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Derivation of irradiation creep constitutive laws for finite element codes

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Author(s)	Maxime Sauzay (CEA), Thomas Jourdan (CEA), Laurent Dupuy (CEA)
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Summary

This report aims at presenting the results obtained in the framework of the first subtask of the task 2.6, dedicated to the derivation of irradiation creep constitutive laws at the crystal and polycrystal scales.

Approval

Rev.	Date	First author	WP leader	Project Coordinator
0	07/2018	M. Sauzay (CEA)	L. Malerba (SCK•CEN) 27/07/2018	P.F. Giroux (CEA) 27/07/2018

Distribution list

Name	Organisation	Comments
All beneficiaries	MatISSE	

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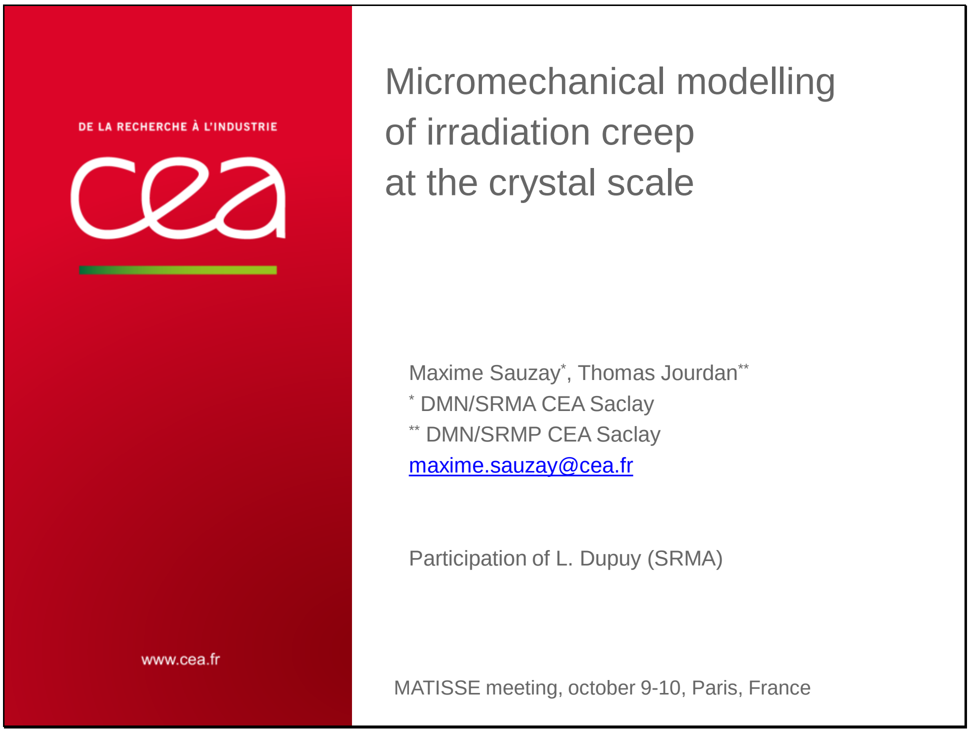
1. Summary of the results

A set of visco-plastic continuum evolution equations ruling free dislocation densities has been written and coupled with point-defects and relevant clusters' evolution as described by cluster dynamics. The goal is to include effects such as:

- elasto-diffusion;
- climb-assisted glide;
- crystal orientation with respect to the tensile axis;
- crystallographic structure etc.

The first results of this modeling approach and an analysis of available experimental observations show that a stationary dislocation density is rapidly reached under irradiation creep, for a viscoplastic strain much lower than without irradiation. It is therefore reasonable to use the density computed by cluster dynamics to simplify the modeling approach. The model also shows that the main contribution to the creep rate comes from dislocation glide assisted climb: the viscoplastic strain is produced by the glide of dislocations between different pinning obstacles (dislocation forest or point-defect clusters produced by irradiation) and the associated time scale by the time needed to unpin the dislocation from these obstacles thanks to dislocation climb. Pure climb mechanisms like stress-induced preferential absorption (SIPA) only marginally contribute to the creep rate. The same is true for the stress-induced preferential nucleation (SIPN) mechanism which considers the coupling between the applied stress and the formation energy of the different point-defect clusters. Finally, it is worth mentioning that the model evidences not only a dependence of the creep rate to the underlying crystal lattice, either bcc or fcc, but also to the orientation of the crystal. Such a dependence will offer in the future a nice way to validate the model by confronting its predictions to experiments performed on single crystals of different orientations.

