The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2137-23

Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and Basic Understanding of Radiation Damage Mechanisms in Materials

12 - 23 April 2010

Multiscale Modelling in the Nuclear Environment

M. Samaras

Paul Scherrer Institut
Villigen
Switzerland

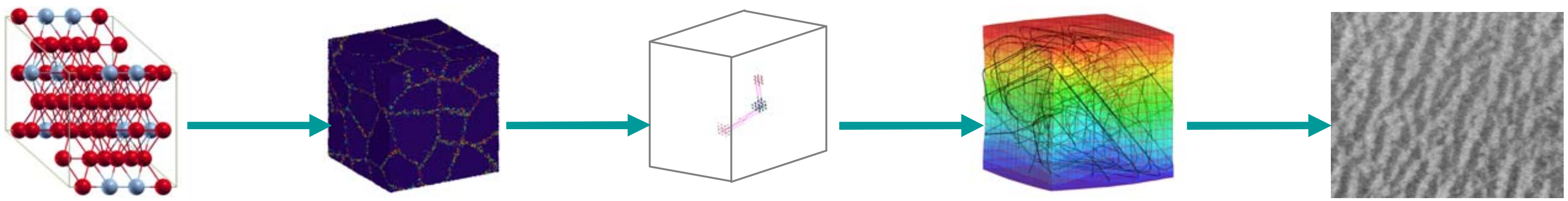
Multiscale Modelling in the Nuclear Environment

Dr Maria Samaras

High Temperature Materials Group
Laboratory of Nuclear Materials
http://lnm.web.psi.ch/ssi/lnm_projects_mod.html

Nuclear Energy and Safety Department
Paul Scherrer Institute

PAUL SCHERRER INSTITUT
PSI

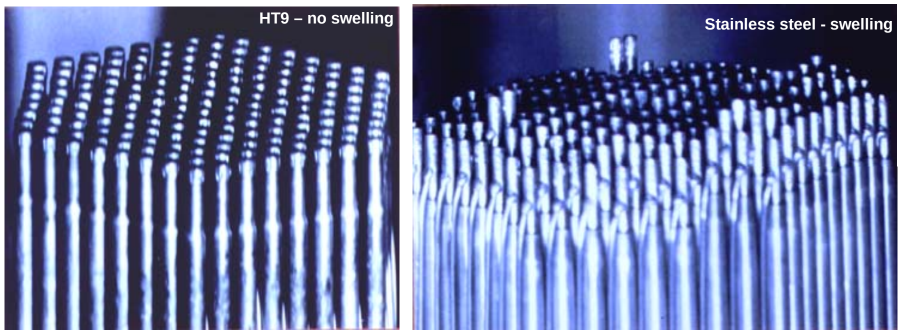


Material Issues

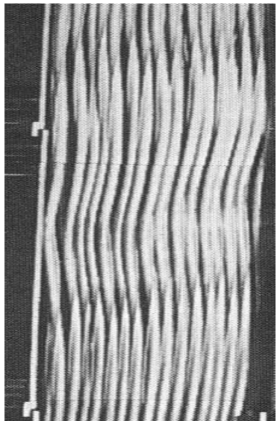
Life Determining Issues

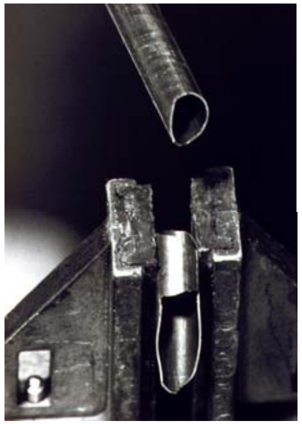
- Strength
- Embrittlement (fracture)
- Swelling-creep
- Corrosion


Corrosion

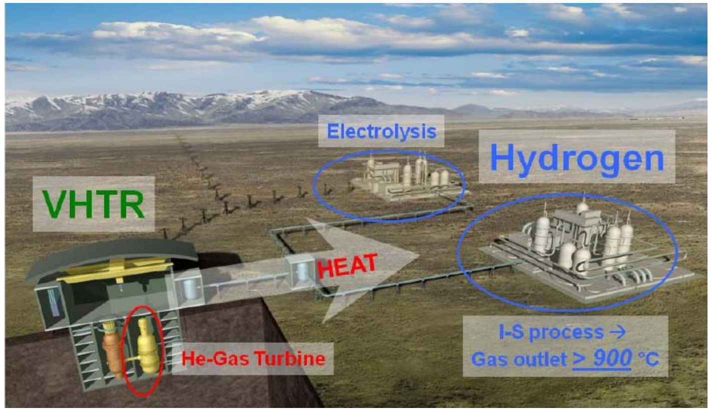


Garner


Swelling-creep: Garner


Fracture: Porter

Gen IV NP



Life Determining Issues

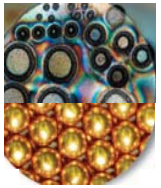
Embrittlement (fracture)

High temperature corrosion

Swelling-creep

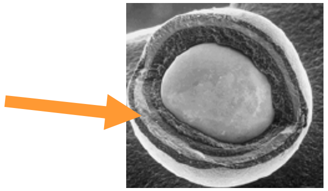
Fuels:

Horvath et al 2004

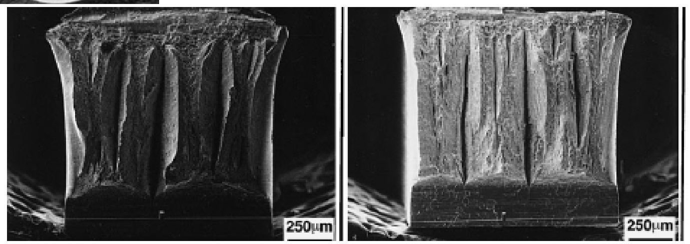


Butler 2004

Claddings:



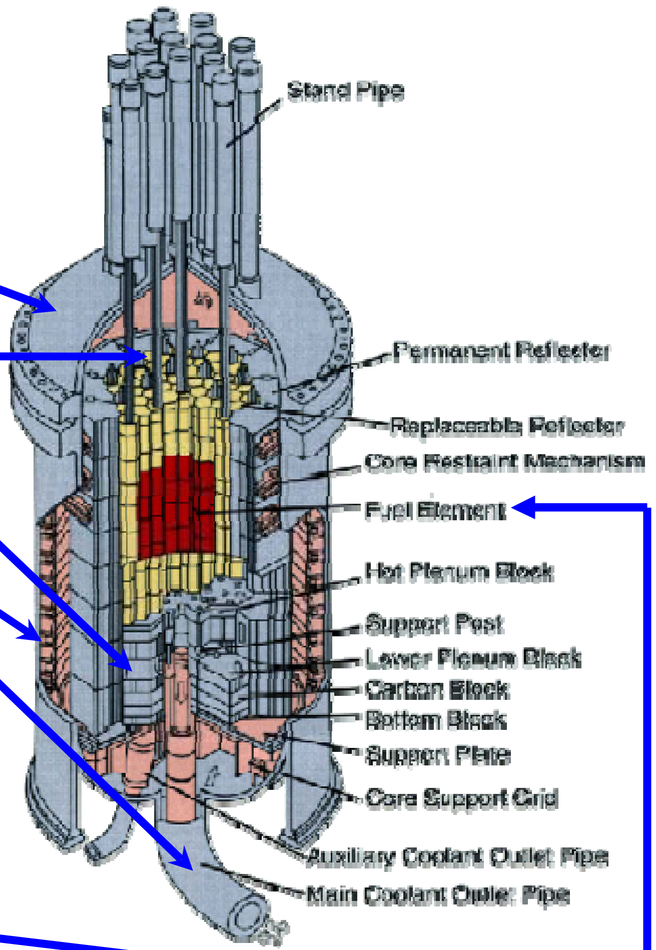
Structural Materials:



Kuwabara 1998

Possible Materials Selection (VHTR)

