Radiation damage in structural materials for GenIV and fusion reactors

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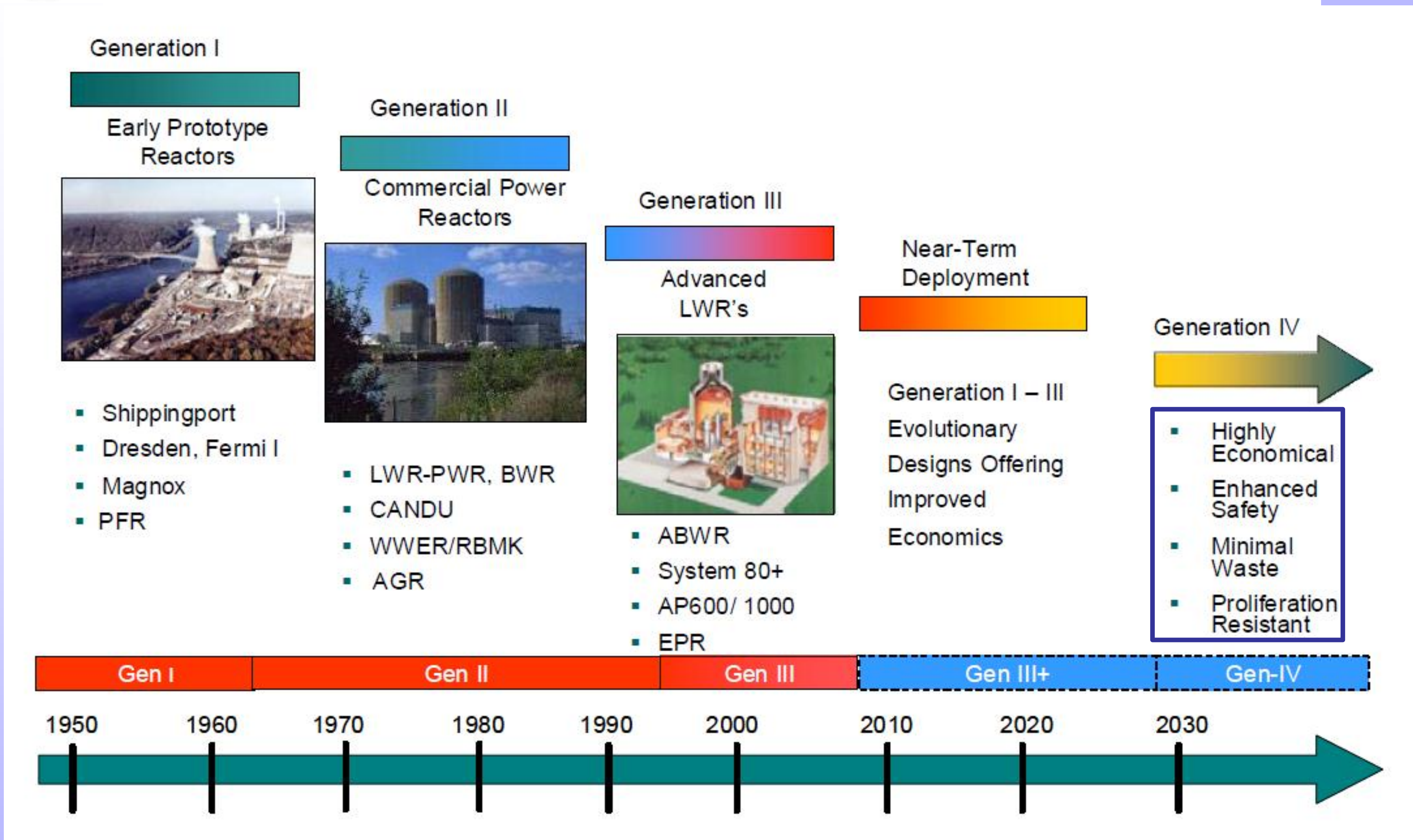
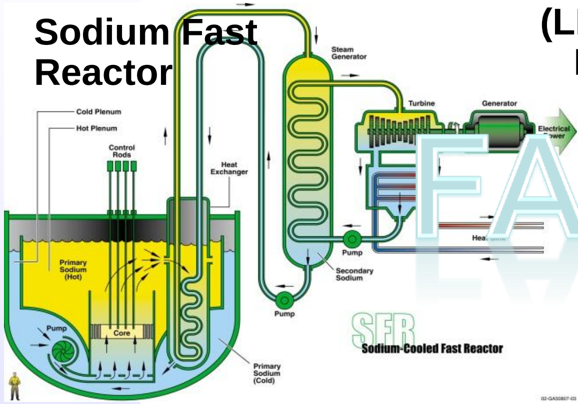
Evolution of nuclear fission reactor concepts



GenIV concepts (as in GIF + ADS)

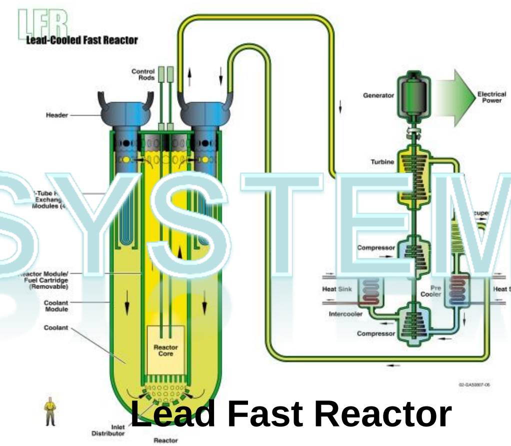
FAST SYSTEMS

Sodium Fast Reactor

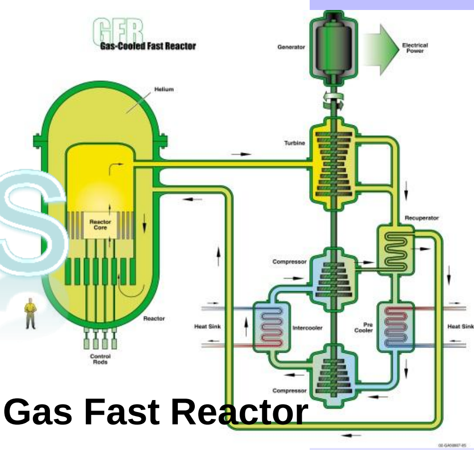


(LBE) Accelerator-Driven System

Lead Fast Reactor

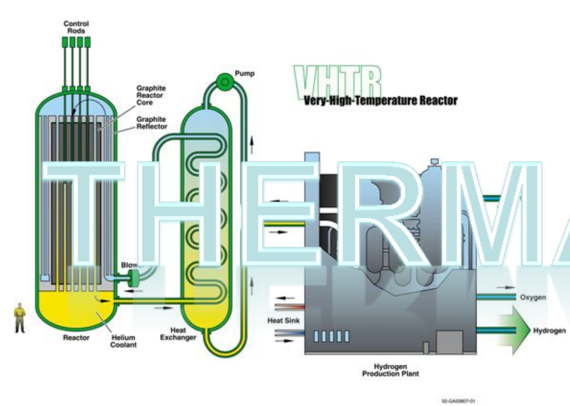


Gas Fast Reactor

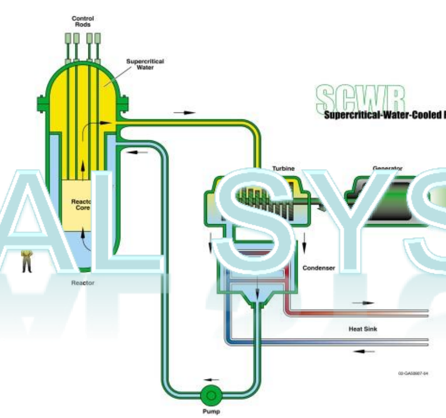


THERMAL SYSTEMS

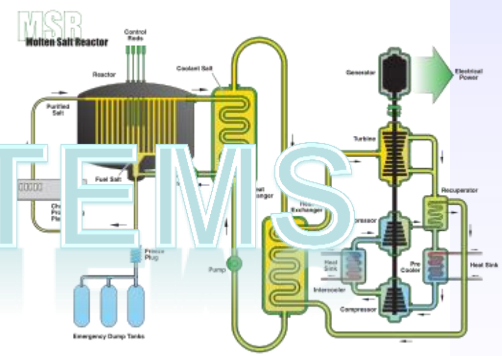
(Very) High Temperature Reactor



SuperCritical Water Reactor



Molten Salt Reactor



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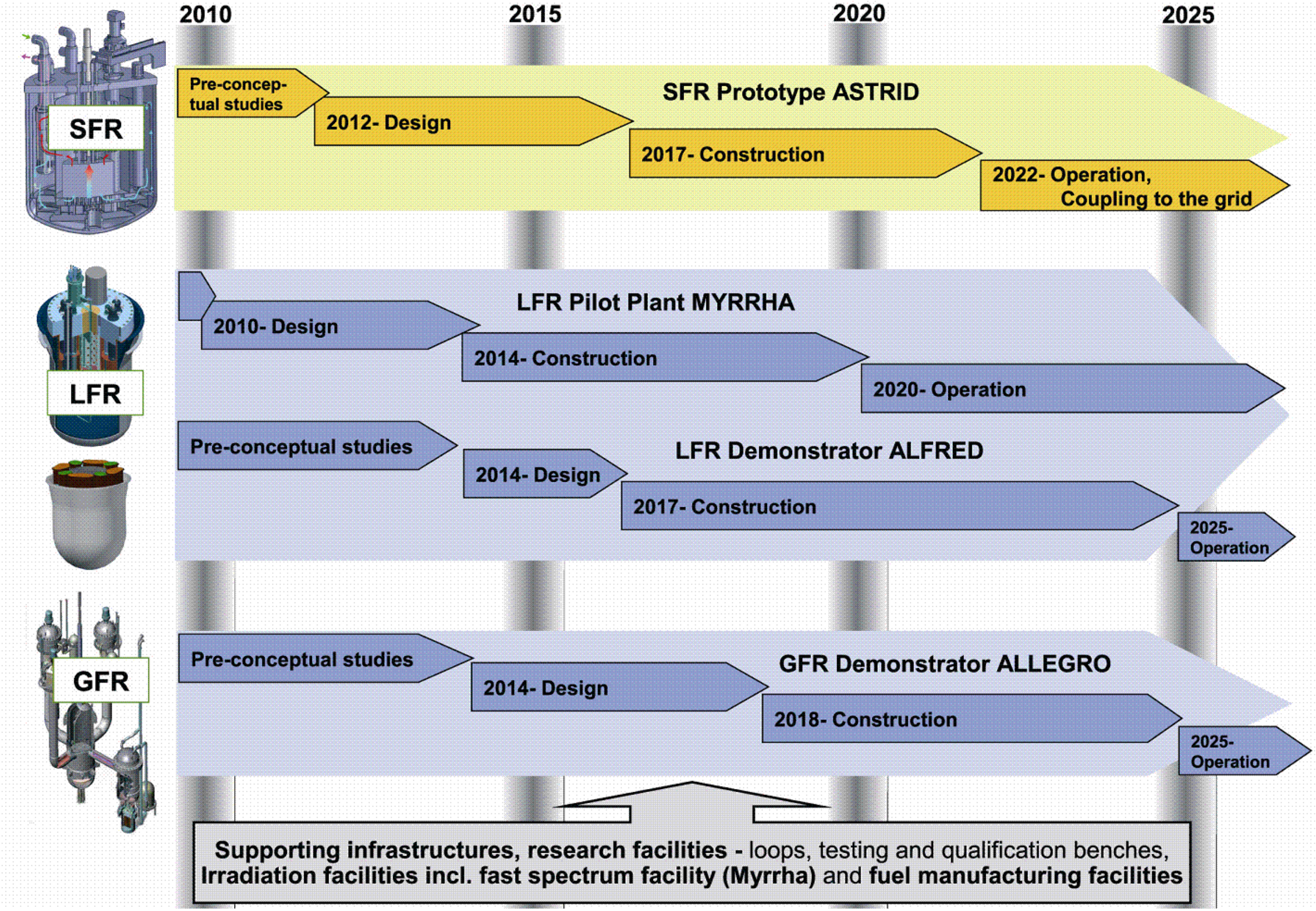
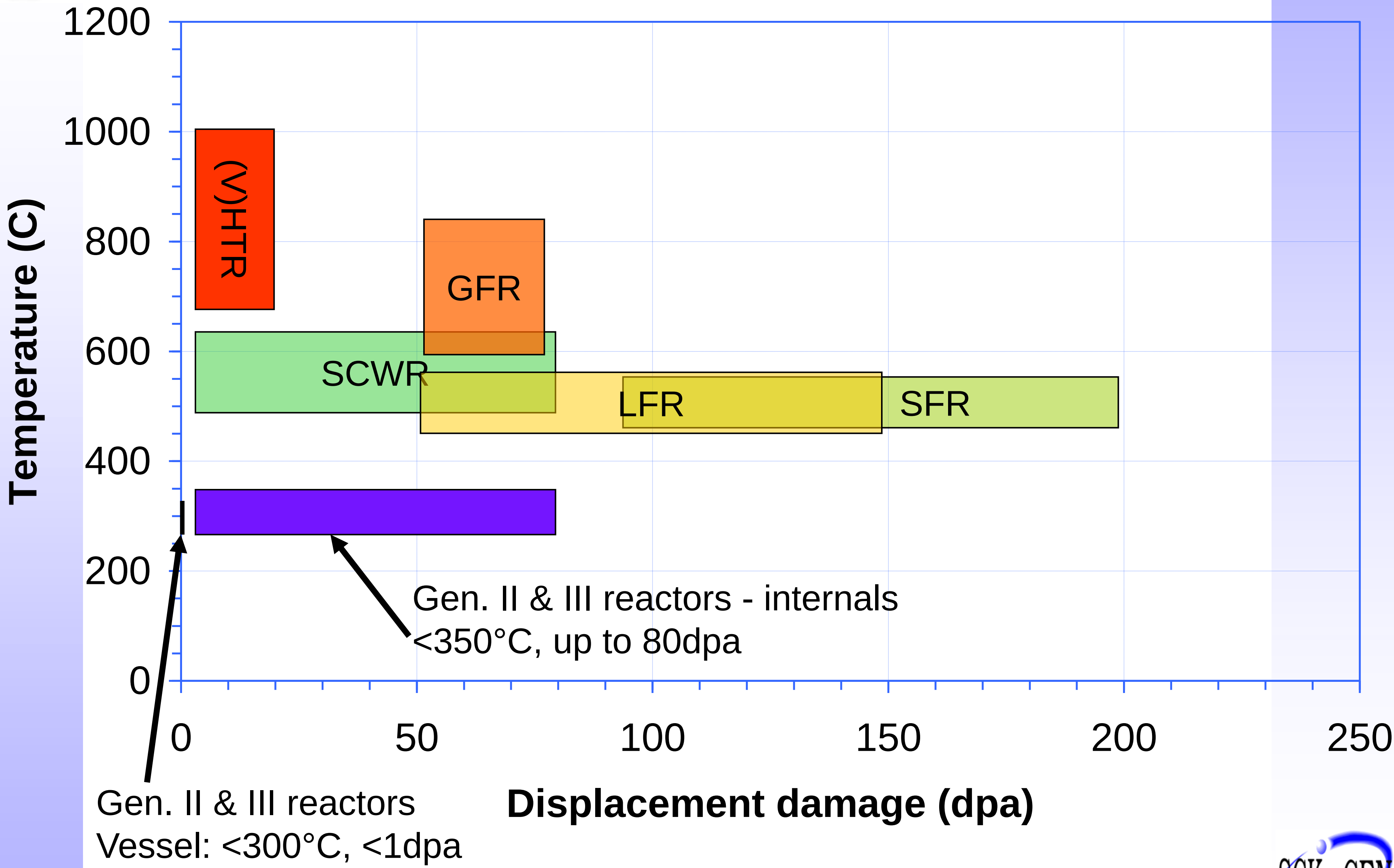
Main features of different concepts

System	LWR	SFR	LFR & ADS	GFR	(V)HTR	MSR	SCWR
Neutron Spectrum	Thermal	Fast	Fast	Fast	Thermal	Thermal / Fast	Thermal / Fast (?)
Coolant	Water	Liq. Sodium	Liq. Lead, LBE	He	He	Fluoride salts	Super-critical water
Outlet temp. (°C)	320	500-550	480-570 / 300-400	850	<1000	700-800	510-625
Fuel cycle	Open	Closed	Closed	Closed	Open	Closed	Open/ Closed
Purpose	Elec-tricity	Elec-tricity	Elec-tricity / Waste inciner-ation	Elec-tricity (high T applic-ations?)	High T applic-ations (elec-tricity)	Elec-trictiy	Elec-trictiy

European Sustainable Nuclear Industrial Initiative (ESNII)



The challenge of structural materials for innovative reactors



GenIV structural materials

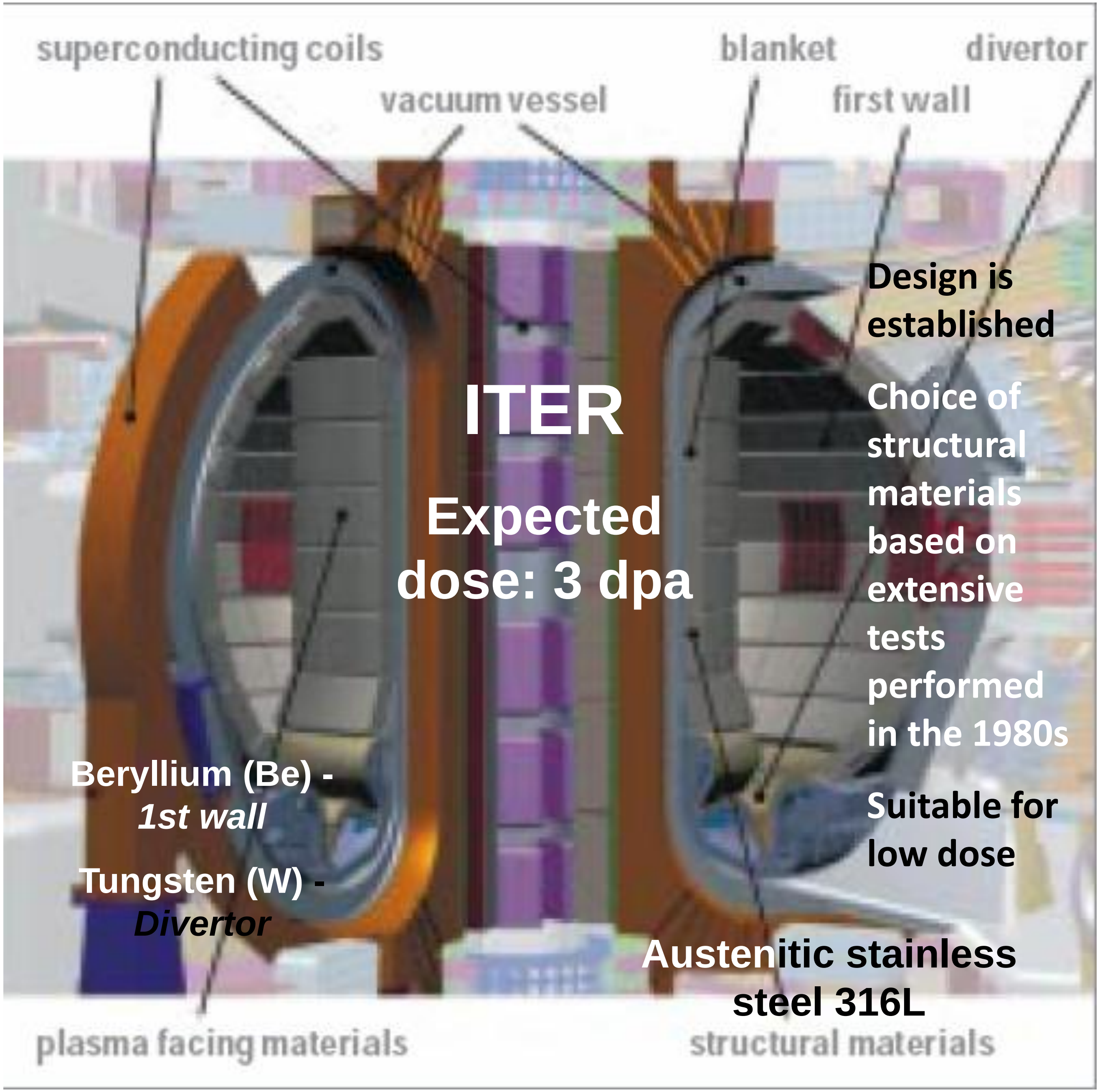
System	SFR	LFR & ADS	GFR	(V)HTR	SCWR
Cladding & Core assemblies	15-15Ti /**ODS** F/M &/or austenitics	15-15Ti /**ODS** F/M	As SFR for low power, else mainly **SiC_f/SiC**	**Graphite &/or C_f/C**	(All previous are possible / still undefined)
Core support structures	316L(N)	316L(N)	SA508 or Mod 9Cr 1Mo	SA508 or Mod 9Cr 1Mo	316L
Above core structures	316L(N)	316L(N)	**SiC_f/SiC or C_f/C** or other ceramic	Alloy 800H or **C_f/C**	(Similar to LWR technology)
Vessel	316L(N)	316L(N)	21/4 Cr-1Mo &/or Mod 9Cr 1Mo/ 12Cr steel	SA508 or Mod 9Cr 1Mo	21/4 Cr-1Mo &/or Mod 9Cr 1Mo/ 12Cr steel
Steam generator	Alloy 800H / 9Cr F/M steel	321 SS or similar	Undefined	SA508 or Mod 9Cr 1Mo	Undefined
Heat exchanger	316 L(N) 9Cr F/M steel	316 L(N) 9Cr F/M steel	IN617, Haynes 230, Hastalloy X or Alloy 800H	IN617, Haynes 230 or Alloy 800H	(None)

Austenitic steel, high-Cr ferritic/martensitic steel, Ni-base alloy, current RPV steel, **ceramic composite**, **oxide dispersion strengthened ferritic/martensitic steel**

GenIV structural materials

“Traditional” nuclear materials to be maybe optimised, for sure **qualified for high dose, high temperature, aggressive environment**	“New” nuclear materials, the industrial scale fabrication of which must be demonstrated, as well as suitability of properties that can be achieved
Graphite	**Oxide-dispersion strengthened high-Cr ferritic steels**
Ferritic-martensitic steels (9-12%Cr)	**SiC fibers in SiC (composite)**
Austenitic stainless steels	Carbon composites / Graphite
Low-alloy bainitic (RPV) steels	

Fusion reactor structural materials : ITER



ITER

Expected dose: 3 dpa

Beryllium (Be) - ***1st wall***

Tungsten (W) - ***Divertor***

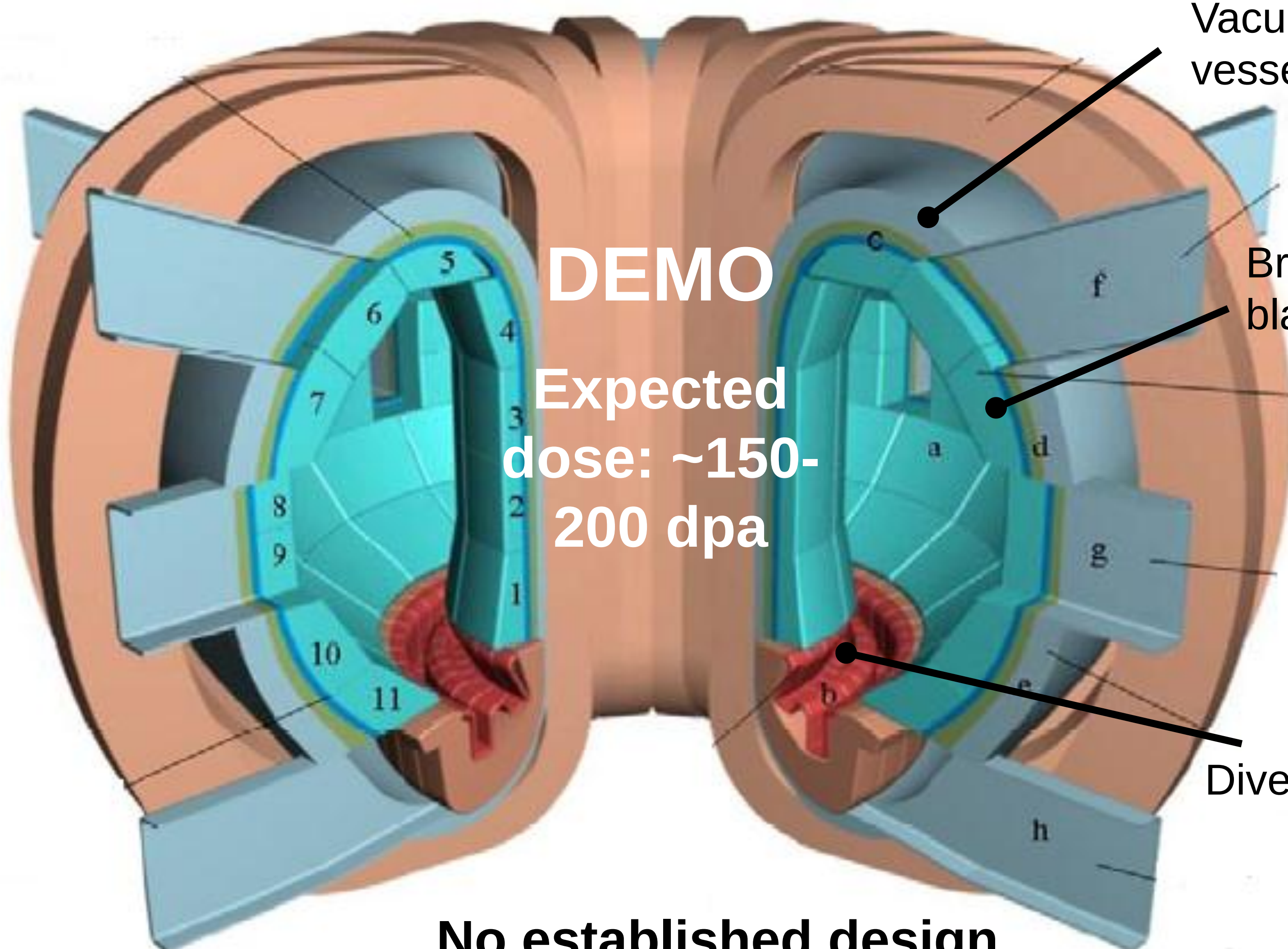
Design is established

Choice of structural materials based on extensive tests performed in the 1980s

Suitable for low dose

Austenitic stainless steel 316L

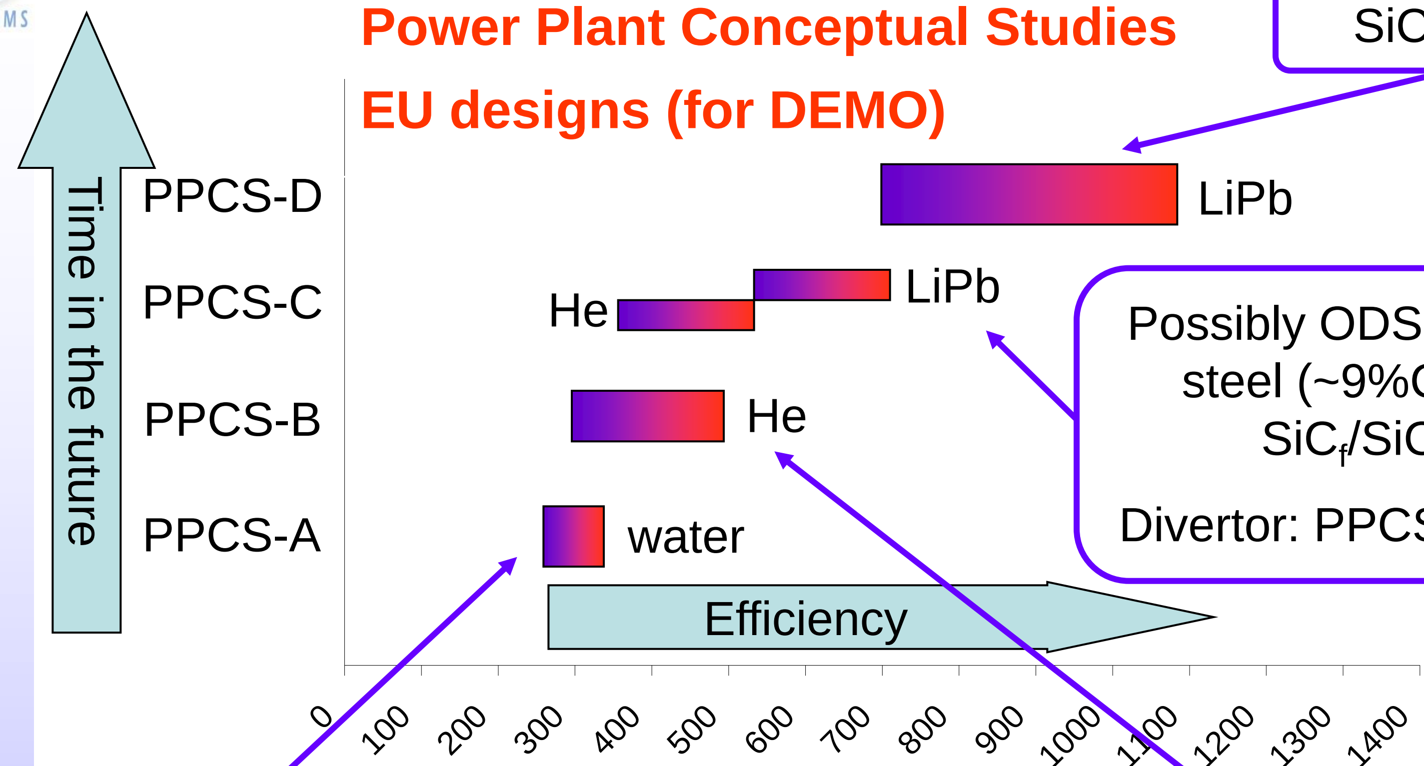
Fusion reactor structural materials: DEMO



