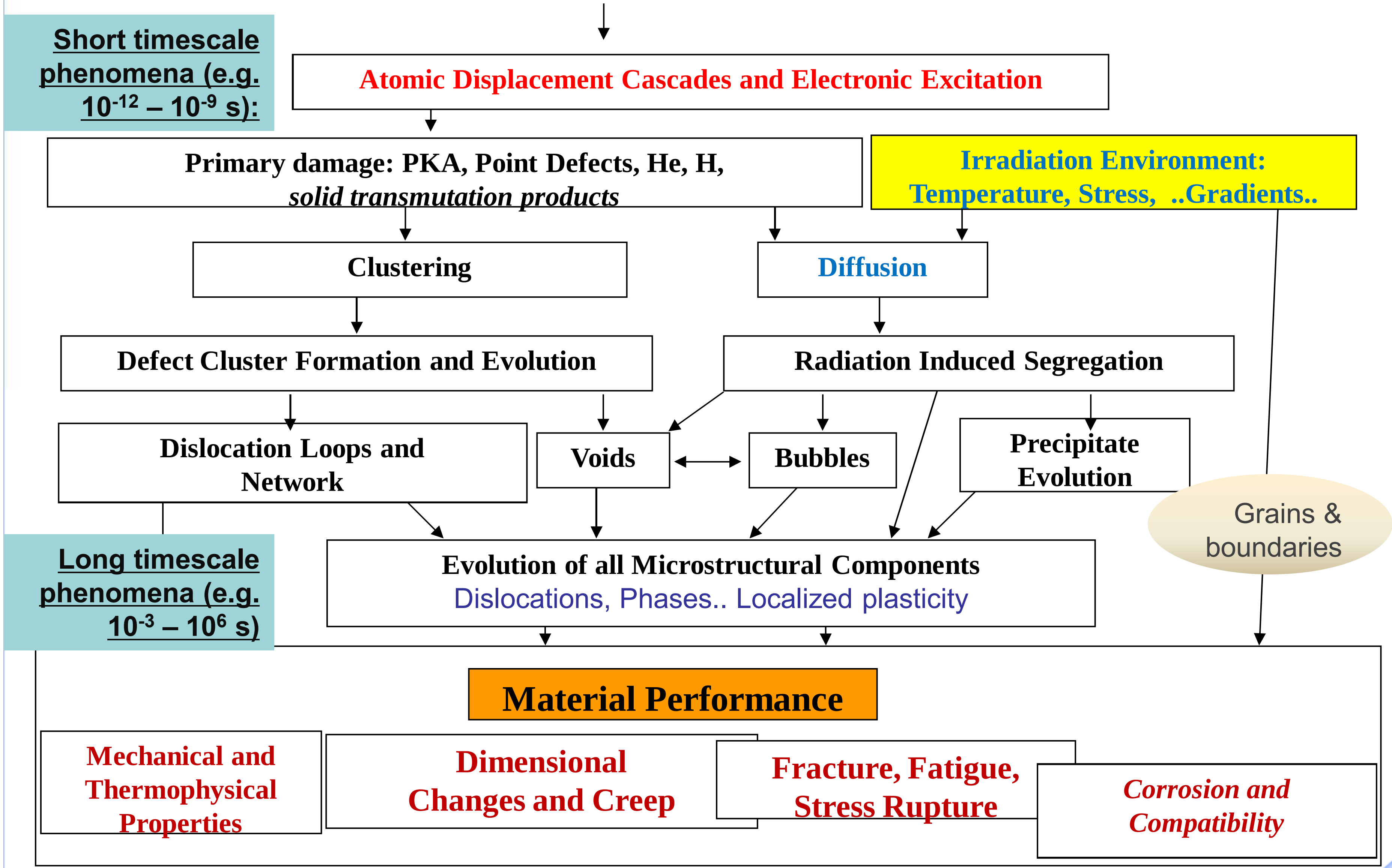
- **Yield strength and strain hardening constitutive laws.**
- **Various types of 'ductility'.**
- **Fatigue crack growth rates.**
- **Fracture toughness.**
- **Irradiation creep rates.**
- **Thermal creep rates.**
- **Void swelling rates.**
- **Creep rupture times and strains.**
- **Thermo-mechanical fatigue stress and strain limits.**
- **Creep crack growth rates.**
- **Creep-fatigue interactions.**
- **Environmentally assisted cracking.**
- **Bulk corrosion, oxidation and compatibility.**

>>> Of course there are other objectives and benefits of modelling

Accelerated material development cycles, i.e. "design" of materials through

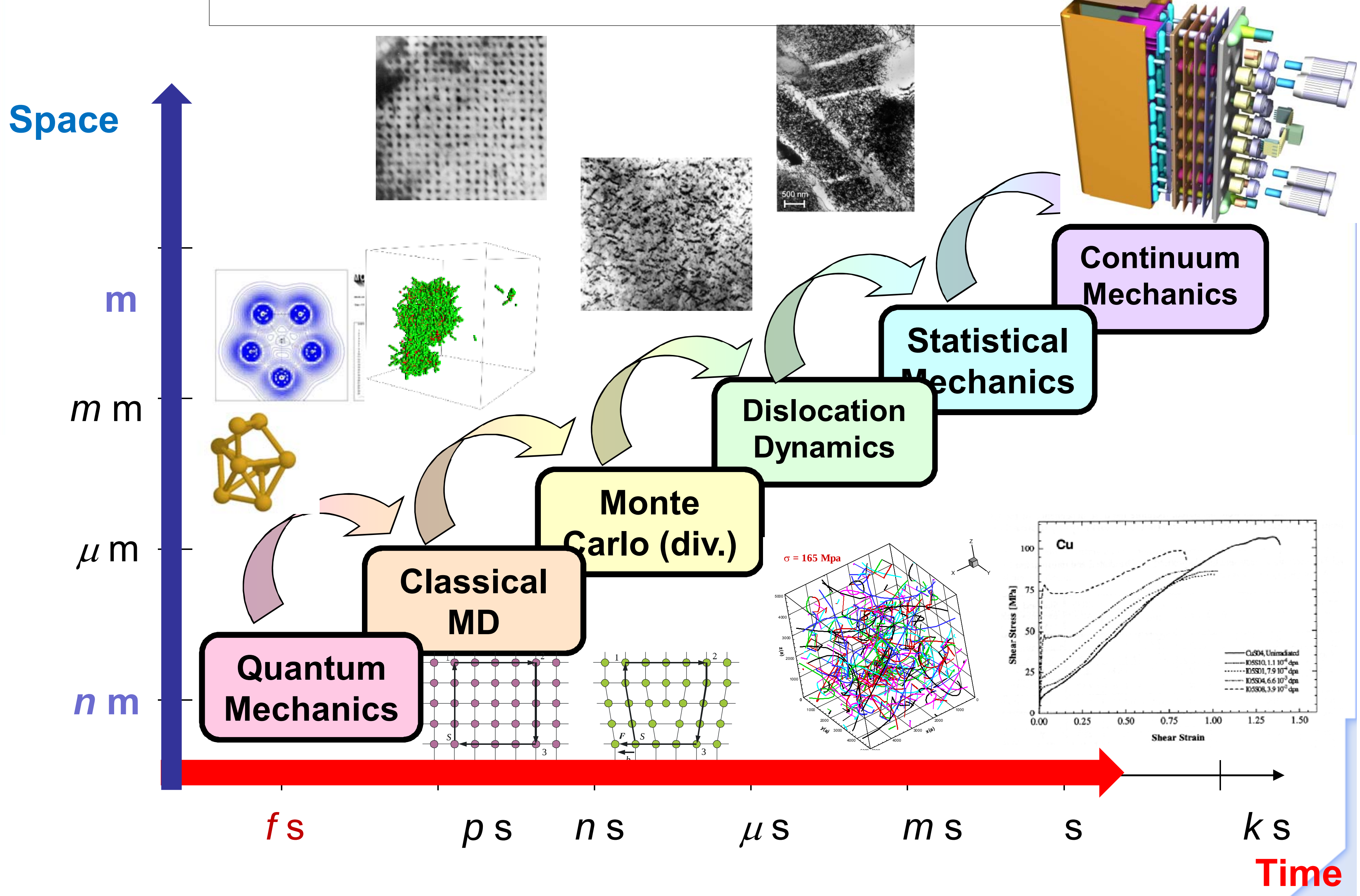
- *Guidelines on improved alloy composition.*
- *Optimized microstructure*
- *Relationship between processing and microstructure........*

Schematic diagram of radiation damage processes

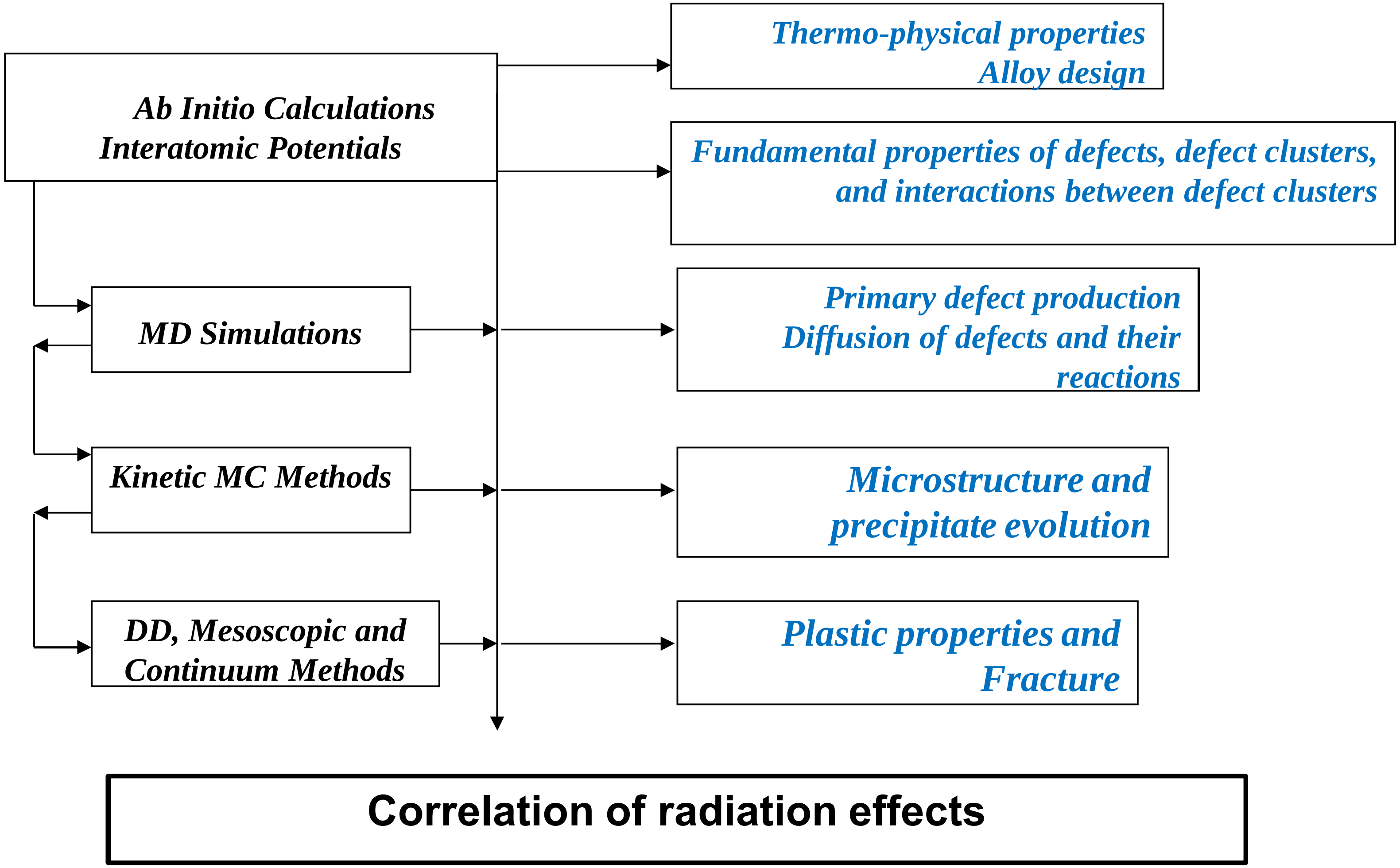


Ref: Workshop on Advanced Computational Materials Science, Washington, D.C. 2004

Multi-scale Modeling Strategy



Summary of computational tools and their uses in radiation damage modelling



"Limitations" and "Potential for improvements"

Limitations

•Computing time

•~ (N) $^{\alpha}$ *[spatial discretisation]* * T /Δt *[time steps]* * Iterations

• Physical complexity of alloys (steels)

• Nature of the radiation damage (time scales..)

"Potential for improvements"

❖ **Model analysis**
(consistency of the problem, physical meaningful input, stability ..)