Tomorrow
Fe- x% Cr alloys
SiC/SiC
Oxide Dispersoid Strengthened
UO2



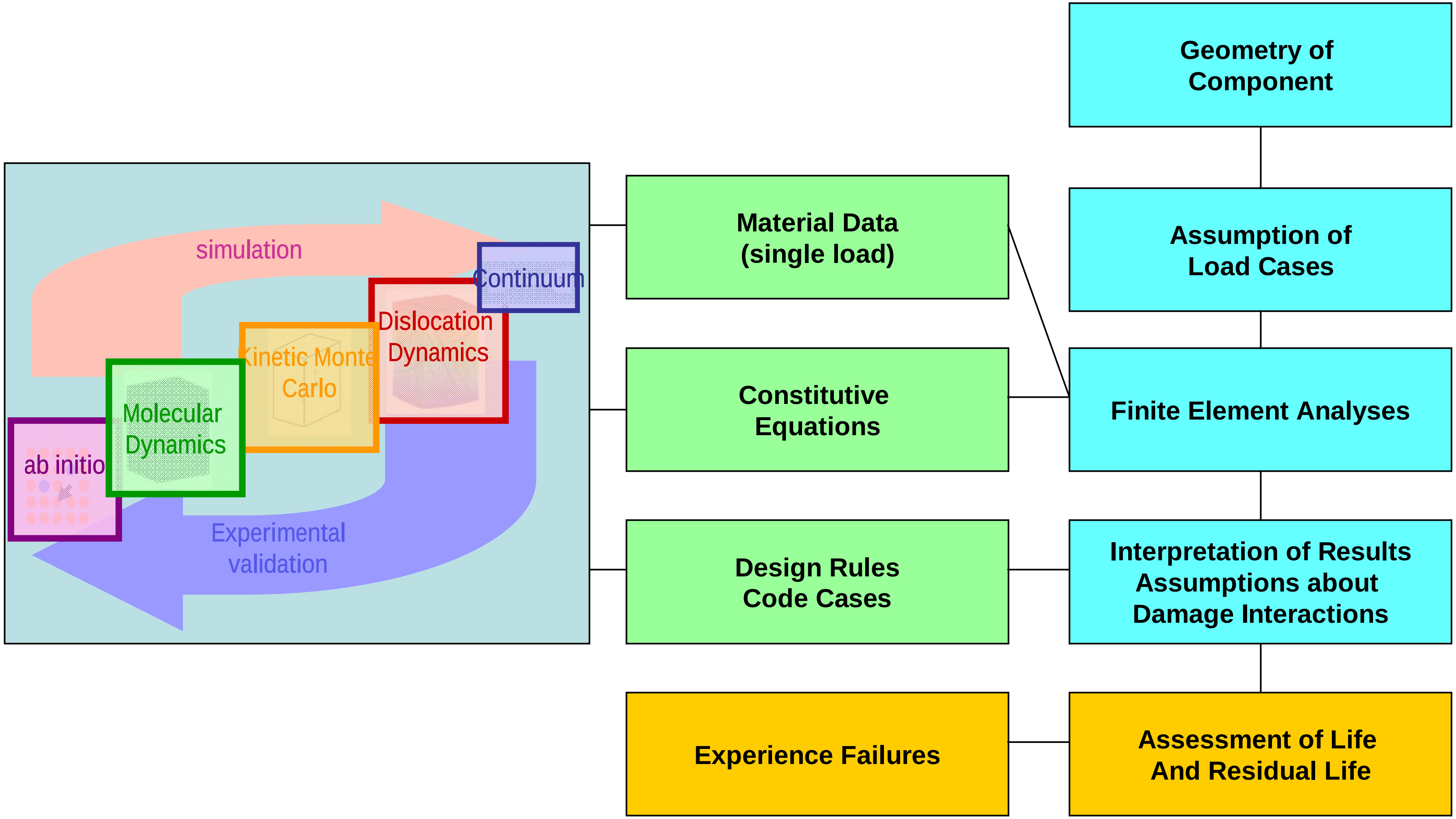
Gen IV reactors

	PWR	SCWR	VHTR	SFR	LFR	GFR	MSR
Coolant inlet temp (°C)	290	290	400-600	370	600	450	700
Coolant outlet temp (°C)	320	500	950	550	800	850	1.000
Pressure (MPa)	16	25	7	0.1	0.1	7	0.1
Max. rad.dose (dpa)	100	10-70	1-10	200	200	200	200
coolant	water	water	Helium	Liqu. sodium	Liqu. Pb/PbBi	He/CO2 supercooled	Molten salt
Critical components	RPV, internals, cladding	RPV, internals, cladding	RPV, core, IHX, heat coupling	cladding	cladding	Fuel/core	core
metals	Ferritic steels, Zircaloy	Ferritic steels, Ni-base,ODS	F-M steels, Ni-base, ODS	F-M steels, ODS	F-M steels ODS	F-M steels (RPV)	Ni-Base
ceramics			Graphite, C/C, SiCf/SiC, SiC			SiC, TiC Other ceramics	graphite
Main damage mechanisms	corrosion, embrittl. LCF	corrosion, embrittl. LCF	HT-corr. creep, LCF	corrosion, creep (th/irrad), LCF, irrad.	corrosion, creep (th/irrad), LCF, irrad.	corrosion, creep (th/irrad), LCF, irrad.	corrosion, creep (th/irrad), LCF, irrad.
Design rules	RCC-MR ASME	RCC-MR ASME to be mod.	RCC-MR ASME (modif. in progress)	RCC-MR, ASME (to be modified/ developed)	to be developed	to be developed	to be developed

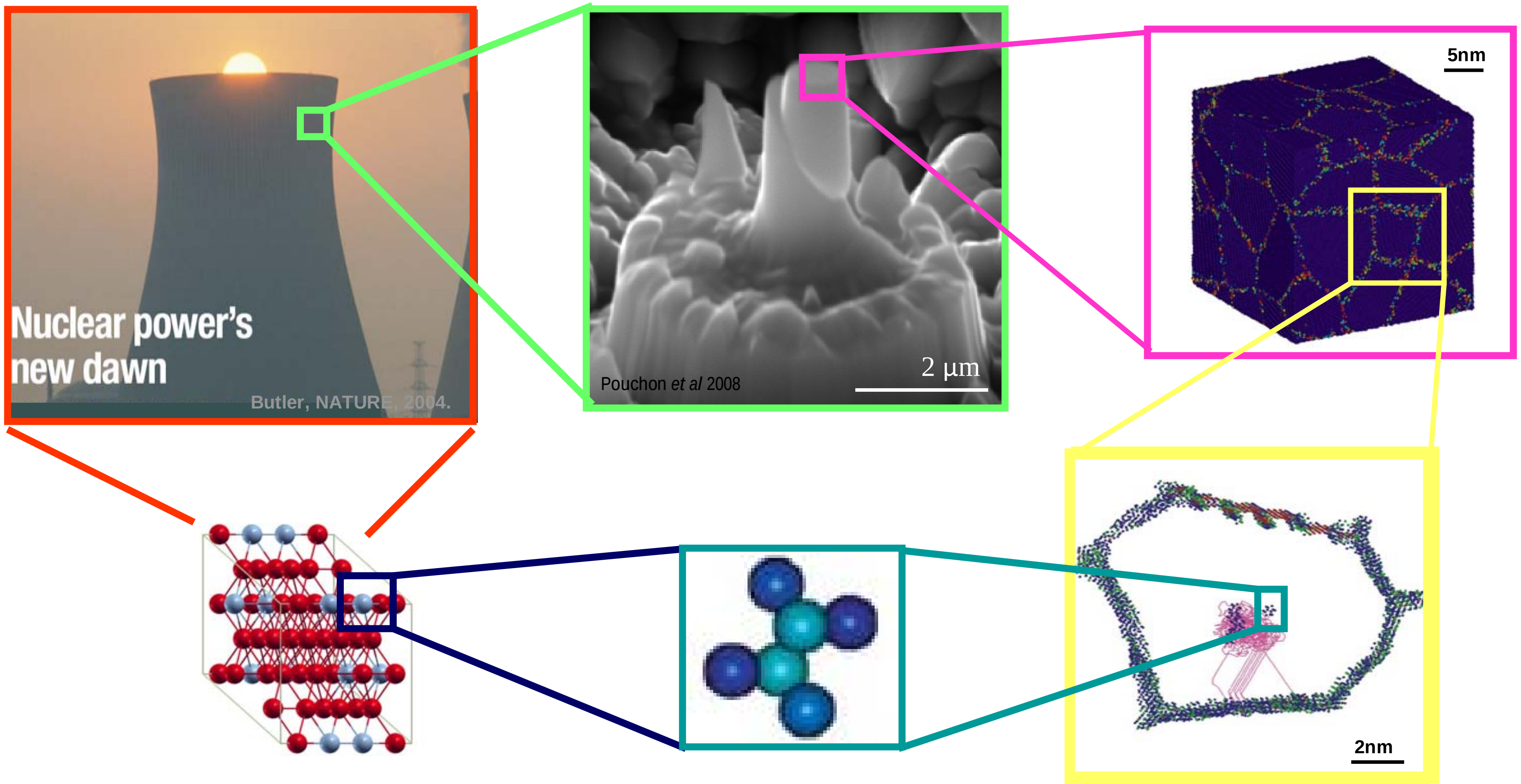
Technical problem and related physical effects