No established design

Different possible choices of structural materials depending mainly on desired operation temperature

Fusion reactor structural materials: DEMO



T (°C)
Coolant temperature

SiC_f/SiC

Possibly ODS RAFM steel (~9%Cr) + SiC_f/SiC

Divertor: PPCS-B-like

Reduced-activation ferritic-martensitic (RAFM) steel (~9%Cr)

Divertor: ITER-like

Other candidate (USA design):

Vanadium (V) alloys

Possibly oxide-dispersion strengthened (ODS) RAFM steel (~9%Cr)

Divertor: W alloy

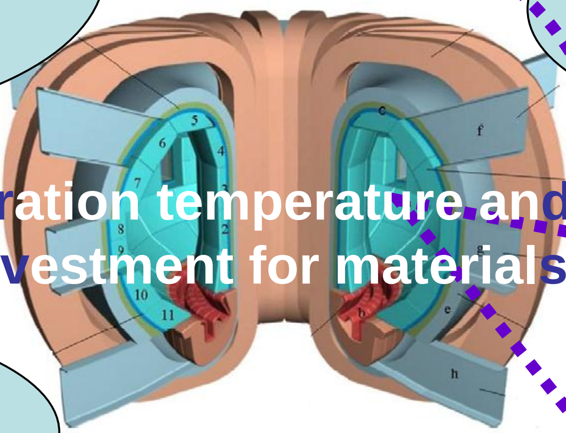
Fusion reactor structural materials

Oxide-dispersion strengthened RAFM steels

Tungsten alloys (divertor)

Reduced-activation ferritic-martensitic steels (9%Cr)

Vanadium alloys



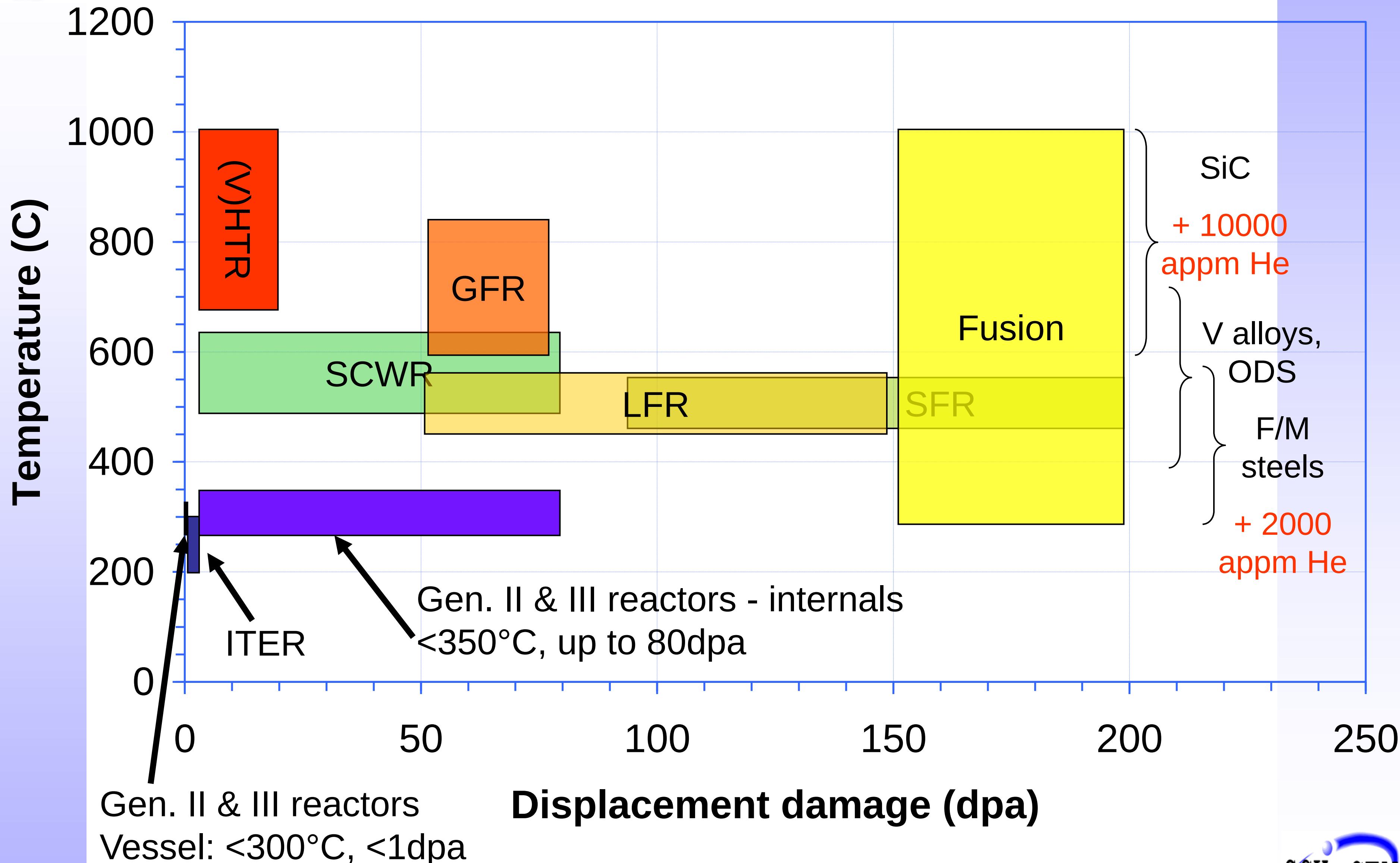
Increasing operation temperature and efficiency

Increasing R&D investment for materials development

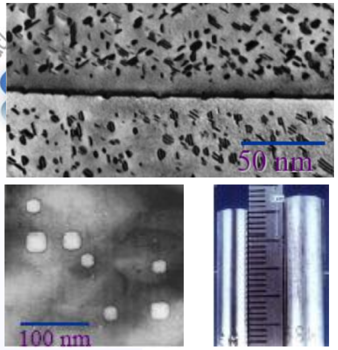
Austenitic stainless steels 316 (ITER)

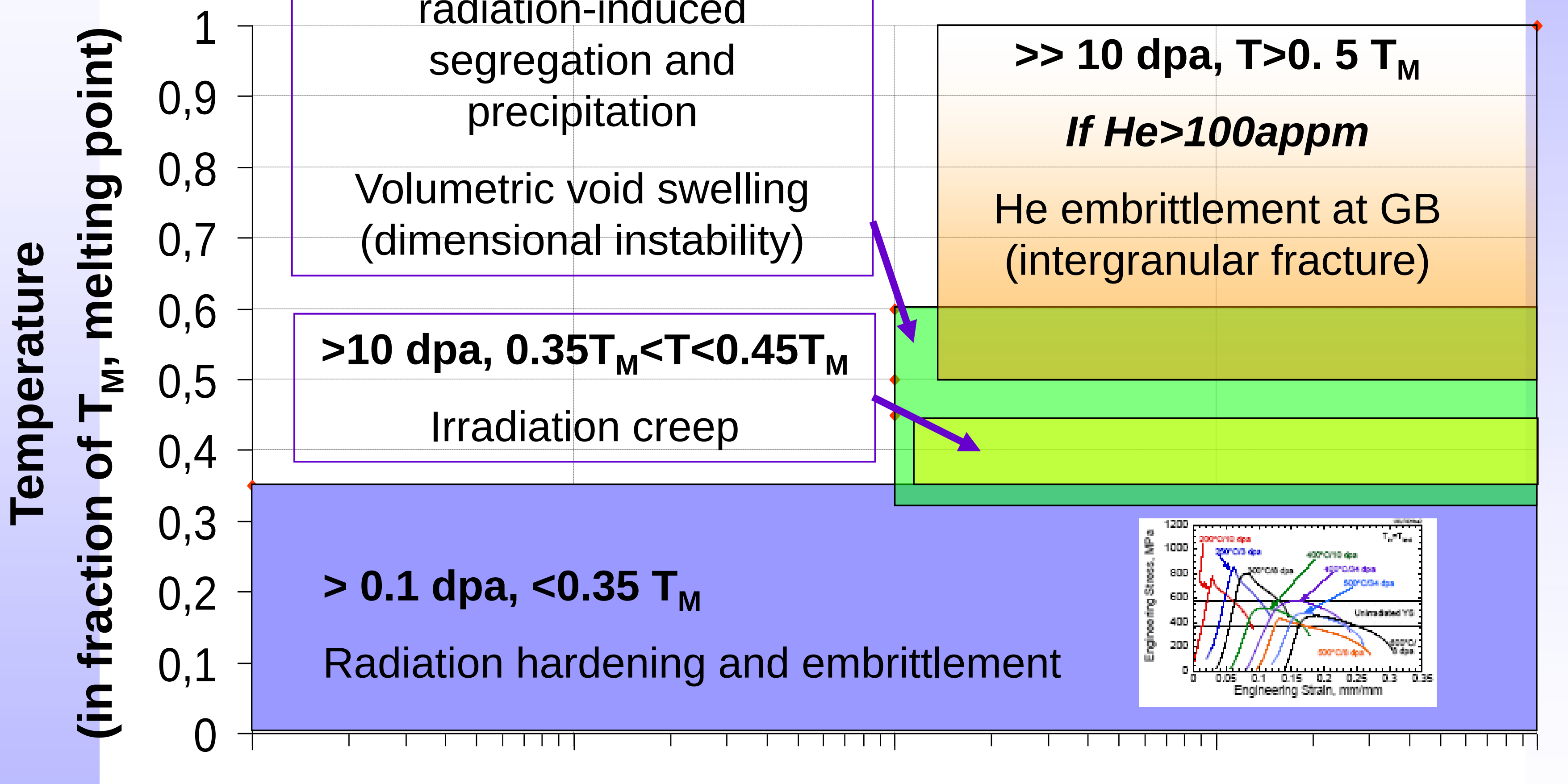
SiC fiber in SiC (composite)

The challenge of structural materials for fusion reactors



Radiation effects in structural materials





The importance of modelling

- The operation conditions expected in innovative reactors are **totally unprecedented**
  - ***No existing facility can reproduce them***
  - ***Construction of adequate facilities lies in the future and will be very expensive***
  - ***Even when facilities are built, it will be impossible to explore all conditions (normal and off-normal)***
- The higher the dose and the temperature, the wider the spectrum of modifications induced in the material by radiation
  - ***The behaviour of a given material under irradiation at the expected conditions cannot be simply extrapolated from tests performed at milder conditions***

⇒ **Valid physical models are necessary** to discriminate between dominant modifications versus dose and temperature and to extrapolate between different irradiation conditions

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Beyond the displacement cascade

Nanostructural evolution in metals under irradiation and correlation with mechanical properties

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How does irradiation change the macroscopic properties of steels?

To understand this we need to see what radiation does at the proper scales involved …

Outline

- Part I – Nanoscopic scale
  - *Production of damage*
  - *Development of a nanostructure*
  - *Microchemistry*
  - *How to model these processes:*
    - Atomistic Monte Carlo
    - Coarse grained models
- Part II – Mesoscopic scale and beyond
  - *Dislocations and hardening*
  - *How to model this:*
    - Dislocation dynamics
  - *Ideas about multiscale modelling*

Part I: Nanoscopic scale

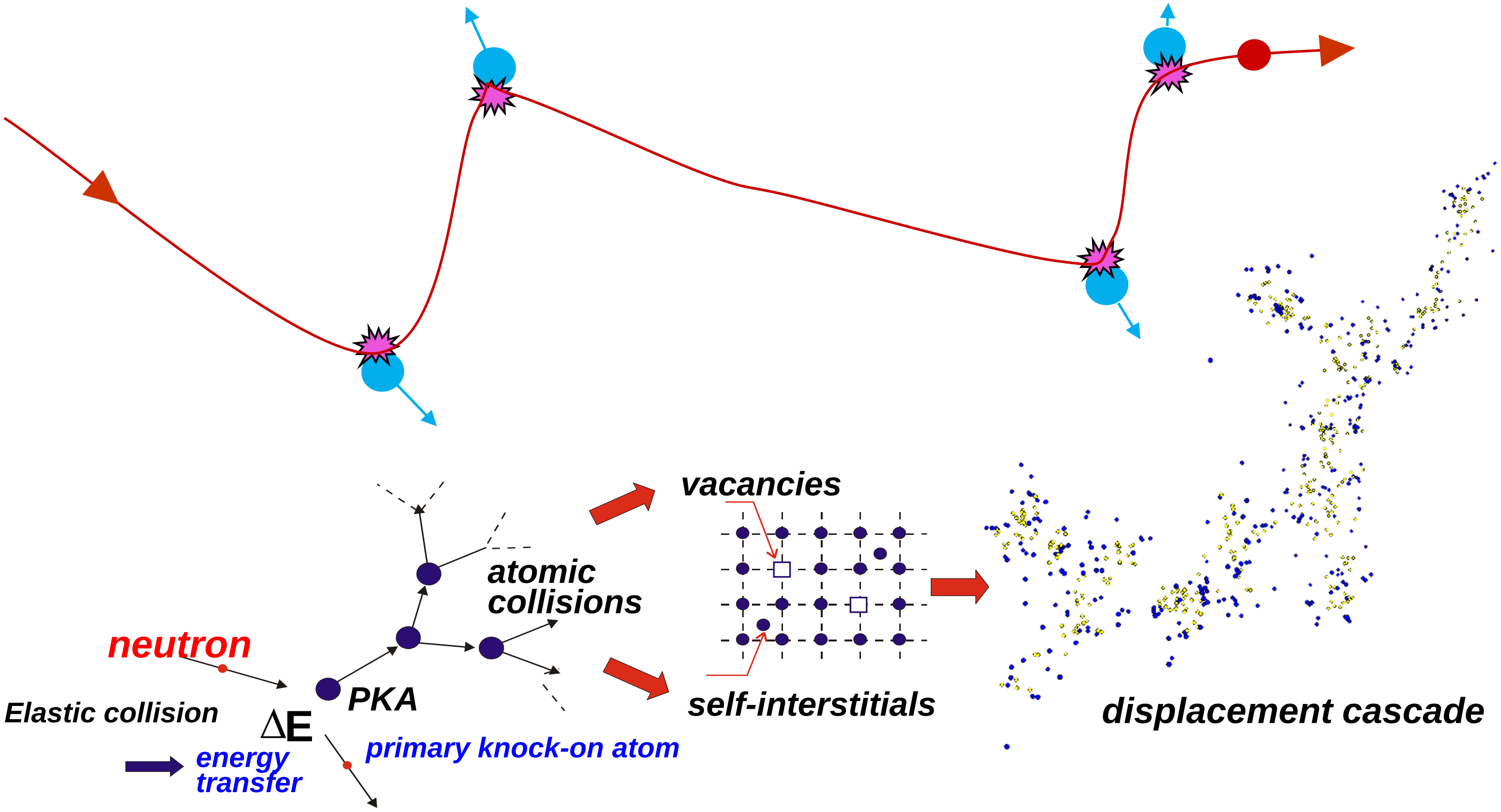
Production of damage:
the displacement cascade

… It all starts with a neutron hitting an atom …

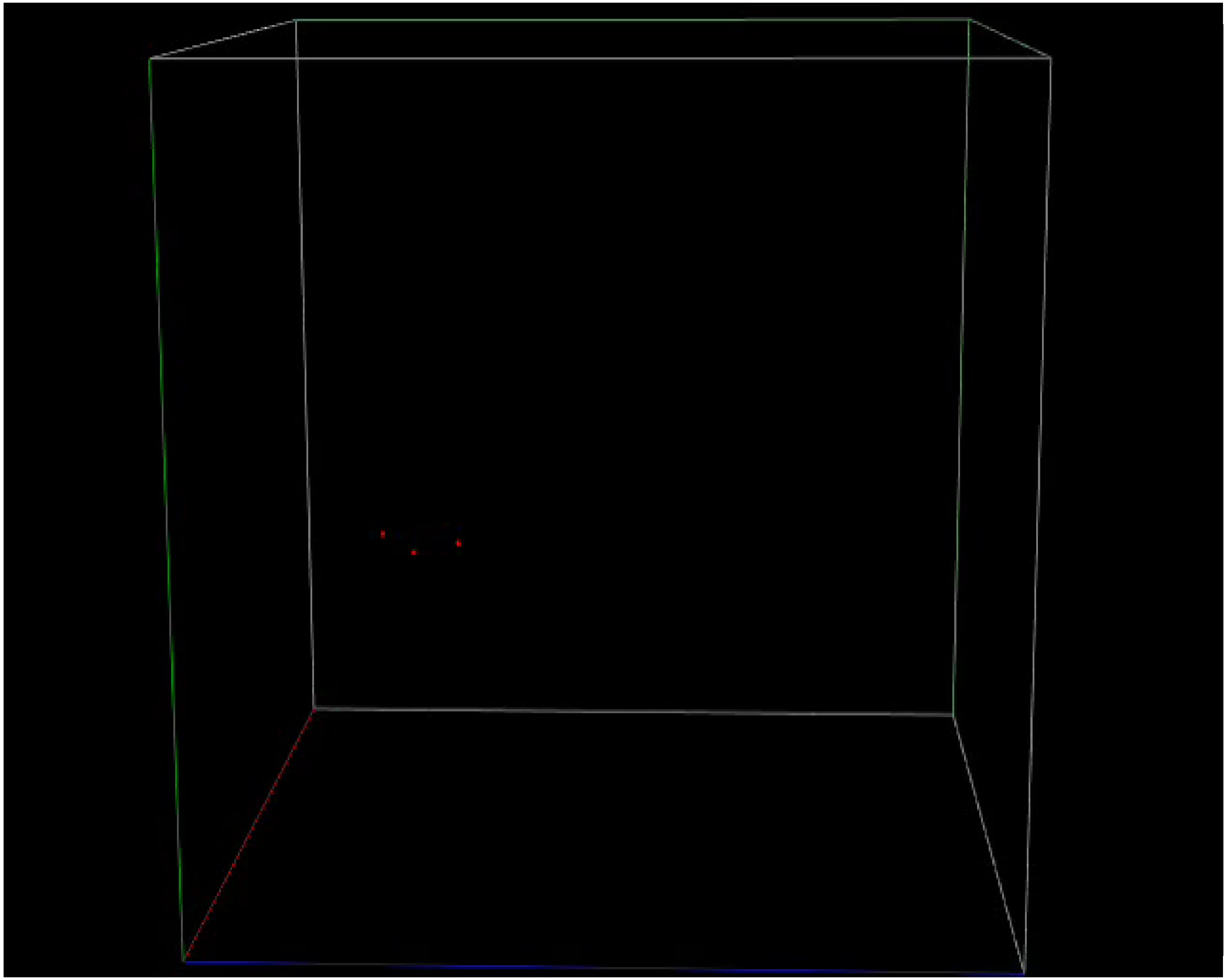
Neutrons = uncharged particles ⇒ can travel long distances in matter

When reacting with nuclei of atoms they can produce

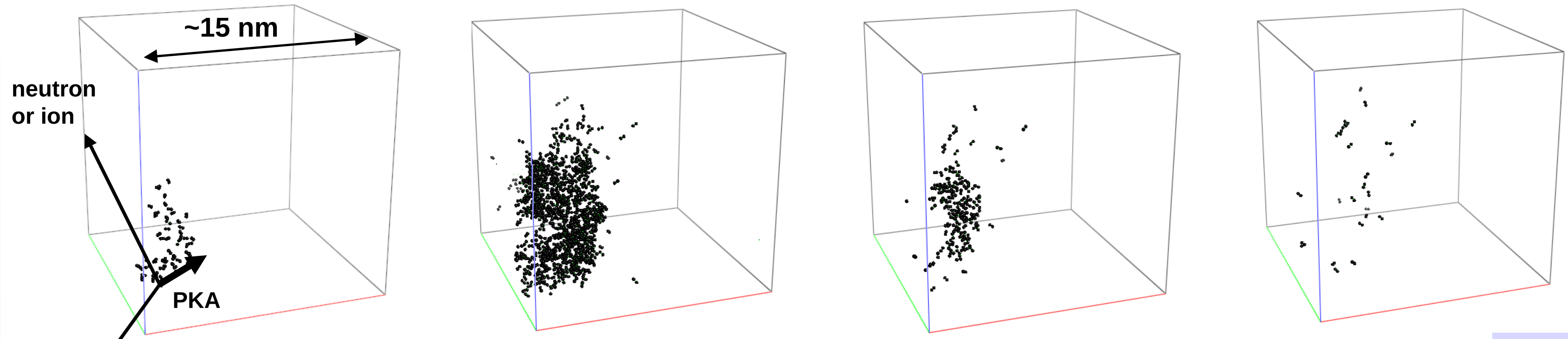
- Activation
- Transmutation (He, H)
- Displacement damage (elastic collisions)



Displacement cascade: the mother of all evils …



A closer look at the cascade phases

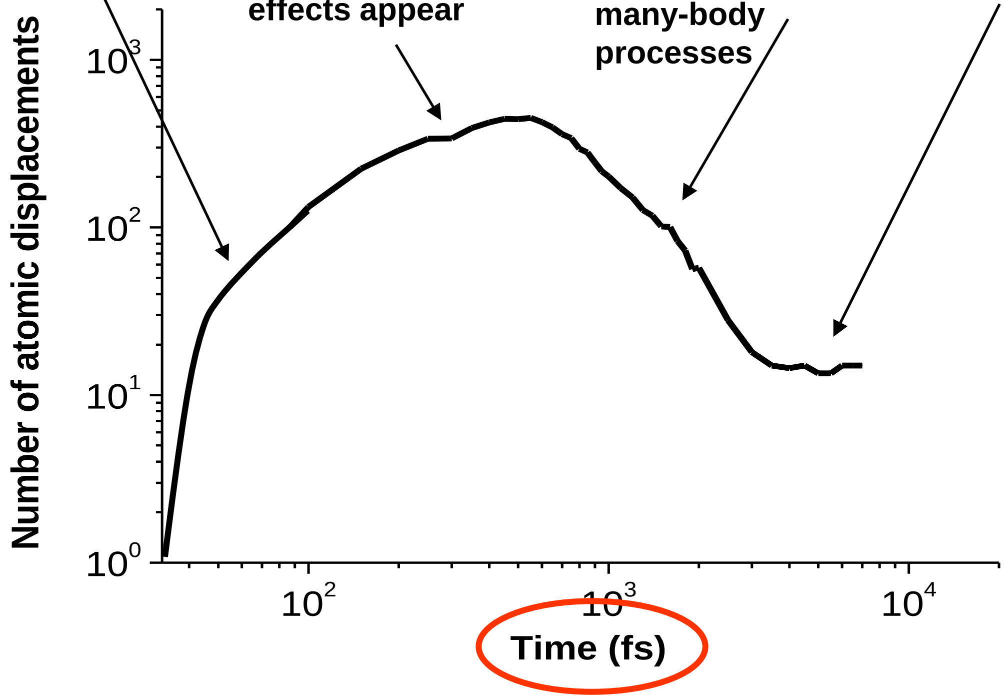


Ballistic phase: atoms behave like colliding hard spheres

Thermal spike: local temperature rises, collective effects appear

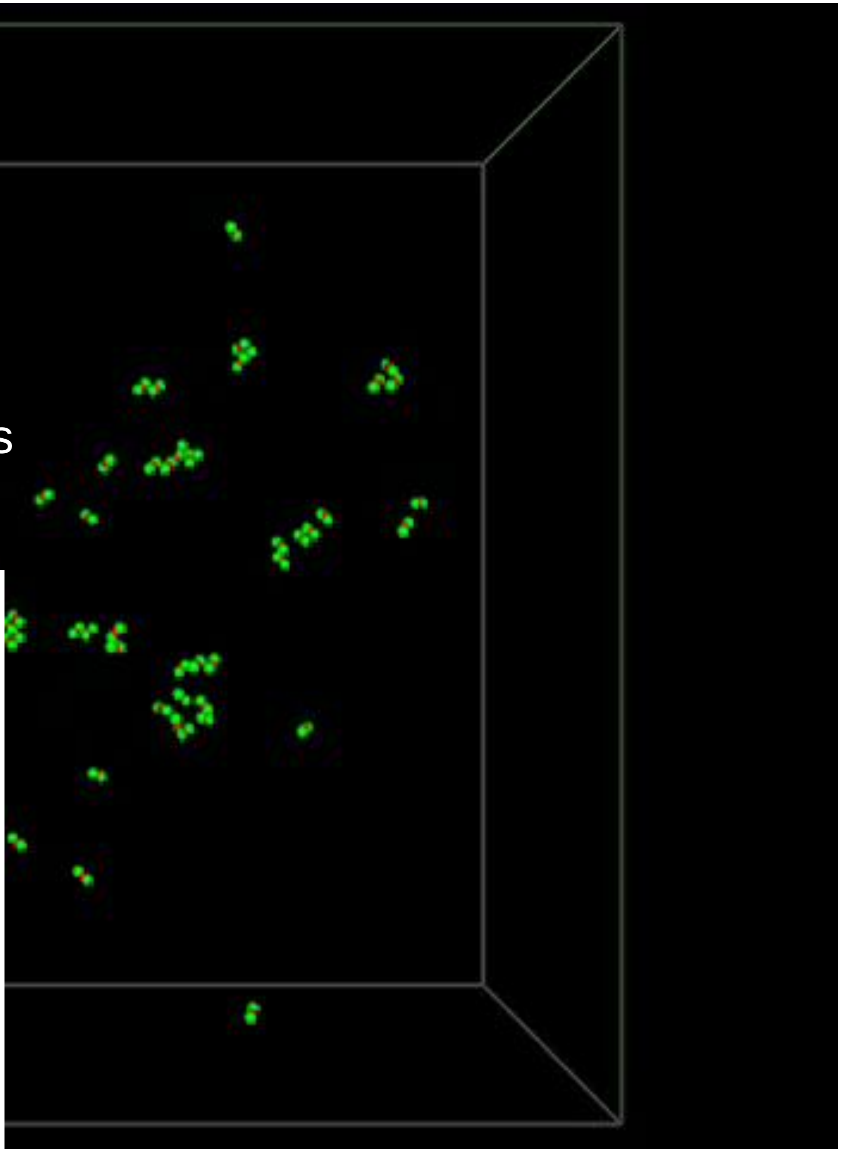
Cooling phase: most defects recombine, following complex many-body processes

Primary damage state: only a few point defects and clusters survive (cascade debris)