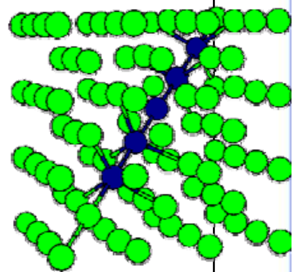
❖**Approximation and discretization**

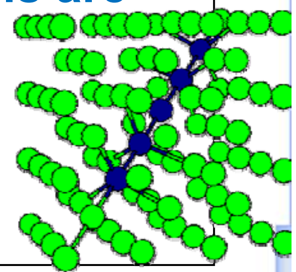
❖**Solvers and software**

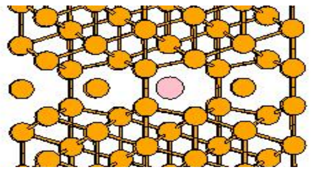
Better physics & science is more important than better computer science and computing power

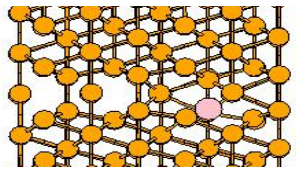
Ab initio, First principle
… Density functional theory .. etc

- **Directly based on quantum mechanics -> EXACT !**
- **Up to today the most exact way to solve multi-particle Schrödinger equations**
- **Significant approximations necessary**
- **Output: all kind of energy calculations results** (binding energies), **point defects, clusters, migration, geometric grain boundaries, phase diagrams magnetism/anomalies, ordering, simple multi-element systems,)**
- **Restriction to zero Kelvin, no temperature involved**
- **Computer power limits number of atoms, today a few hundred atoms are the rule, up to about a few thousand is the cutting edge**
- **In 30 years: possible number of atoms might increase significantly, methods for including temperature might be developed**









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Molecular Dynamics (MD)

- Directly based on Newton's equation of motion
- Discrete solution of many particle equation system (with initial defect distribution)

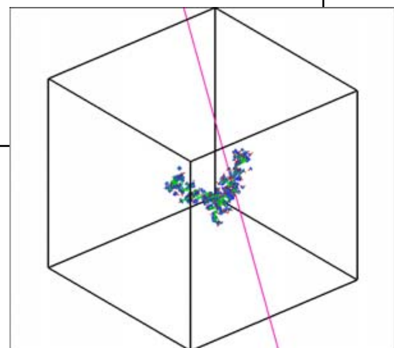
- Time-step ~ 1 fs; Short-range forces;

  (N) $^{\alpha}$ *[spatial discretisation]* * T /Δt *[time steps]* * Iterations

- Application to all <u>kind of defects</u> &

  <u>polycrystalline materials, alloys</u> ….

- Big advantage: <u>Parallelization</u> by spatial decomposition
- Output: time-dependent atomic positions, i.e. the total information of the whole system (temperature, distribution/correlation functions, etc. can be easily derived)



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Molecular Dynamics (MD) *-cont*

- Restriction: Severe approximations/simplifications necessary → particle interactions (potentials) have to be semi-empirically, i.e. fitted to the simulation problem/study.
- Restriction of number of atoms and of the simulation period due to computer power: (1-100 million atoms, < 100 ns).

  Billion atom calculations are demanding, but possible with cluster computing..
- Short-range forces implication: The total number of atoms in the simulation strongly depends <u>on the range of the interaction forces</u>, i.e. the more complex a material the less effective the method → best suited for simple metals
- In 30 years: possible simulation periods might increase by some orders of magnitudes → but still μs range (below mm sec!)

*To model 3 D 3x3x3 grains of ferritic steels on needs ... **10 000 000 000 * Billion** atoms*

Monte Carlo (MC)

- Directly based on statistical mechanics.
  - Freeze atomic degrees of freedom;
  - Track defects only;
  - Microstructure evolution of defects
  - Spatial inhomogeneity
  - Time is introduced to calculate transition probabilities
- Different approaches of Kinetic Monte Carlo, eg
  - Lattice MC
  - Object MC
- Restriction: for interaction forces of the atoms the same restrictions mentioned for MD are true (semi-empiric potentials with reduced range of application)
- Model size depends on computer power, but is less demanding compared to MD
- Output: evolution from initial system to equilibrium,

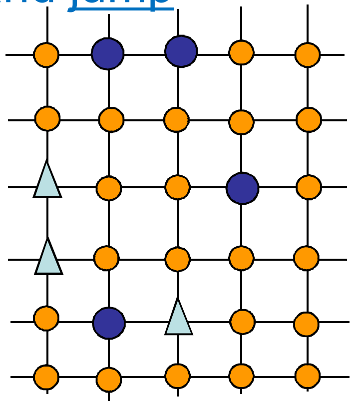
  Limitation: no “real time scale”

  → equilibrium conditions only, temperature is a constant input parameter

Lattice Monte Carlo (LMC)

- Monte Carlo method that uses fixed lattice positions for the atoms and jump frequencies of the atomic species involved in the calculation

  (this may be vacancies, interstitials, or substitution elements)



- Output: evolution from initial system to equilibrium,

  limitation: The models does not include a "real time scale"

  → equilibrium conditions only, temperature is a constant input parameter

- Output: transition/evolution from initial system **to equilibrium**. The system time can be estimated for the intermediate steps.
- Diffusion, decomposition, precipitation, growth, mixing, and other processes with long time scales
- Restriction: fixed lattice positions, jump frequency principle is a global simplification
- In 30 years: no significant improvements are expected. The method includes intrinsic limiting factors

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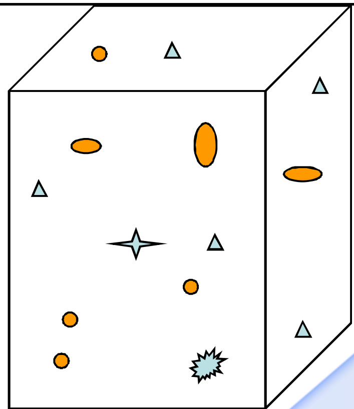
Object Monte Carlo (OMC)

- Modified Monte Carlo method were objects (not atoms) and transition probabilities are used to describe the evolution of a system
- Objects can be everything like point defects more complicated clusters or dislocation loops
- Output: annealing processes, recovery stages
- Drawback: each object has to be described separately, i.e. the number of possible interactions between different objects increases fast (exponentially) and makes the model setup rather difficult. De facto, only well known phenomena can be modelled.
- In 30 years: the method will most probably not improve by orders of magnitude.

200nm



Discrete Dislocation Dynamics (DDD)

- Directly based on the equations of motion (Dislocations are created, move, join and change shape as a consequence of applied stress and mutual interactions)
- The only method which directly deals with dislocations → capable to model important deformation mechanisms (fracture, strain localization)
- Output: time dependent evolution/motion of dislocations in a simulation box
- Drawbacks: each possible interaction of a dislocation with other dislocations and/or defects (grain boundary, point defects, etc. but also lattice anisotropy) has to known and described separately.
  - *Thermo-dynamical magnitudes such as temperature and pressure cannot be easily controlled in virtual specimen*

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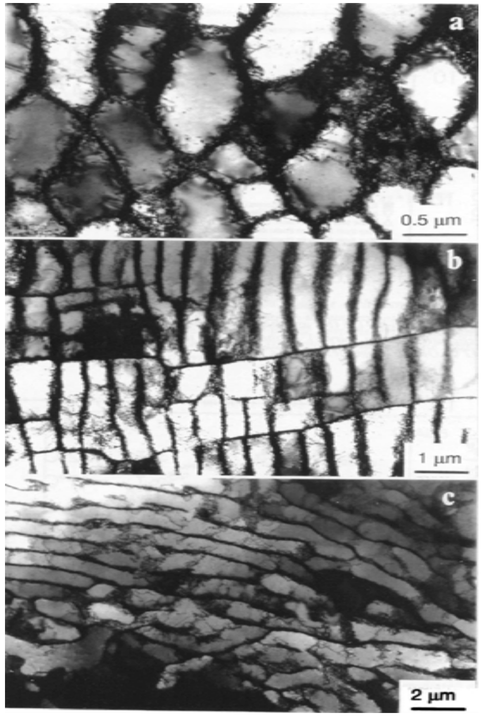
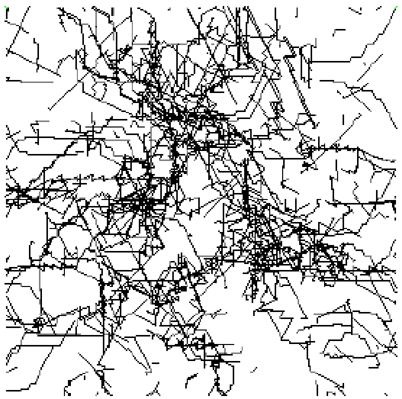
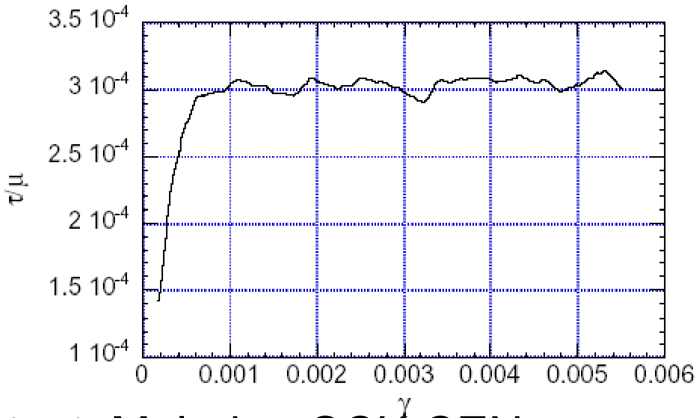
Discrete Dislocation Dynamics (DDD) *-cont*

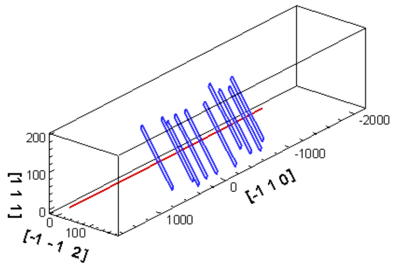
- ❑Timescale and simulation volume are depending on computer power. Relevant single crystal straining (comparable to a tensile test) is possible on high end super computers.
- ❑In 30 years: there will most probably a significant improvement (in volume and detail). However, predictions without prior experimental input are unlikely.







Tensile test, Malerba, SCK.CEN



Fatigue (cracks)
N.Ghoniem, UCLA

Finite Element Methods (FEM)

- Based on the solution of linear equation systems which result from the description of a volume, devided into small fractions with elasto-plastic deformation behavior
- Input: material model (a variety of possible description, the most simple is an elastic model, described by Young's modulus and Poisson's ratio), temperature dependend (thermal expansion, conductivity, etc.), if useful.
- Output: equilibrium deformation as a result of mechanical and/or thermal load.
- In 30 years: the degree of complexity and detail definition will certainly increase by orders of magnitude (today the simulation of car crash tests are possible with ultra-high performance computers)

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Modelling on the level of continuum mechanics Or DDD- continuum mechanics

- *Approach taken in the 1980-ties in developing constitutive equations (eg Chaboche model) for austenitic steels that unified creep and plasticty in viscoplastic constitutive equations*
- ***Physically based models** **with "internal" variables to describe evolution of yield stress / kinetic hardening & isotropic / strain rate effects ...***
- ***These models are the basis for calculations/simulations***
  - ***to understand test results, (Interpretation &a ssessmen of results)***
  - ***to transfer between different conditions***
  - ***to evaluate simplified rules***
  - ***to define verification experiments and their assessment***

They are essential for

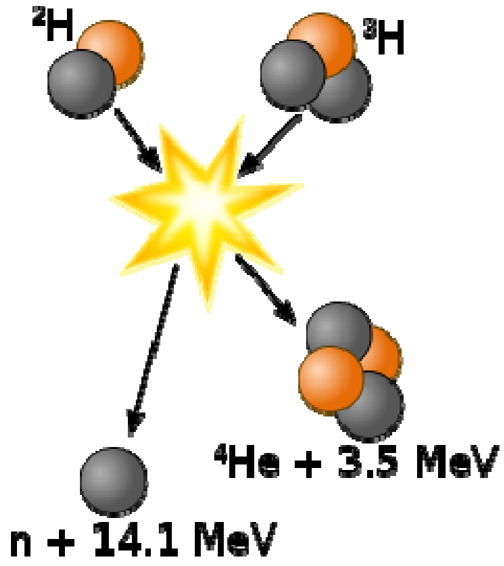
- ***"formulation of rules" to describe complex "cyclic [creep-fatigue-relaxation]" loads superimposed by effects from n-fluence / n-flux, generation of transmutations***
- ***"justification of rules"***