2. MatISSE Final Meeting presentation



SUMMARY

1/ Irradiation-creep properties of metals & alloys

2/ Experimental discussion of the SIPA model

3/ Effect of the spatial distribution of loops and lines –
Effect of the crystallographic orientation

4/ Weak / strong coupling with cluster dynamics

5/ Conclusions and perspectives

| PAGE 2

1- IRRADIATION CREEP PROPERTIES

Studied materials:

- Austenitic stainless steels
- Zirconium alloys
- FCC metals: copper, aluminium, nickel
- Ferritic and martensitic steels
  and more recently ODS (ferritic / martensitic)

Stationary creep deformation under stress and dose.

Compliance definition: strain proportional to dose and stress

Rather low material effect and T effect (in a given range)

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IRRADIATION CREEP COEFFICIENT

A phenomenological equation describing the evolution of the creep strain is generally used:

$\varepsilon = B_0 \sigma \Phi$ with σ the von Misès stress (Mpa) and the dose (dpa)

For ferritic / martensitic steel, the measured creep compliance values of B0 (unit: 10^{-6} $Mpa^{-1}dpa^{-1}$) are:

HT9: 0,95 D57: 0,4-0,5 MA957 (ODS): 0,25-0,6
(Tolockzko et al., 98)
11Cr ferritic martensitic steel: 0,5-0,75 (Uehira et al., 2000)
T91: 3-7 (Xu & Was) ! Surface effects? Minimum creep strain rate?

Garner et al, (2000), typically measured values: 0,25-1

Temperature range: 400-550°C → B_0 is rather stable with respect to T,

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IRRADIATION CREEP VERSUS THERMAL CREEP?

ODS steel

300 / 400 / 500°C

(Chen et al., 2008)

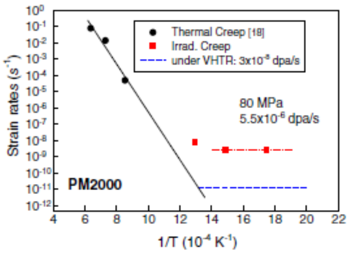
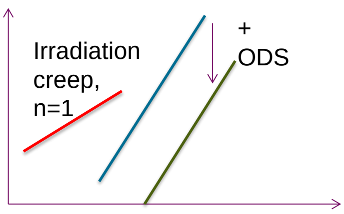


Fig. 6. Temperature dependence of creep rates of PM2000 without irradiation (solid line), under He-implantation (dash-dotted), and expected for VHTR conditions (dashed line).

Up to 500°C, irradiation creep seems to be dominant but we should take care to:

*Stress magnitude
*ODS particles
*non stationary creep



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1- CLASSICAL MODELLING (SEVENTIES)

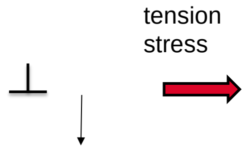
- Stress-induced preferential absorption (SIPN)
- Stress-induced preferential absorption (SIPA),

→ proposed during the seventies

Usually largely underestimate the creep strain rates with respect to experimental data (Was, 2009; Garnier, 2009; Jourdan, 2012).

And the predicted microstructure changes are generally not observed

(Was, 2009, Garnier, 2009, Chen, 2013; Renault et al., 2016).



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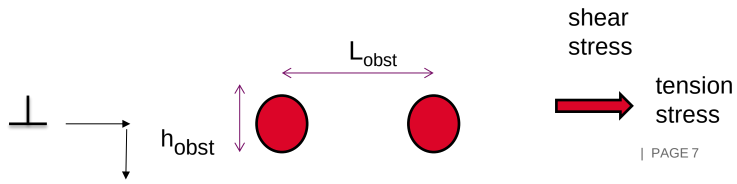
1- RELEVANT MECHANISMS

Probably involved mechanisms to be accounted for:

- irradiation defects / dislocation line evolution under flux, with/without stress (cluster dynamics) ;

- climb (bias without/with stress) → climb assisted glide (Mansur, Gittus);

- dislocation line glide through irradiation defects /and the dislocation forest.