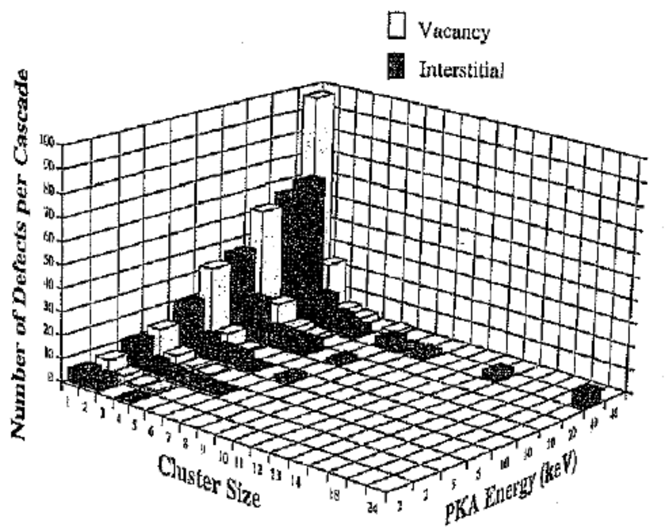


Primary state of damage

- At the end of cooling phase only a few defects remain:
  - Surviving Frenkel pairs
  - Clusters of both self-interstitials and vacancies



Bacon et al, Nucl Instr & Meth B, 1999

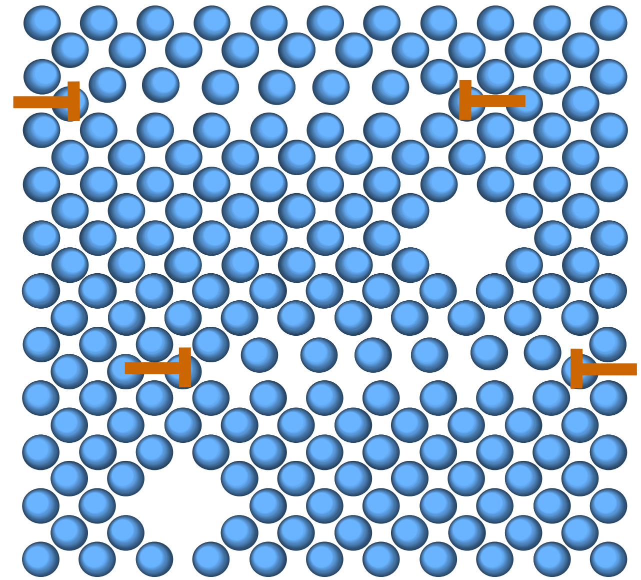


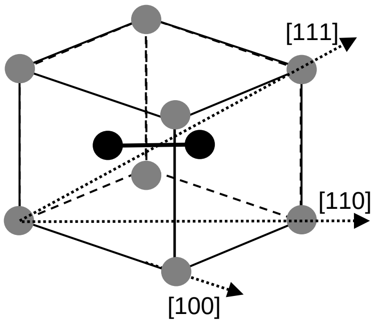
What happens next?
Development of a nanostructure

Clustering of point defects

- Clusters of vacancies
  - *nano-cavities*
  - *vacancy dislocation loops*

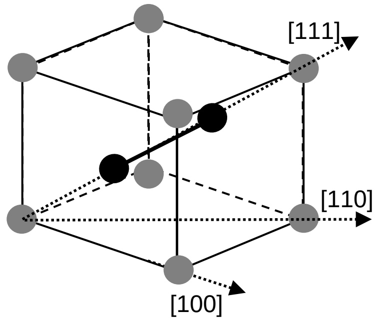
- Clusters of self-interstitials
  - *interstitial dislocation loops*





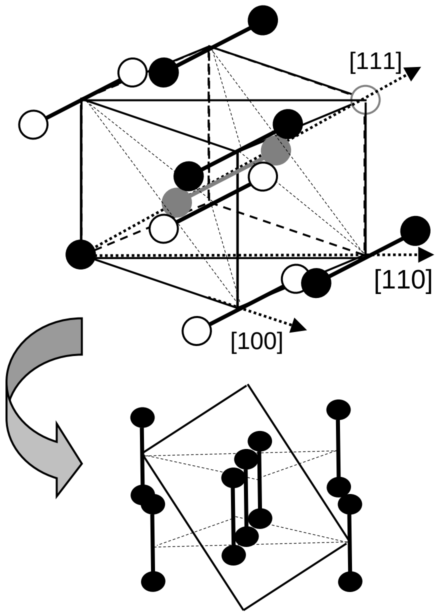
[110] dumbbell

Stable in Fe if isolated or in small clusters

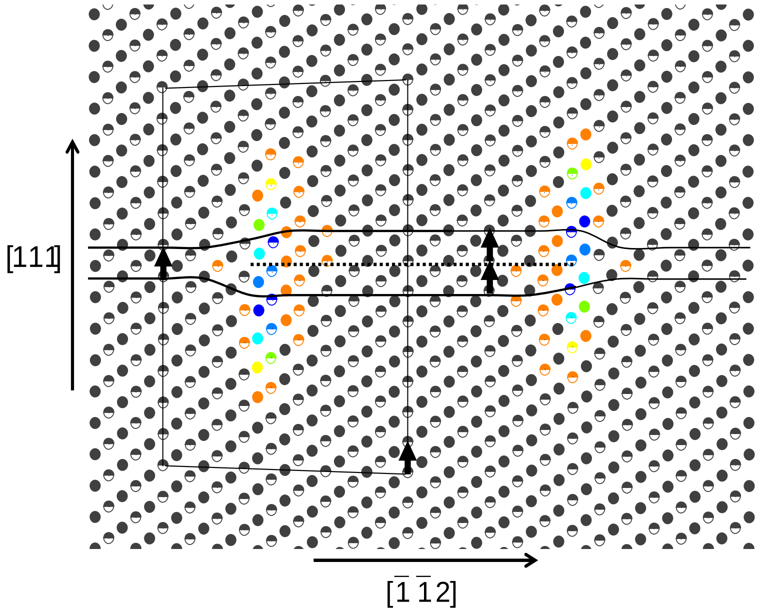


[111] dumbbell or crowdion

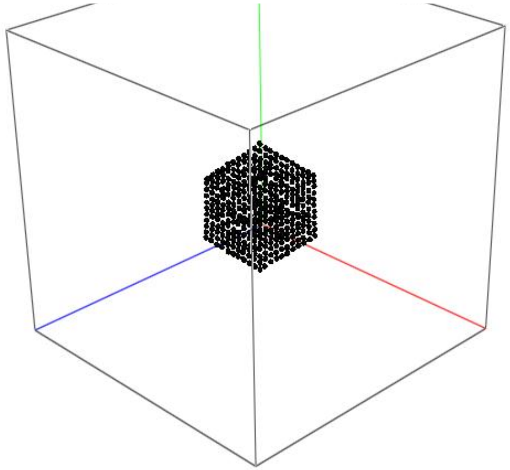
Unstable in Fe if isolated but unit of large clusters

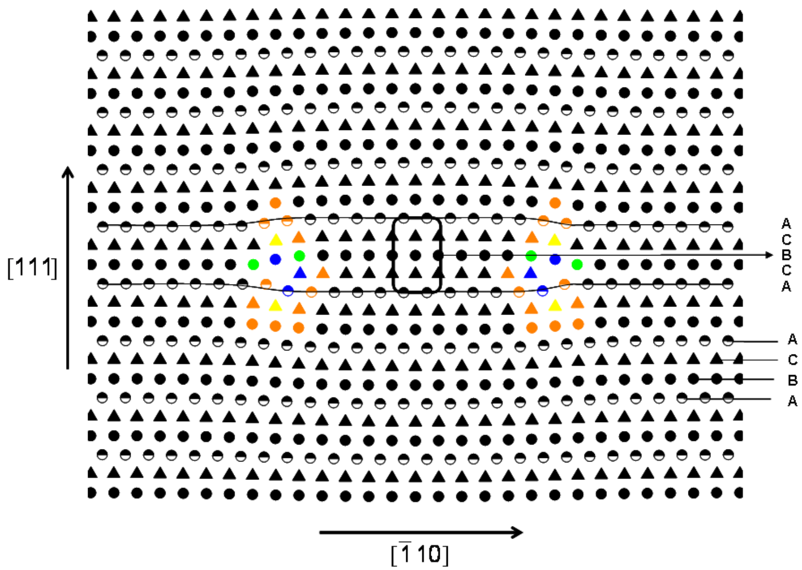


Self-interstitial loops *('prismatic loops')*

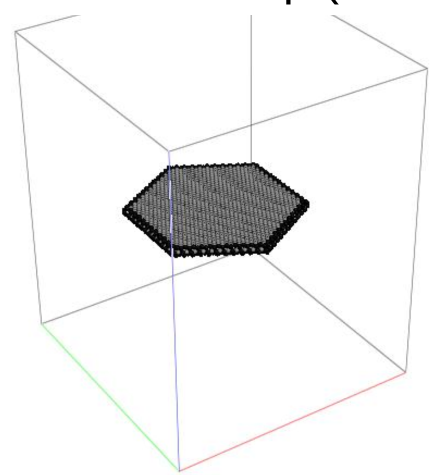


½(111) loop (bcc metals)

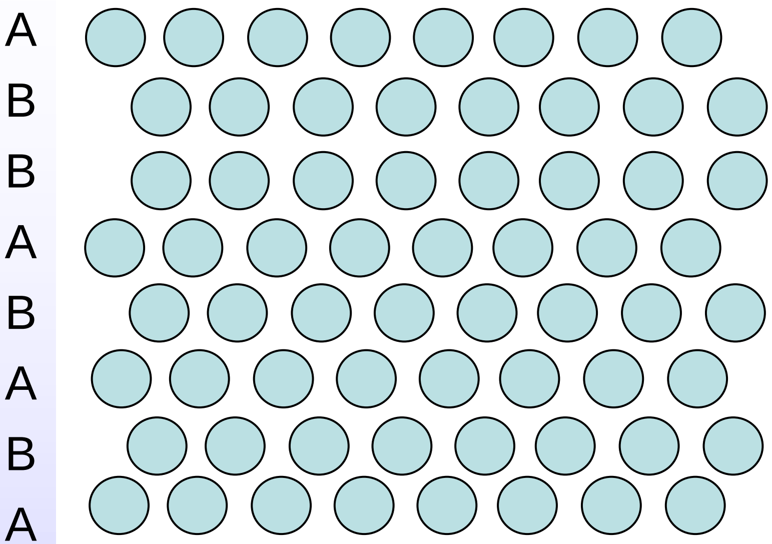


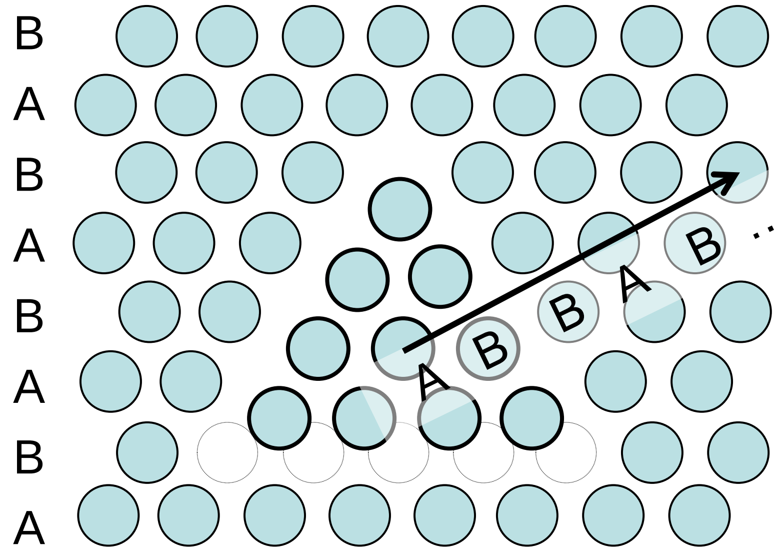


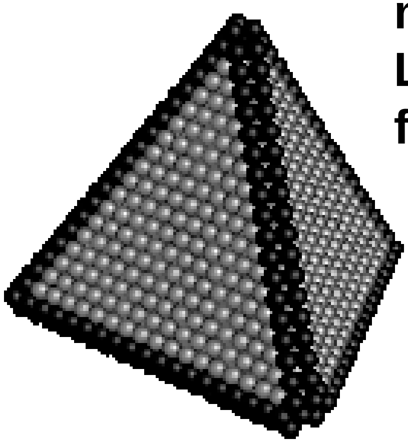
Faulted Frank loop (fcc metals)



Stacking-fault tetrahedra

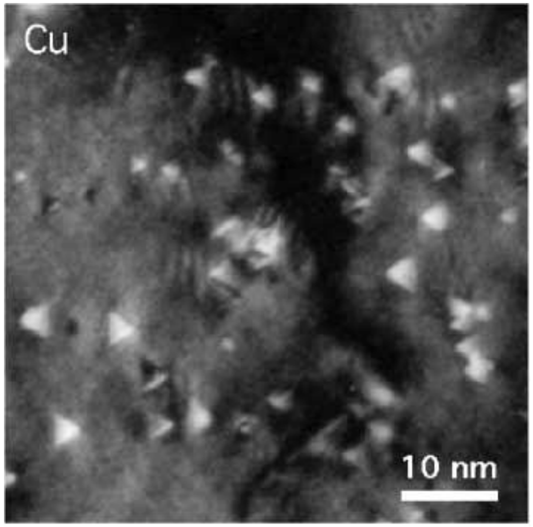






3D result

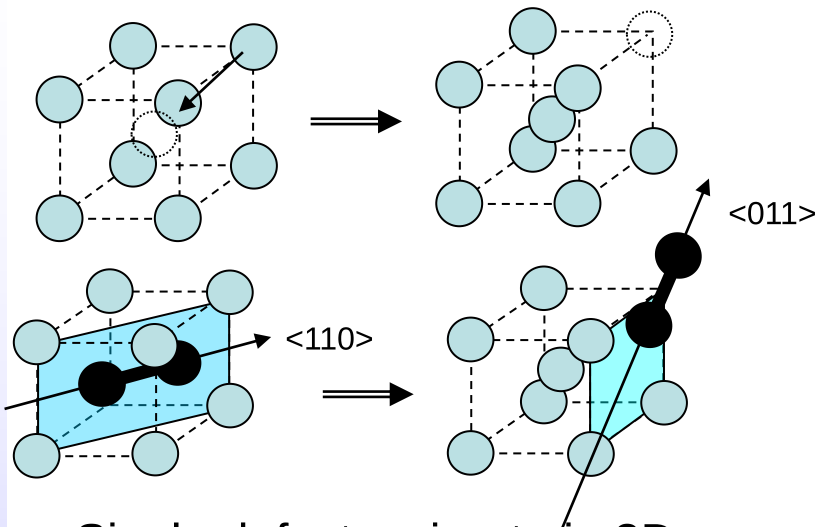
Typical of FCC metals with LOW stacking fault energy



Schaublin *et al.*, Phil. Mag., 2005

Defect migration and cluster growth

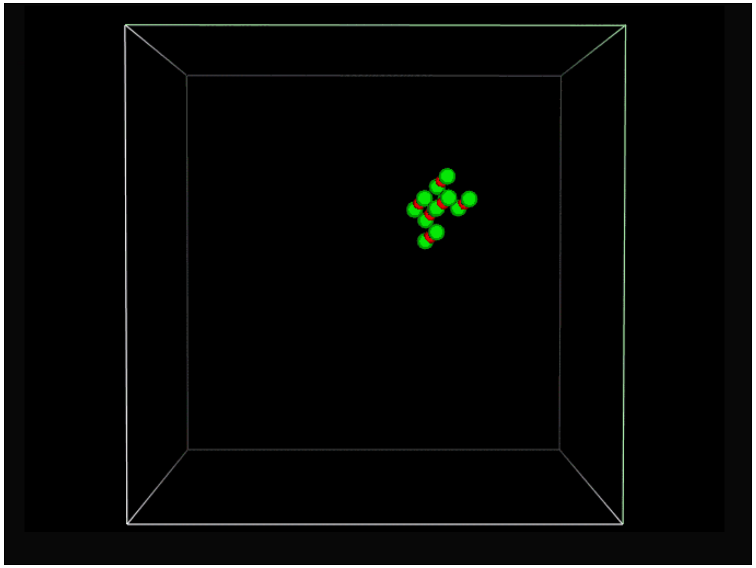
SIA clusters

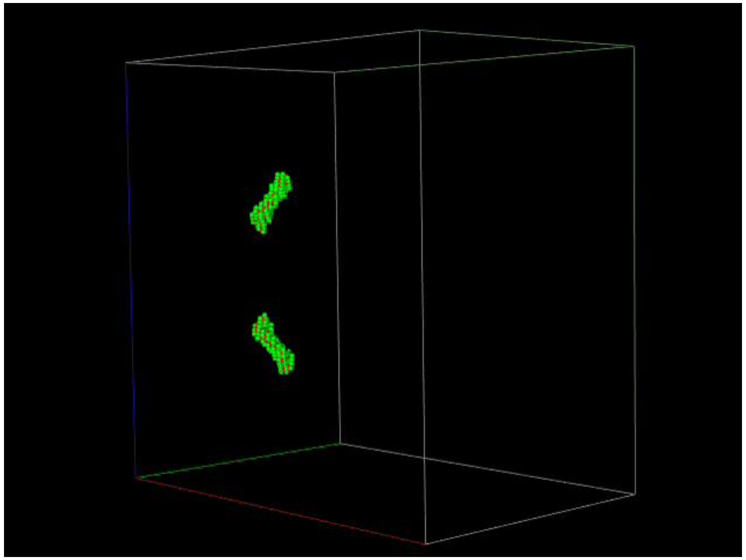


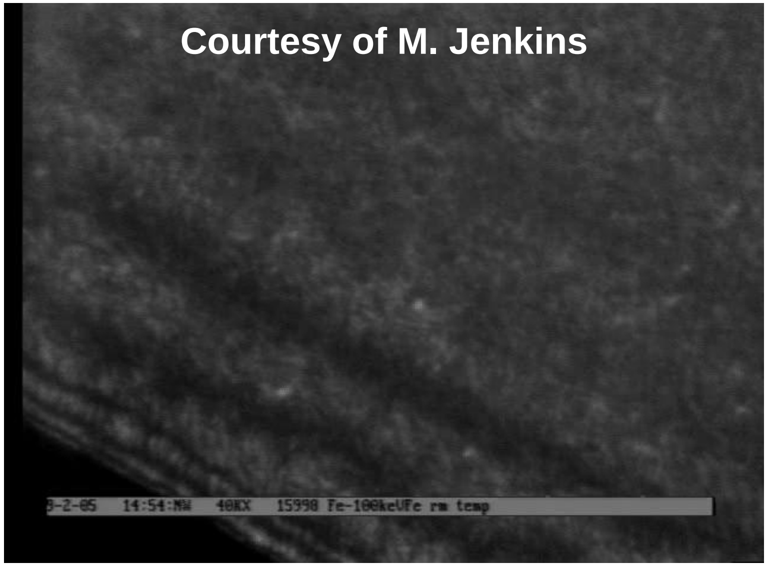
Single defects migrate in 3D

SIA faster than vacancies

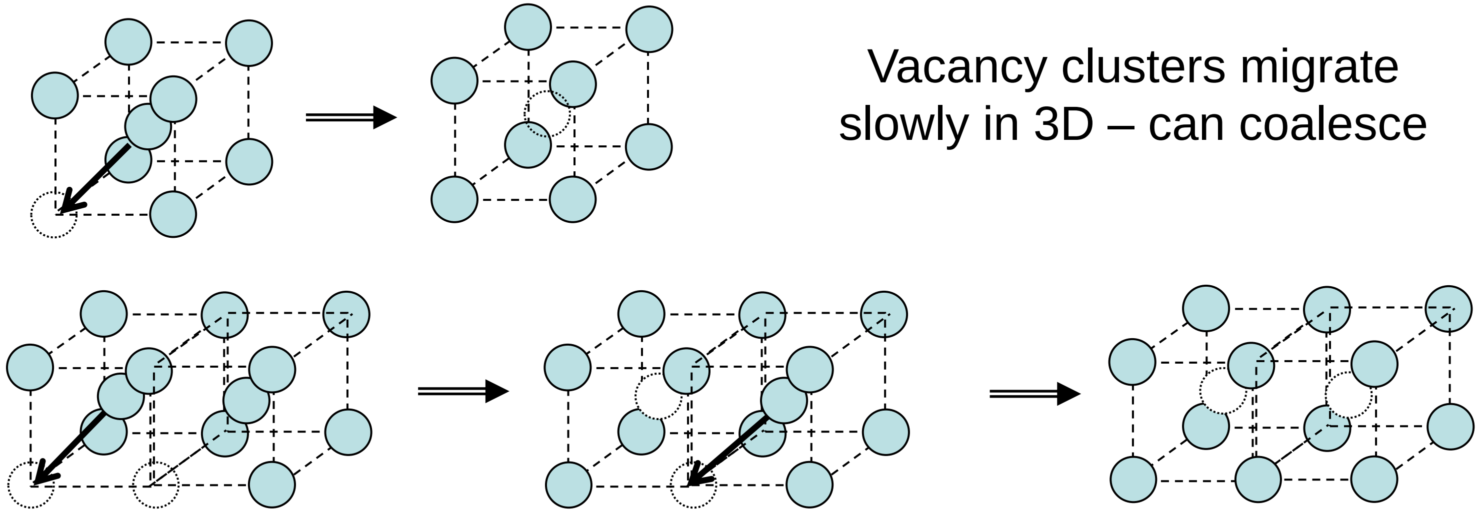
SIA clusters migrate fast in 1D



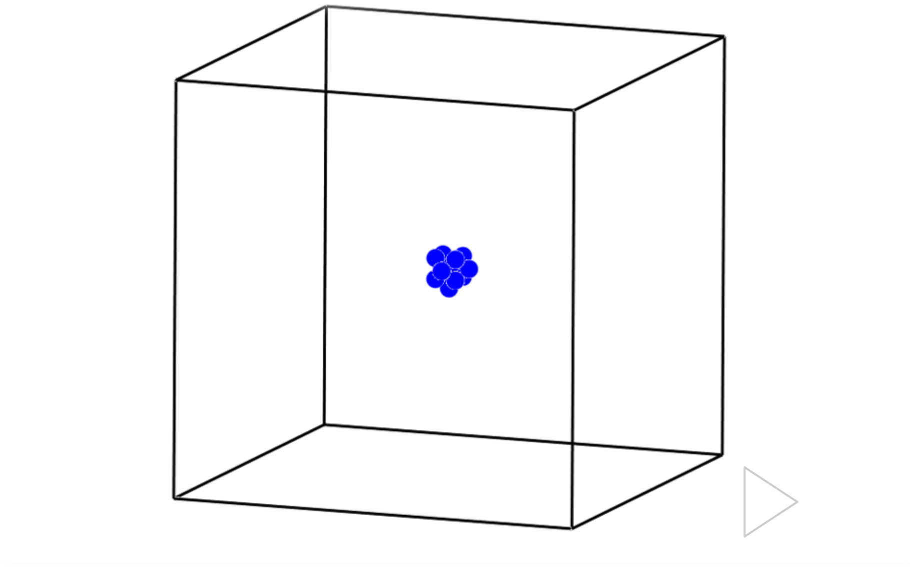




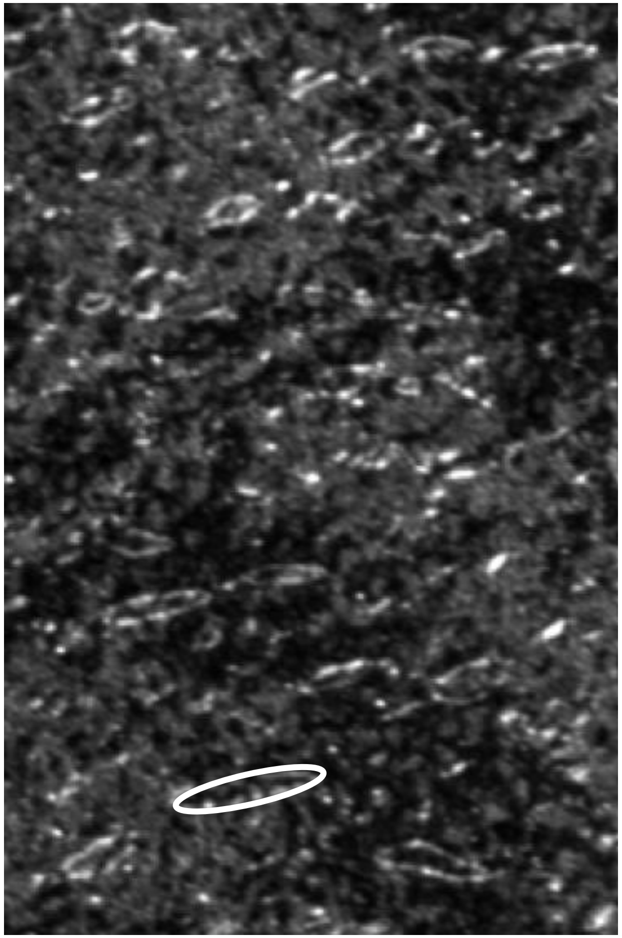
Defect migration and cluster growth
Vacancy clusters



Vacancy clusters migrate slowly in 3D – can coalesce

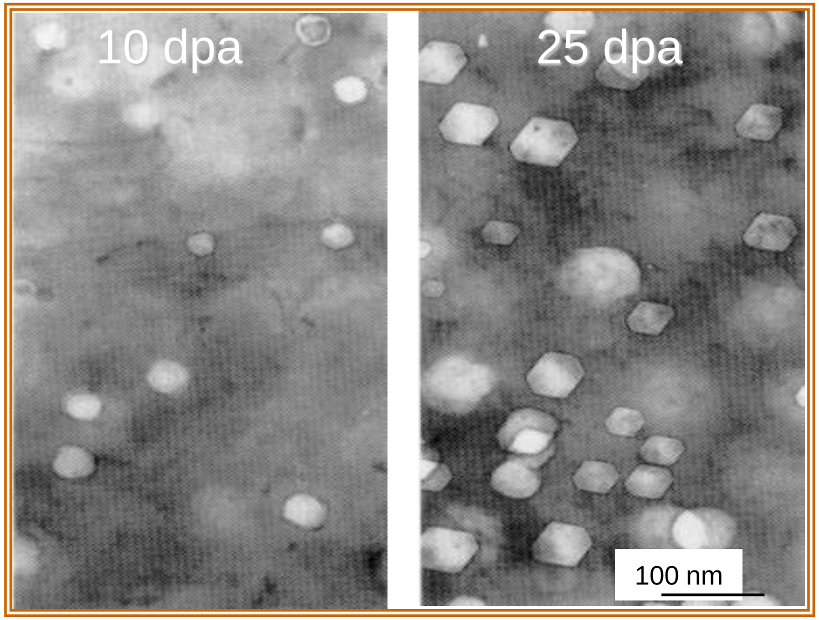


Evidence of point-defect cluster growth

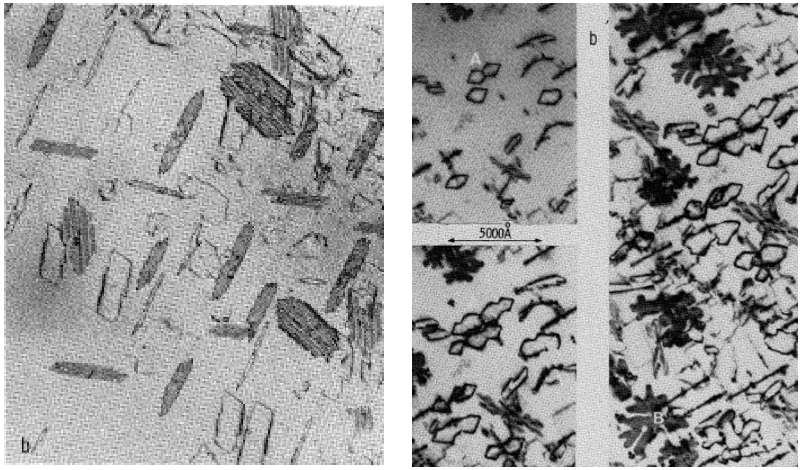


Loops in 150 keV Fe^{+} irradiated ultra-high-pure Fe at 300°C

Courtesy of M. Hernández Mayoral



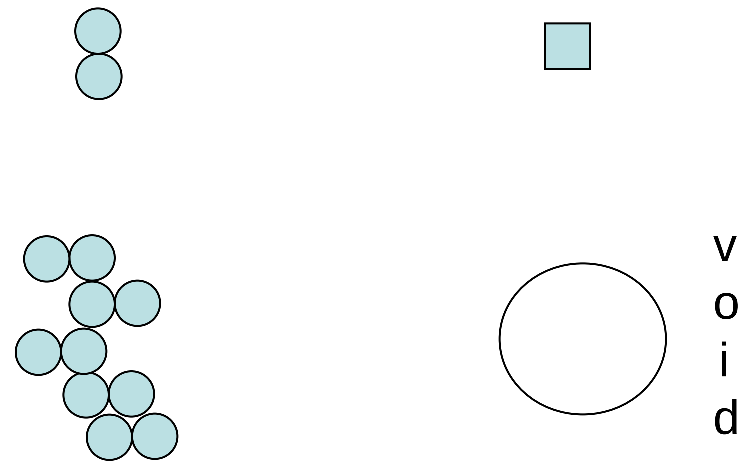
Cavities (above) & Frank loops (below) in irradiated 316 SS at high T



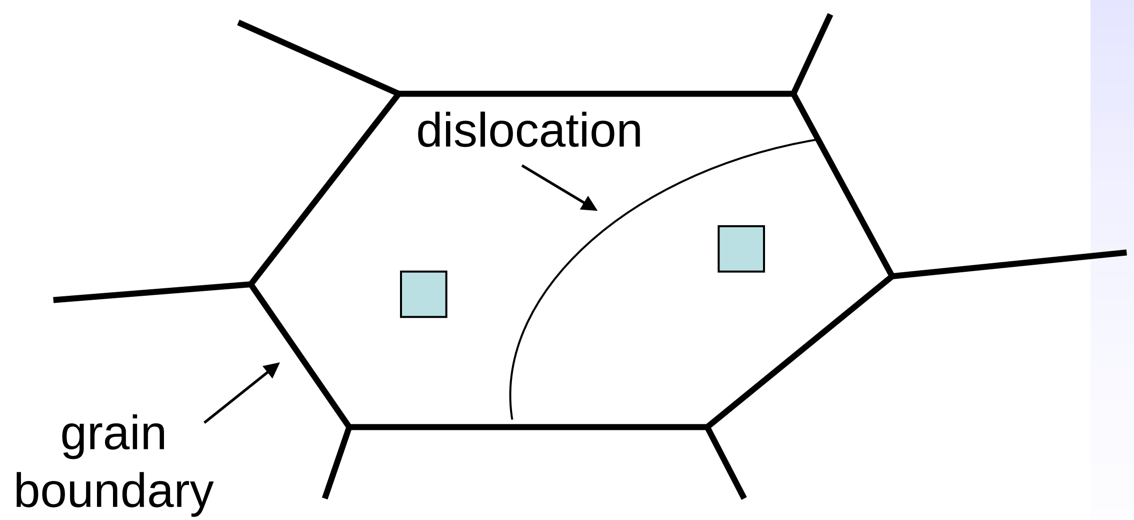
Garner & Gelles, JNM 159 (1988) 286

Defect recombination and disappearance at sinks

Recombination of SIA with Vacs



Disappearance at sinks



Does everyone know what a dislocation and a grain boundary are?