This includes knowledge and results from any of the other tools addressed before

- ***Ab initio, Molecular Dynamics (MD),***
- ***Lattice Monte Carlo (LMC), Object Monte Carlo (OMC)***
- ***Discrete Dislocation Dynamics (DDD)***

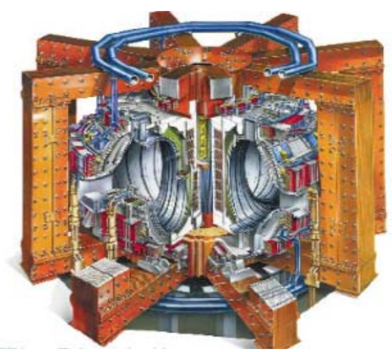
Damage in a Fusion machine: validation experiments

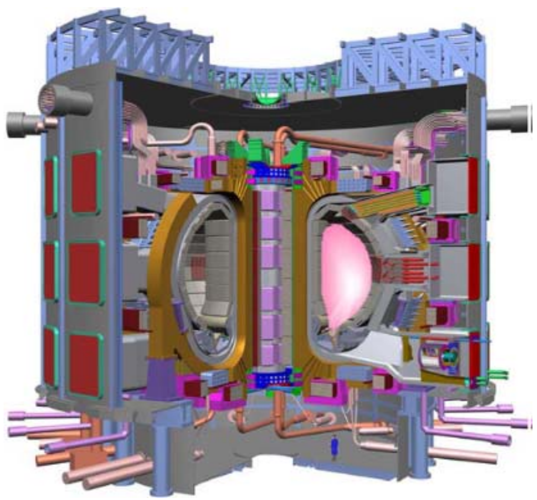
All these tools have to be used to simulate damage evolution

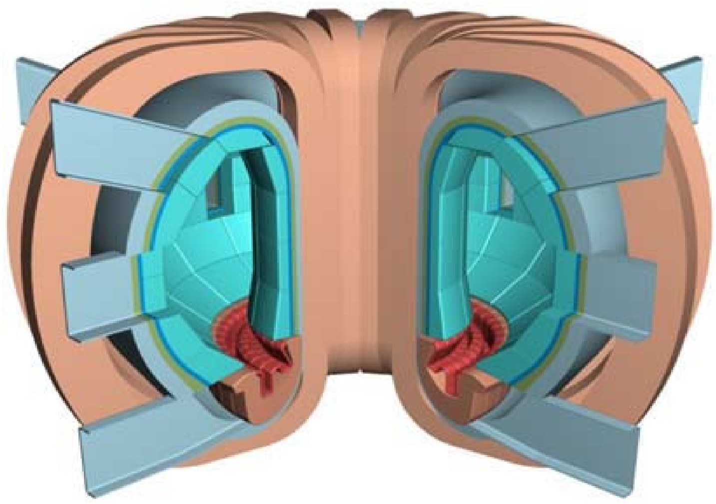


- Gamma ray
- Ion Bombardment
- Electron irradiation
- Neutron irradiation

Within a Fusion machine







Radiation Simulation Experiments

At present no entirely suitable Irradiation Test Facility for materials in a suitable representative "environment"

So use --->

fission reactors
particle accelerators
gamma and X-ray sources

Each have their advantages and disadvantages

Irradiation Conditions

Must simulate --->

displacement and ionization damage rates
(i.e. n + γ flux and spectrum)

radiation environment (vacuum and temperature)

operating conditions (voltage, mechanical stress)

For insulators in-situ testing is essential
For metals simple PIE (Post Irradiation Examination) insufficient

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REMINDER!

Effects of radiation on insulators

- **Ionizing** ⇨ **e-h pairs are created**

(NON PERMANENT Effect) ⇩ **ΔConductivity, ΔTan δ, RL**

• Also changes charge states of present defects (+ radiolysis)

- **Displacement** ⇨ **Point Defects**

(PERMANENT) ⇩ **Clusters**

⇩

Dipolar losses, ΔConductivity
Optical Absorption, Photo-Luminescence,
ΔThermal Cond., Swelling…

⇧

- **Transmutation** = **Impurities + Intrinsic Defect**

(PERMANENT)

Experimental fission reactors

- Have advantage of producing a radiation field
- of both neutrons and gammas

- But radiation volume inaccessible
- and problem of irradiating in vacuum

- Also nuclear activation means PIE in hot cell
- or postpone until the material can be safely handled

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Comparison of possible neutron sources

Neutron Source	Advantages	Disadvantages
Fission Reactors	Well-characterized spectra Allows medium-high damage regimes to be investigated in bulk specimens Operating funds provided by multiple users (non-fusion)	Low He/dpa ratio
Spallation	Allows high-He irradiation conditions to be explored Operating costs may be largely provided by non-fusion agencies	Not designed for materials irradiations (physics/ neutron scattering facility) He/dpa,H/dpa ratio too high Pulsed irradiation; requires detailed analysis
D-Li	Correct He/dpa ratio, etc. Dedicated materials irradiation facility	Operating funds completely provided by fusion

Particle accelerators

- Ideal for in-situ experiments in vacuum
- well controlled temperatures

- High levels of displacement damage and ionization can be achieved with little or no nuclear activation

- But radiation field non-nuclear, and non-uniform

- Limited irradiation volume

Irradiation facilities - Van de Graaff UAM

Typical test facility:

- 5 MV Tandem Van de Graaff
- High energy ion beams: material modification and radiation damage

Neutron damage

Neutrons Irradiation Damage:

There are 2 elementary reactions

- **Displacement Damage („dpa“)**
- **Nuclear Reactions. Transmutation**

Consequences of neutron Irradiation Damage: He/H Production. After irradiation some materials show an increased He/H content due to transmutation processes during neutron irradiation.

Key parameters:

- **Damage production (dpa)**
- **Ratio H/He production per dpa**

Current Irradiation Facilities for Fusion applications

- The existing sources of 14 MeV neutrons have a small intensity and do not allow us to get important damage accumulation in a reasonable time.
  - Fusion Neutron Source (FNS): $3 \cdot 10^{11}$ and $3 \cdot 10^{12}$ n/s; JAERI
  - Frascati Neutron Generator (FNG): 10^{11} n/s; ENEA

- It is necessary to simulate irradiation by 14 MeV neutrons, by using either fission neutrons, or high energy protons, or heavy ions.

Present Approach

- Materials are irradiated with fission neutrons on the one hand and with high-energy protons on the other hand. The obtained results are tentatively interpolated for fusion irradiation conditions.
- It is difficult to separate effects of particle type, particle energy, temperature, accumulated damage, damage rate and rates of production of impurities.
- Materials have to be submitted to actual fusion irradiation conditions in order to be fully qualified for designers and engineers.

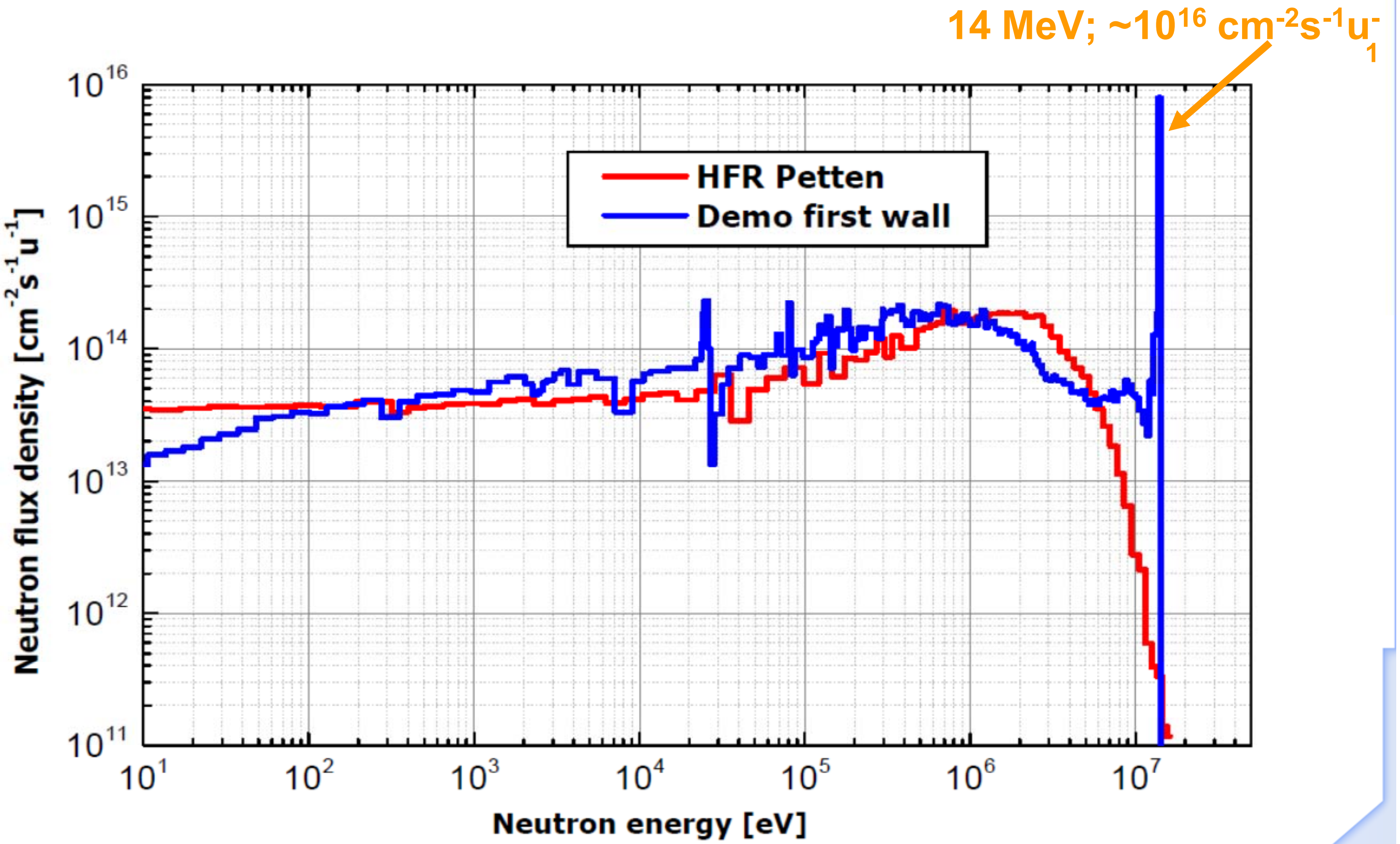
Irradiation Modes

- Fusion neutrons, fission neutrons:
- Strong differences in the production rates of impurities

Defect poduction (in steels)	Fusion neutrons (3-4 GW reactor, first wall)	Fission neutrons (BOR 60 reactor)
Damage rate [dpa/year]	20-30	~ 20
Helium [appm/dpa]	10-15	≤ 1
Hydrogen [appm/dpa]	40-50	≤ 10