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1- GOALS

Aims:

- carry out precise comparisons of strain rates predicted by the SIPA model with experimental strain rates (SIPA strain > SIPN strain);
- take into account both crystal structure and crystal orientation in the stress-induced bias computations (Woo, 1979);
- combining cluster dynamics and crystal viscoplasticity flow law. Compare to measured stress rates (austenitic stainless steel, BCC iron);
- propose parts of a combined work program to:
  - assess the adopted hypothesis;
  - go further in the modelling approaches at different scales;
  - validate experimentally the preliminary multiscale approach of the project

2- Experimental discussion of the SIPA model

2- SIPA AXIAL PLASTIC STRAIN RATE (LINES, LOOPS)

SIPA: the applied stress tensor induces an anisotropy in the V/I absorption efficiencies of dislocations lines / loops. Pure climb,

- Dislocation climb velocity for the edge slip system, k, uniaxial tensile loading: $v_{cl,k} = b\sigma(\delta z_i^{dk} D_i c_i - \delta z_v^{dk} D_v c_v)$

- Assuming a cubic partition of dislocation lines and loops (three {100} planes: $\frac{d\varepsilon}{dt} = \sum_{k=1}^{3} \rho_k v_{cl,kb}$

- Finally, the hydrostatic part should be substracted for getting the isovolumic plastic strain rate and considering the <100> tensile axis:

$$\frac{d\varepsilon^{vp}_{SIPA}}{dt} = \frac{4}{9}\rho b\sigma((\delta z_i^{d,1} - \delta z_i^{d,2}) \quad D_i c_i - (\delta z_v^{d,1} - \delta z_v^{d,2}) \quad D_v c_v)$$

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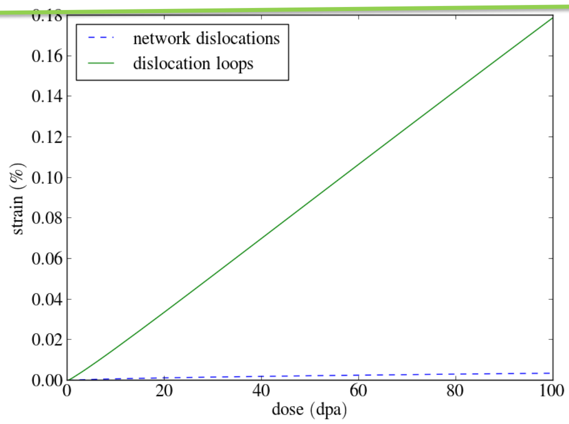
3- FRANK LOOPS: SIPA DEFORMATION

Different irradiation creep tests, different SSs (Garnier, 2009; Grossbeck, 1196): strain close to 4,3%!

Fact 25!!



i- FL density Ok
ii- cristallography : /2
iii- Climb assisted glide (BCC iron)
iv- elastodiffusion

Th. Jourdan, P60, 2012, dislocation line density: 10^{14}m^{-2}, remote axial stress: 220MPa, 330°C

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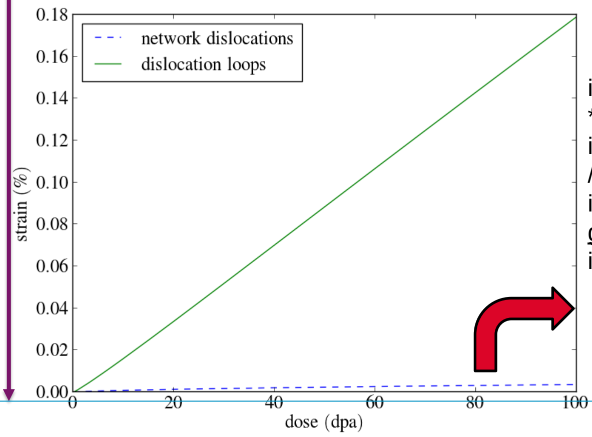
3- DISLOCATION LINES: SIPA DEFORMATION

Sur trois essais de fluage ss irrad, sur trois aciers diff, auteurs diff, mesures concord (Garnier, 2009; Grossbeck, 1196) : 4.3%!

Fact

1400!!



i- line density *5
ii- cristallography : /2
iii- climb assisted glide?
iv- elastodiffusion

Th. Jourdan, 2012, dislocation line density: $10^{14}m^{-2}$, remote axial stress: 220MPa, 330°C

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3/ Effect of the spatial distribution of loops and lines

Effect of the crystallographic orientation

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2- APPLICATION OF THE WOO FORMULAE (1979), FCC/BCC STRUCTURE

Two different assumptions concerning dislocation line network:

- Cubic partition of the edge dislocation lines as usually assumed in the irradiation creep modelling. Three identical densities (<100> lines);

- Partition between the twelve easy slip systems {111}<110> of the FCC structure. Twelve identical densities (<112> lines). BCC structure: {110}<111>

→ Effect of the FCC / BCC slip systems?