Take home messages

- Either by diffusion or directly in displacement cascades, point-defects tend to join to form clusters
  - *Vacancies: cavities, loops, other (stacking fault tetrahedra)*
  - *SIAs: loops only*

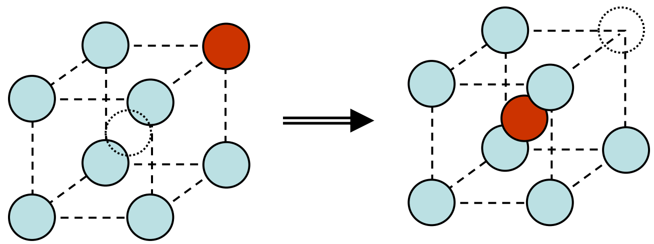
- SIA clusters migrate fast in 1D and are highly stable
- Vac. clusters migrate slowly in 3D and are less thermally stable

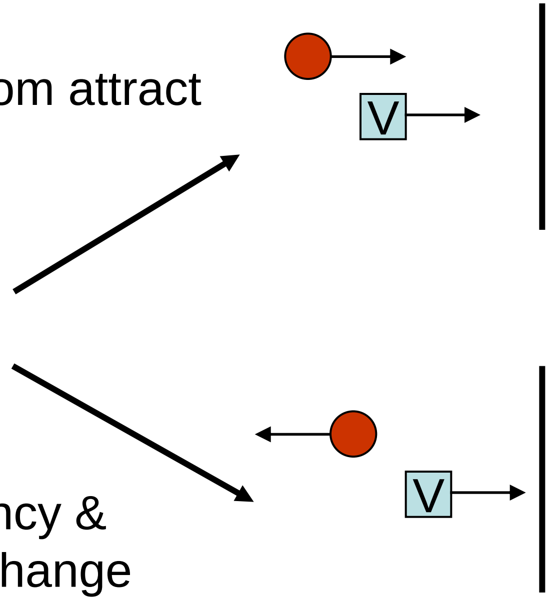
- Migrating defects eventually recombine or disappear at sinks
  - *Visible defects are there because they do not move*

What happens next?
Microchemical changes

Transport of chemical species

Vacancy & solute atom attract each other

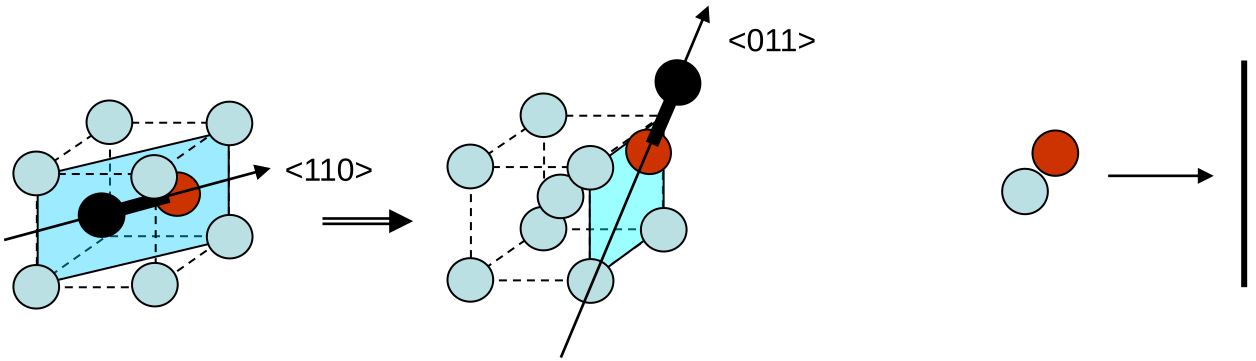




No attraction: vacancy & solute atom only exchange position

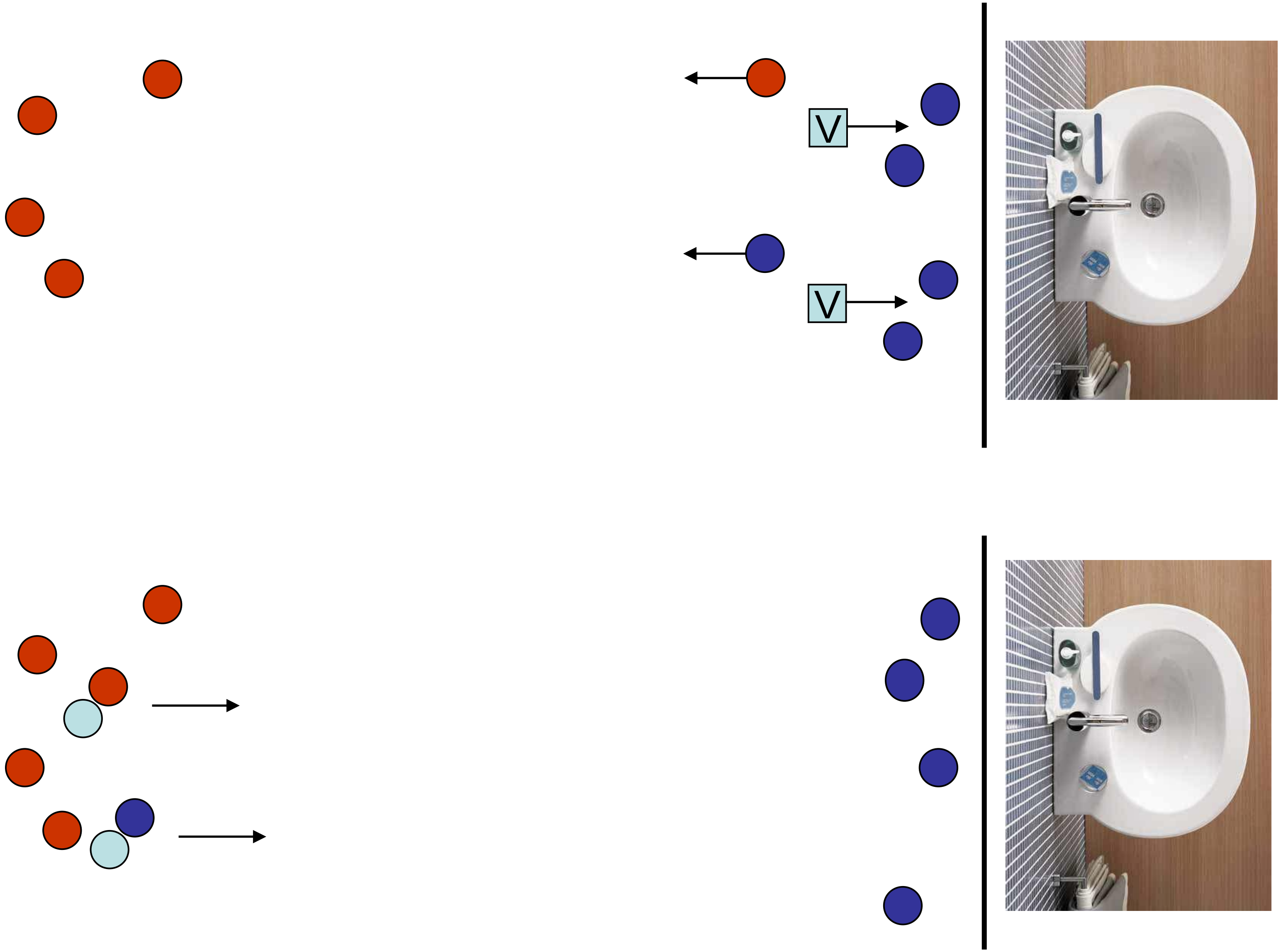
Sink for Vacs

Sink for SIAs



If stable, mixed dumbbell transports solutes to sinks

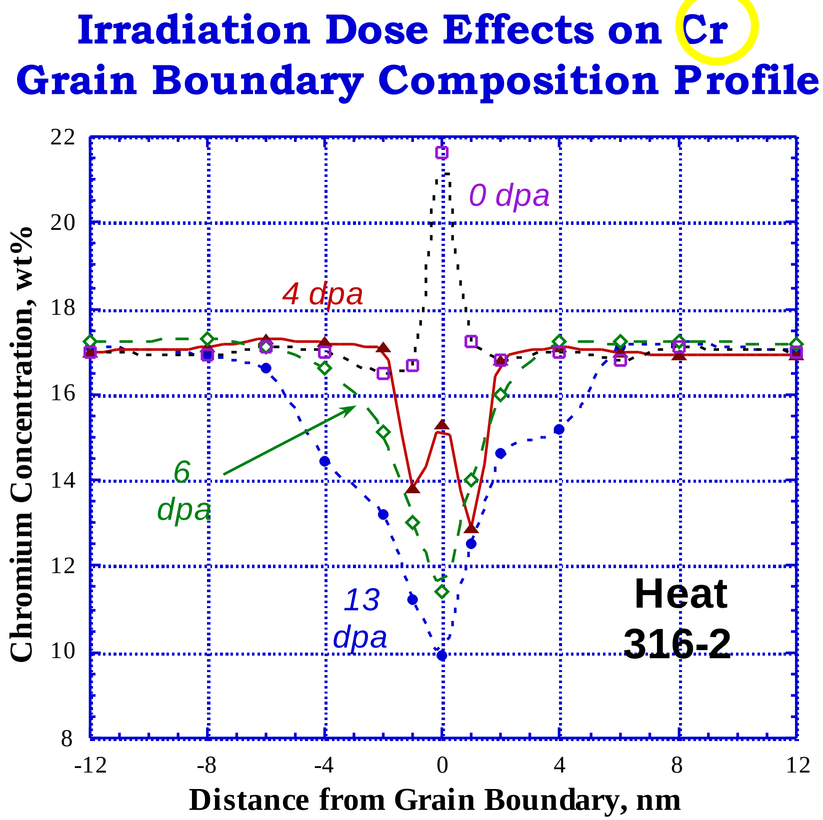
Competition between chemical species

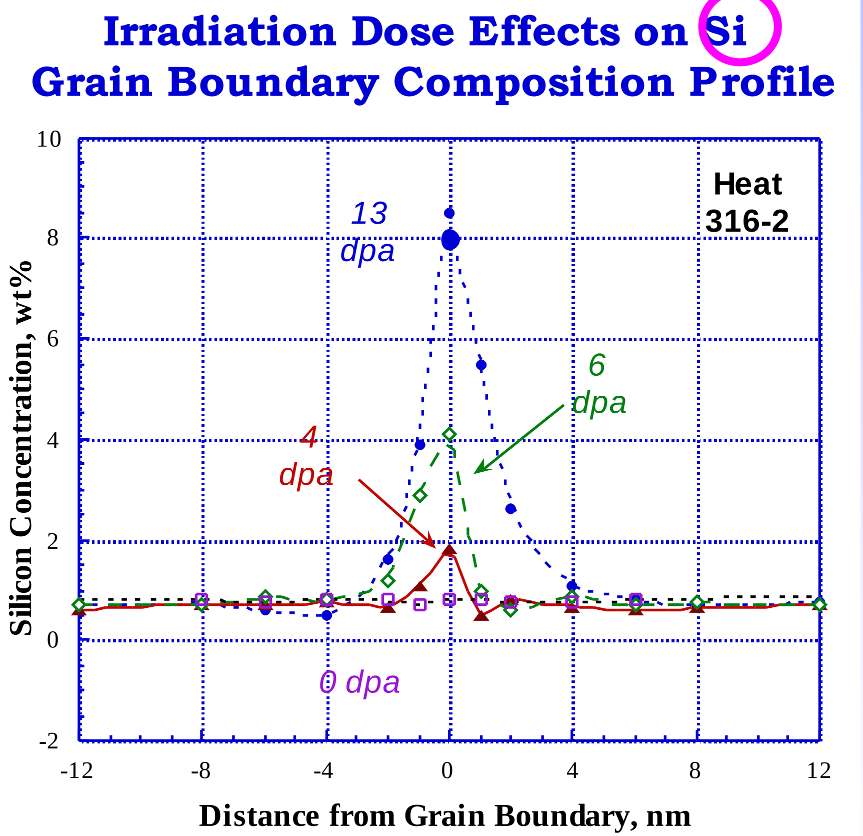


Typical example: radiation-*induced* segregation

Observed in <u>austenitic steels</u>

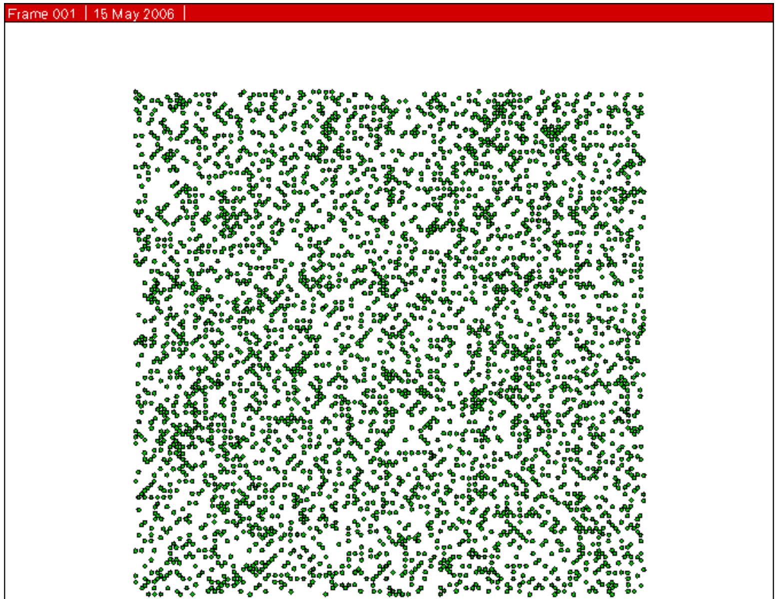
Determines higher susceptivity to stress corrosion cracking





Radiation-enhanced and radiation-induced

Enhanced

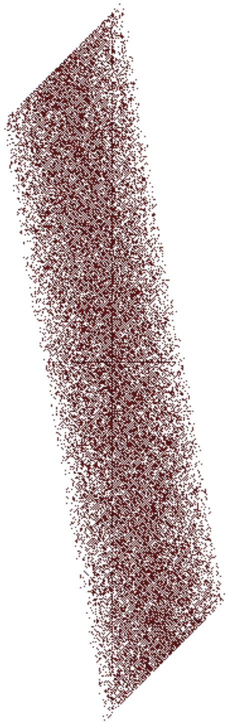


Courtesy A. Caro

Precipitates form because higher number of point defects under irradiation enhances transport and accelerates their formation

They would form also under high T annealing

Induced



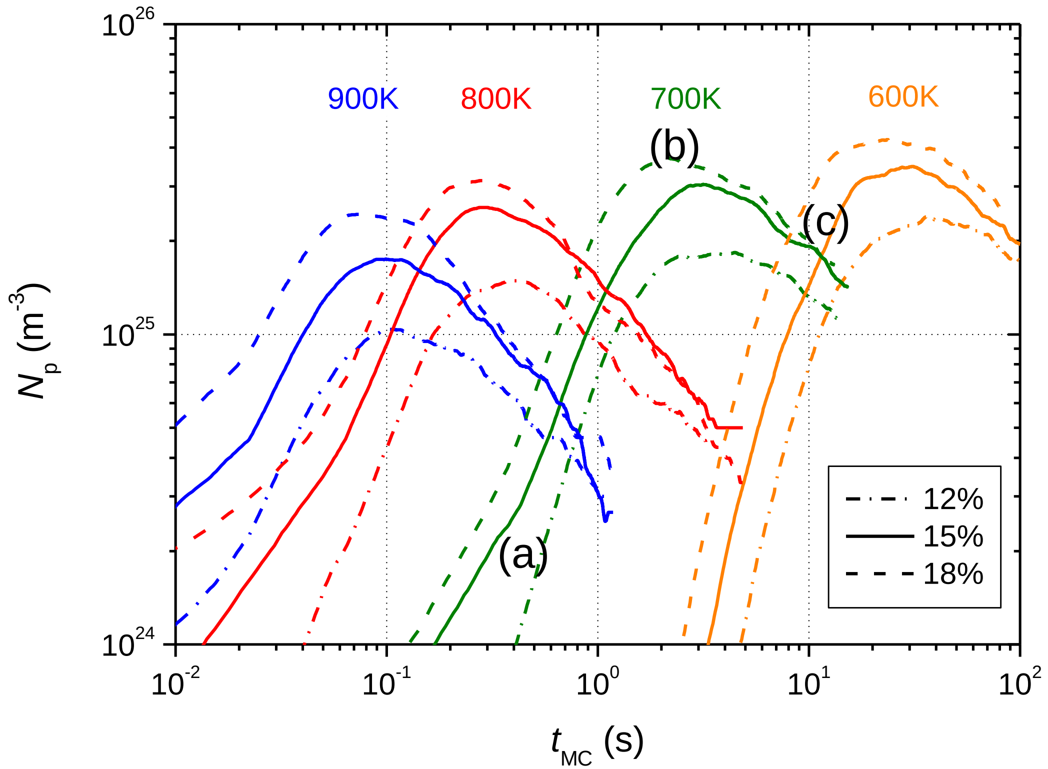
Courtesy F. Soisson

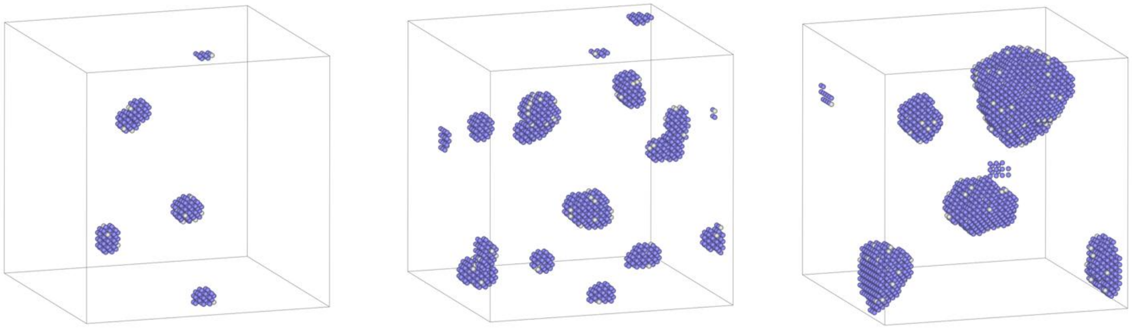
Precipitates form because continuous flux of point defects to sink increases local solute concentration, until solubility limit is locally exceeded

This would not happen without irradiation

Phases of precipitation

Nucleation, Growth and Coarsening

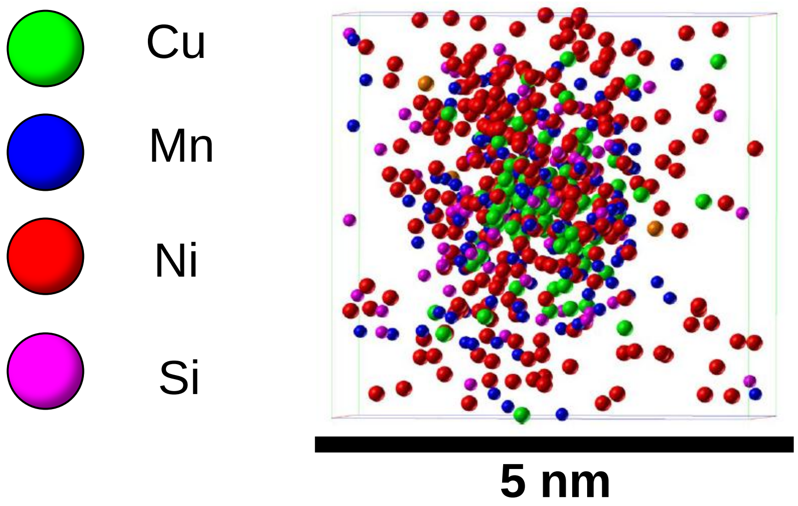


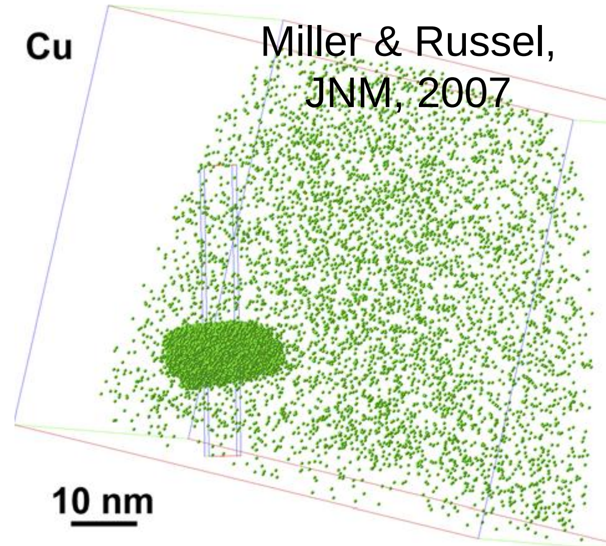


(a) (b) (c)

Example of radiation-enhanced phenomena

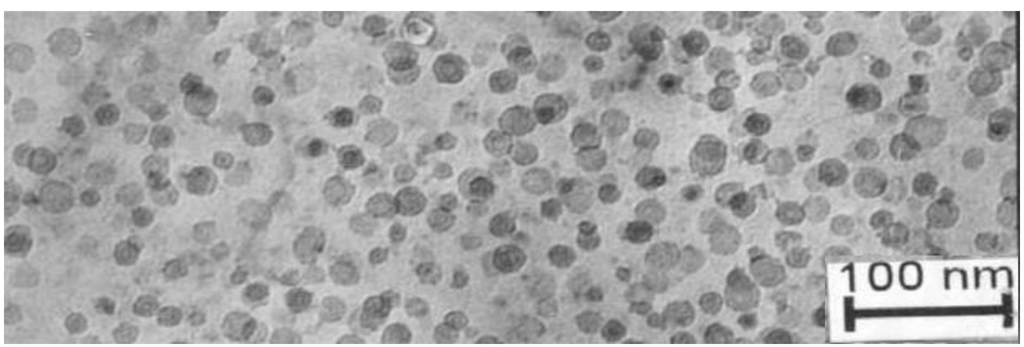
Cu-rich precipitate formation in RPV steels





Miller & Russel, JNM, 2007

Cu-free Ni-Mn-rich precipitate formation in RPV steels: radiation-*enhanced* or radiation-*induced*?

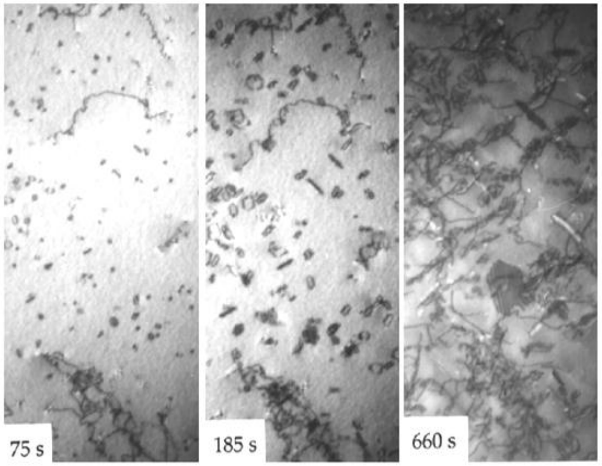


Konobeev et al., JNM, 2006

Cr-rich precipitate formation in high-Cr steels

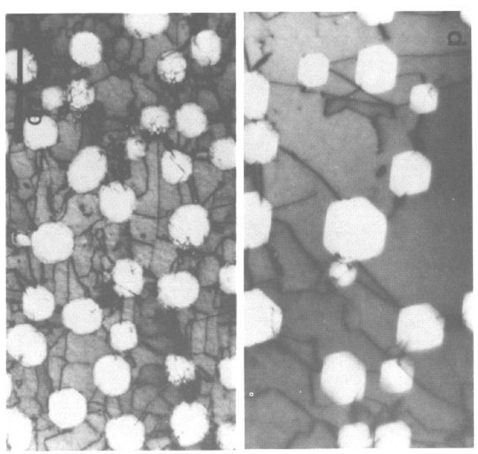
Summary: Nanostructural evolution under irradiation

Point defect evolution



Dislocation network

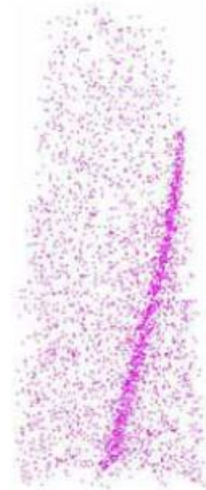
Nucleation, growth and coarsening of dislocation loops



Void swelling

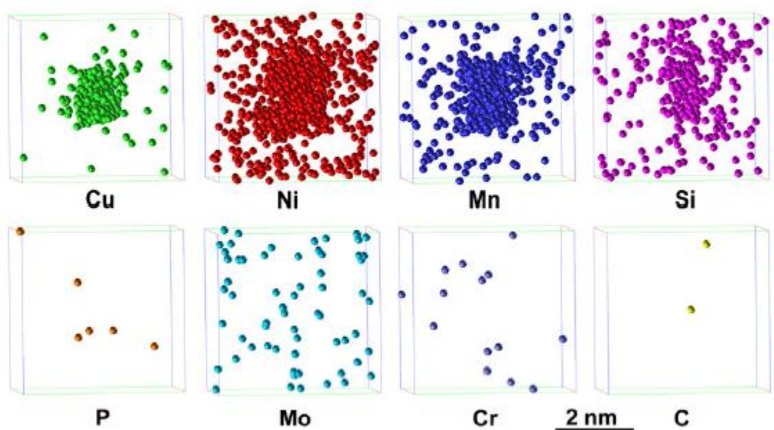
Nucleation, growth & coarsening of voids

Microchemical evolution



Nagai et al.,

Radiation induced segregation at sinks (grain boundaries, dislocations, ...)