Fusion neutrons / Fission neutrons

Neutron flux spectra: fusion vs. fission



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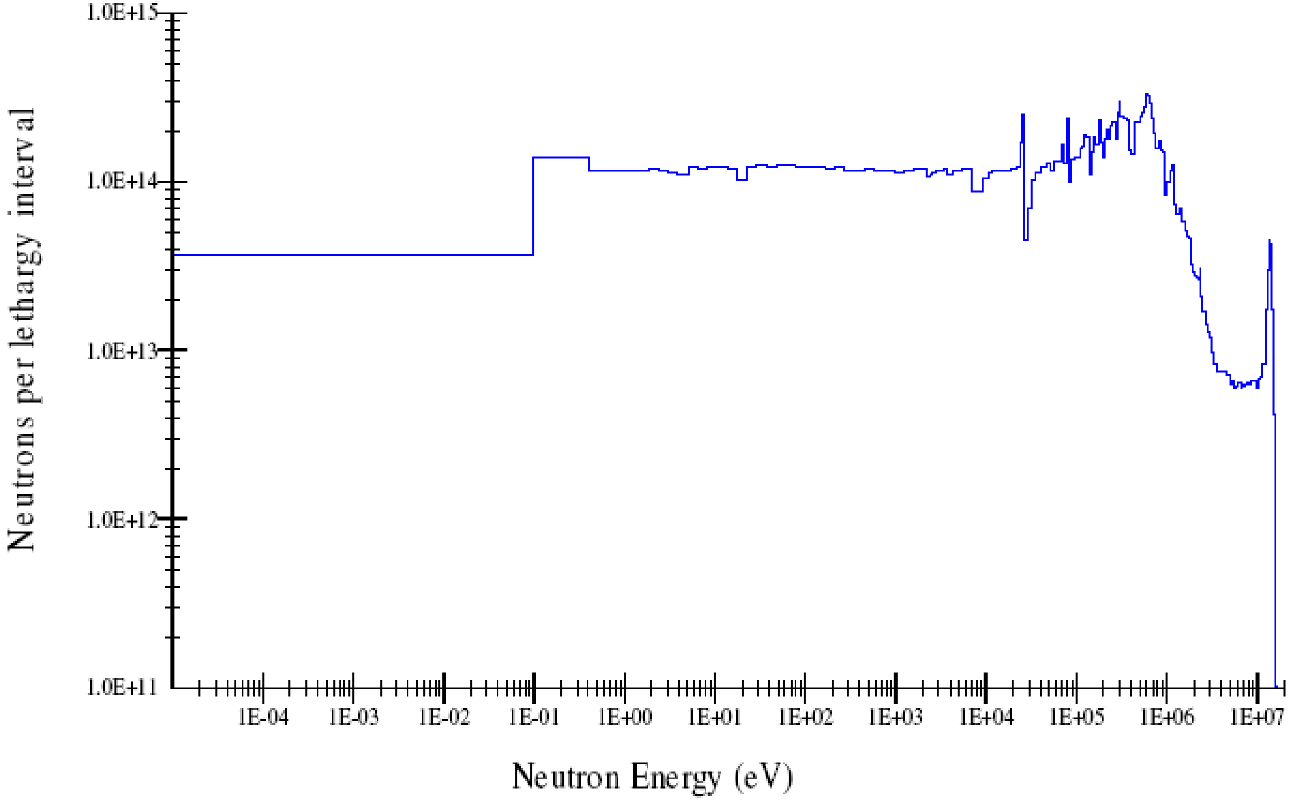
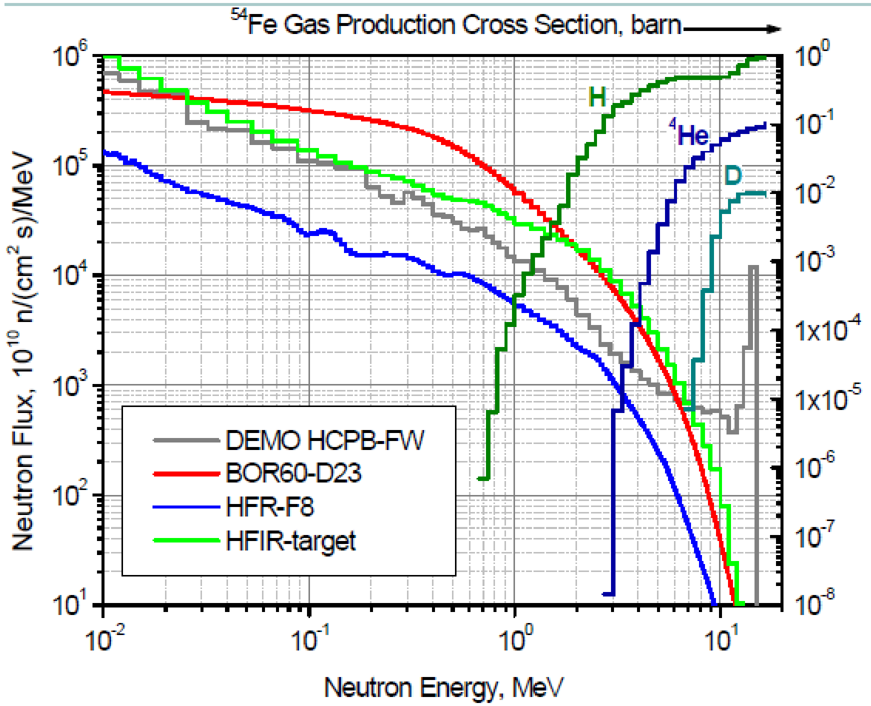
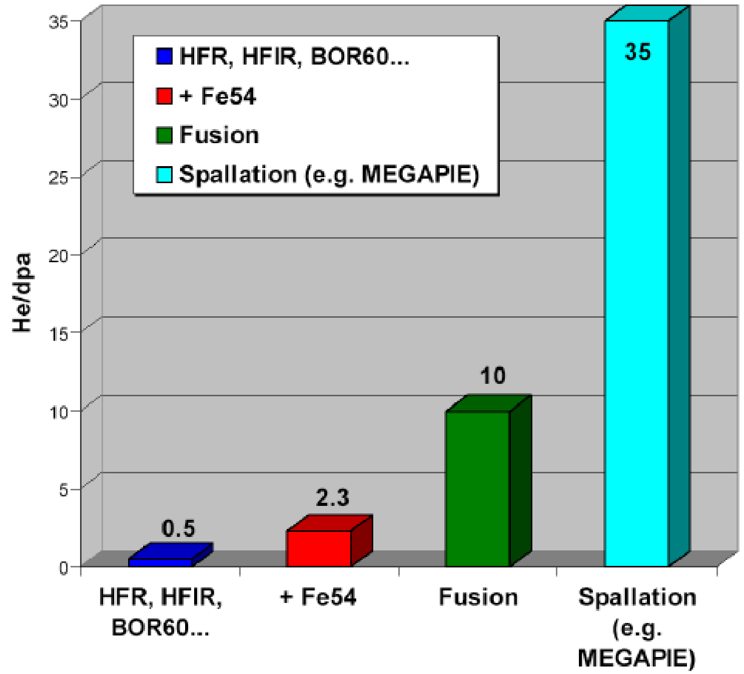
Neutron spectrum behind 1st wall



Fusion neutrons / Fission neutrons

Neutron Spectrum & He/dpa Ratio





- In fusion applications, beside displacemnt damage („dpa“), neutrons generate also:
  - Transmutation products like H, D, He above typical threshold energies Eth.
  - Most important is the so-called „He/dpa ratio“. For the „First Wall“ the value is about 10, i.e., during
- the damage generation of 1 dpa there is a He production of about 10 appm.

Ion damage

- **Simulating neutron damage: JANNuS Facility**

<u>Ion irradiation:</u> An example, JANNuS

JANNuS - Joint Accelerators for Nano-science and Nuclear Simulation

JANNuS is designed to supply a large range of ion irradiation and implantation conditions, allowing in-situ Transmission Electron Microscopy (TEM) and ion beam analysis with single, dual or triple beam combinations. Such a facilty has no equivalent in Europe and will play an essential role for multi-scale modelling of irradiation effects in materials.

Ion beams → to simulate the whole neutron-induced damage effects and its main consequences on both microstructure and mechanical properties.

Advantages of this simulation process → the versatility of the available experimental irradiation conditions (temperature, dose rate, fluence, damaged thickness) and the possibility to carry on in situ or ex situ physico-chemical and structural characterization.

USES:

Evolution of the microstructure of the material during irradiation and its physical and mechanical consequences+ cumulative effects of simultaneous multi-irradiation.

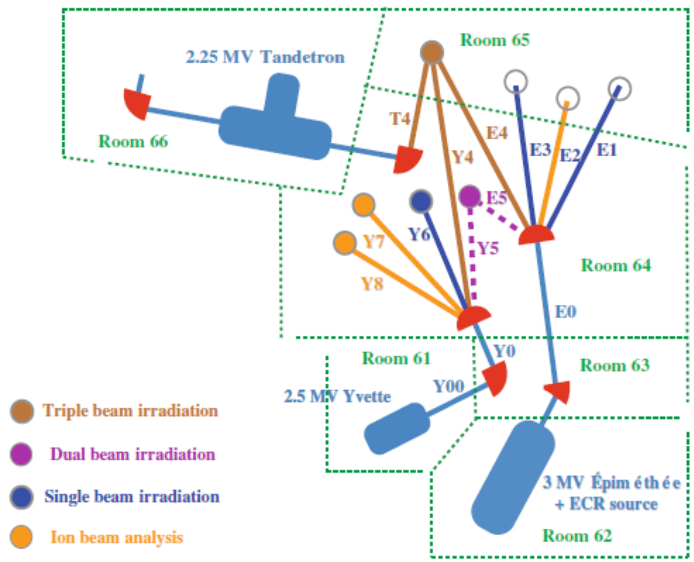
For fusion application:

- The study of the evolution of the microstructure of model materials (ultra pure Fe, Fe–C and Fe–Cr alloys, silicon carbide).
- The experimental validation of kinetic Monte Carlo and chemical kinetics modelling approaches based on dual irradiation of diluted ferritic alloys.
- The combined effects of damage accumulation/helium incorporation/hydrogen incorporation on ferritic alloys and silicon carbide.

JANNuS

The JANNUS project gathers two independent ion beam facilities:

A triple irradiation facility at Saclay:



3 MV PelletronTM from NEC (Épiméthée)

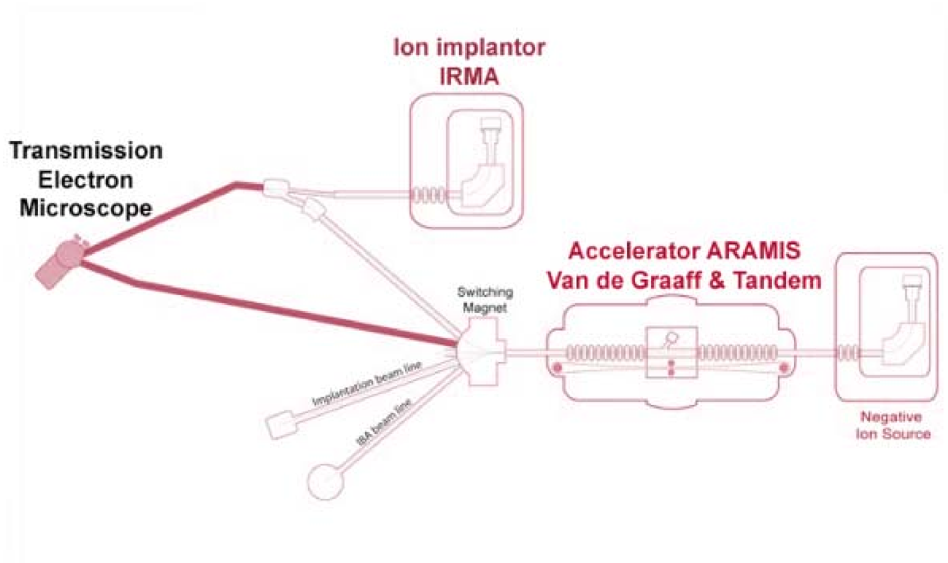
+

2.5 MV Van de Graaff (Yvette)

+

2.25 MV tandem (Tandetron)

A TEM-coupled dual beam facility at Orsay:



200 kV TEM TECNAITM from FEI

+

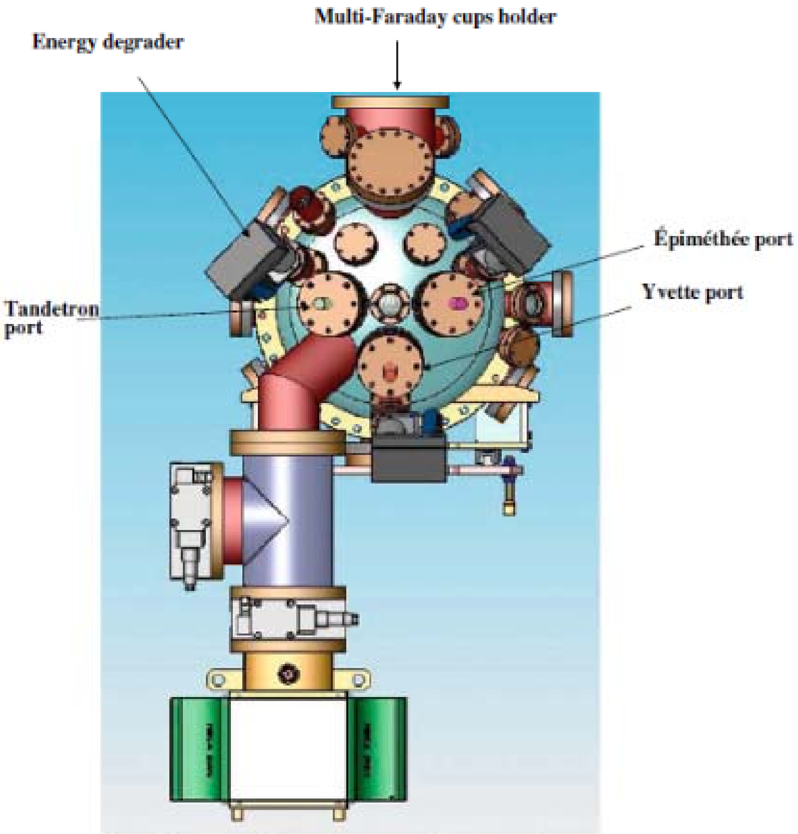
2 MV Van de Graaff/tandem (Aramis)