Physical Phenomena	Technical Relevance
Condensation and diffusion	Phase Diagram, time-temperature-phase diagram, microstructural stability,
Dislocation – obstacle interactions	Effects of precipitates, dispersoids and point defect clusters on yield strength, stress rupture stress, and creep strength
Dislocation-dislocation interactions	Dislocation arrangements, Yield stress (shear stress), fatigue, creep-fatigue
Point defect – defect and boundary interactions	Effects of irradiation on existing voids at boundaries (void growth, void shrinkage)
(Grain) boundary diffusion	creep damage, segregation, toughness/embrittlement
Decohesion of lattice	Crack formation and rupture
Surface phase formation	Oxidation and Corrosion
Effect of He	Bubble formation, swelling cracking, embrittlement
Fission gas release	Fission gas transport, swelling, fatigue, cracking
Actinide and oxygen redistribution	Thermo-chemical stability
Effect of Minor actinide	Stability, phase diagram, waste disposal

Modelling Schemes



Small Sample Condition Monitoring



Study small samples to understand much larger components

Outline

Fundamentals- Structure

Hardening

Creep

IASCC – Sink Strength

Voids, Swelling, Cracking

Corrosion

Coarse Graining

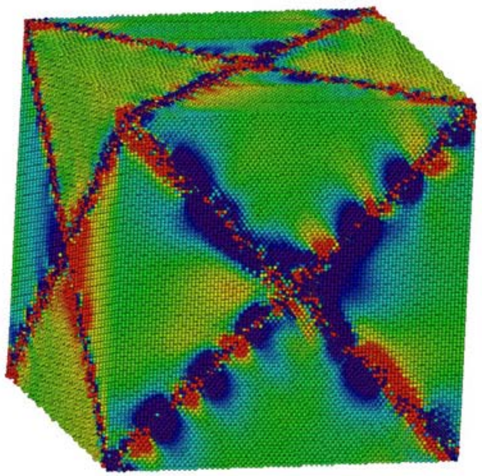
Lifetime Predictions

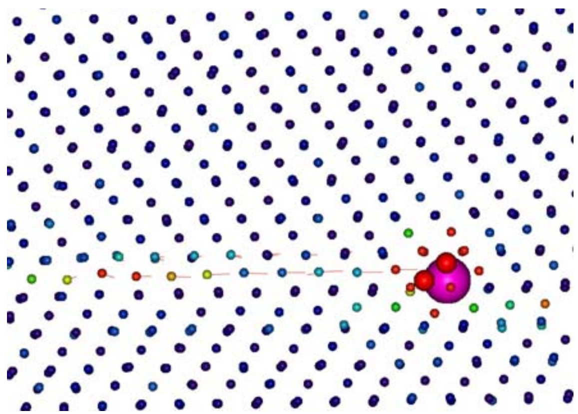
Structure

Phase Stability; Clustering and Segregation

– binary Fe-Cr alloys

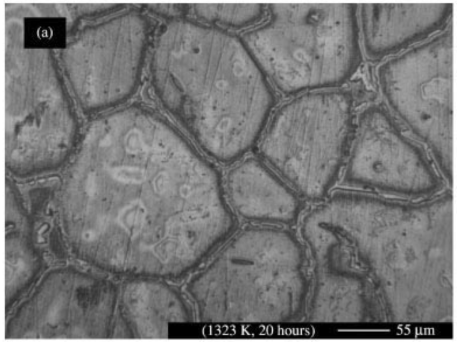
Grain Boundary structure/packing



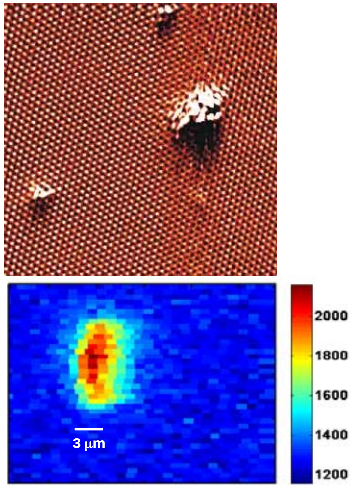


Types of Defects