Miller & Russel, JNM, 2007

Radiation enhanced/induced precipitation

How do we model these processes?
Atomic-level modelling: Molecular dynamics

Molecular Dynamics

➢ Principle

- *The classical equations of motion for a set of N atoms are timestepwise solved, using finite difference integration algorithms, so as to know atomic positions and velocities at each timestep:*

$$m\frac{d^2\bar{r}_i}{dt^2} = -\nabla V\left(\bar{r}_1, \bar{r}_2, ..., \bar{r}_N\right) \rightarrow \left\{\bar{r}_i, \bar{v}_i / i = 1, ..., N\right\}$$

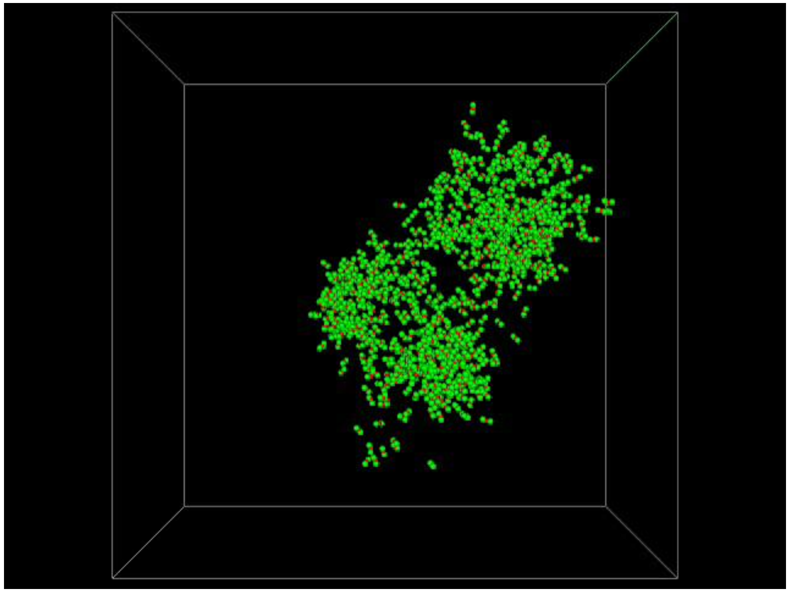
- *From the knowledge of atomic positions and momenta all statistical mechanics magnitudes are directly accessible*

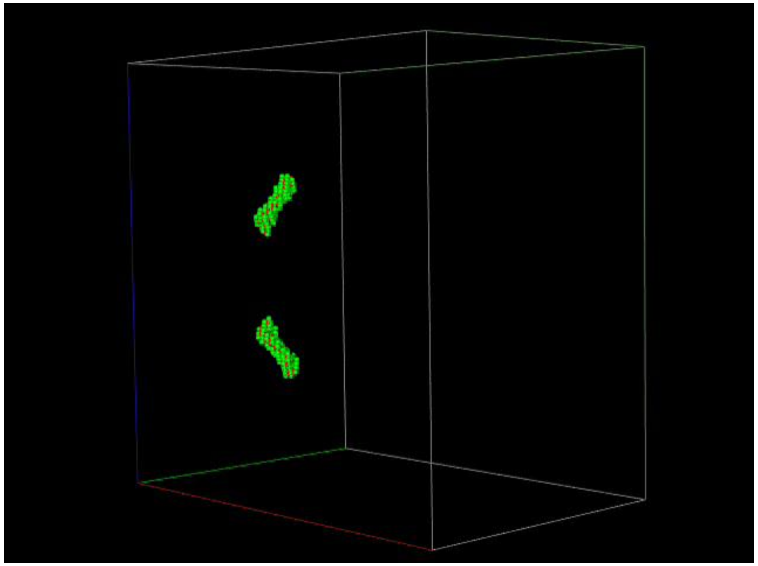
- *The core of the method, containing all the physics, is the interatomic potential, V(**r**$_i$),from which the interatomic forces are derived*

Applications of MD for irradiation problems

- MD is the technique "par excellence" for displacement cascade simulations:
  - *one atom is given kinetic energy*
  - *the dynamic evolution of the system is followed*
- MD also allows stability and mobility of (fast enough) defects to be studied
- Finally, MD can be used to model the interaction between dislocations and defects

20 keV cascade (peak time) in Fe





Pros & Cons of MD

- Advantages
  - *Wide applicability (bulk, surfaces, crystals, amorphous, liquids, ...)*
  - *No analytical simplifications or approximations*
  - *Treats spontaneously complex systems and phenomena at equilibrium or far from it, not accessible to analytical approaches*
- Limitations
  - *Evolution of the system calculated by timesteps of ~1 femtosecond*
  - *Limited timescale (tens of nanoseconds, trade-off size/time)*
  - *Limited volumes (up to 10^7 atoms): not big enough for e.g. extended defects*
  - *All the physics is contained in the interatomic potential*

How do we model these processes beyond MD scale?
Atomic-level modelling: Monte Carlo

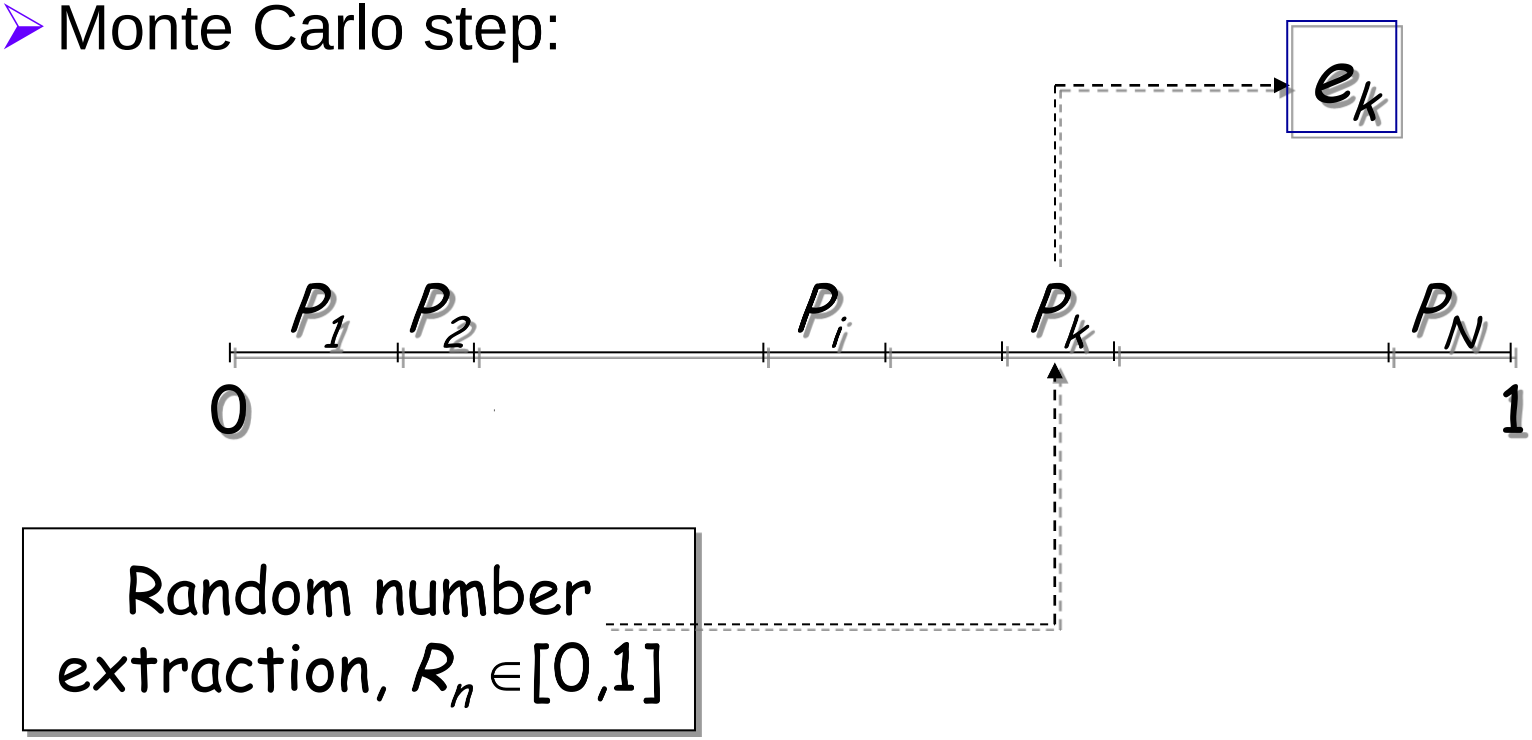
Stochastic Monte Carlo Algorithms

- MD cannot deterministically reproduce the evolution of a system to equilibrium if the kinetics is slower than nanoseconds

- MC methods can be used for this purpose or more generally to extend the timespan of radiation damage simulations:
  - *Metropolis Monte Carlo*
  - *Kinetic Monte Carlo*
    - Atomistic KMC
    - Object KMC

The Monte Carlo Algorithm

- List of possible events: e_i / $i=1, \ldots, N_e$
- A probability P_i is associated to each event
- $\Sigma_i P_i = 1$
- Monte Carlo step:



Metropolis Monte Carlo

- System of *N* atoms, defects can be included
- Total energy must be calculable, e.g. using an interatomic potential
- One trial event is chosen between:
  - *atomic position exchange*
  - *small atomic displacement*
  - *global expansion or contraction*
- If $E_{after} - E_{before} = \Delta E < 0$, the trial is accepted
- If $\Delta E > 0$, the trial is accepted with probability

$$\exp(-\Delta E/kT) < 1$$

(by extracting a random number, which can fall only in one out of two possible probability intervals)

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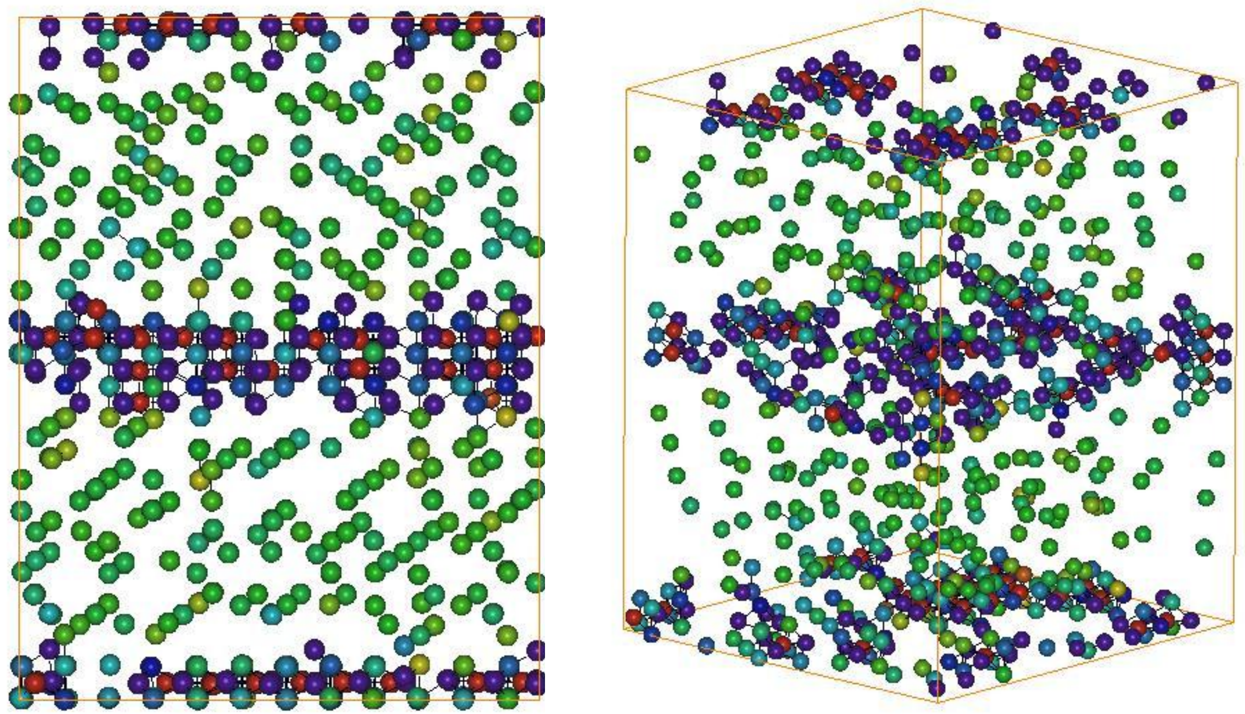
Application of Metropolis MC

Study Cr redistribution in presence of a grain boundary: is segregation favoured or not?

Cr atoms only:

{111}



Cr 2D distribution **Cr 3D distribution**

E. Zhurkin et al.

Metropolis Monte Carlo

Advantages

- *Phenomena such as segregation or precipitation, out of scope for MD, can be studied*
  - ✓ (given a suitable hamiltonian and on the condition that these correspond to equilibrium states)
- *All contributions to the free energy can be included in the calculation*
  - ✓ Powerful tool to evaluate phase diagrams

Problems:

- *Evolution does not involve physical mechanisms, only total energy*
- *Intermediate configurations are physically not meaningful*
- *No information is given about time necessary to reach equilibrium*

Kinetic Monte Carlo

Kinetic $\Rightarrow$ time is introduced !

- Probabilities are calculated for physical transition mechanisms as Boltzmann factor frequencies :

$$\Gamma_i = \nu_i \exp\left(-\frac{E_{a,i}}{kT}\right)$$

- After a certain event is chosen, time is in[...]as[...] amount:

$$\Delta\tau = \frac{-\ln(rand)}{\sum_{i=1}^{N_e}\Gamma_i} \overset{average}{=} \frac{1}{\sum_{i=1}^{N_e}\Gamma_i}$$

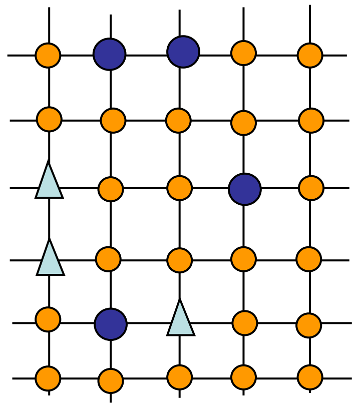
Most physics (kinetics and thermodynamics) contained in the activation energies !

(residence time algorithm)

Kinetic Monte Carlo Families

KMC
residence time algorithm

Atomistic KMC

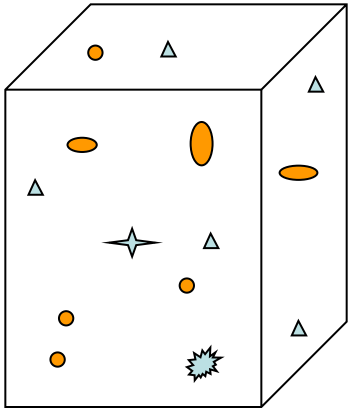


Atoms (alloy) on rigid lattice

Mainly vacancy jumps (SIA in 1st approx.)

Energy parameters from interatomic potentials or DFT

Object KMC

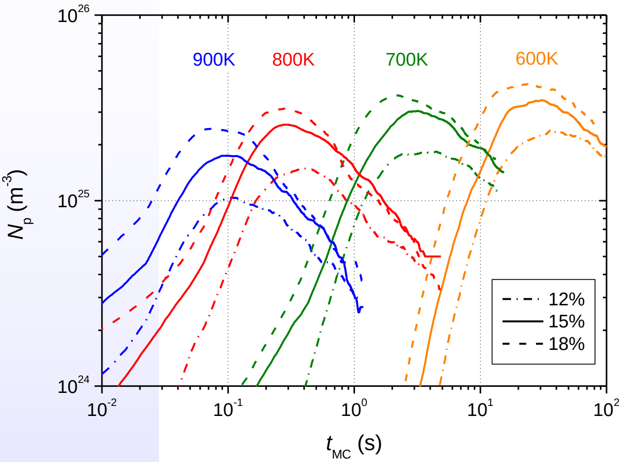


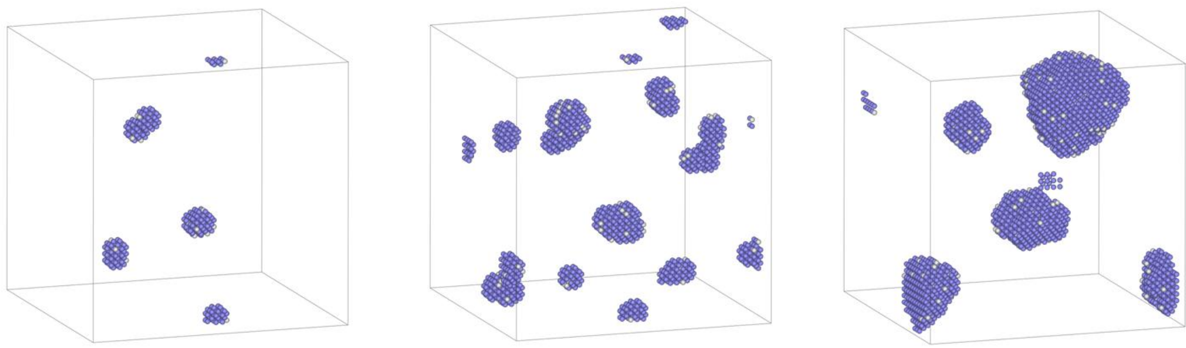
"Objects" on *non-atomic* lattice (V, SIA, clusters, …)

Many possible reactions between "objects"

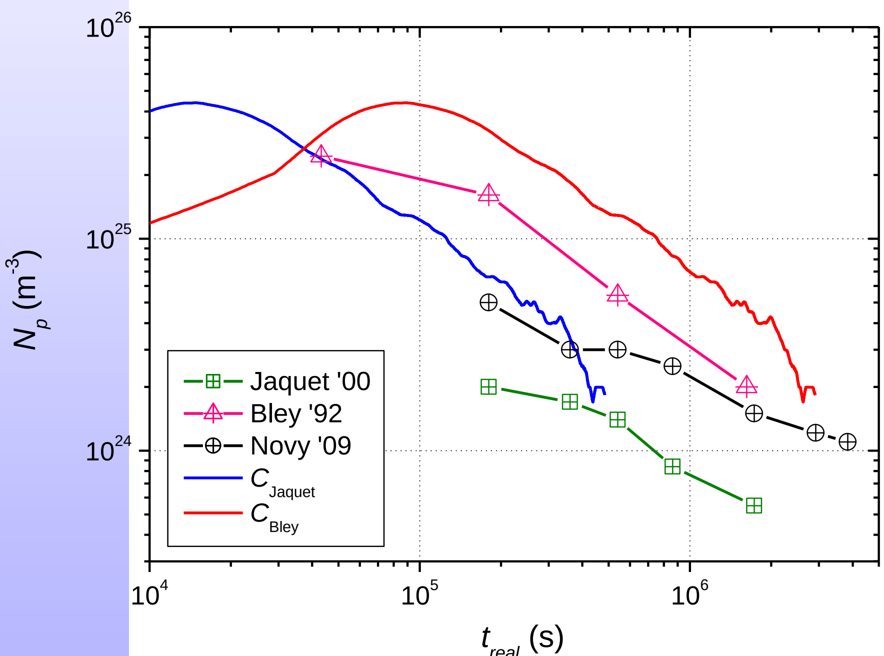
Large set of parameters covering all possible reactions is needed

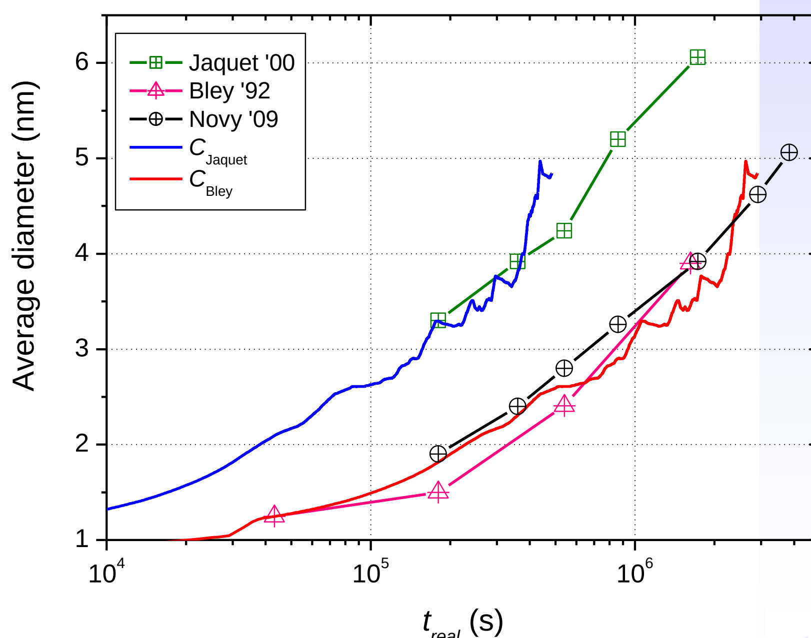
Example of application of AKMC: precipitation in FeCr





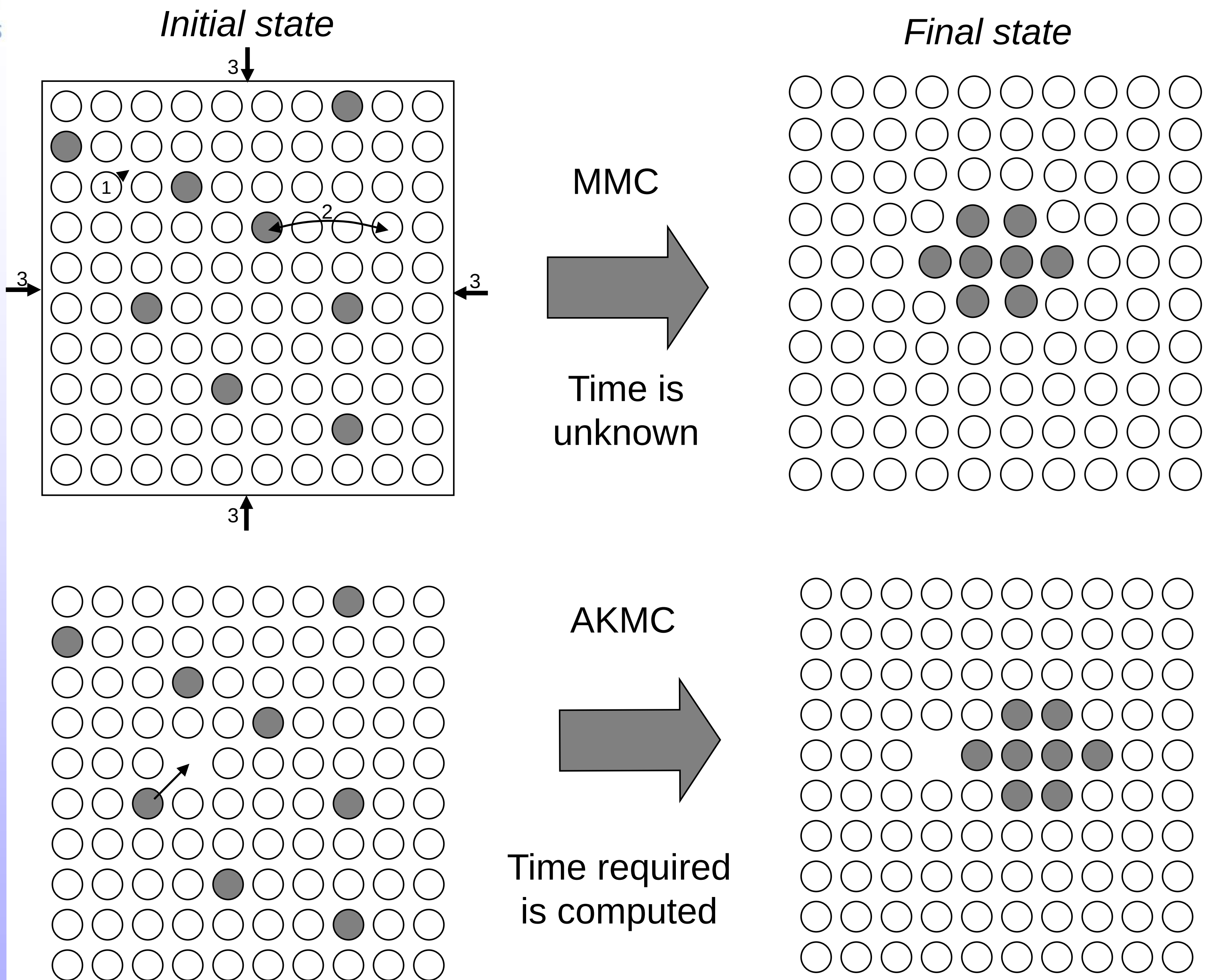
(a) (b) (c)





G. Bonny et al., Phys. Rev. B, 2008

Difference between AKMC and MMC



AKMC: Pros & Cons

- **Advantages:**
  - *Atomic-level method: can treat diffusion processes including proper atomic level mechanisms*
  - *Can be extended to relatively long timescales (it depends on the problem), much longer than MD any way (seconds easily)*

- **Limitations:**
  - *Computationally expensive: the volumes that can be simulated remain fairly small*
  - *At the moment, the treatment of SIA is only tentative*

How do we model these processes to their full timescale? Nanostructure evolution models

Coarse-grained microstructure evolution models

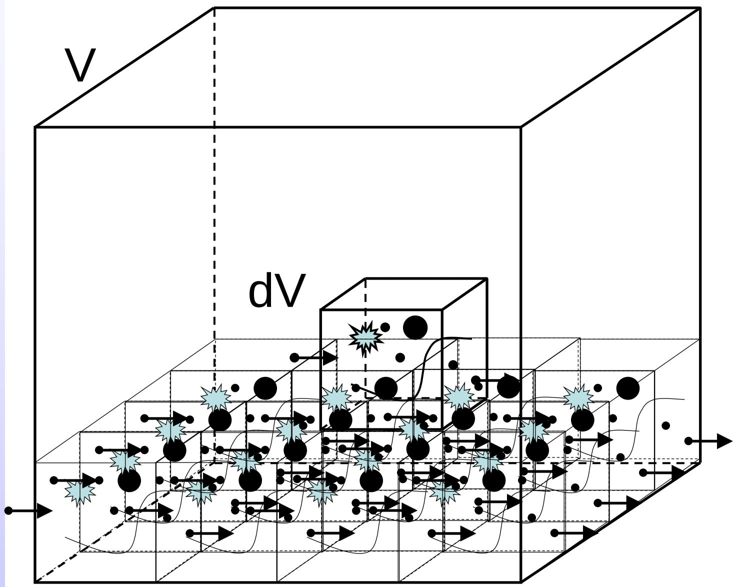
- Coarse-grained → no atoms
  - *The "elements" or "grains" of the simulation are not atoms:*
    - ✓ Defects (point-defects, clusters, precipitates) → nanostructure evolution models
    - ✓ Dislocations → dislocation dynamics models
    - ✓ Grain-boundaries → texture models
    - ✓ …

- Nanostructure evolution models for radiation damage are those that in principle allow direct comparison with experiments:
  - *Rate theory*
  - *Object kinetic Monte Carlo (and similar)*

Nanostructure evolution models: Rate Theory

- Mean-field approximation:

  Defects are created, react and disappear at sinks everywhere at the same rate



- The same thing happens in each infinitesimal volume dV
- Different from periodic boundary conditions:
  - ✓ dV → 0 (infinitesimal)
  - ✓ There is no real simulation volume
  - ✓ Only variables are concentrations

- Example:

Source term

Flux term

Reaction term

$$A + B \underset{k_C^-}{\overset{k_{A+B}^+}{\longleftrightarrow}} C \qquad \frac{\partial C_B}{\partial t} = G_B + D_B \nabla^2 C_B - \left(k_{A+B}^+ C_A C_B - k_C^- C_C\right)$$