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3- APPLICATION OF THE WOO FORMULAE (1979), EFFECT OF THE CRYSTAL ORIENTATION

- SIPA strain rate:
pre-factor depending on the crystallographic orientation through the <u>climb tensile axis</u> which depends on the slip system and orientation of the tensile axis the standard crystallographic triangle.

- CAG (climb-assisted glide) strain rate:
pre-factor depending on the crystallographic orientation through the <u>climb tensile axis</u> and the <u>Schmid factor</u> which depend on the slip system and orientation of the tensile axis the standard crystallographic triangle.

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3- CLIMB ASSISTED GLIDE (~ MANSUR)

Crude viscoplastic flow law equation:

Irradiation creep uniaxial strain rate:

$$\rho \frac{L_{obst}}{h_{obst}} v_{climb}(orientation) bSF(orientation)$$

L_{obst}

h_{obst}

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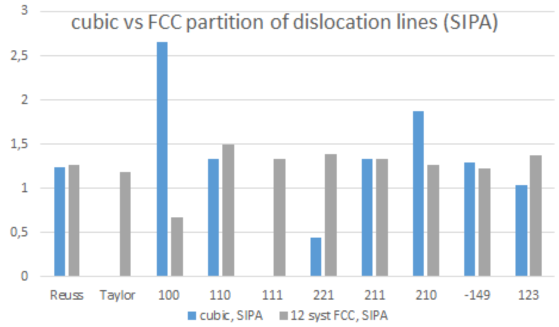
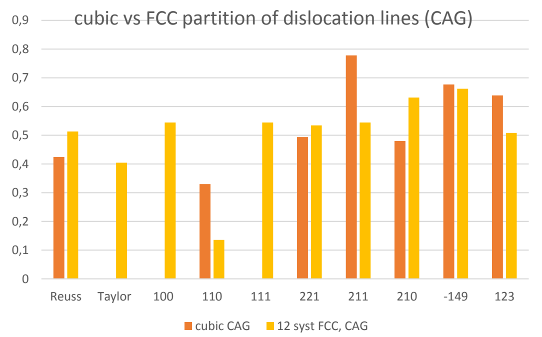
3- APPLICATION OF THE WOO FORMULAE (1979), FCC STRUCTURE



SIPA: the cubic partition induces a very strong anisotropy which is usually not accounted for. The Reuss assumption of homogenous stress in the polycrystal leads to a pre-factor lower than one-half the one computed for a tensile loading along a <100> direction.

As expected the FCC partition leads to a much lower anisotropy. The Reuss average pre-factor is similar for the two distributions.

APPLICATION OF THE WOO FORMULAE (1979), FCC STRUCTURE



Climb Assisted Glide (CAG): the cubic partition still induces a very strong anisotropy which is usually not accounted for. The Reuss assumption of homogenous stress in the polycrystal leads to a pre-factor lower than one-half the one computed for a tensile loading parallel to the <211> direction.
As expected the FCC partition leads to a much lower anisotropy. The Reuss average pre-factor is similar for the two distributions.

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CONCLUSIONS ABOUT CRYSTALLOGRAPHY (I)

- **Macroscopic scale** (Reuss and Taylor polycrystalline homogenization)

Negligible effect of the partionning of the edge dislocation densities:

Cubic ~ FCC structure ~ BCC structure (12 slip systems)

SIPA pre-factor: 1.24-1.3 CAG pre-factor: 0.42-0.51

- **Single crystal scale**: which anisotropy depending on structure?

SIPA: rather high (*2.3, FCC) and very high anisotropy (∞, BCC)

CAG (climb assisted glide): high crystal anisotropy (*5, FCC & ∞, BCC)

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CONCLUSIONS ABOUT CRYSTALLOGRAPHY (II)

- **SIPA:** Both cubic distribution and <100> tensile axis are usually considered, which leads to a pre-factor as high as 2.66. That is more than twice the homogenized value computed for both FCC and BCC structures,

→ the strain rates predicted by Garnier (2009) and Jourdan (2012) should be divided by a factor 2., leading to strain rates definitively much lower than the measured values.