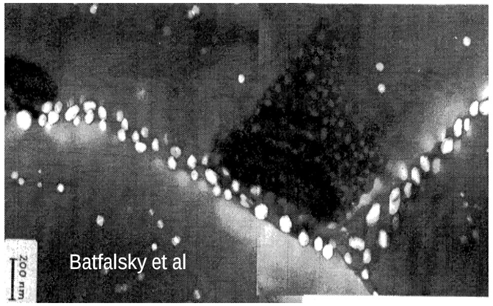
Types of defects present in a material



Grain boundaries

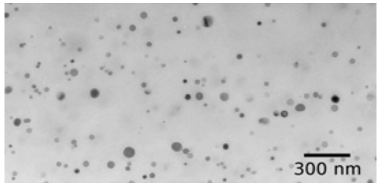


clusters

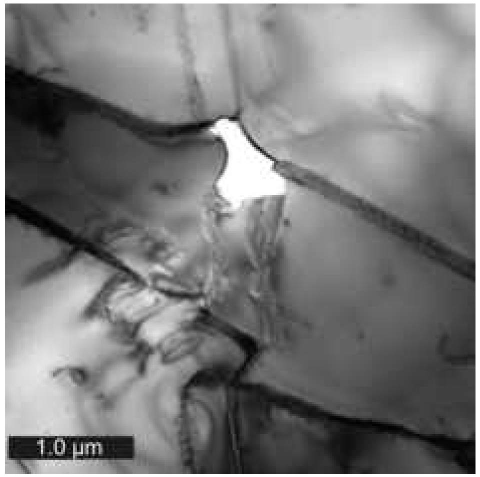


bubbles

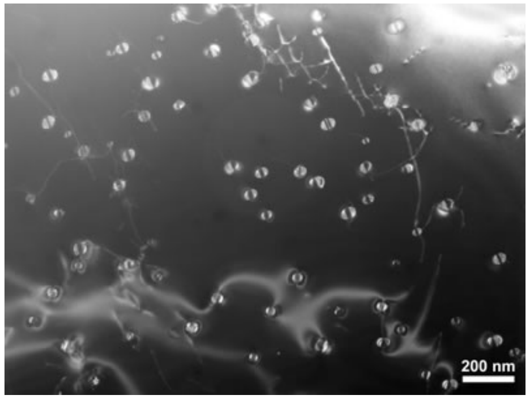
dislocations



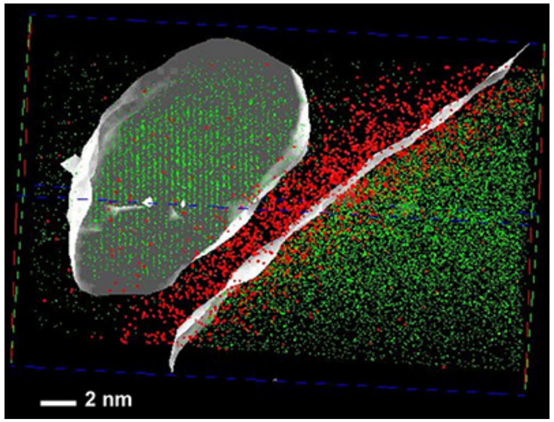
ODS



voids



loops



segregation

Experimental Visualisation Techniques

Microscope techniques- TEM, SEM

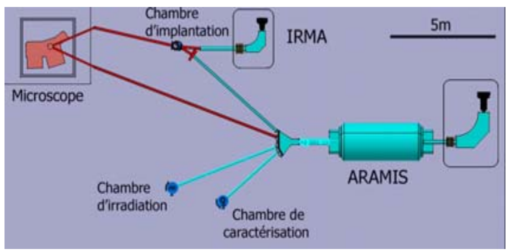
Atom Probe

Positron Annihilation

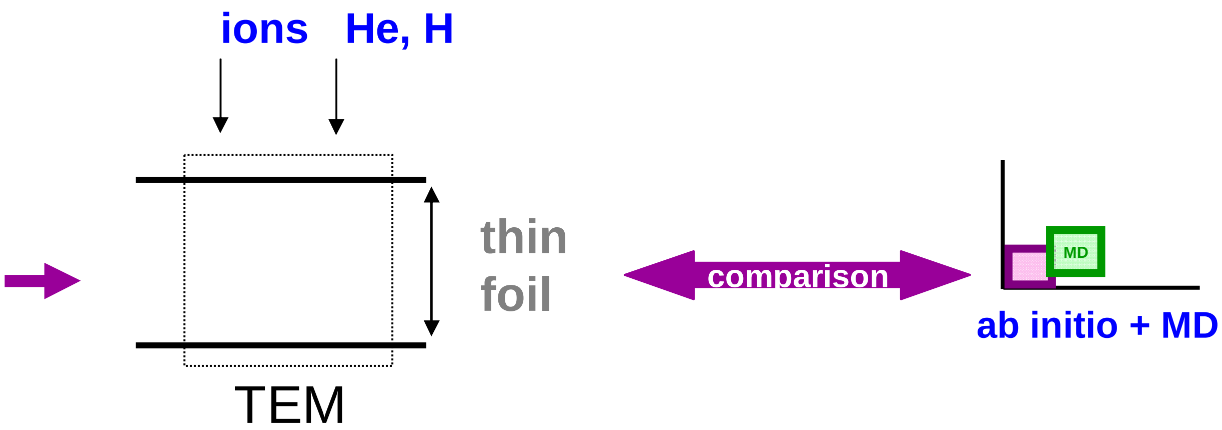
Synchrotron Irradation techniques

JANNUS Facility to study

- **clusters, segregation**
- **loops**
- **bubbles, voids**
- **precipitates**



Jannus facilty, CEA



Structure: Types of Defects

Interaction of defects with the matrix and one-another affects the properties of the material

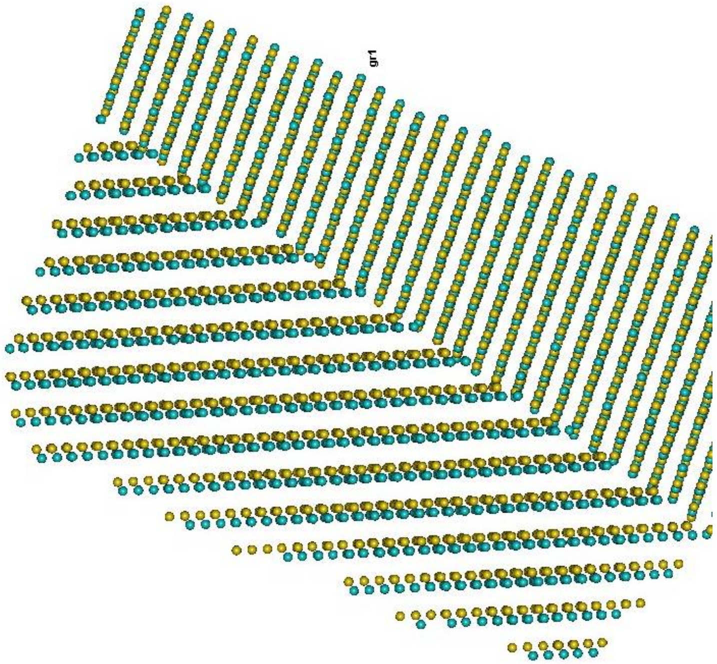
Clusters- lead to segregation
Voids/bubbles can grow and lead to cracking

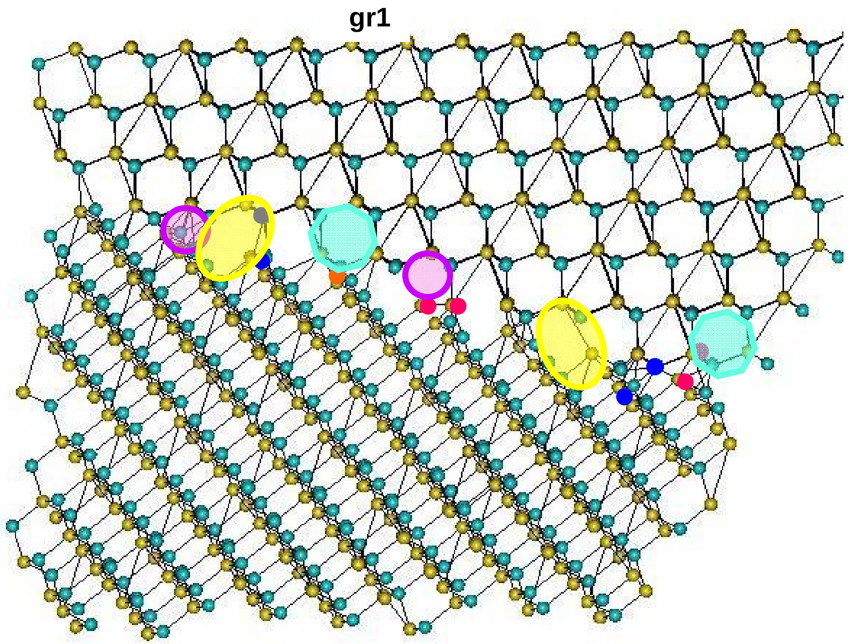
Dislocations act as sinks to defects
Defect- dislocation interactions
Defect- GB interaction

Defects can be introduced to change the material properties in order to optimise them for a particular use

GB structure: nc β-SiC (MD)

GB structrure- ordered, disordered, amporphous?





Ab initio **bi-crystal calculations have found:**

Wrong-bonds lead to formation of 5-member and 7-member rings

Hardening

Simplest steel: inclusion of carbon into the matrix

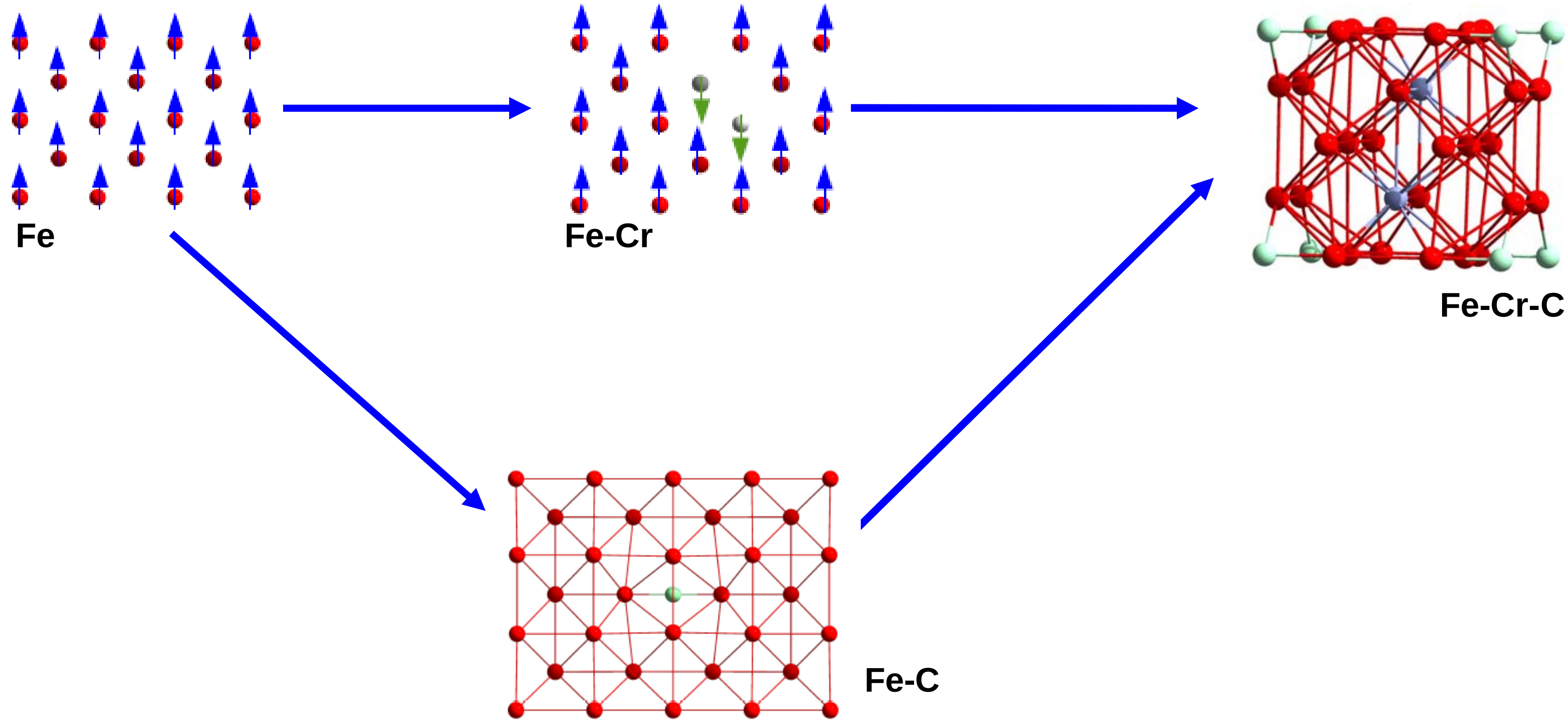
Dispersoid strengthening: dislocation-particle interaction