Nanostructure evolution models: Rate Theory

$$A + B \underset{k_C^-}{\overset{k_{A+B}^+}{\longleftrightarrow}} C \qquad \frac{\partial C_B}{\partial t} = G_B + D_B \nabla^2 C_B - \left(k_{A+B}^+ C_A C_B - k_C^- C_C \right)$$

- *N* (10s to 100s) coupled differential equations of this type need to be written, one for each defect species
- The actual *rate* theory concerns the determination of the "rates" at which the reactions occur
  - E.g., through the theory of diffusion-limited reactions and based on mass-action law we know that:

$$k_{A+B}^+ = 4\pi (r_A + r_B)(D_A + D_B) \qquad k_C^- \propto k_{A+B}^+ \exp\left(-\frac{E_b}{kT} \right)$$

- Thus, given the source terms, **the basic ingredients of nanostructure evolution models are**
  - **Diffusion coefficients**
  - **Capture radii**
  - **Binding energies**

Nanostructure evolution models: Rate Theory – Pros & Cons

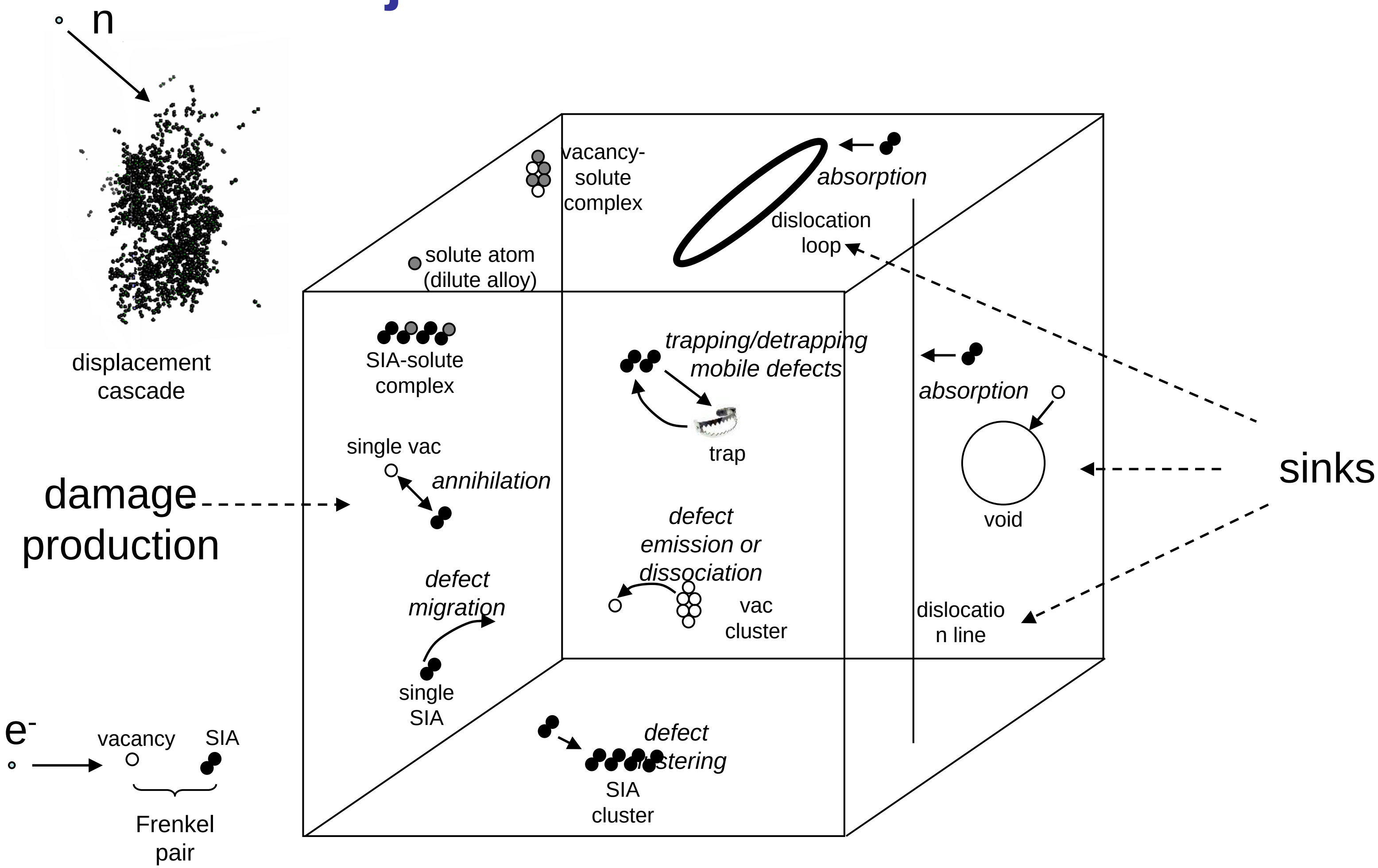
Advantages:

- Computationally cheap :
  - *Sensitivity studies easily performed*
  - *Fitting of parameters to experiments is possible*
  - *Large fluences and volumes are no problem*
  - *Steady-state or simplified expressions can be analytically obtained*
- Fully theoretical framework within which radiation effects can be addressed
  - *It is not a "simulation"*
  - *Computer solves system of eqs.*

Drawbacks:

- Random inhomogeneities and geometrical effects (e.g. coalescence) not taken into account
- Introduction of new mechanisms requires specific theoretical developments
- Solution of these eq. systems when large easily leads to numerical crashes
- All acting mechanisms and parameters must be known
  - *The model does not provide them, like e.g. MD*
- Atomic-level configurations are not provided, either
  - *As compared to e.g. AKMC*

Nanostructure evolution models: Object kinetic Monte Carlo



$$\Gamma_i = \nu_i \exp\left(-\frac{E_{a,i}}{kT}\right)$$

$$\Delta\tau = \frac{1}{\sum_i \Gamma_i + \sum_j P_j}$$

Nanostructure evolution models: Object kinetic Monte Carlo

- Volume containing "objects" exists:
  - *Point-defects and their clusters*
  - *Precipitates, solutes, …*
  - *Traps and localised sinks*
  - *Dislocations*
  - *(Grain boundaries)*
- Each "object" is defined by:
  - *Type*
  - *(centre-of-mass) position*
  - *Migration parameters*
  - *Possible reactions*
  - *Reaction radius*
- Events can be
  - *Thermally activated → activation energy (migration, emission)*
  - *External of known rate P_i (cascades, …)*
  - *Effect of geometry (recombination, trapping, clustering)*

- **As for the rate theory, the basic ingredients are**
  - **Diffusion coefficients**
  - **Capture radii**
  - **Binding energies**
  - **…**

Nanostructure evolution models: Object kinetic Monte Carlo: Pros & Cons

- Advantages:
  - *Flexibility in introducing objects, mechanisms and parameters, taken from any source of information (DFT, MD, AKMC, experiments, …)*
  - *No theoretical developments required for each new mechanism*
  - *Spatial inhomogeneities and correlations (including sink strengths) are spontaneously accounted for*
  - *Defects behave in a realistic way*

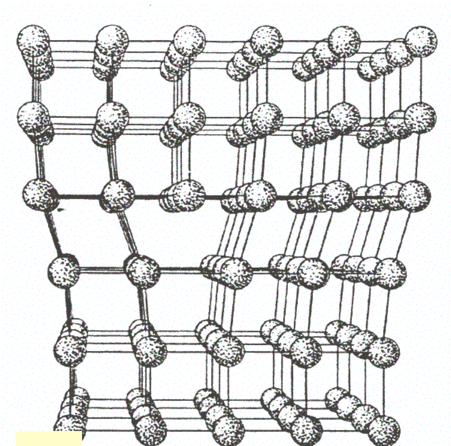
- Drawbacks:
  - *No atomic configurations*
    - ✓ As compared to *atomistic* KMC
  - *All mechanisms and parameters must be known in advance*
    - ✓ The model does not provide them, like MD does
  - *Computationally expensive*
    - ✓ (as compared to rate theory)
    - ✓ Small volumes reduce statistical significance, especially for low densities
    - ✓ Fitting not possible; sensitivity studies possible, but at high cost

Part II: Mesoscopic scale and beyond

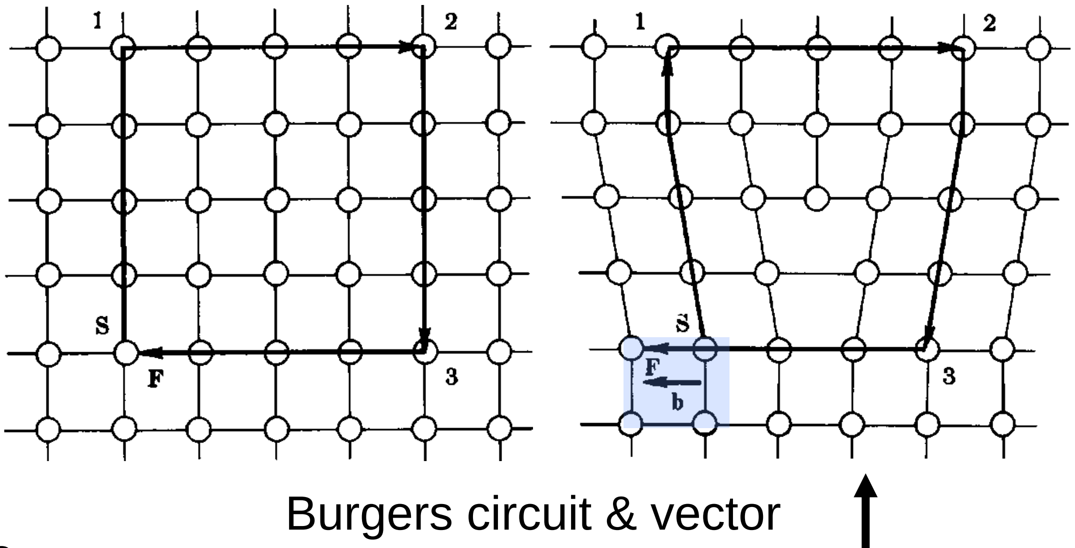
Dislocations and hardening

Dislocations

Edge type

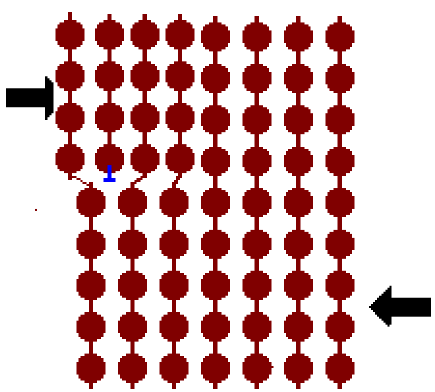


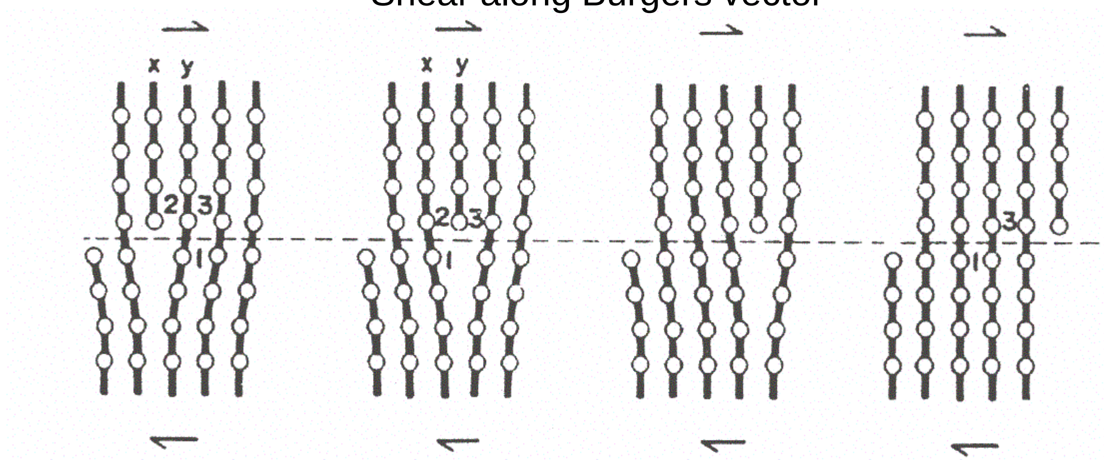
$\hat{\xi}$ Edge dislocation:
line normal to slide



Burgers circuit & vector

Shear along Burgers vector

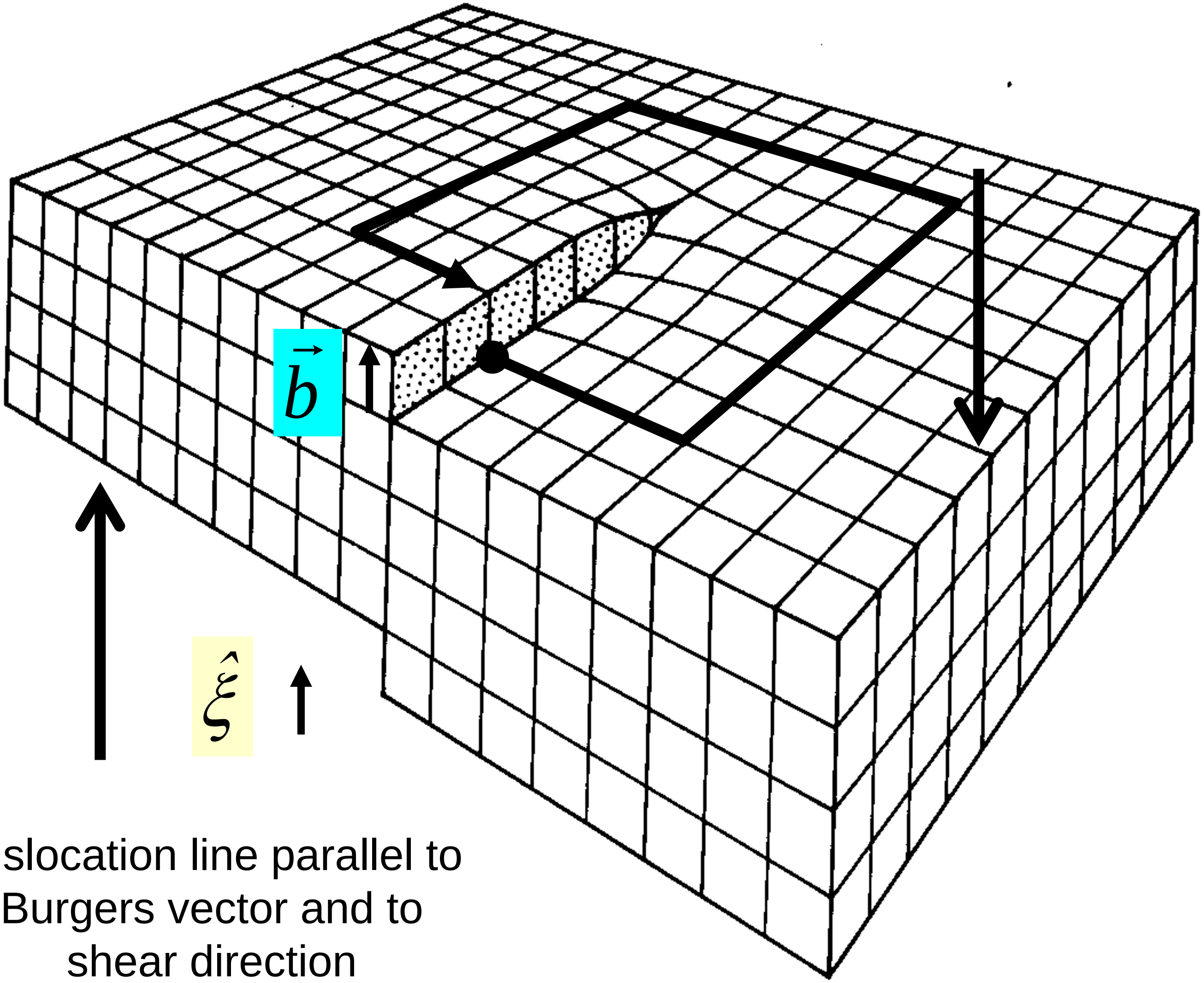




Dislocation glide under shear is the most frequent mechanism whereby metals are <u>irreversibly deformed</u> (<u>plastic deformation</u>)

Dislocations

Screw type



Dislocation line parallel to Burgers vector and to shear direction

Dislocations

Mixed type

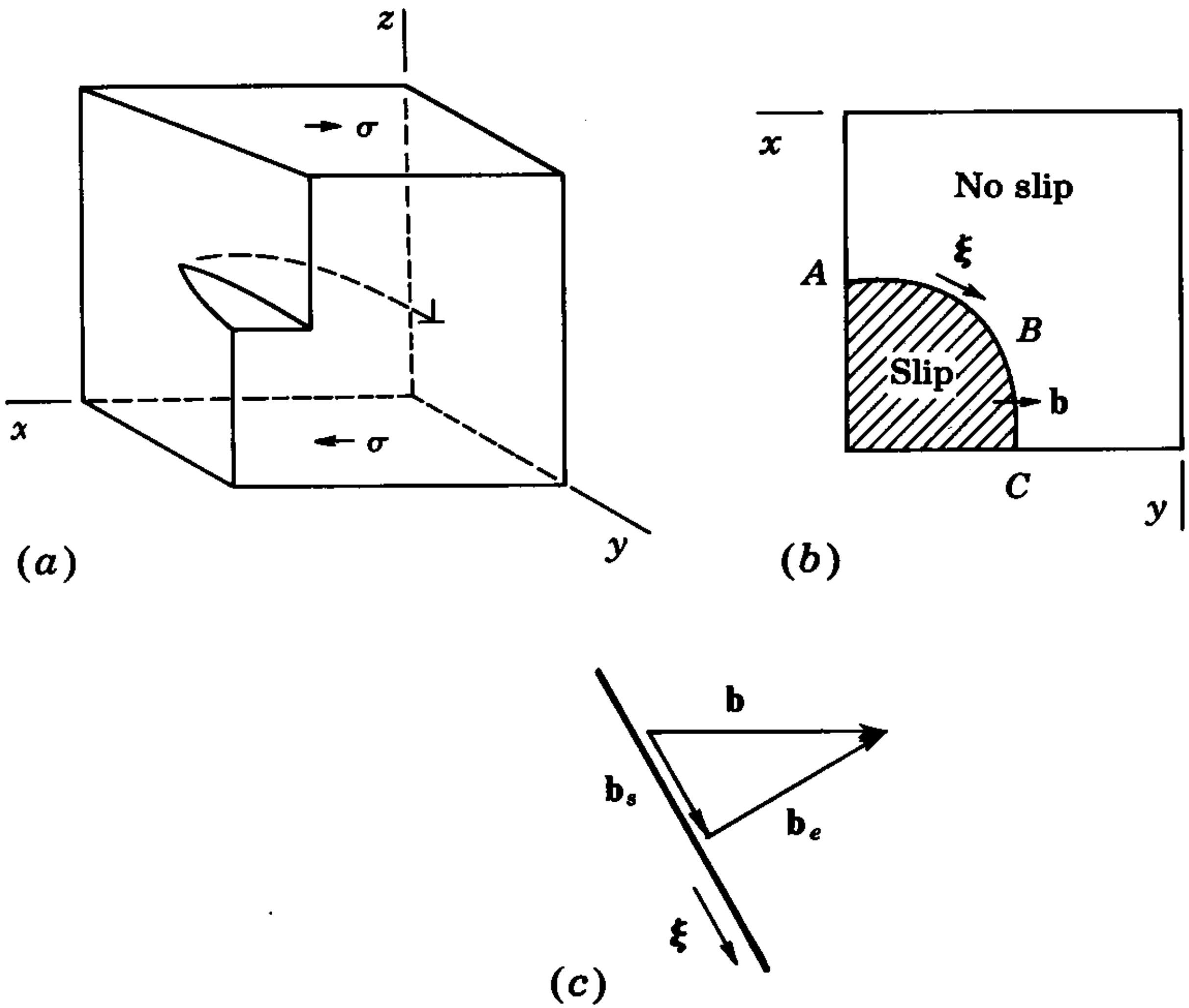
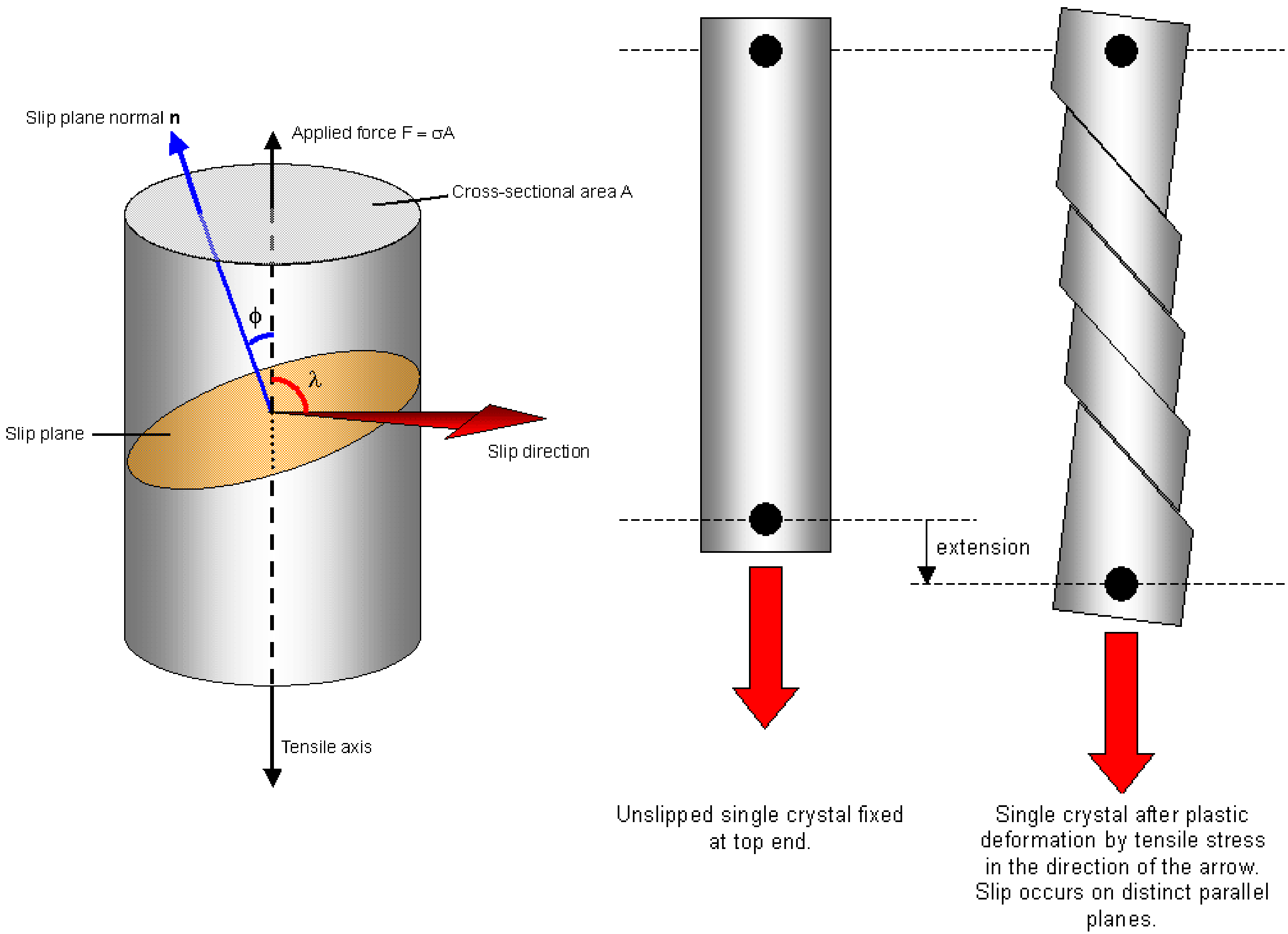


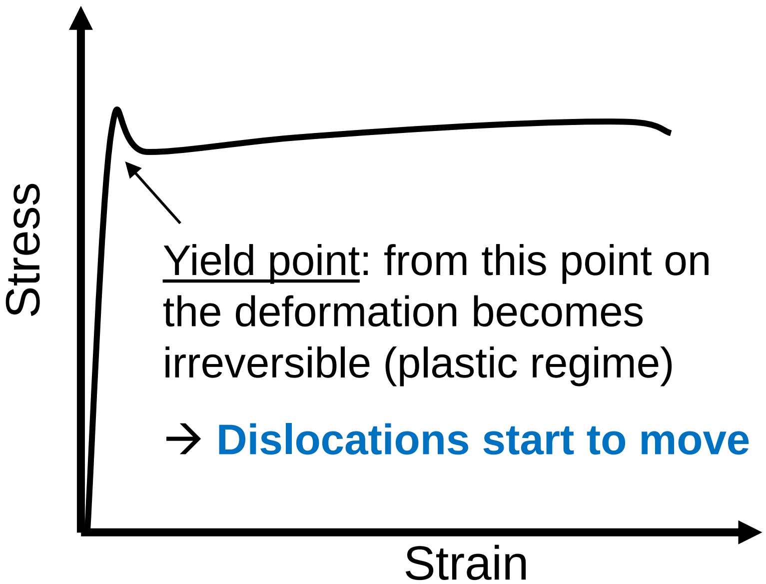
FIGURE 1-23. (*a*) Shear of a perfect crystal to form a mixed dislocation. (*b*) Projection normal to the glide plane in (*a*). (*c*) Resolution of (*b*) into components at point *B*.