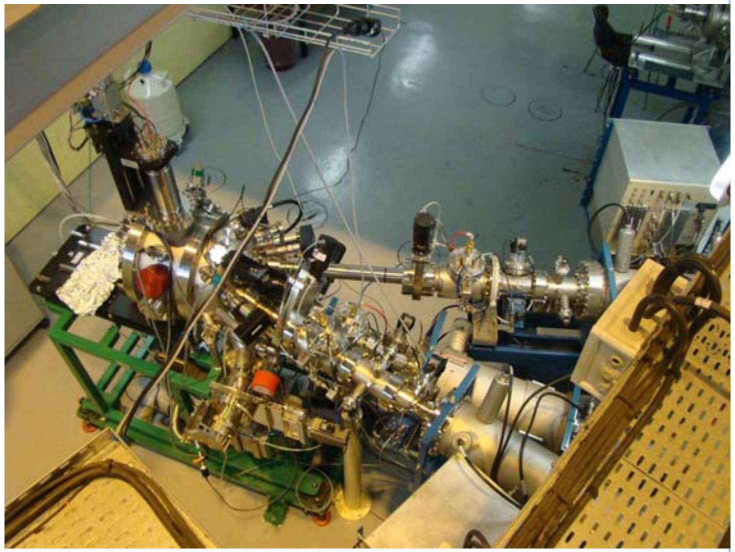
+

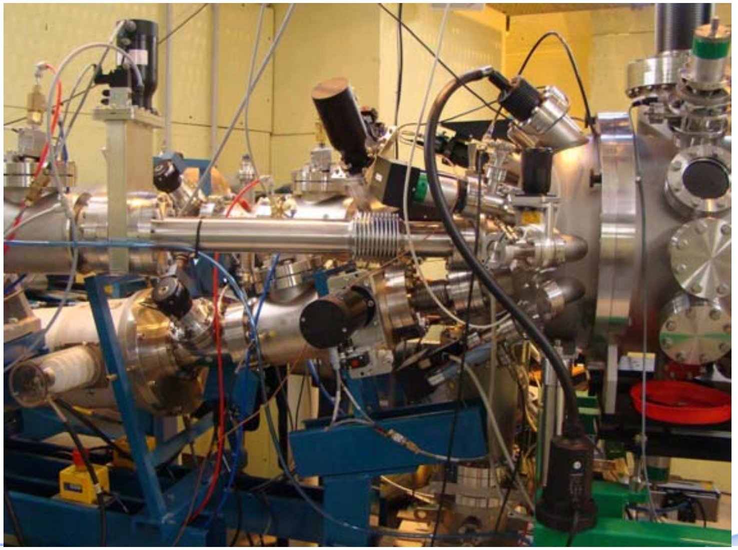
190 kV ion implantor (Irma)

JANNuS

The triple beam vacuum chamber installed at CEA Saclay





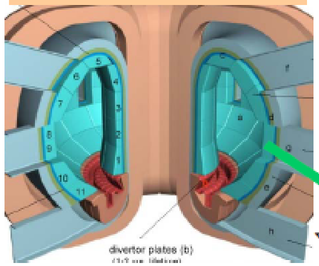


The sample holder mounted on the rear part of the chamber covers the temperature range liquid nitrogen to 800 C

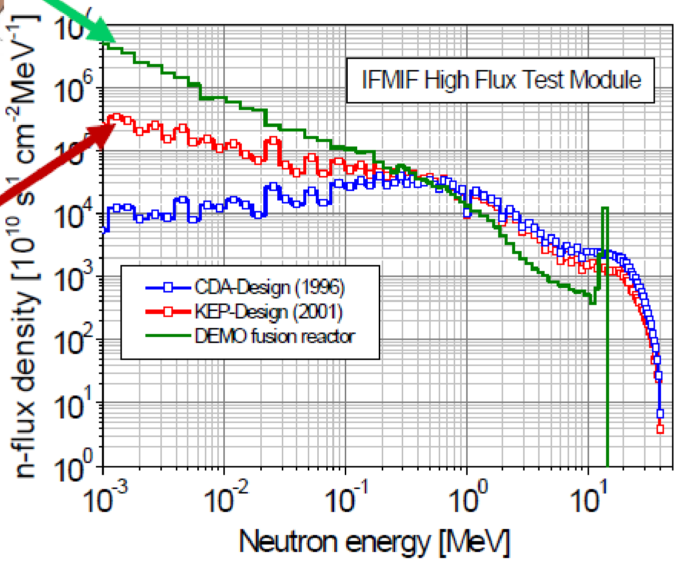
Fusion neutron source

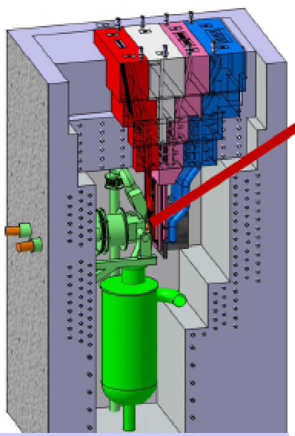
Fusion neutron source

Fusion reactor DEMO



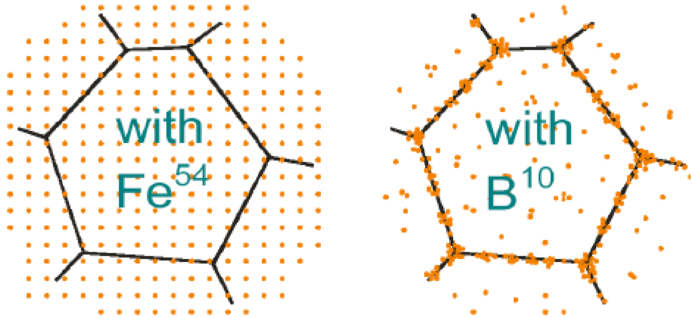
IFMIF is tailored to the fusion specific neutron spectrum and He production rate …





IFMIF test cell

He distribution after irradiation



$Fe^{54} + n \rightarrow Cr^{51} + \alpha$

$B^{10} + n \rightarrow \ldots \rightarrow$ **2** α

… while using fission reactors as irradiation source still needs artificial “He sources“ and the neutron spectrum is not as high energetic as in fusion.

Critical Issues

How to account for actual irradiation conditions: fusion-relevant neutron spectrum, temperatures, accumulated damages (dpa), damage rates (dpa/s), production rates of impurities (e.g. appm He/dpa, appm H/dpa) ?

Modelling of radiation damage and radiation damage effects

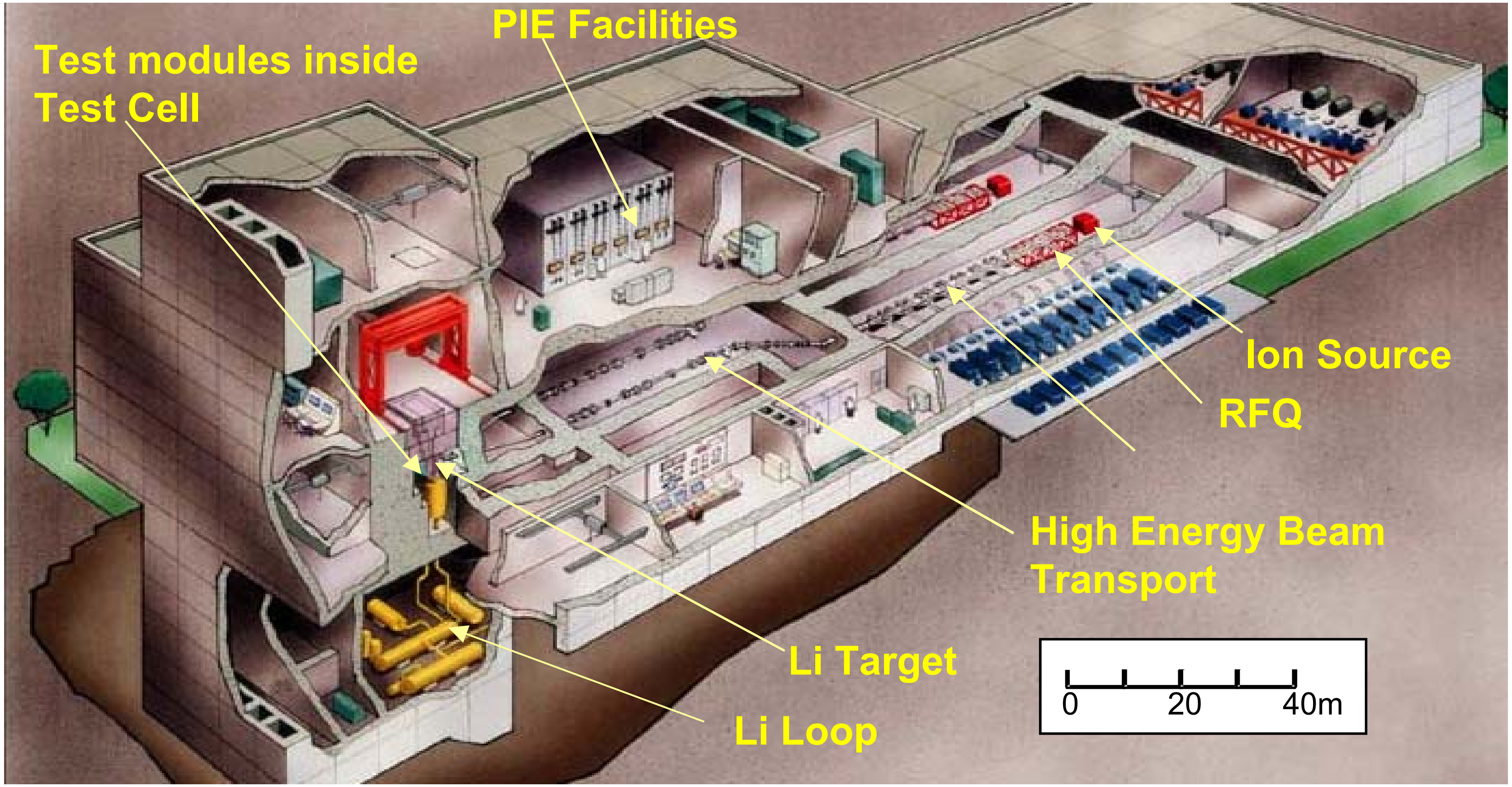
Construction of the International Fusion Materials Irradiation Facility (IFMIF)

What is IFMIF?

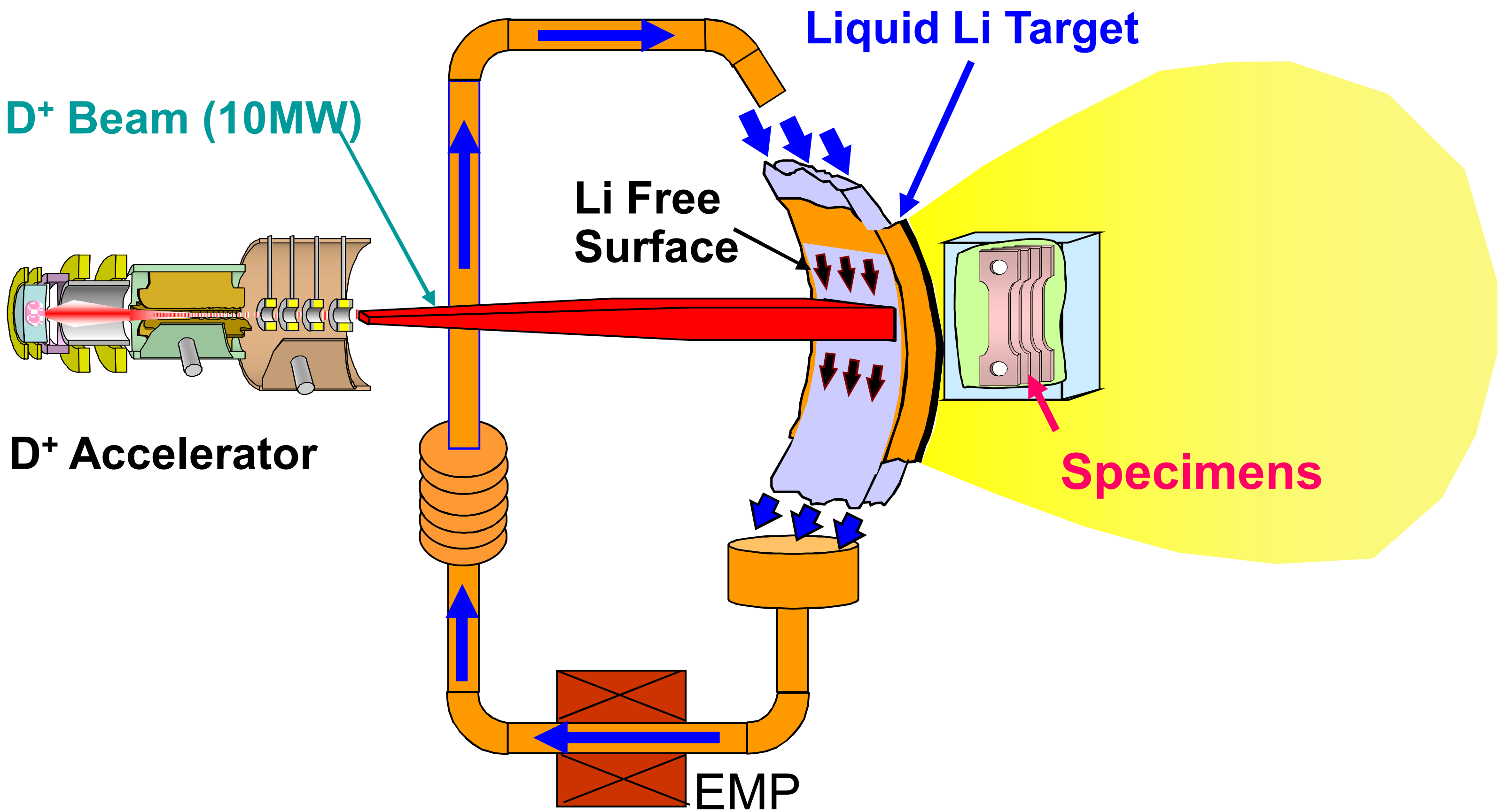
Intense source of 14 MeV neutrons (250 mA): the neutron spectrum should meet the first wall neutron spectrum as near as possible.