PSB Fatigue: dislocation-dislocation interactions

Grain Size effects (Wednesday 14th)

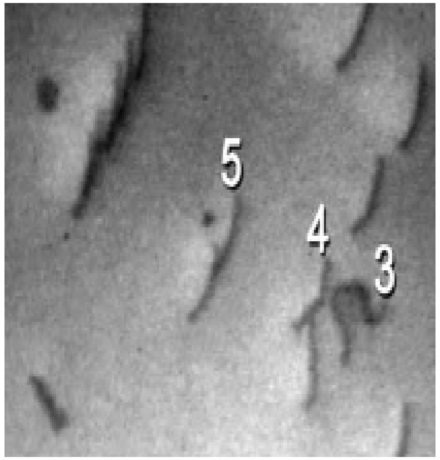
From binary Fe-alloys to steel

DFT study of Fe-Cr, Fe-C, Fe-Cr-C

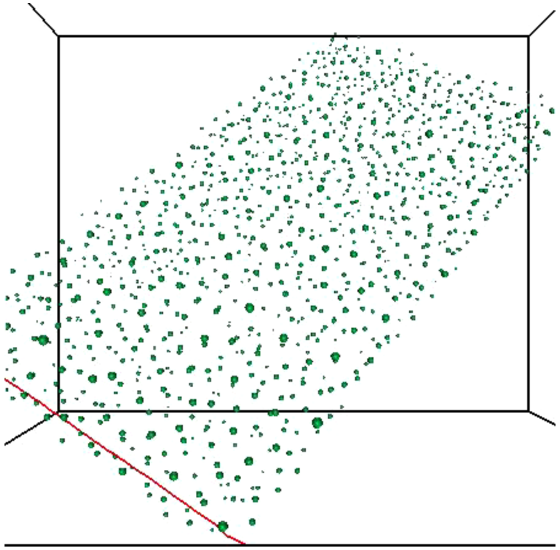


ODS Strengthening

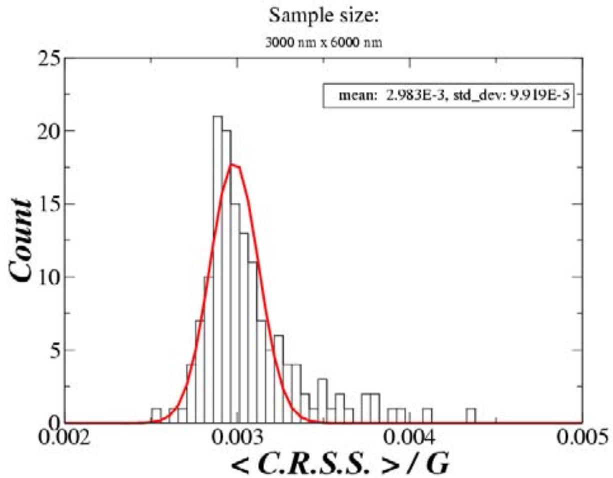
Dislocation-dispersoid interaction in Fe- 3D DDD



Zinkle et al 2004



3μm



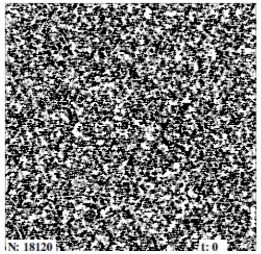
PM2000 single dislocation CRSS~ 240MPa
Experimental value CRSS~ 265MPa

ODS particle is the main contributor to critical resolve shear stress

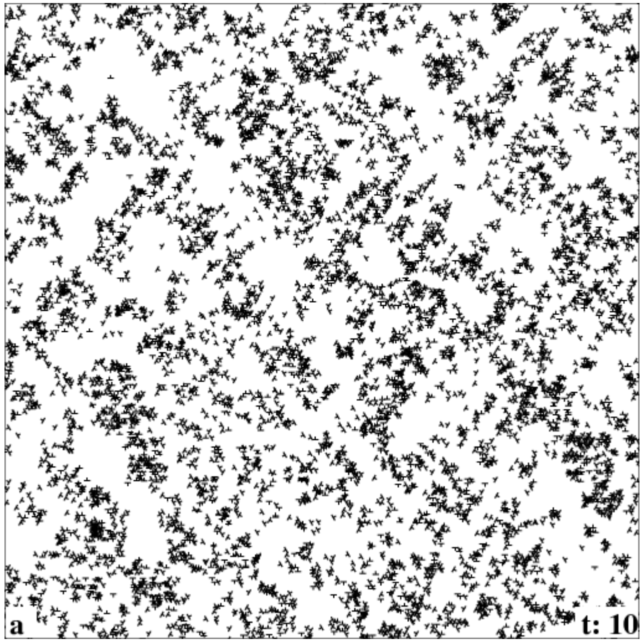
Fatigued Dislocation Systems

2D DD dislocation-dislocation interactions

Original structure

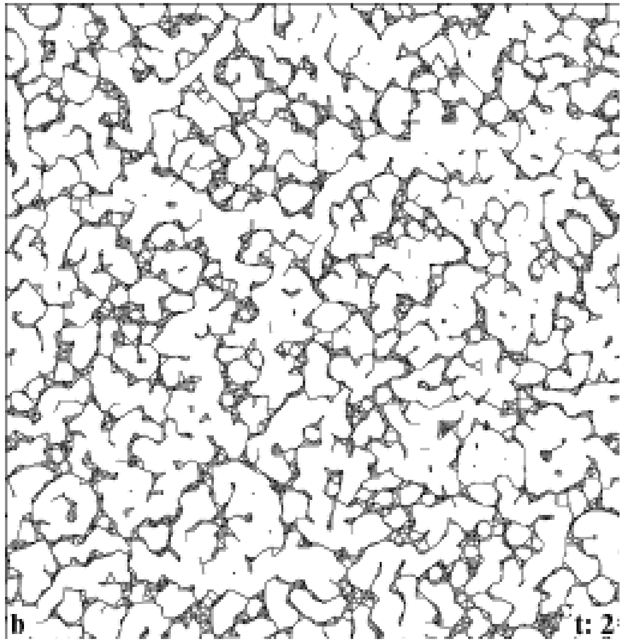


No climb



Fractal patterning

Climb

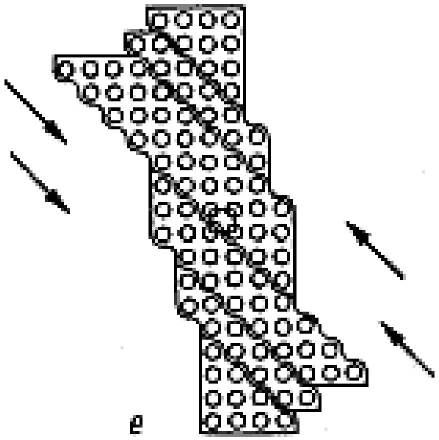


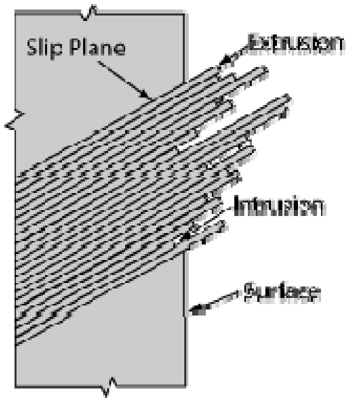
Cellular patterning

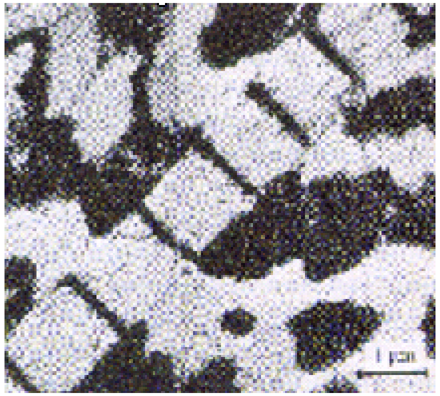
Bako et al

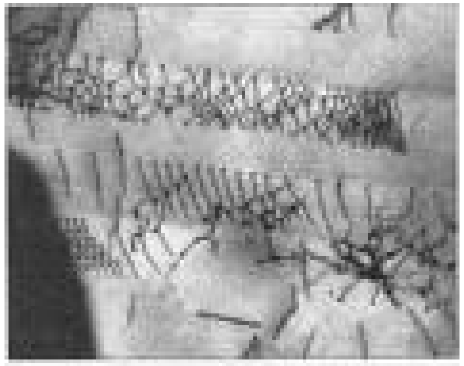
PSB Fatigue (DD)