→ **<u>Irradiation creep tests carried out on single crystals are of high interest (PSI and CNRS Orléans)</u>**

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4/ Weak / strong coupling with cluster dynamics

Climb-assisted glide modelling

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3- CLIMB ASSISTED GLIDE

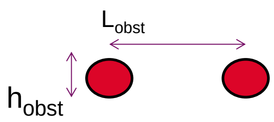
Crude viscoplastic flow law equation:

Irradiation creep strain rate = $\rho \frac{L_{obst}}{h_{obst}} v_{climb} b$

Low dependence ? low dependence

With respect to T with respect to T

(Was, Garnier, SS)



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4- CLIMB ASSISTED GLIDE

4-1 Glide distance after depinning from irradiation defects

Mansur (SIPAG) and Gittus (I-creep) : pure elastic deflection which is indeed proportionnal to the applied stress (Friedel). Nevertheless that strain is fully reversible!

Glide distance of dislocations through arrays of obstacles (Forman and Makin, 1960, Kirasov et al, ; Landeiro dos Reis et al., MRS Spring 2017, + article submitted):

$L(\tau, c_{obst}, f_{obst})$

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4- CLIMB-ASSISTED GLIDE MODELS

4-2 Climb velocity

- Mansur (SIPAG): stress induced changes in the sink efficiencies biases, k^{th} (slip system)

$$v_{cl,k} = b\sigma(\delta z_i^{dk} D_i c_i - \delta z_v^{dk} D_v c_v)$$

similar as SIPA

- Gittus (I-creep): use of the total efficiencies of the dislocation sinks.

Because of other sinks less favorables to I absorptions than dislocations are (grain boundaries, particle interfaces, nanocavities…)

Following the many computations: the stress perturbation of the total efficiencies is rather low.

$$v_{cl,k}^{tot} = b\sigma(\delta z_i^{dk} D_i c_i - \delta z_v^{dk} D_v c_v) + b(z_{i,0}^{d} D_i c_i - \delta z_{v,0}^{d} D_v c_v)$$

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4- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

Cluster dynamics allow the prediction of the evolution of many microstructure characteristics with dose and eventually stress:

- Irradiation defect density and size (average, distribution);
- Interstitial and vacancy densities;
- Dislocation line density

A weak coupling consists in using outputs from cluster dynamics computations to predict irradiation creep strain rate.

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4- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

Simplified assumptions to provide orders of magnitude of the strain rates for 316L steel and BCC iron.

- weak coupling between cluster dynamics and crystal viscoplasticity (active slip syst i).

- dislocation climb velocity: $v_{cl,i} = b^{-2}(z_{i,0}^{dj} D_i c_i - z_{v,0}^{dj} D_v c_v)$

(dominant term with respect to the SIPA climb velocity)

- glide distance:

mean distance between distance between irradiation defects (density and mean loop size) → to be discussed later

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4- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

Weak coupling between cluster dynamics and crystal viscoplasticity (active slip syst i)

Viscoplastic flow law: $\frac{d\varepsilon_k^{vp}}{dt} = \sum_{k\ actif} F_k \rho_k \frac{L}{h} b v_{cl,k}$

To get simple analytical estimations, it is assumed that:

i) the dislocation lines are equally distributed on the slip systems (low effet of stress on bias and dislocation distributions, CD and TEM)

ii) a critical shear stress of 30MPa is used for austenitic stainless steels (tensile tests of well-oriented single crystals of 316L, Gorlier, 1989)

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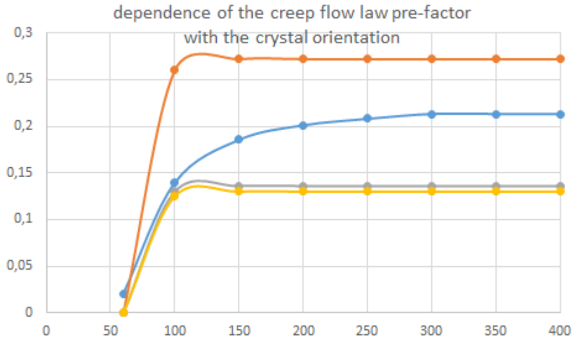
5- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

A non negligible crystal orientation effect on the plastic flow law pre-factor is found: $A(orientation) = \frac{1}{N_{syst}} \sum_{k\ actif} F_k$

It is only due to the Schmid factor distribution (FCC / BCC structures)