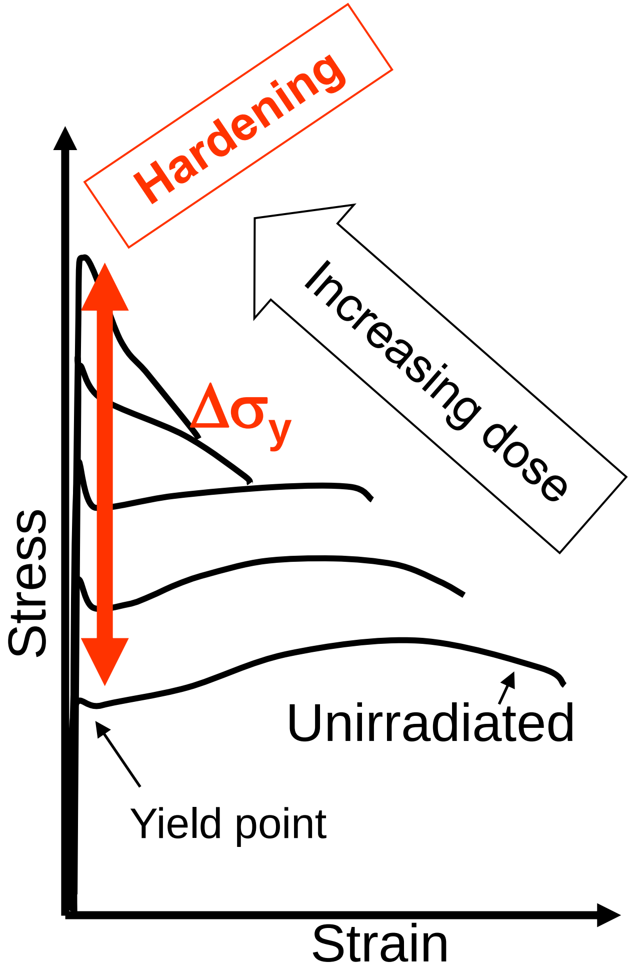
From Hirth and Lothe, Theory of Dislocations

Dislocations, slip planes and deformation

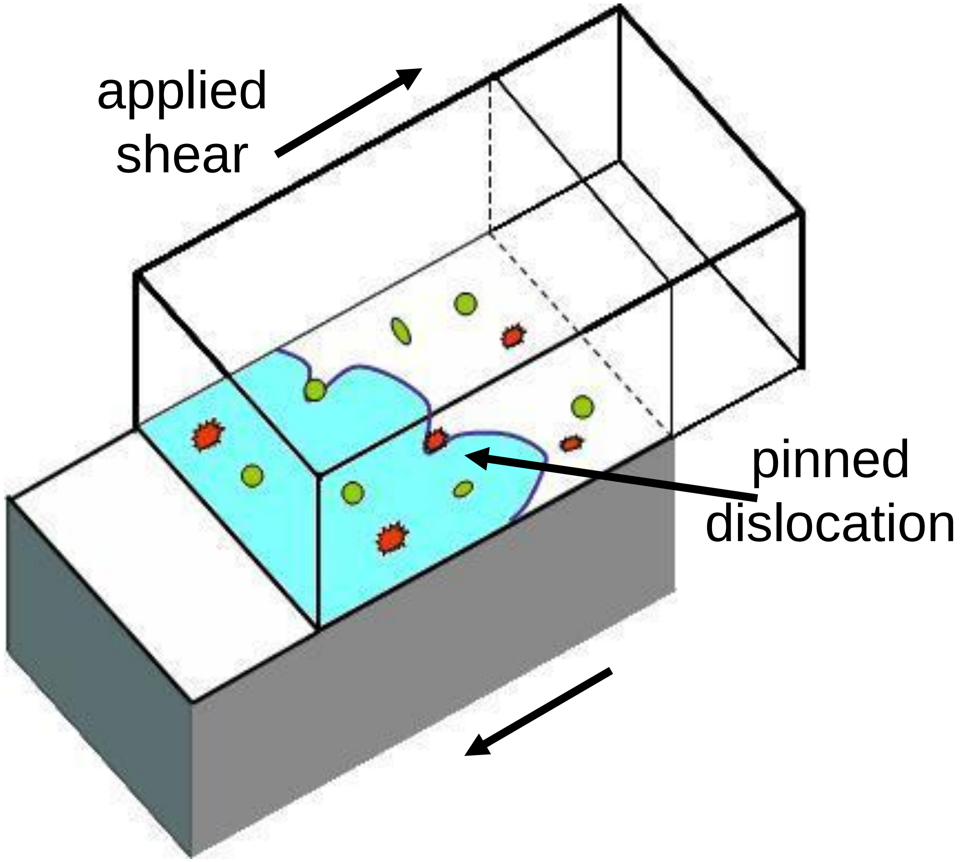


Hardening = Yield strength increase





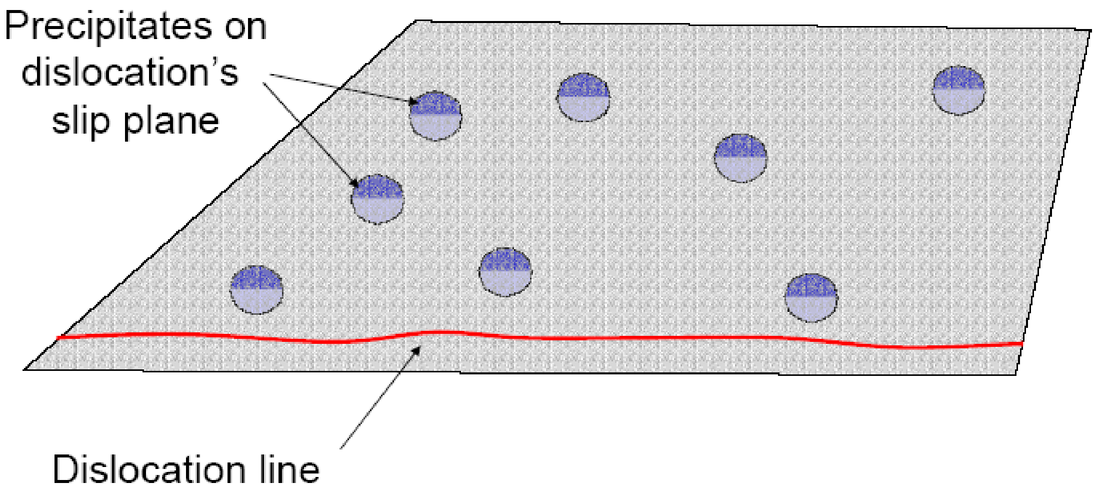
Why does the yield strength increase after irradiation?



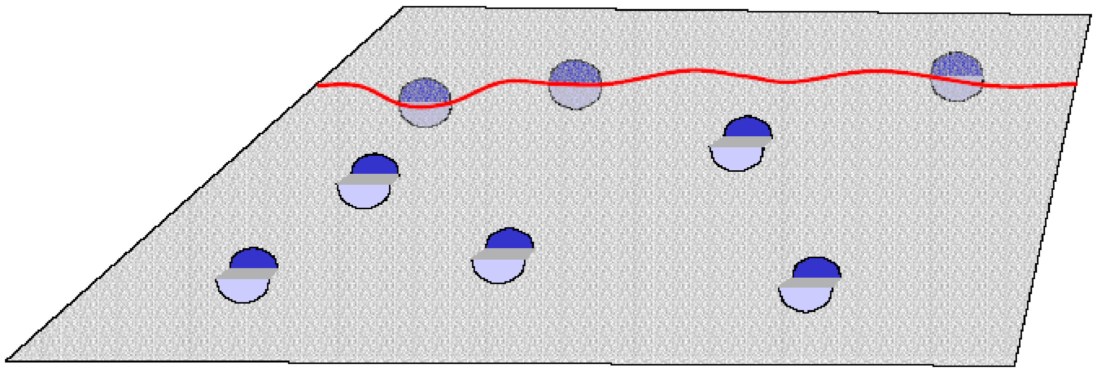
Defect populations act as obstacles for dislocations

There are different classes of obstacles …

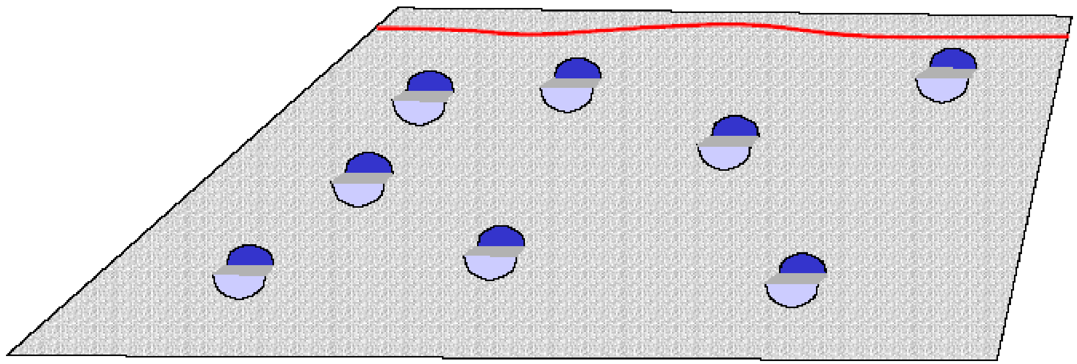
Shearable obstacles



Shearable obstacles

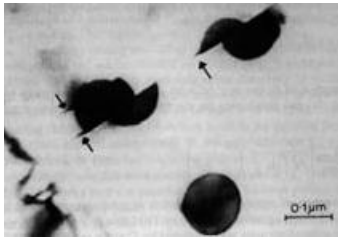


Shearable (weak) obstacles



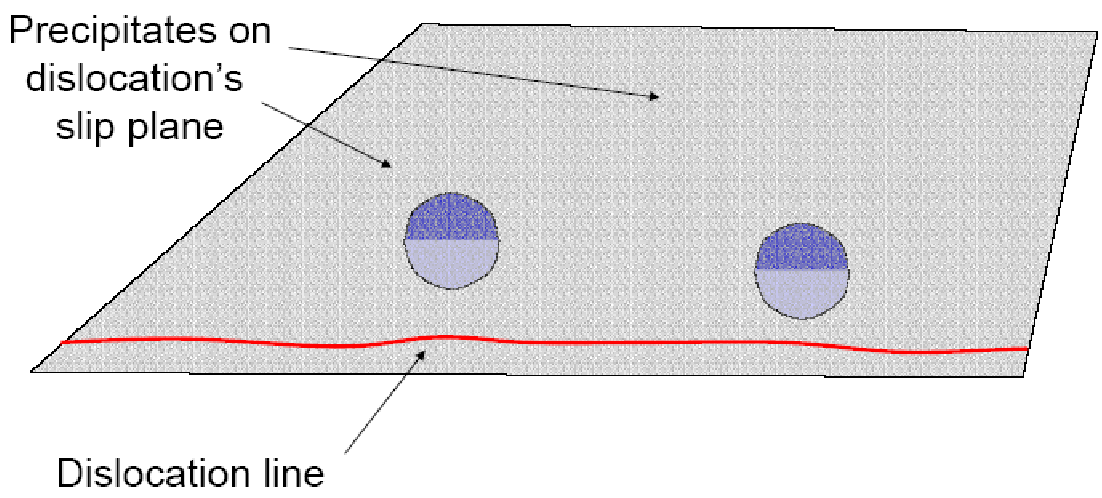
Dislocations can cut through the obstacle: the bigger, the more difficult to cut it through

Elastic, chemical, and phase stability effects also play a role to determine obstacle strength

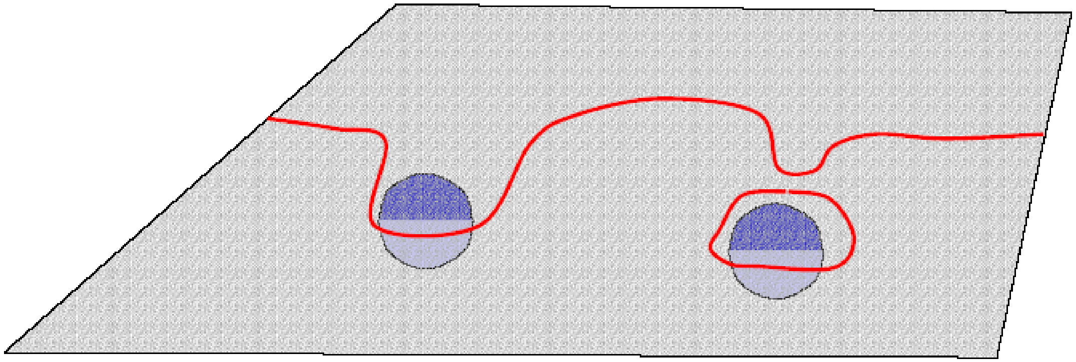


Increasing strain ‘chops up’ sheareable obstacles

Impenetrable obstacles

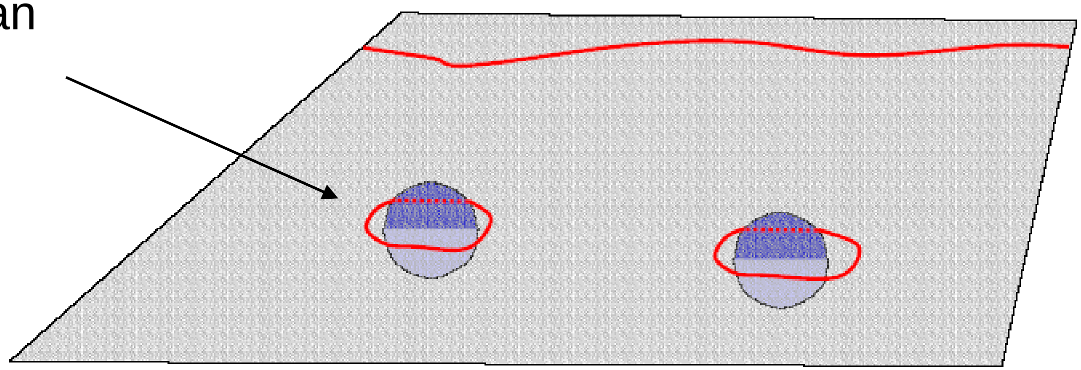


Impenetrable obstacles



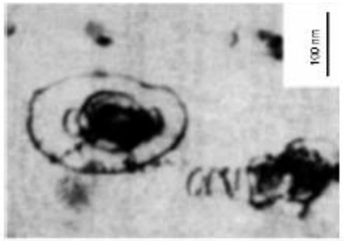
Impenetrable obstacles

Orowan loop



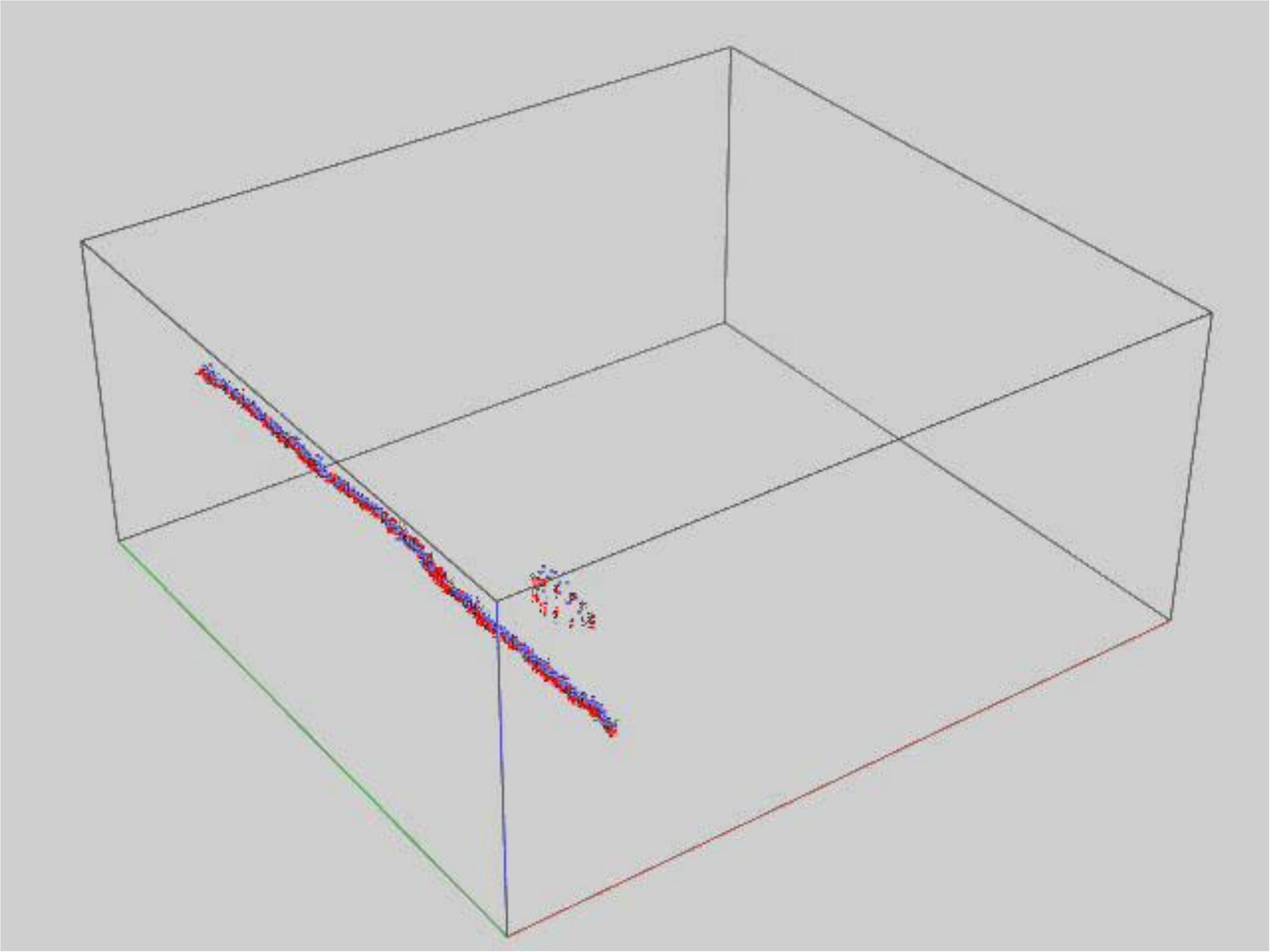
The bigger the spacing between obstacles, the easier for the dislocation to squeeze through the gaps.

Each 'bypass' event leaves a dislocation loop behind, narrowing the gaps and increasing hardening.



Prismatic loops are ***absorbable*** obstacles

This is a peculiar feature of irradiated materials



Edge dislocation interacting with SIA loop at 600 K

Take home messages

- Dislocations are defects that always exist in metals (and other materials) and make irreversible (plastic) deformation possible
  - ☞ *This is why metals are ductile: they can deform before breaking*

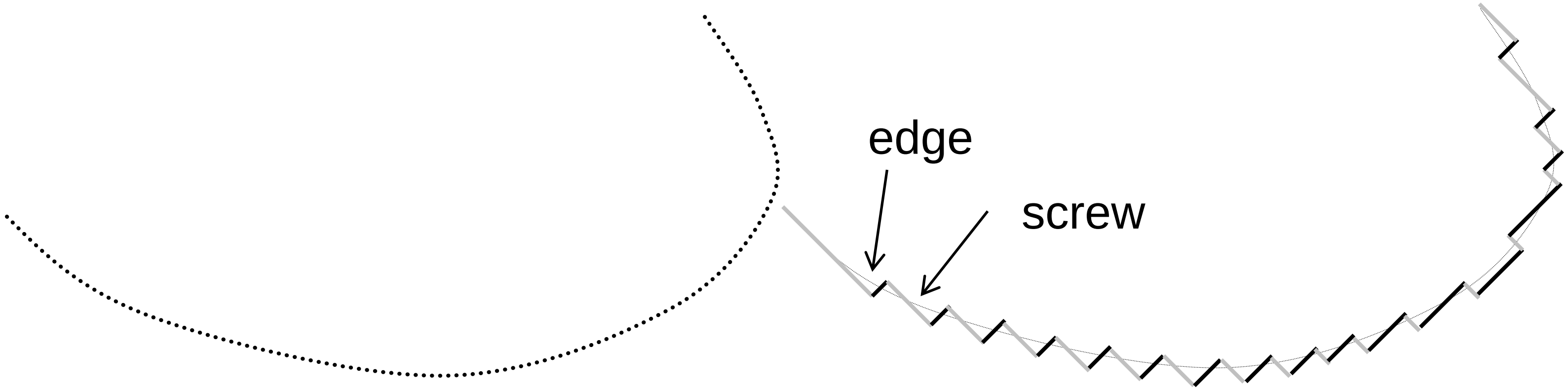
- The yield strength is the stress to be applied to make dislocations move in a material

- The presence of defects (loops, voids, precipitates, …) from irradiation makes dislocation glide more difficult → the yield strength increases, the material becomes <u>harder</u>

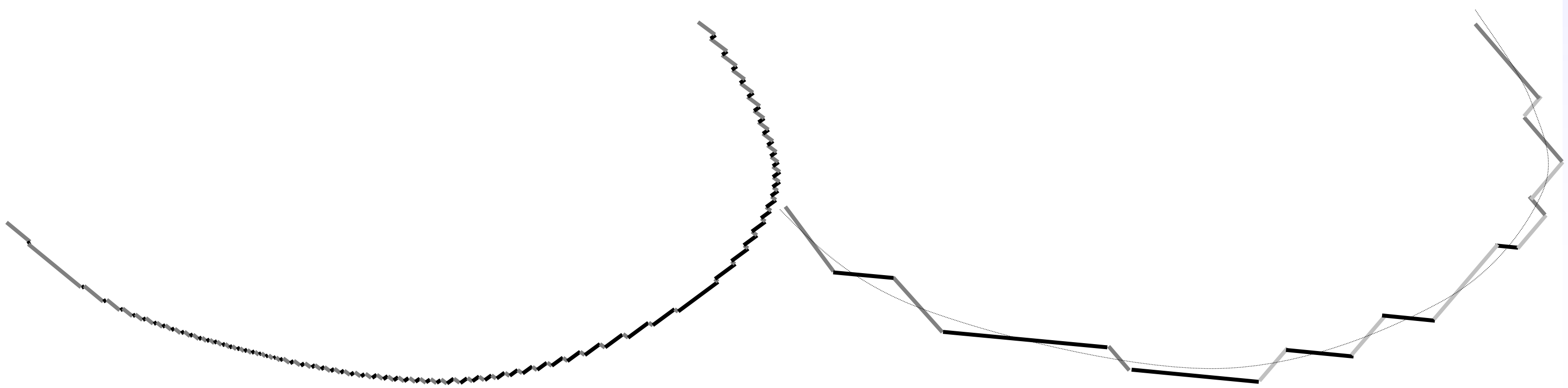
How do we model these processes?
Strengthening models

Dislocation dynamics: basics

In a DD model, a curved and continuum dislocation line is discretised as small segments, e.g. normal to each other (edge/screw)



To refine description, length of segments can be reduced (increase of computational time), or more than two species of segments, including slanted ones with mixed dislocation properties, can be included

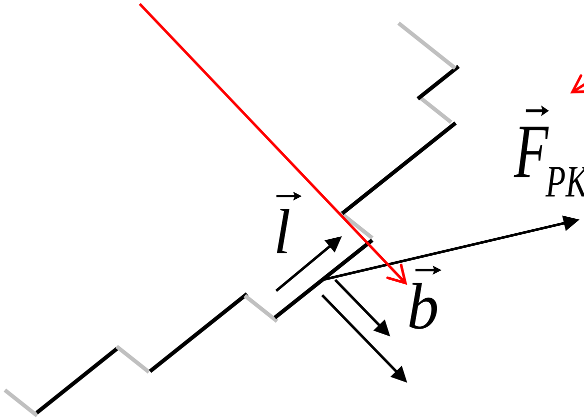


Dislocation dynamics: basics

Elements of simulation are dislocation segments that are displaced according to the forces acting on them

Burgers vector : normal to edge segments, parallel to screw segments

Peach-Koehler force: depends on applied & internal stress field



$$\vec{F}_{PK} = \vec{\tau}|b| = \left\{ \left[\left(\overline{\overline{\sigma}}_{app} + \overline{\overline{\sigma}}_{int} \right) \cdot \vec{b} \right] \wedge \vec{l} \right\}$$

$$\tau^* = \tau_{PK} + \tau_l + \tau_f$$

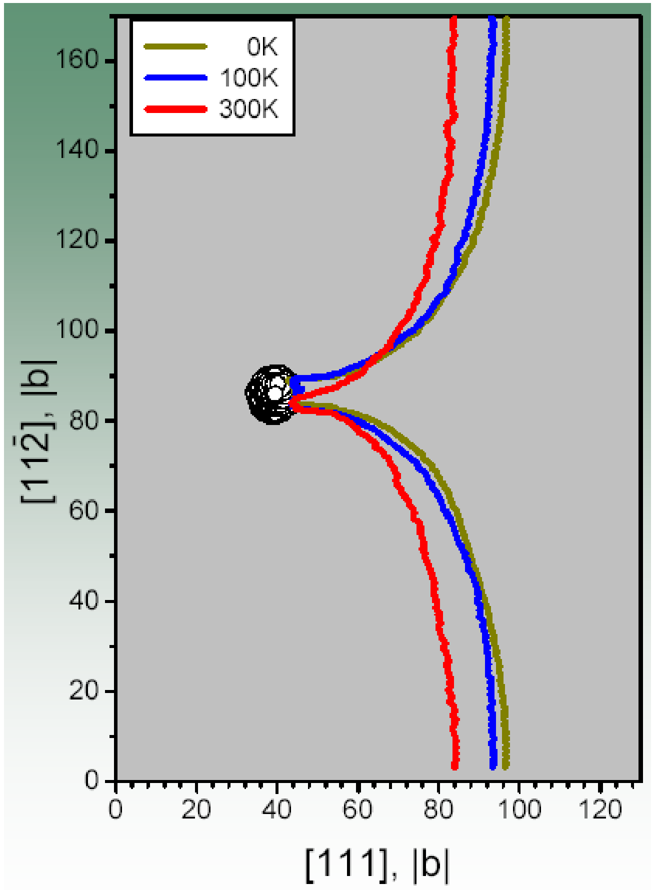
stress on the glide plane, sum of Peach-Koehler stress, τ_{PK}, line tension stress, τ_l, and lattice friction stress, τ_f

$$\tau^* \rightarrow v \rightarrow \Delta s$$

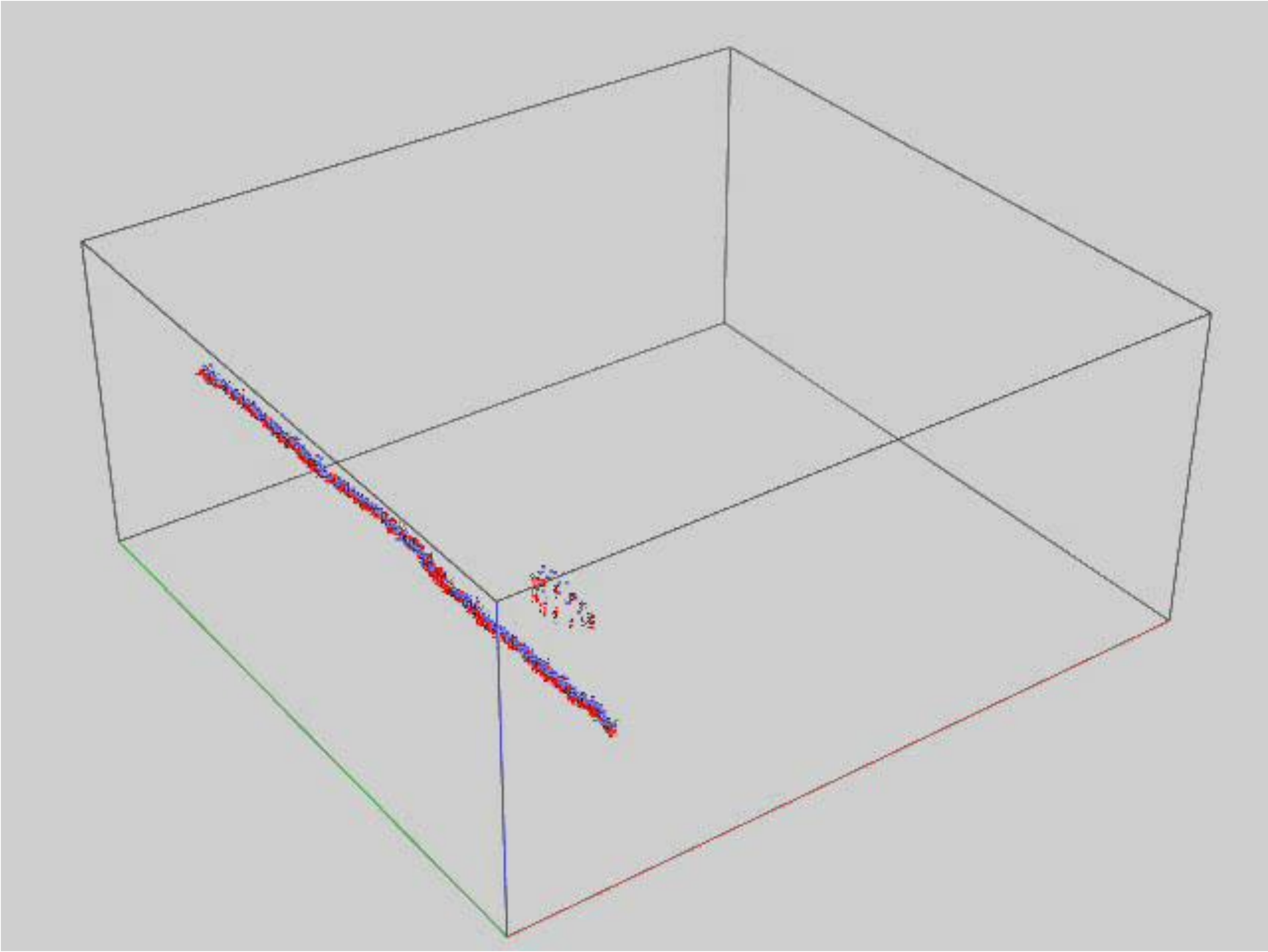
knowing τ^*, the velocity *v* of the segment is deduced and it its displacement Δs on the glide plane

Dislocation dynamics: basics

- Elasticity theory provides the background formulation
- Any mechanism that cannot be described in terms of elasticity must be introduced as <u>special local rule</u>
  - e.g. pinning of dislocation by precipitate or radiation defect)



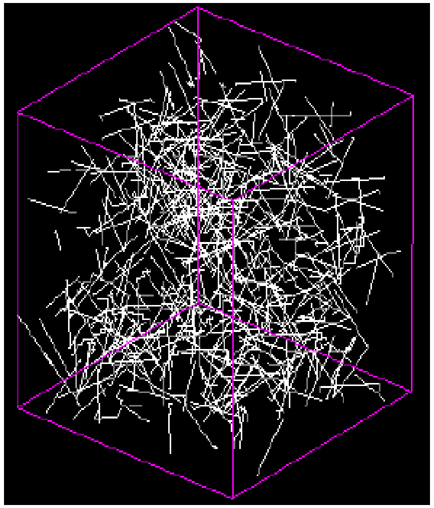
MD as tool to study dislocation/defect interaction



Edge dislocation interacting with SIA loop at 600 K

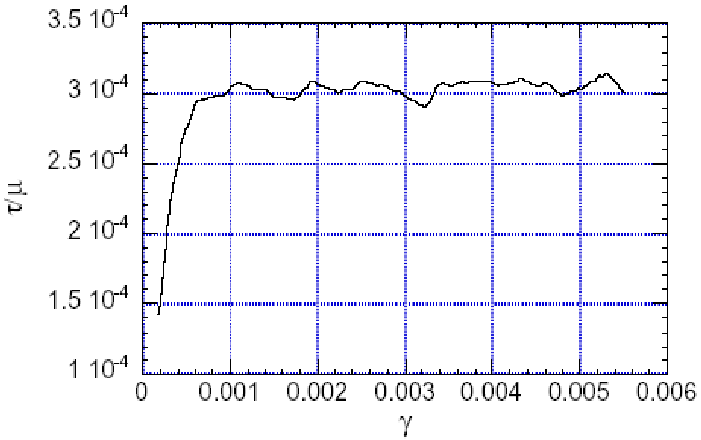
Dislocation Dynamics: pros & cons

- Complex dislocation line patterns can be reasonably well predicted



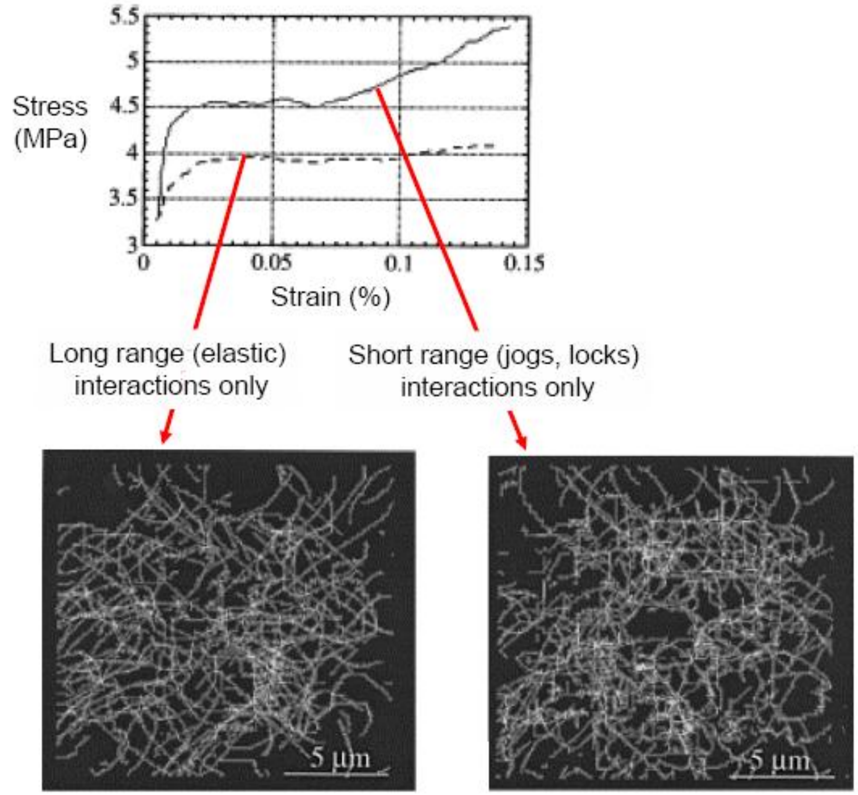
Deformation of a fcc single crystal (Cu) of linear dimension 15 µm. The stress tensile axis is [100], the imposed strain rate is 50 per second and the plastic strain reached at the end of this sequence is 0.1%.