First step- Dislocation Pile-up



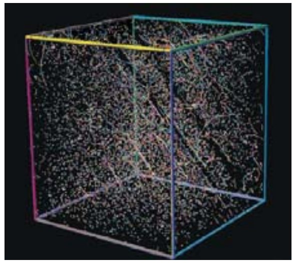






Metal becomes harder and stronger through plastic deformation

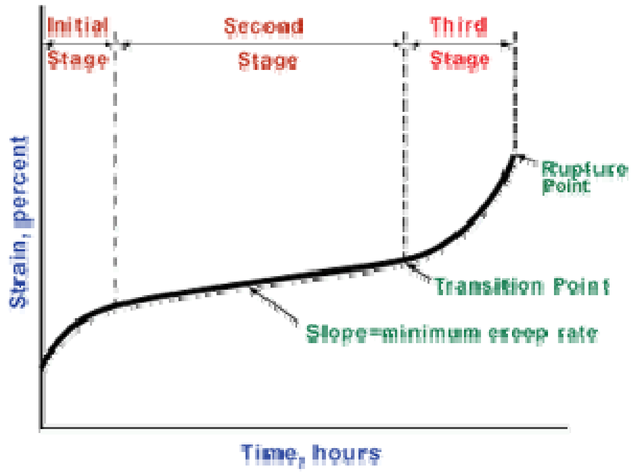
The more dislocations, the more they will interact and become pinned or tangled leading to pile-up.



3D simulations until now have not been able to reproduce PSB

2D single slip nonlinear effects may lead to the instability (fcc Groma et al)

Creep



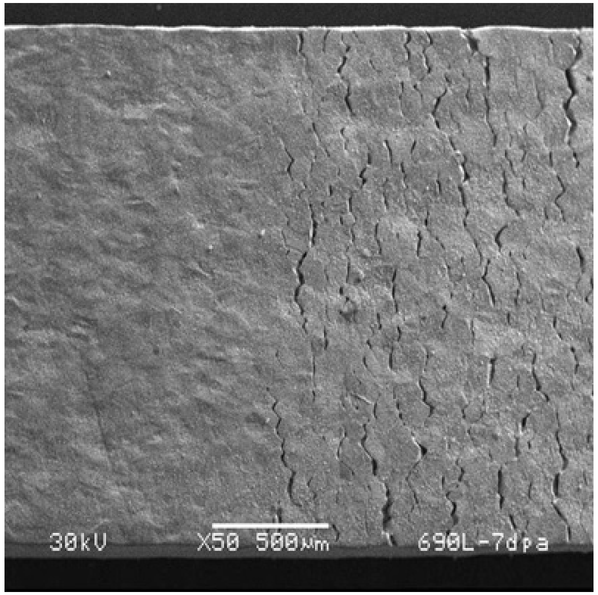
Time-dependent material deformation under applied load that is below its yield strength.

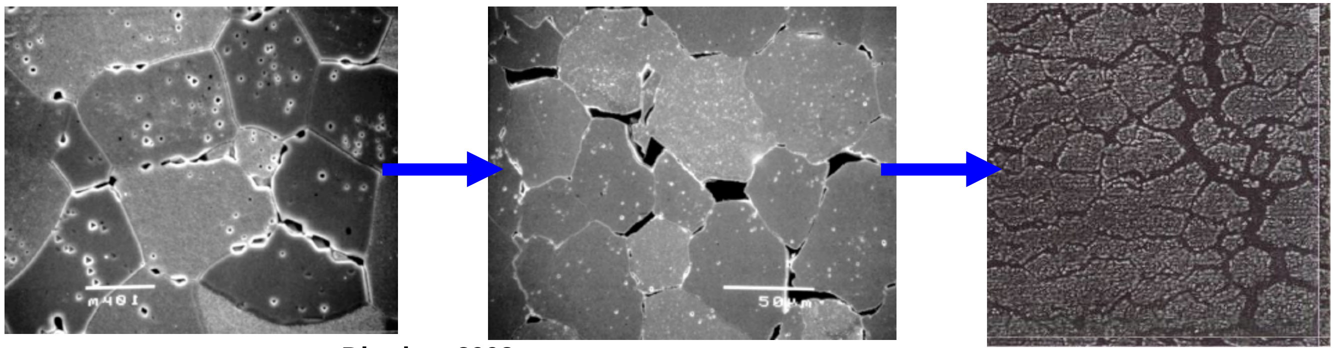
Creep terminates in rupture

Often occurs at elevated temperature, but some materials creep at room temperature.

IASCC

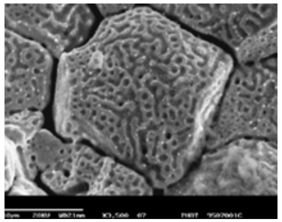
Radiation Damage (throughout the next 2 weeks)
sink strength (MD)