Considering one-half of well-oriented grains and one-half of multiple slip, an average value of 0.2 is used for FCC materials (low effect of more accurate evaluations)

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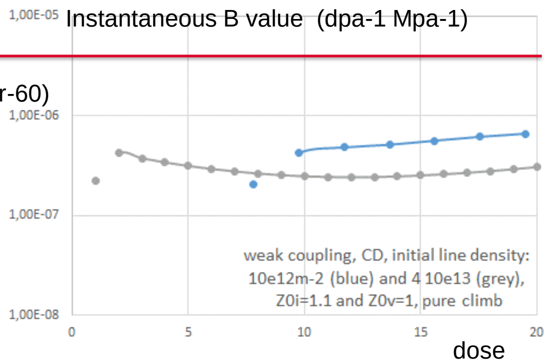
5- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

Weak coupling between cluster dynamics and crystal viscoplasticity.
Crescendo outputs obtained with two sets of parameters (CD),

measured compliance value
3-4 10^{-6} dpa^{-1} MPa^{-1}
(SA 304L, CW 316, OSIRIS and Bor-60)

<u>PURE CLIMB (SIPA)</u>
Zi0=1.1 and Zv0=1 → vcl (incoherence)
L : irrad defect dist



Even if the bias used in the evaluation of the climb velocity amounts to 0.1, the predicted SIPA compliance is 6 to 14 times lower than the experimental compliance. How enhanced computations of the stress influence on biais may reduce such gap?

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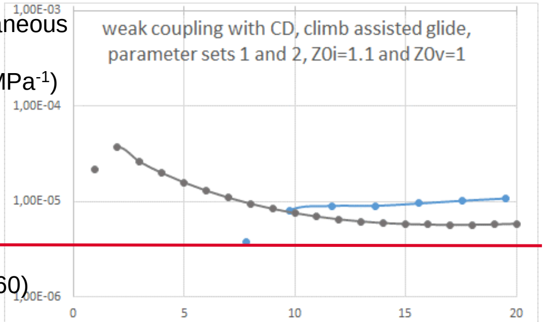
5- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

Weak coupling between cluster dynamics and crystal viscoplasticity
Crescendo outputs using two sets of parameters (CD)

CLIMB ASSISTED GLIDE
Zi0=1.1 and Zv0=1 → vcl (incoherence)
L : irrad defect dist

measured compliance value
3-4 10^{-6} dpa^{-1} MPa^{-1}
(SA 304L, CW 316, OSIRIS and Bor-60)

instantaneous B value (dpa^{-1} MPa^{-1})



dose (dpa)

The predicted Climb assisted glide compliance about the double the experimental compliance. A CD computations up to 50dpa may be useful. Introducing the stress influence on bias may not be fully avoided. Is the use of Zi0=1.1/Zv0=1 in the vcl computat valid?

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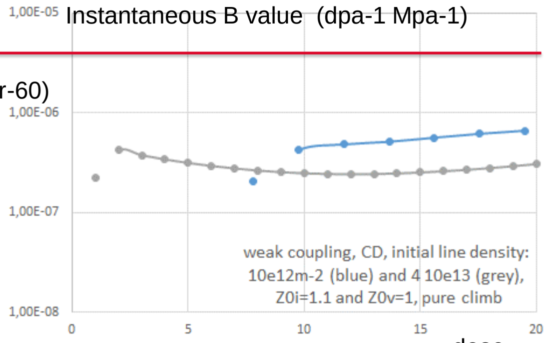
5- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

Weak coupling between cluster dynamics and crystal viscoplasticity.

measured compliance value
3-4 10^{-6} dpa^{-1} MPa^{-1}
(SA 304L, CW 316, OSIRIS and Bor-60)

PURE CLIMB (SIPA)
Zi0=1.1 and Zv0=1 → vcl (incoherence)
L : irrad defect dist



Even if the bias used in the evaluation of the climb velocity amounts to 0.1, the predicted SIPA compliance is 6 to 14 times lower than the experimental compliance. How enhanced computations of the stress influence on biais may reduce such gap?