- Stress-strain curve for single crystal of defined material can be acceptably predicted for small deformations



Dislocation Dynamics: pros & cons

- Possible to separate variables and identify mechanisms mainly responsible for given effects



- **Main limitations**
  - ***Computationally still very heavy***
  - ***No standardized approaches (such as in MD or KMC)***
  - ***Limited to single crystals***
  - ***No generalized method to introduce irradiation induced defects, <u>though progresses have been made</u>***

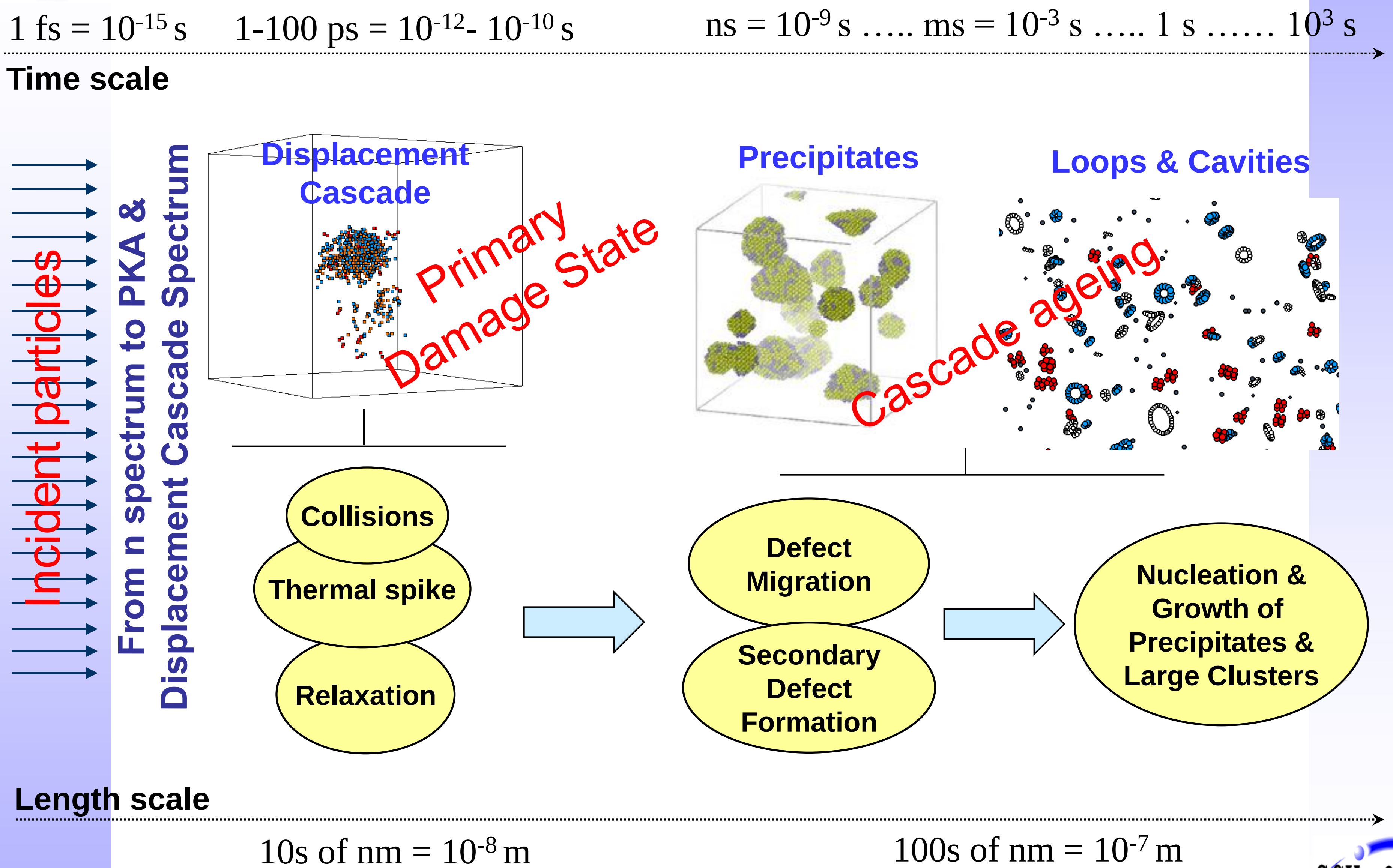
Other models at higher scales based on FE (not described here)

- Crystal plasticity
  - *Describes how aggregates (portions of polycrystals) behave mechanically, given crystalline constitutive laws*
  - *Most immediate way to transfer dislocation dynamics results to finite elements*
- Homogenisation
  - *Allows a single, average constitutive law to be obtained for an aggregate, to be used for larger scale calculations where grains and crystallography are not explicitly treated*
- Reference volume element scale calculations
  - *RVE is the biggest volume for which the homogenisation is possible without loosing too much information*
- Component scale calculations
  - *Those used for the design of components, as simple as possible*

Closure: Multiscale modelling

What does “multiscale” mean?

Irradiation effects are inherently a multiscale problem



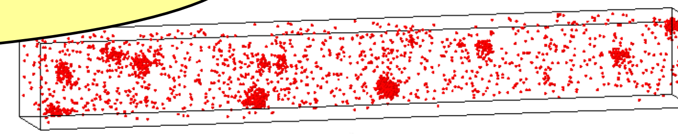
Irradiation effects are inherently a multiscale problem

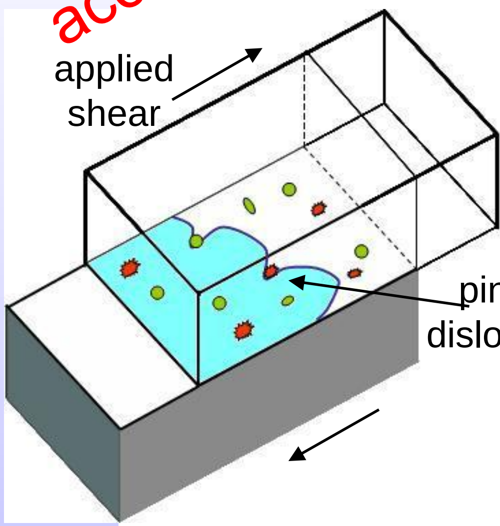
μs = 10^{-3} s.. Years = 10^{7} - 10^{9} s

Time scale

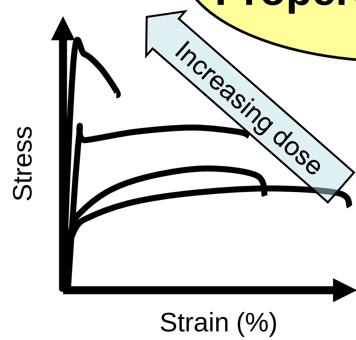
Cascade accumulation

Growing Concentration of Radiation Induced Defects while the Irradiation Proceeds



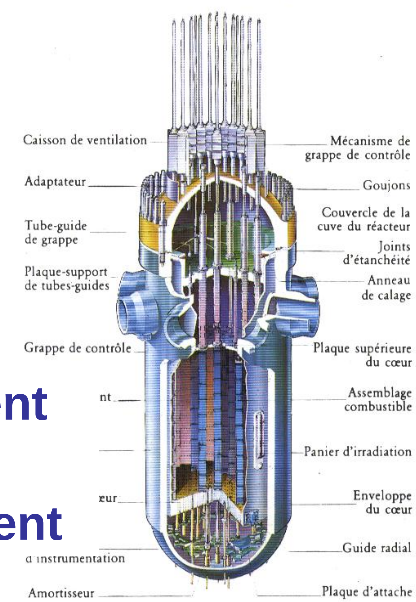


Mechanical Property Changes



Dislo/Defect Interaction
Yield Strength Increase
Loss of ductility

Component lifetime management



Length scale

10s of μm = 10^{-5} m cm = 10^{-2} m

What is multiscale modelling?

Use of the proper experimental examination and modelling technique to study each phenomenon of interest *at the correct scale*

Combination of experimental and modelling techniques to describe phenomena at different scales

Intensive and extensive use of not only advanced theory and experimental techniques, but also, and especially, computer simulation

Radiation effects studied by multiscale modelling

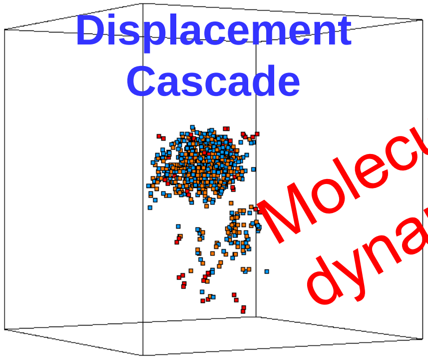
1 fs = 10^{-15} s 1-100 ps = 10^{-12}- 10^{-10} s ns = 10^{-9} s ….. ms = 10^{-3} s ….. 1 s …… 10^{3} s

Time scale

Incident particles

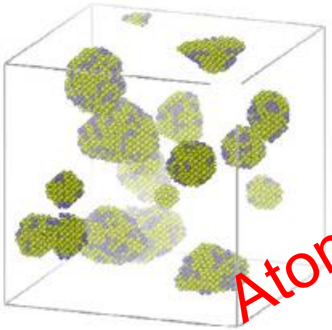
From n spectrum to PKA &
Displacement Cascade Spectrum

Displacement Cascade

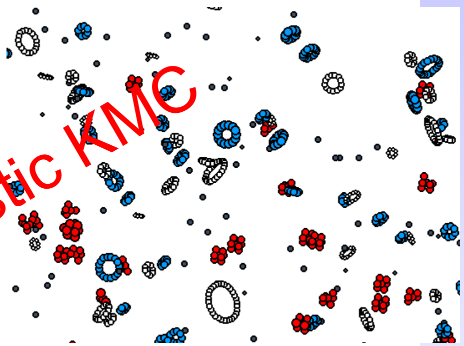


Molecular dynamics

Precipitates



Loops & Cavities



Atomistic KMC

- Collisions
- Thermal spike
- Relaxation

→

- Defect Migration
- Secondary Defect Formation

→

- Nucleation & Growth of Precipitates & Large Clusters

Length scale

10s of nm = 10^{-8} m 100s of nm = 10^{-7} m

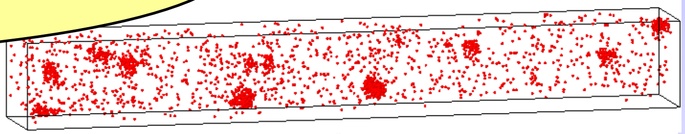
Radiation effects studied by multiscale modelling

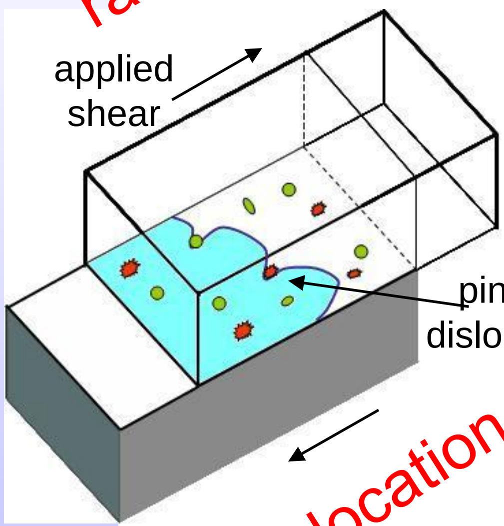
μs = 10^{-3} s…………………………………… Years = 10^7 - 10^9 s

Time scale

Object KMC, rate theory

Growing Concentration of Radiation Induced Defects while the Irradiation Proceeds



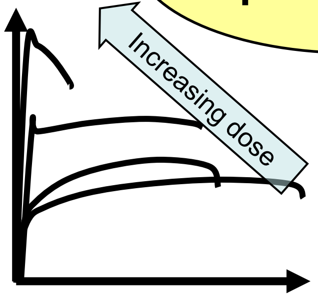


Mechanical Property Changes

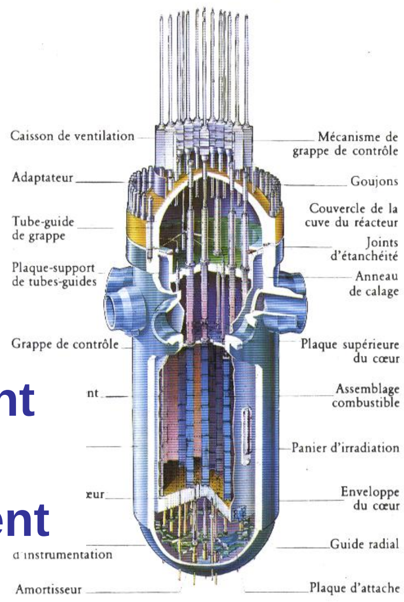
Dislocation dynamics

Bridge to crystal plasticity

Dislo/Defect Interaction
Yield Strength Increase
Loss of ductility



Component lifetime management



Length scale

10s of μm = 10^{-5} m cm = 10^{-2} m

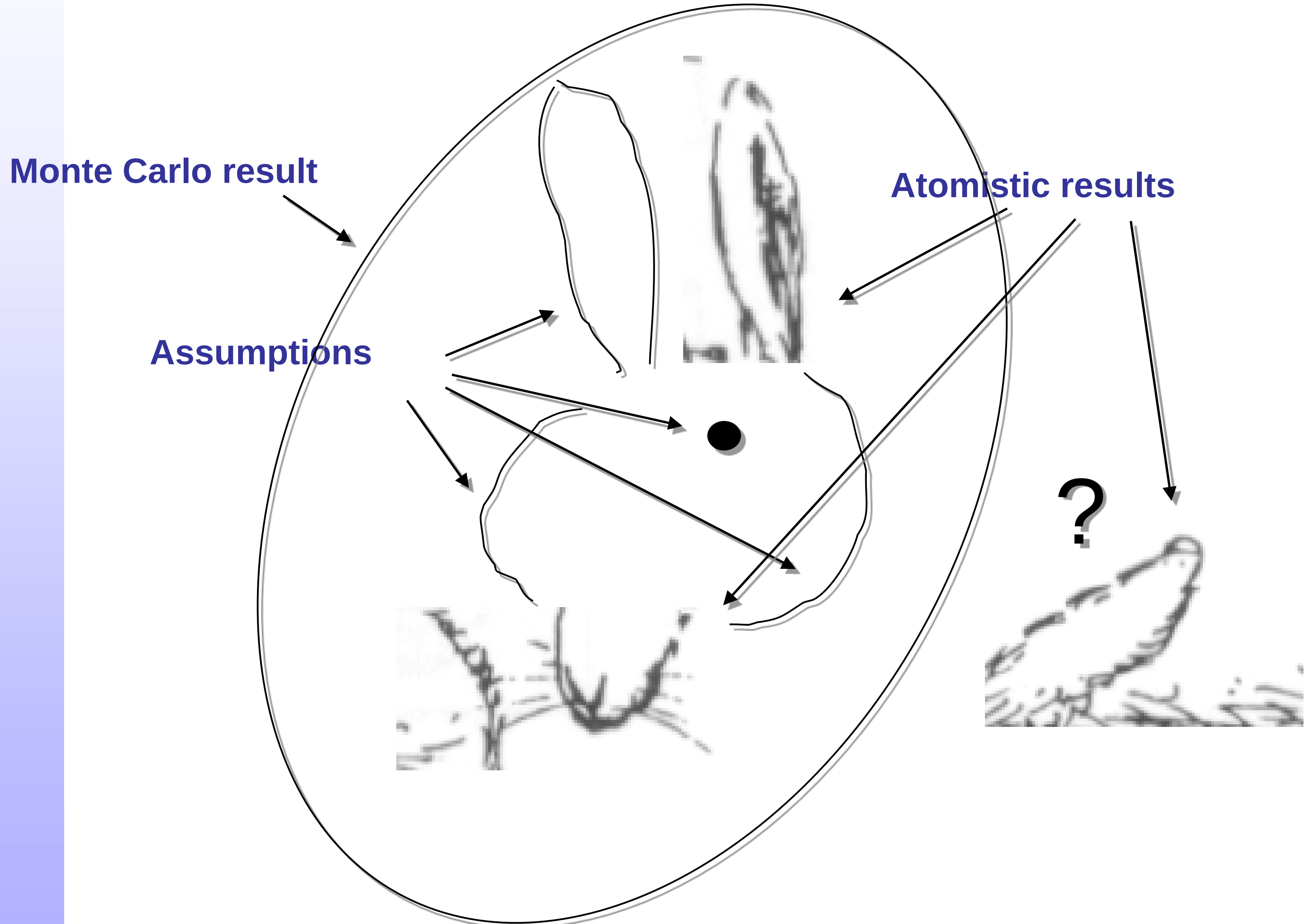
Main open issues

- Atomistic simulations in multi-component systems
  - *Possible only with DFT, within size limits*
  - *Interatomic potentials still challenging*
  - *AKMC models possible by paying prices*
- Treat in one model microchemical and nanostructural evolution
  - *Difficult to treat self-interstitials in AKMC models*
  - *Difficult to treat chemical complexity in OKMC or RT models*
- Bridge between MD and DD
  - *Progresses made recently towards a standard approach to transfer information*
  - *Hampered by non unified standard for DD approaches*
- Bridge between discrete and continuum models
  - *Especially from DD to crystal plasticity*

<u>Biggest open issue</u>: the comparison between models and experiments is not easy (in the case of radiation effects at least) …

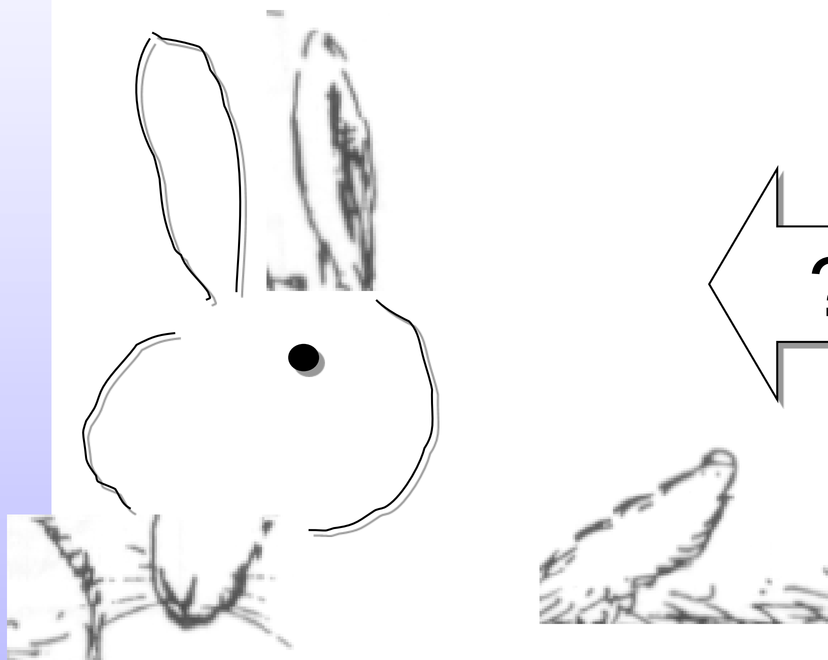
“Experimental validation”

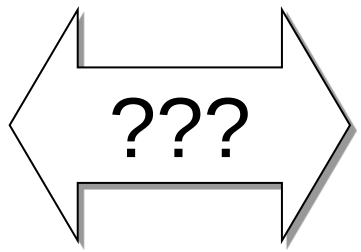
Build a picture: Simulation results

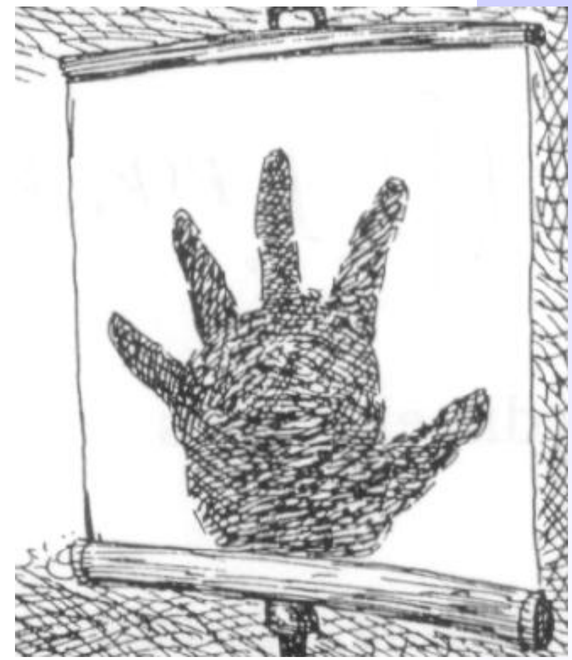


“Experimental validation”

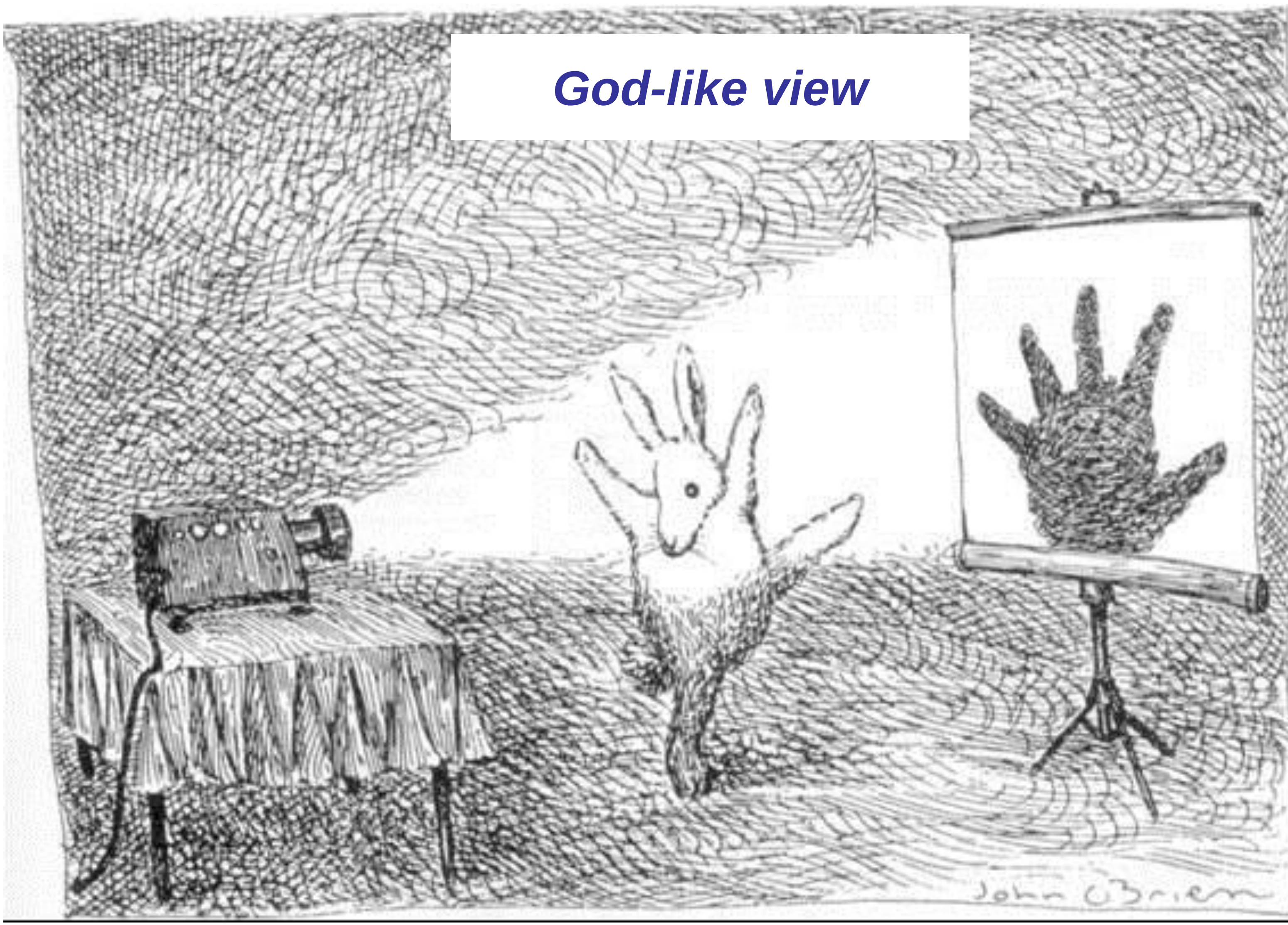
Build a picture: Experimental result







“Experimental validation”



The End