- Missions:
- Qualification of candidate materials up to about full lifetime of anticipated use in a fusion DEMO reactor
- Calibration and validation of data generated from fission reactors and particle accelerators
- Identify possible new phenomena which might occur due to the high energy neutron exposure

IFMIF (International Fusion Materials Irradiation Facility)

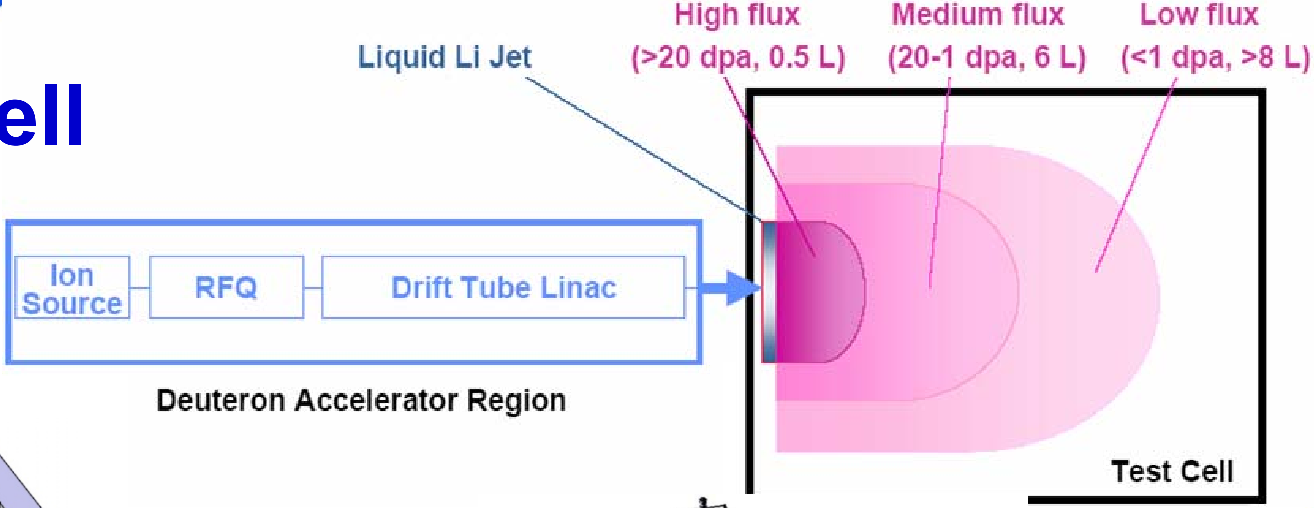


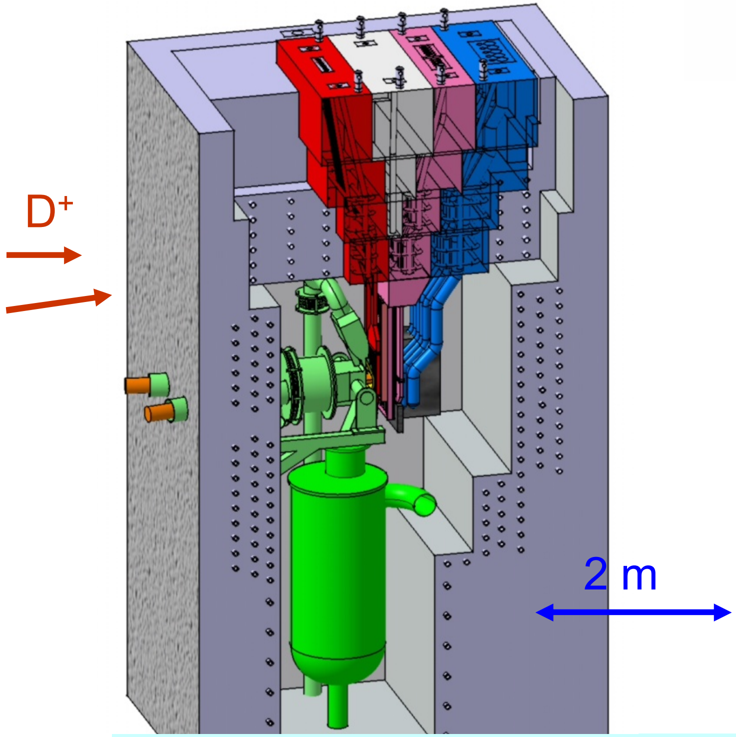
IFMIF uses the reaction: $^{7}Li\ (d, n)\ ^{7}Be$

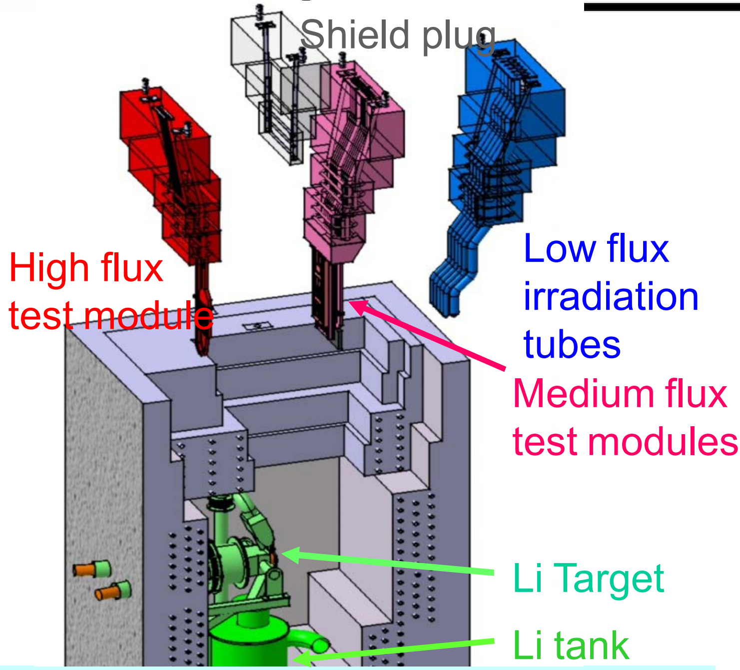


Mission:
Obtain stable and high speed Li flow during 10 MW D^+ beam loading

IFMIF Test Cell







- Gas coolant for all test modules
- Modular and highly flexible

Easy user access
Capacity for upgrades

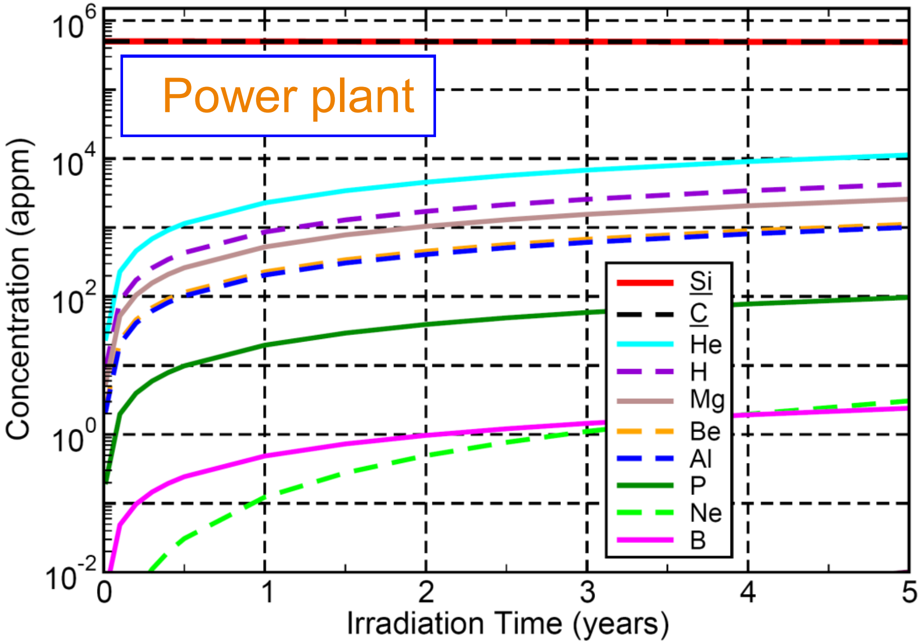
Example of modelling + validation (still pending)

SiC composition evolution under fusion n irradiation

EFDA
EUROPEAN FUSION DEVELOPMENT AGREEMENT

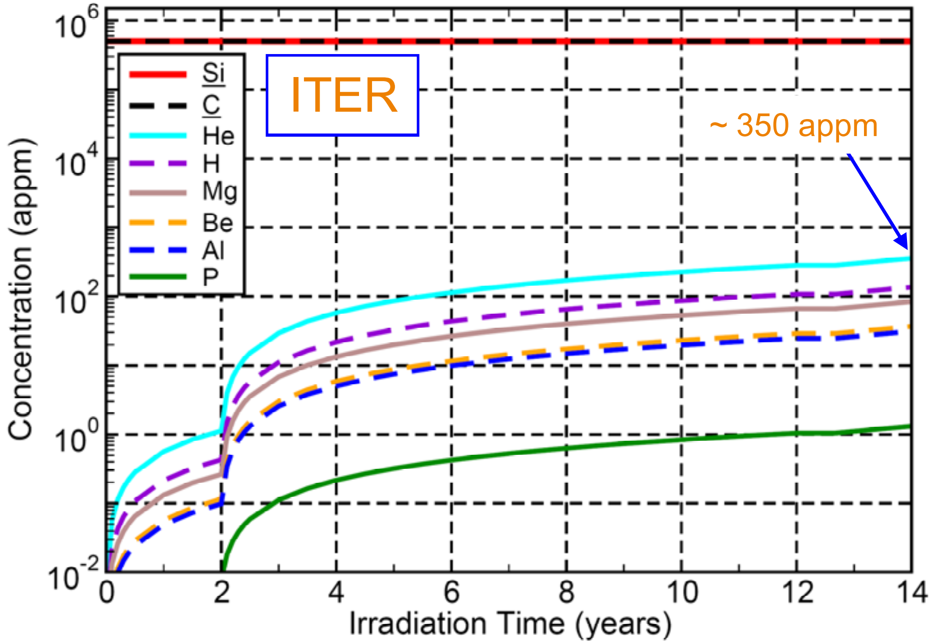
Transmutation: SiC

- Gas production dominates the burn-up (transmutation) of SiC under neutron-irradiation, but there are several other elements produced in low concentrations
- Under power plant conditions Mg, Be, and Al all reach concentrations greater than 1000 appm after 5 years
- But even after 14 ITER-years not even He or H reach 1000 appm



Final composition: 48.99% C, 48.98% Si, 1.13% He, 0.42% H, 0.25% Mg, 0.11% Be, 0.10% Al, …

100 appm in W



Final composition: 49.97% C, 49.97% Si, 0.036% He, 0.014% H, …

1 appm in W

CCFE, M. Gilbert

Summary + conclusions

- For insulators the ab-initio approach is indispensable if electronic effects are to be taken into account, in particular the damage due to particles other than high-energy neutrons, electrons, and photons

- Predictions of long-term microstructural evolution kinetics, rely on already highly developed models, that have shown good performance with respect to metals, application of which to ceramics, however, is only just beginning.

- For insulators **in-situ testing** is essential for validation!