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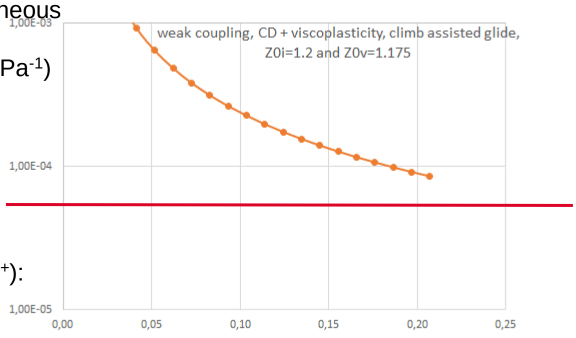
5- WEAK COUPLING WITH CLUSTER DYNAMICS

BCC iron, irradiated by e-, <100> loops

instantaneous B value (dpa^{-1} MPa^{-1})

CLIMB ASSISTED GLIDE
Zi0=1.2 and Zv0=1.175
→ vcl
L : irrad defect dist

measured compliance value (0.2 dpa, 180MPa, 773K, He^{2+}): $5\ 10^{-5}$ dpa^{-1} Mpa^{-1}, (Chen et al, 2013)



dose (dpa)

The predicted Climb assisted glide compliance is close to the experimental compliance.

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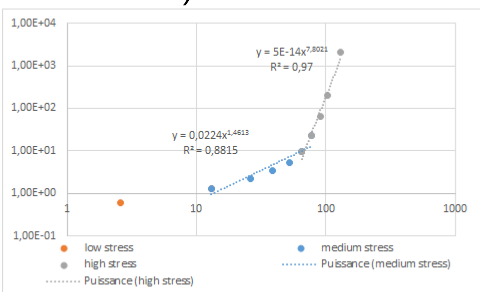
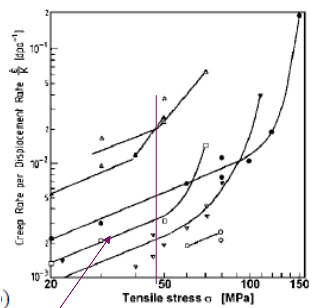
5- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

Towards a more general model: what about the strain rate dependence with respect to stress dependence?

- Glide distance after unpinning induced by climb if the kth system is activated ($|\tau_k| > \tau_0$ allowing glide between dislocation/loop obstacles) : $L_k = L(\tau_k, c, h)$





From the work of M. Landeiro dos Reis (MRS Srping, 2017;
Landeiro dos Reis, Proville & Sauzay, submitted)
Copper, f=12eV/nm, c=2 10^{-5}) *copper*
Very preliminary results

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5- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

Would a strong coupling between cluster dynamics and crystal viscoplasticity affect strongly the predicted microstructure and irradiation creep strain rate evolution?

Concerning the microstructure evolution: the stress effect on the stress induced changes in the sink efficiently is low whatever the accuracy of their computations (Garnier, 2009; Jourdan, P60, 2012)

→ stress would not affect directly microstructure evolution.

Concerning the irradiation creep strain rate: the negligible changes in microstructure features (irradiation defect density and size, I/V concentrations) would affect marginely the strain rate.

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5- WEAK / STRONG COUPLING WITH CLUSTER DYNAMICS

Finally the plasticity-based equation evolution terms (Kubin et al, ; Giordana et al., 2012; Monnet et al.) are negligible with respect to the irradiation based terms (loop production and unfaulting…)

→ To be confirmed by a full coupling which is time consuming on the implementation point of view.

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5/ CONCLUSIONS

-Huge underestimation of strain rates by the SIPA model in the case of 316L steel
(factor 25 for FLs, factor 200 for dislocation lines

- Non negligible effect of the FCC / BCC structures with° respect to the usual <100> cubic distribution of loops and lines. Large effect of the crystal orientation with respect to the tensile axis

→ Importance of irradiation creep tests to be carried out on single crystals of various orientations

- Accounting for the total sink efficiencies (not much affected by the applied stresses and climb assisted glide leads to predicted strain rates close to experimental data for 316L steel and BCC iron

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5/ PERSPECTIVES, PARTIAL RESEARCH PROGRAM

- Computation of dislocation glide for various materials and loading conditions

- Full coupling between cluster dynamics and continuum viscoplasticity

- Elasto-diffusion → acceleration of climb rate under stress?

- Importance of irradiation creep tests to be carried out on single crystals of various orientations (PSI and CNRS Orléans)

- Mean-field / full-field polycrystal computations (crystal elasticity and viscoplasticity anisotropy).