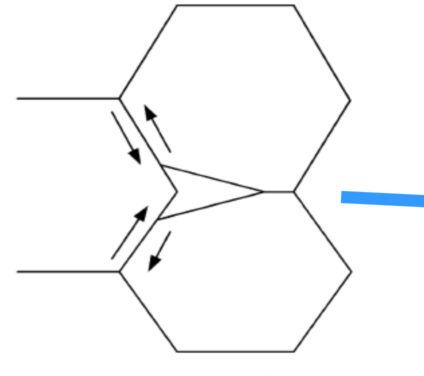


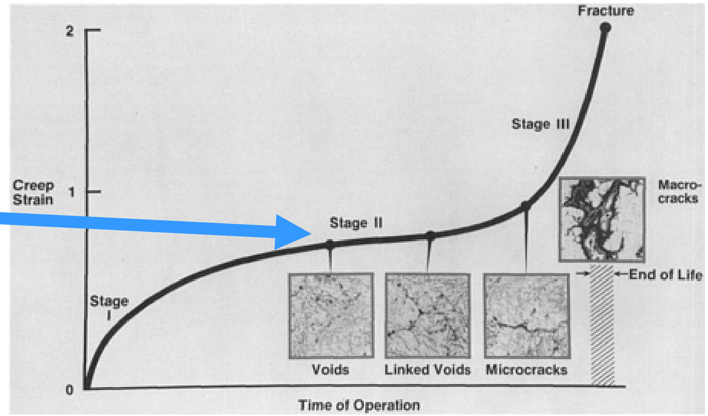
Dherbey 2002

Voids, Swelling and Cracking

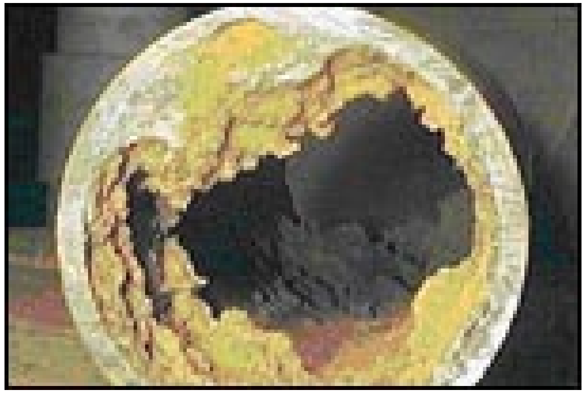


White 2004

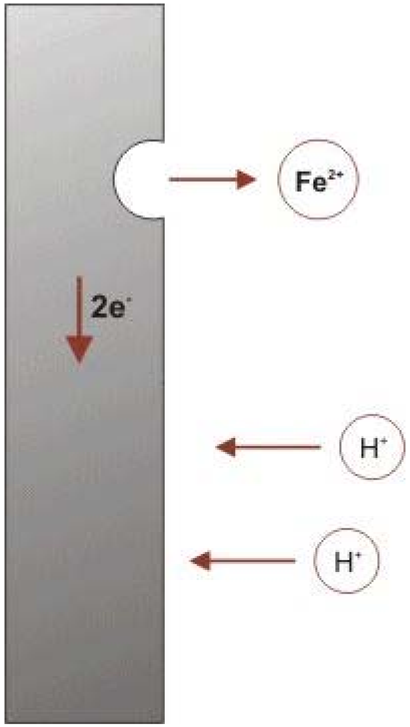




ASM Materials Handbook, online version 2005



Corrosion



Corrosion: Studying Metal Oxides

MD simulations

Need Fe-O, Zr-O potentials

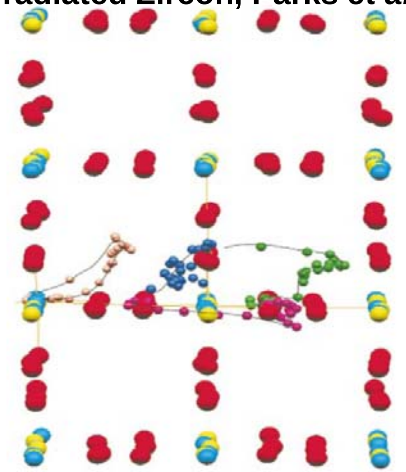
- Requires DFT calculations of defect energies
- Requires fitting the potential

Oxygen in the system

- Require shell model or charge transfer model

Study mobility of oxygen in GBs

Irradiated Zircon, Parks *et al*



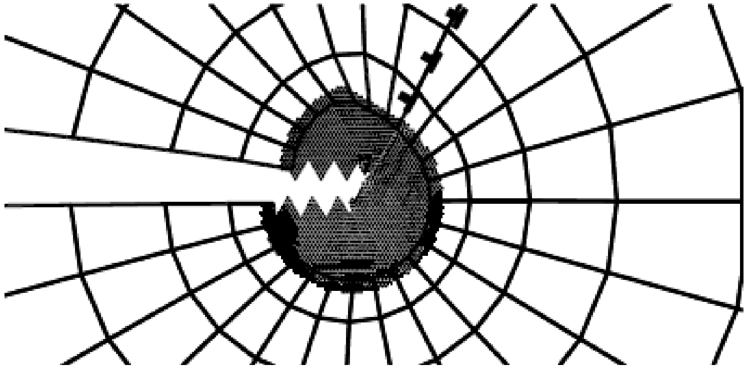
blue=Zr
yellow = Si
red= O

KMC: Diffusion

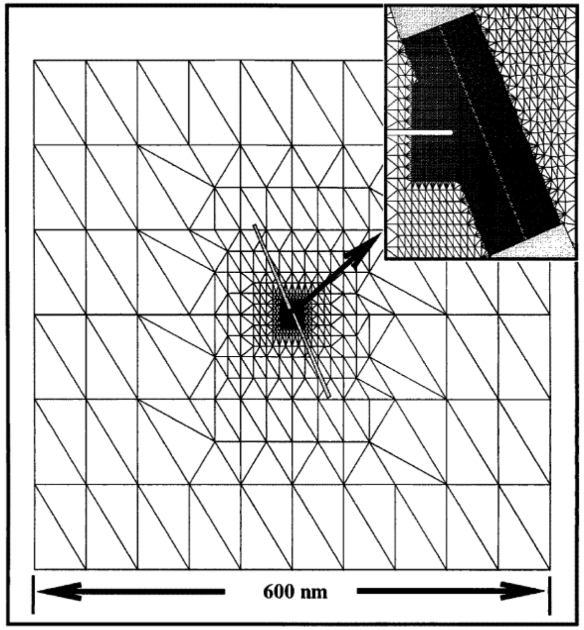
Experimental Validation

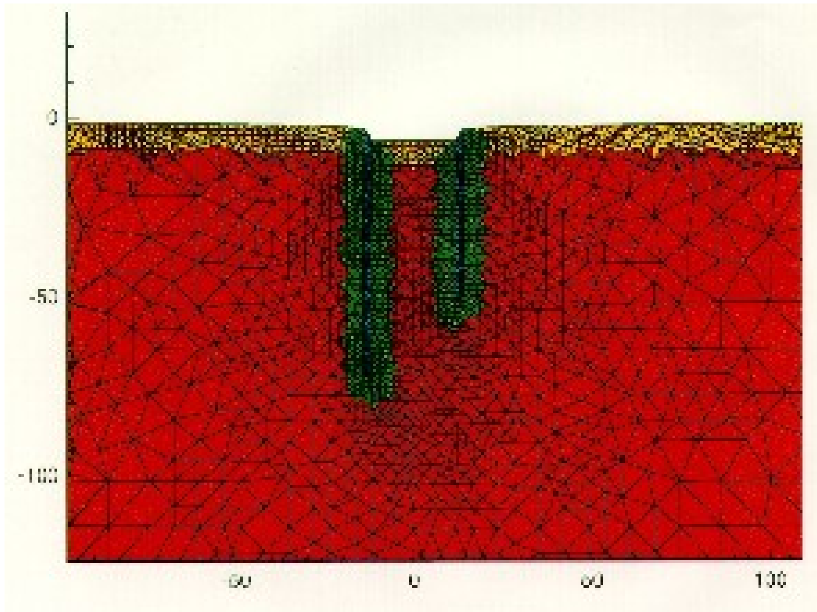
EXAFS, XRD

secondary ion mass spectroscopy (Brossman et al)



Coarse Graining



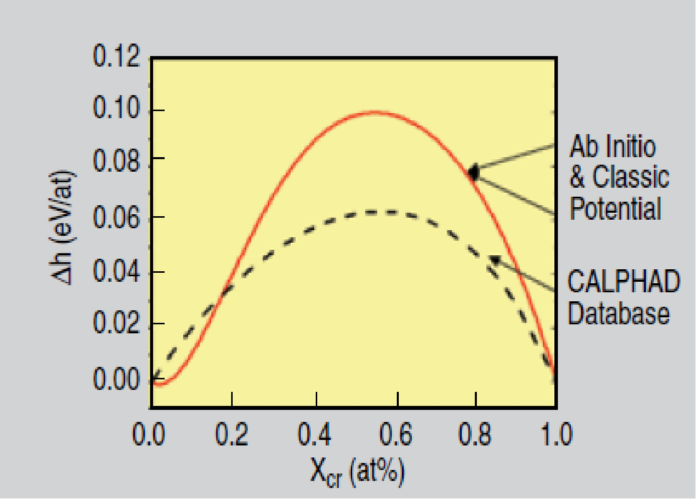


Coarse Graining

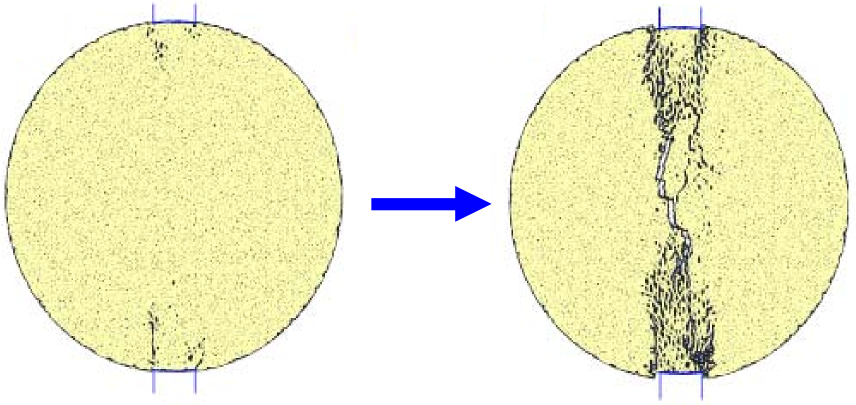
Implementation of possible continuum methods