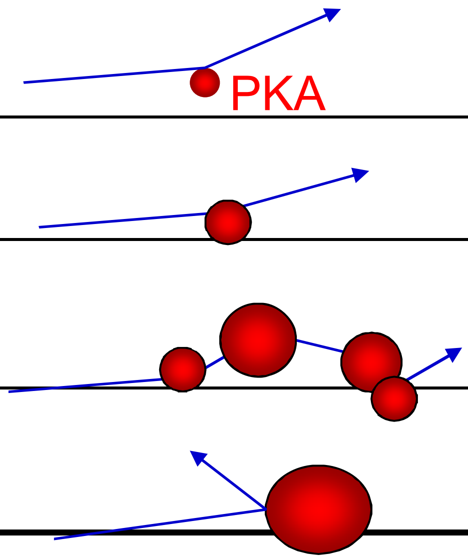
Thank you for your attention!

Courtesy of C. Alejaldre

background

Irradiation effects: Displacement damage

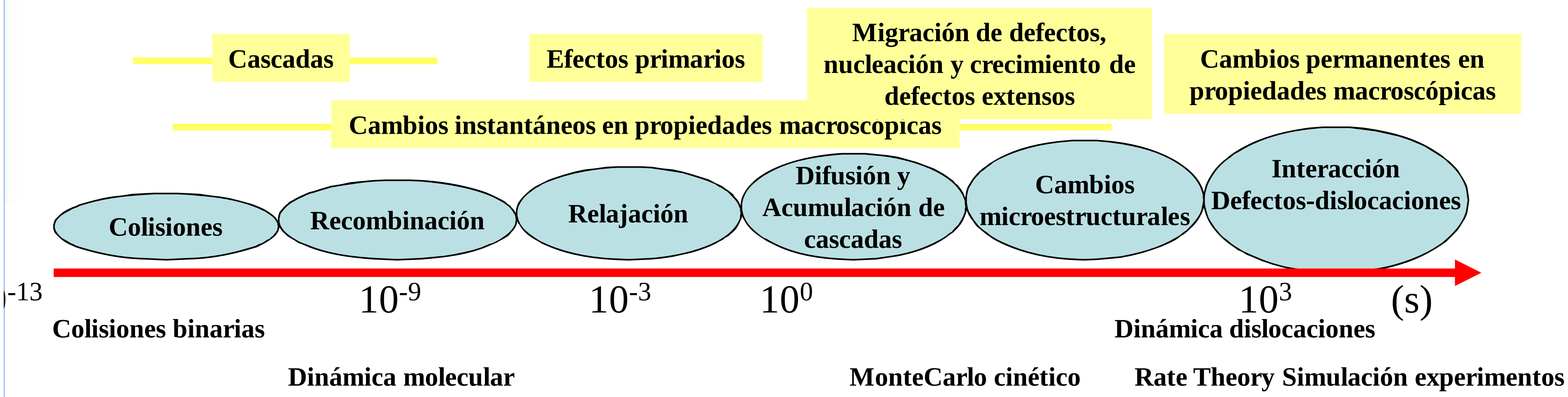
Sensitivity of energetic particles to recoil energy distribution

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

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

Escalas de Modelización

Cálculos analíticos complicados salvo que se hagan grandes simplificaciones



Sin embargo, gracias al aumento de potencia de los ordenadores empieza a ser posible simulaciones del efecto de la radiación partiendo de primeros principios, aunque también es necesario disponer de datos experimentales que puedan utilizarse como datos y para la "calibración" del sistema

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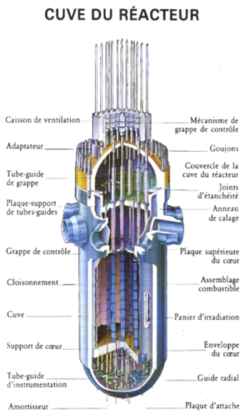
Which type of simulation ? It depends…

40 yrs

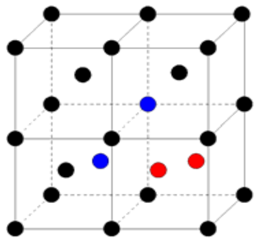
m^3



Ab initio

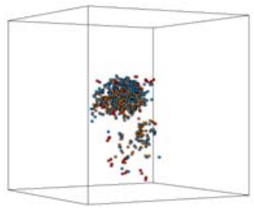
atomistic

0 - ps $1nm^3$

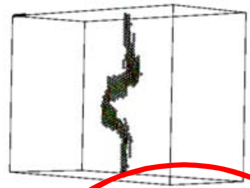


Molecular Dynamics

ns

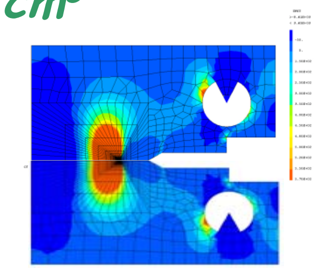


$(10\text{-}30nm)^3$



Finite element

cm^3

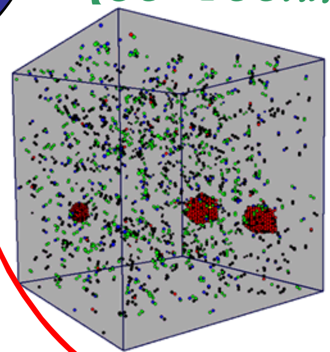


Irradiation implies a Multi-scale modeling

Kinetic Monte Carlo

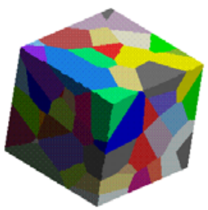
s-year

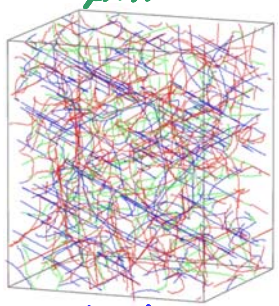
$(30\text{-}100nm)^3$



Micro-macro

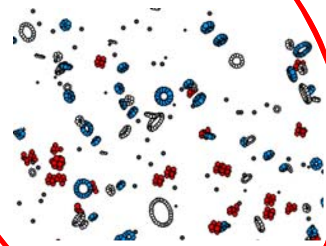
μm^3





Dislocation dynamics

Rate theory



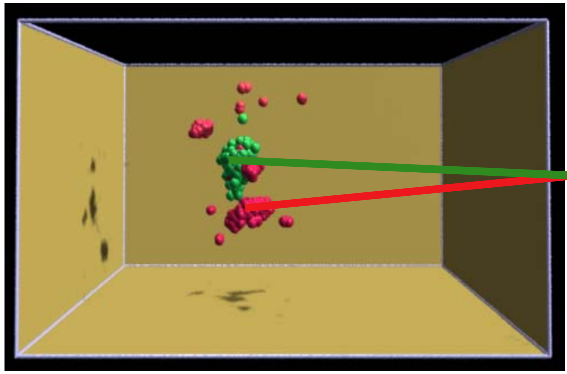
Mesoscopic

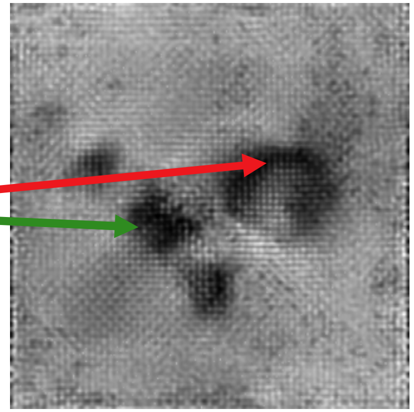
Métodos de simulación: capacidad y limitaciones

Método	Aproximación	Átomos	Tamaño	Tiempo
Ab initio DFT	E. Schrödinger a traves de aproxi.	Todos	Unos pocos cientos de atomos	Estatico Car-Parinello << ns
Tight-binding	Repulsion - empirica	Todos	Unos miles de atomos	< ns
Dinamica Molecular clasica	Potenciales Empiricos	Todos	Millones de atomos ~ $(100nm)^3$	~ ns
Monte Carlo cinetico	Probabilidades de reaccion	Solo defectos	~ $(1000nm)^3$	Horas - años
Rate theory	Campo medio	Solo defectos	Sin limites	Horas - años
Dinamica de dislocaciones	Elasticidad + reglas corto alcance	Solo dislocaciones	~ $(1000nm)^3$	----
Elementos finitos	Ecuaciones constitutivas	Discretización del sistema	-----	-----

Validación experimental

Au
20keV
in Au





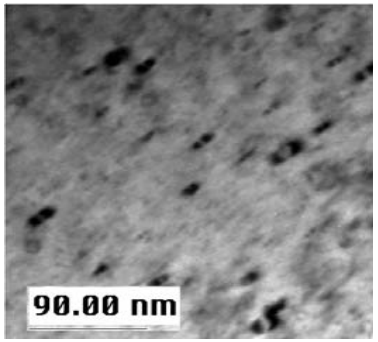
High-resolution TEM image simulation Robin Schäublin, CRPP-EPFL, CH

Microscopía
- ✓ Optical microscopy
- ✓ X-ray diffraction
- ✓ Scanning electron microscopy
- ✓ Transmission electron microscopy
- ✓ Auger electron microscopy
- ✓ Atomic force microscopy

Espectroscopía
- ✓ X-ray spectroscopy
- ✓ X-ray photoelectron spectroscopy

Test mecánicos
- ✓ Nanoindentation

Otros: Resistividad…**por mencionar algunas …**

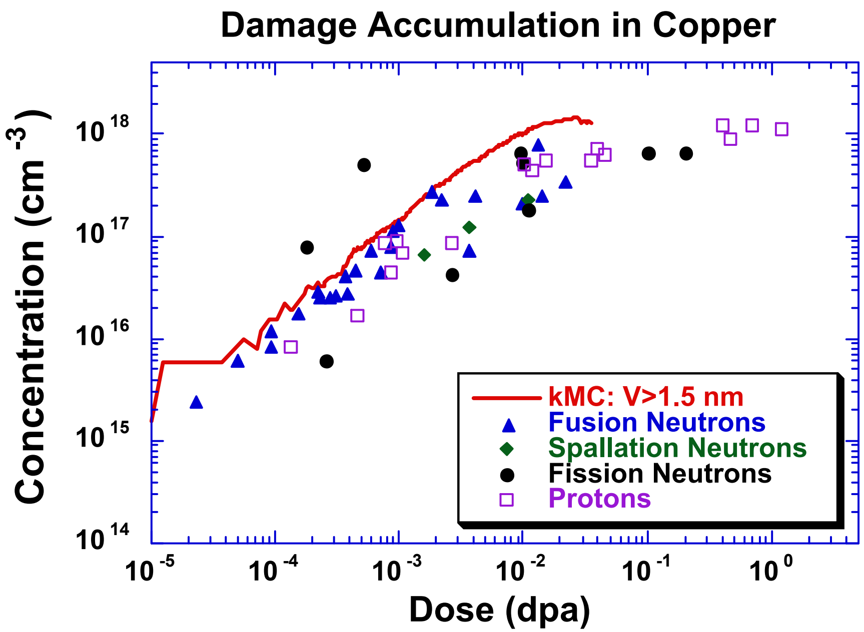


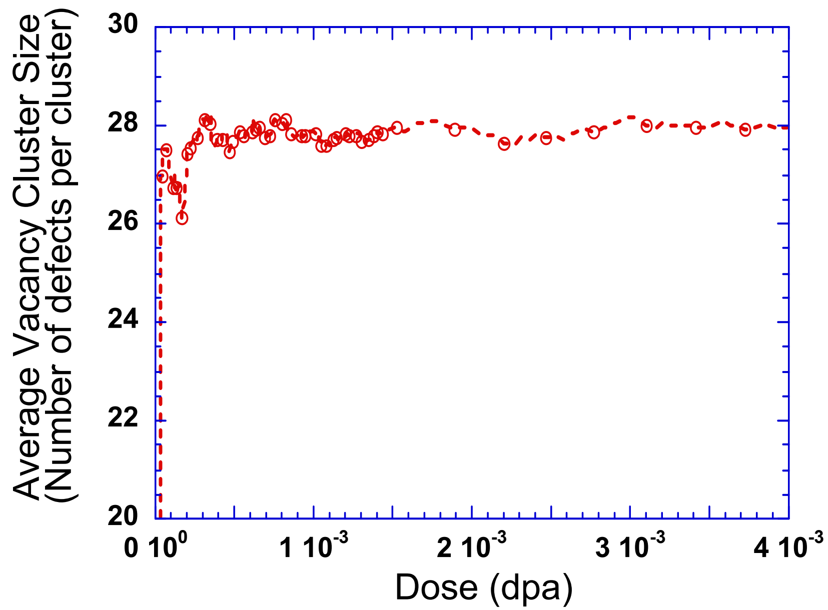
Pb (M. Law & M. Fluss)

Validación a todos los niveles escalares y temporales
Nuevos métodos de caracterización de materiales

Damage evolution from kMC can be directly compared to experimental measurements

Cluster density of Visible clusters





• All defects are of V type

Experiments: *Y. Dai and M. Victoria, MRS V. 439 (1996) p. 319*

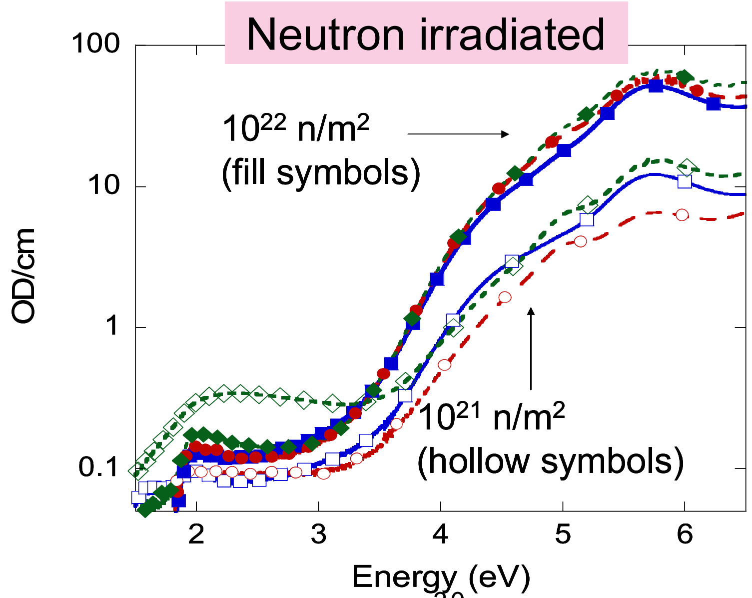
•Average size (~1.7 nm) of V clusters constant with dose in agreement with experiments.