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5/ Conclusions and perspectives

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3- ACCOUTING FOR ATOMISTIC-BASED ESTIMATIONS SINK EFFICIENCIES AND BIAS

Dislocation line sinks, without stress

3-4 DFT computations (Clouet, 2017; Marinica and Jourdan, 2017)

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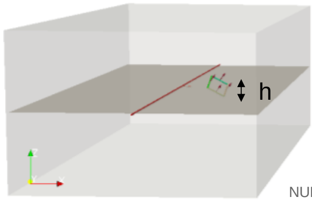
Modelling of irradiation creep

MINOS

Viscoplasticity flow law
(SIPAG, Mansur, 1979)

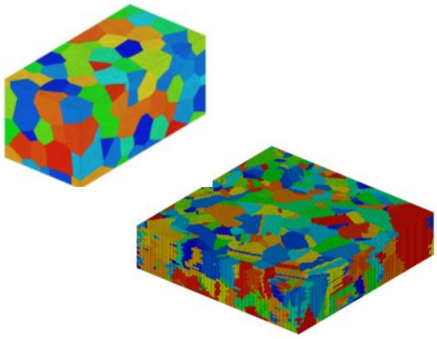
- For instance; glide of dislocation line assisted by climb :
  - Climb time for an obstacle height h?
  - Mean distance between two characteristic obstacles to dislocation glide
  - Friction stress or any other minor obstacles



From the grain scale to the macroscopic scale:

- Crystalline FE computations carried out on large scale aggregates

Polycrystal meshes: collaboration with L. Signor (P', ENSMA Poitiers)
→ « real » 3D mesh of an austenitic steel (numerous EBSD measurements/ repolishings)
→ Meshes for ferritic/bainitic microstructures



- Influence of crystal elasticity anisotropy?

--> may affect the primary creep stage

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4- CLIMB-ASSISTED GLIDE MODELS

4-2 Climb velocity

- Mansur (SIPAG): stress induced biases k[th] (slip system)

$$v_{cl,k} = b\sigma(\delta z_i^{dk} D_i c_i - \delta z_v^{dk} D_v c_v)$$

- Gittus (I-creep): use of the total efficiencies of the dislocation sinks.

Because of other sinks less favorables to I absorptions than dislocations are (grain boundaries, particle interfaces, nanocavities…)

Following the previous computations: the stress perturbation of the total efficiencies is rather low, OTHER WRITTING KIRASOV ET AL, SWELLING

$$v_{cl,k}^{tot} = b\sigma(\delta z_i^{dk} D_i c_i - \delta z_v^{dk} D_v c_v) + b(z_{i,0}^{d} D_i c_i - \delta z_{v,0}^{d} D_v c_v)$$

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3- ACCOUTING FOR ATOMISTIC-BASED ESTIMATIONS SINK EFFICIENCIES AND BIAS

3-1 Classical formulae: effect of the applied stress tensor

J. Garnier :	+0.7	-0.2
Th J 2012	+0.7	-0.2

Relative change in the isotropic elasticity moduli (?):

shear modulus, µ:	+0.5	-0.5
Bulk modulus, K:	+0.5	-0,5

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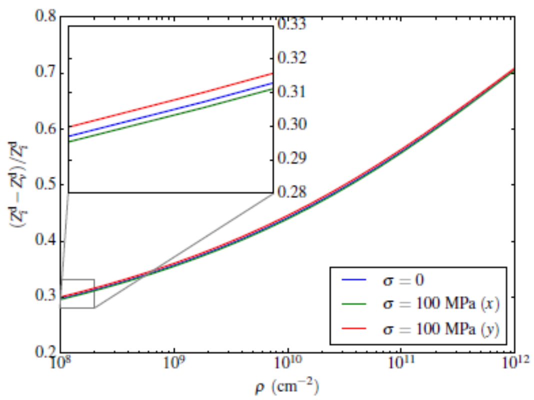
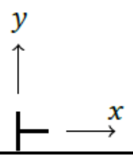
TH JOURDAN, MATISSE, 2014





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3- ACCOUTING FOR ATOMISTIC-BASED ESTIMATIONS SINK EFFICIENCIES AND BIAS

3-4 Molecular Dynamics computations using empirical potentiels (Ackland, 1997; Baraev et al., 2017)

Ackland, 1997: copper	+1.2 (I)	-0.22 (V)
	$\frac{\Delta C_{44}}{C_{44}} = -35.4$	-8.5
$\frac{\Delta K}{K} = -28.6$	-5.4	
$\frac{\Delta C'}{C'} = -16.5$	-7.2	

3-3 DFT computations (Clouet, 2017; Marinica and Jourdan, 2017)

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