Thermodynamic Phases Diagrams – Calphad

2D Discrete Element Fracture Model – to study fracture

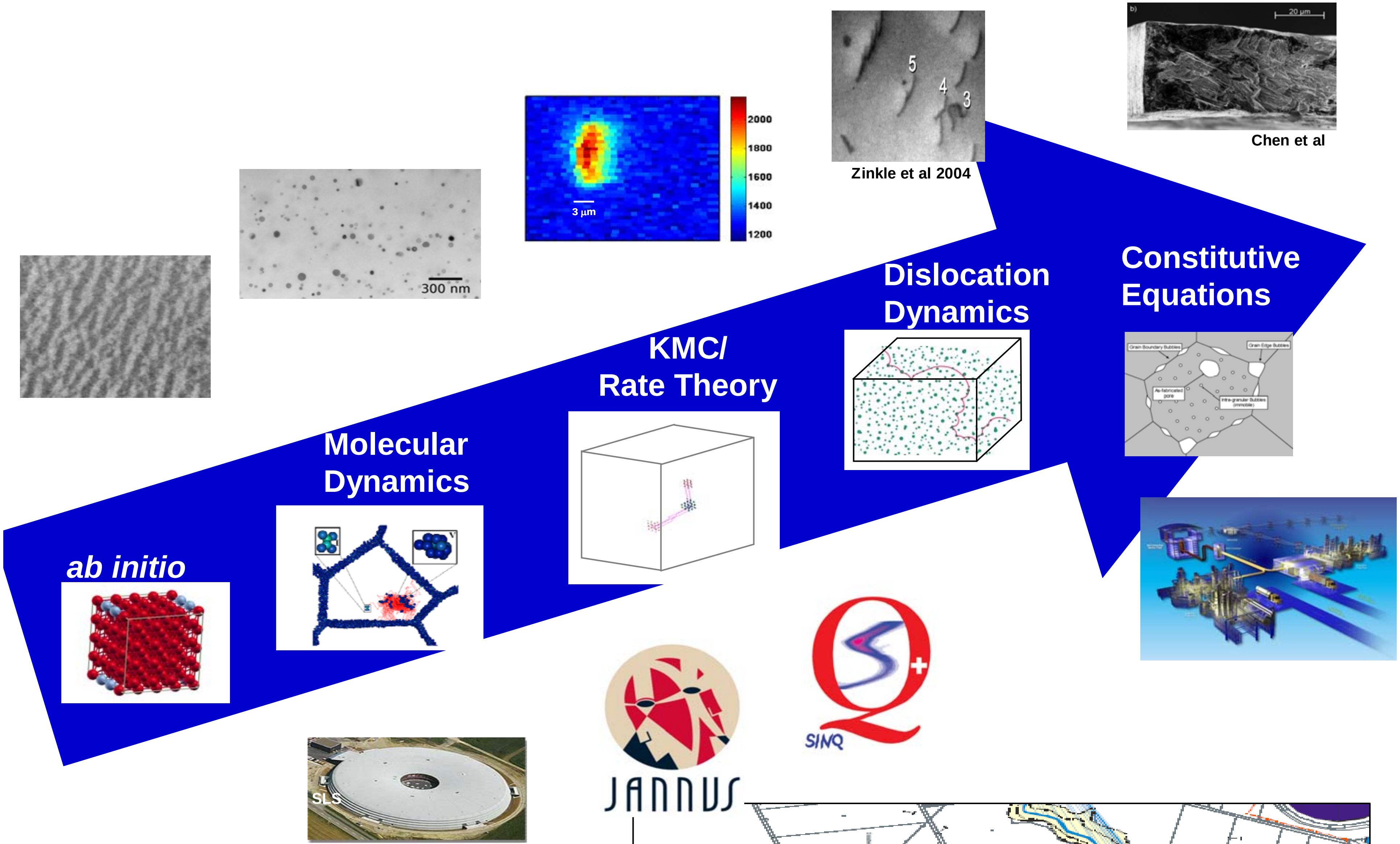


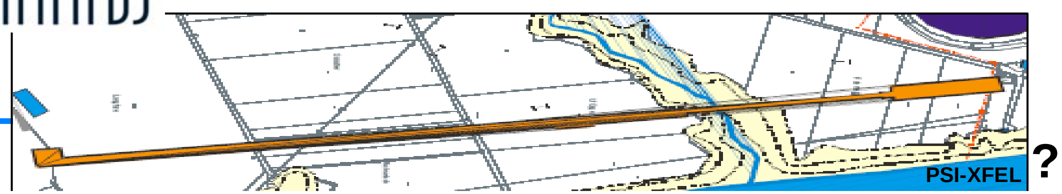
Phase Diagrams: Caro *et al*



Fracture: Carmona *et al*

Design with a Model Toolbox





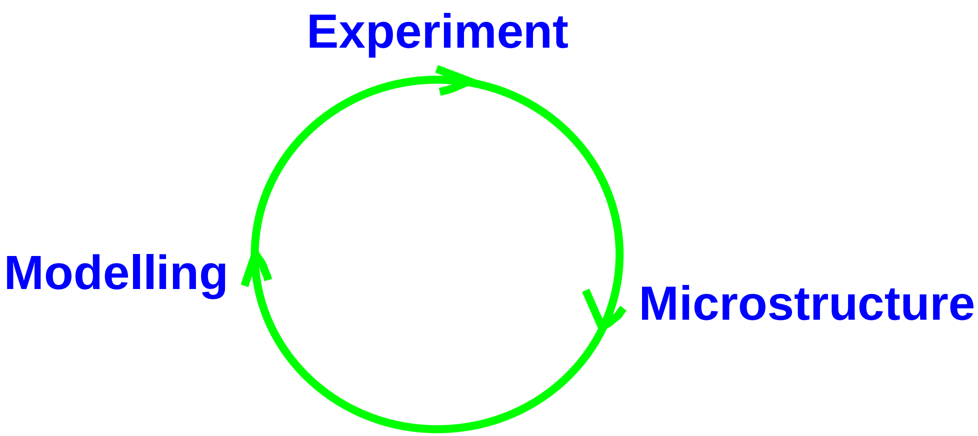
Understanding Material Properties from Simulation

Implement a multiscale, multicode approach to:

- **answer critical issues**
- **reduce time and cost of evaluating materials**
- **understand phenomena not visible by experiment**
- **obtain a lifetime prediction of materials**

Bridge experiment and simulation

Future: design optimal materials



Modeling: Current limitations and drawbacks

- Mostly pure materials

- Almost no carbon in alloys

- Temperature not always included

- Grain boundaries not included in meso-scale models

- **Charge transfer difficult to add to interatomic potentials**

- Numerical accuracy is limited

- **Measurement techniques for validating simulations**

- Need of model materials (to compare with theory)

- Need experimental support to models

- Important that the modeling can drive the experiments

Computational Capability

Simulations need a lot of computational capacity.
Each code needs an optimised platform.
Need a combination of local clusters, supercomputers and local pcs

Code issues:

DFT: parallelisation might be an issue (depends on the code)
Local clusters
Supercomputers

MD: Often good parallelisation
Local clusters and supercomputers

DD: Mostly serial (ParaDIS –parallel)
Local pcs, local clusters

Visualisation: Worth investing in commercial codes

Memory: Can be an issue- simulation capacity doesn´t increase indefinitely or linearly

Building up a Modelling Paradigm

Construct a Modeling Scheme relevant for research issues of interest

Create local expertise through education

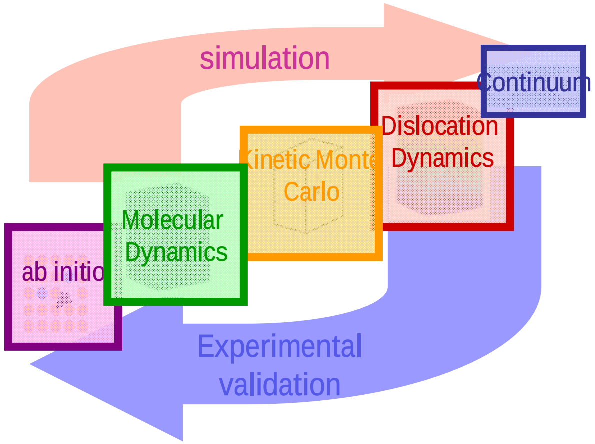
Investigate Material Properties on the multiscale

Toolbox to predict material properties

Experimental Validation of results

Build up modelling consortia

Incorporate experitse of many labs



Modeling Future - predict material properties

- optimise alloys

- materials design