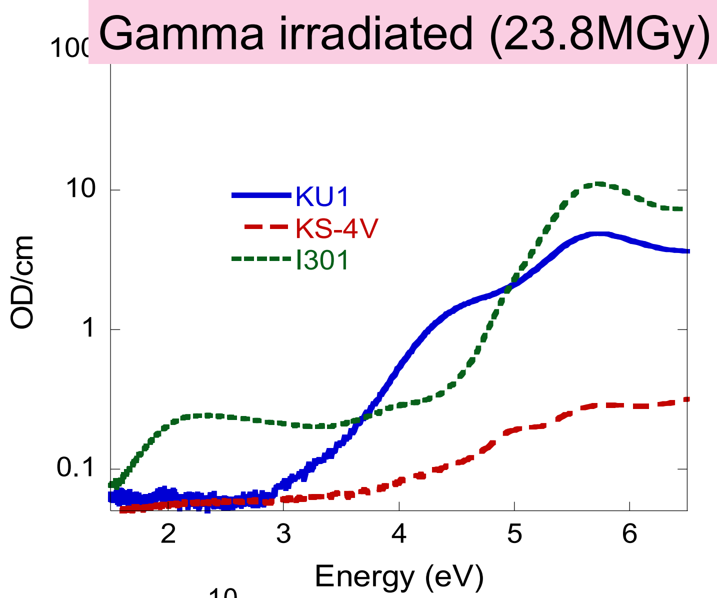
•Experimental value ~ 2 nm

Key input parameter: clustering of vacancies in the cascade

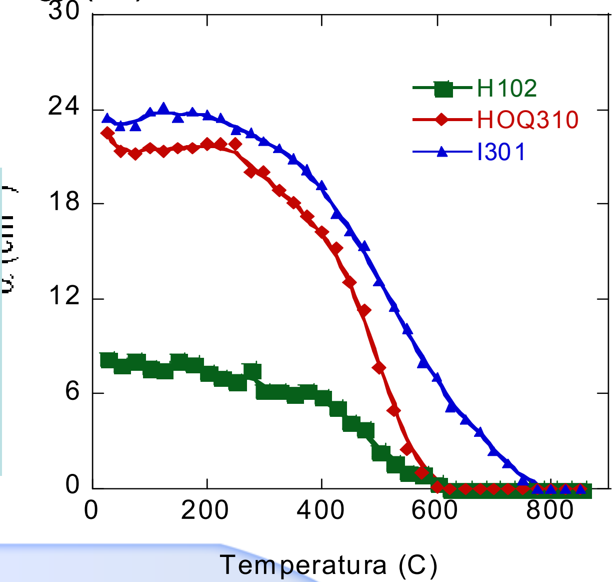
Importance of the <u>source term</u> in damage accumulation

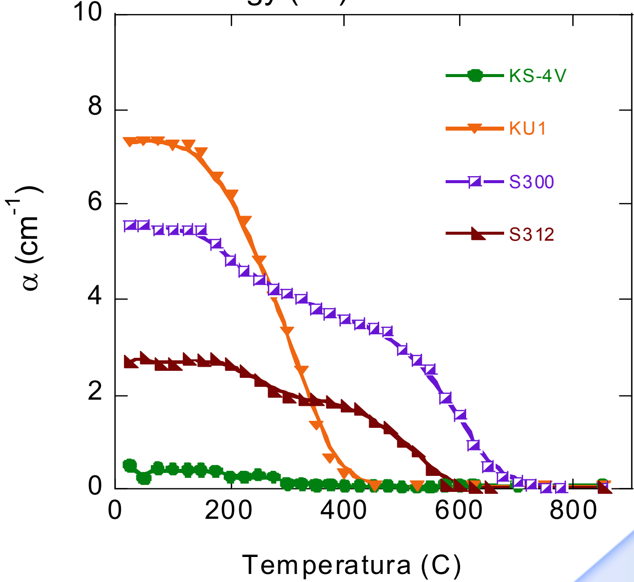
Fused silica: Optical Absorption comparison



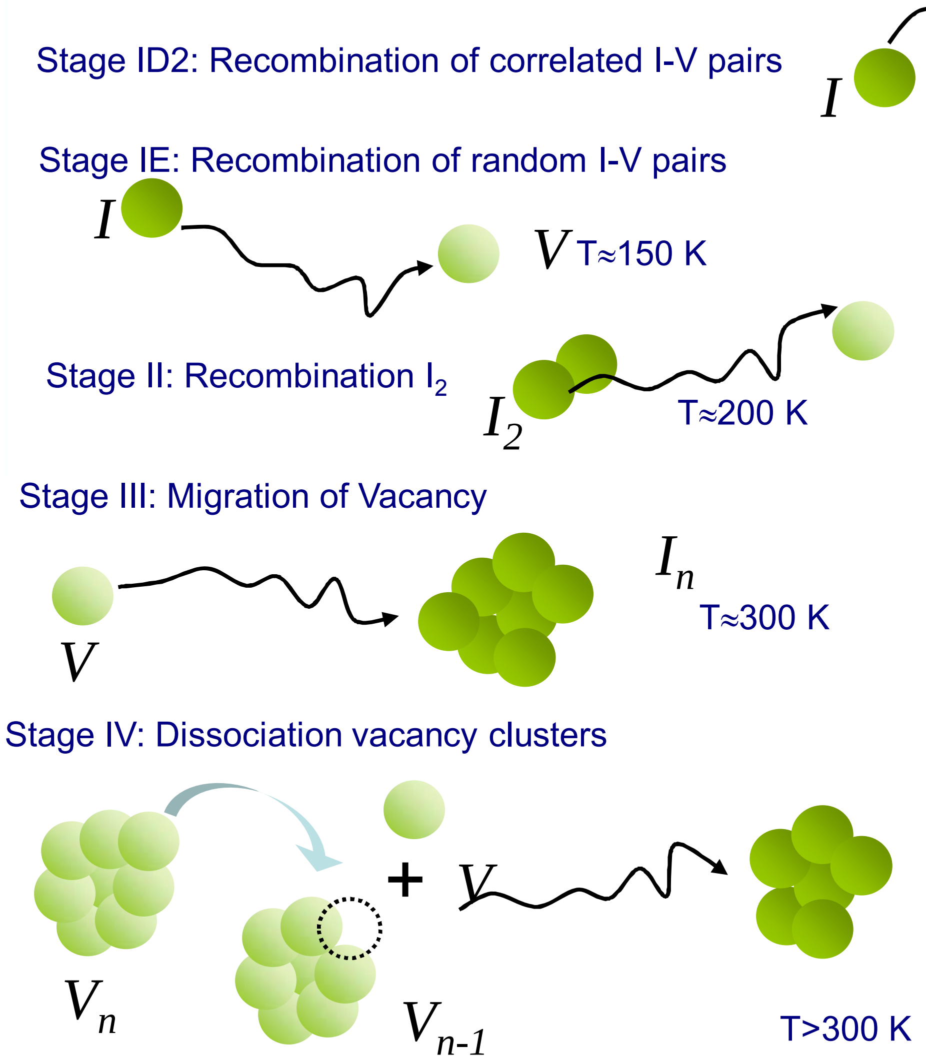


Thermal stability of gamma irradiation induced E´ defect (5.8eV) for different fused silicas

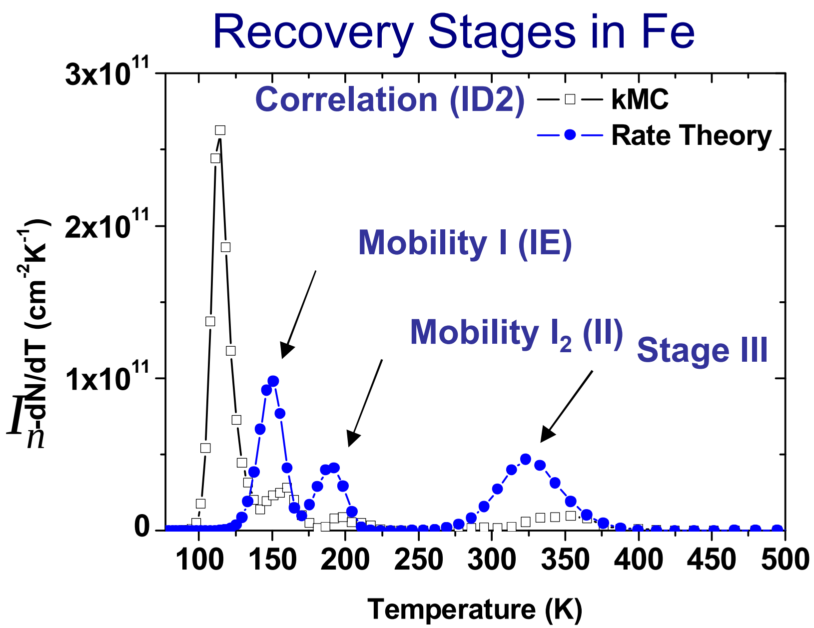




Determination of basic atomistic processes in materials: Simulation of resistivity recovery experiments in Fe



Combination of kinetic Monte Carlo and Rate Theory simulations to investigate basic atomistic mechanisms.



New irradiation facilities

- Participación en el proyecto IFMIF-EVEDA

- Línea de irradiación en el acelerador del CMAM (UAM)
- Línea de irradiación en el proyecto del ESS-CVA
- Proyecto ICTS TechnoFusion

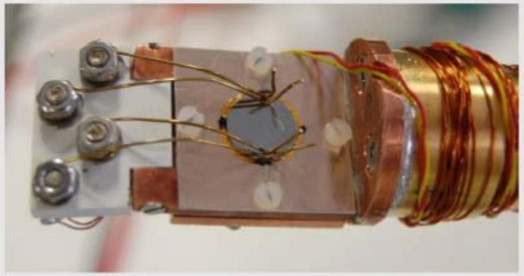
OBJETIVO: Simular algunos aspectos del daño que producen los neutrones mediante iones y otros métodos de irradiación

Desarrollo de cámaras multipropósito en línea:

✓ **CMAM** - reflectividad, ionoluminiscencia, IBAs ...

✓ **CIEMAT** - resistividad vs Tª. Objeto de la tesis de Begoña Gomez-Ferrer (dirección de R. Vila). Enmarcado en proyecto EFDA.

Objetivo: Estudio de la evolución de defectos producidos por radiación. Parametrización de mecanismos de difusión y migración. Como *inputs* para la correcta modelización y validación de simulaciones. Primera aproximación en Fe ultrapuro y aleaciones de $FeCr_x$. Extensión a otras aleaciones futuras.



Dispositivo experimental para medidas de variación de resistividad inducida por radiación con la temperatura. Muestras de Fe de 60μm irradiadas con H^+ 6 MeV en criostato

- In W the transmutation rates are significantly greater than in Fe and other light elements
- High burn-up also observed for Ta, Re, etc
- Gas production much lower than in Fe

Element	Concentration (appm) after:	
	14 ITER years	5 power plant years
W	9.98×10^5	9.40×10^5
Re	1.77×10^3	3.80×10^4
Ta	4.04×10^2	8.09×10^3
Os	2.47×10^1	1.38×10^4
H	2.29	7.63×10^1
Hf	2.24	1.41×10^2
He	1.04	3.36×10^1