MSM
M.M.S Metallic Materials Science
LIÈGE université Sciences Appliquées
ĐẠI HỌC THỦ DẦU MỘT
THU DAU MOT UNIVERSITY

Colloque Aussois 2024 de l'association MECAMAT
Cours du lundi 22 01 2024 sur invitation

Méthodes numériques pour la simulation des procédés

AM Habraken,
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Contents

- A survey of scales and methods

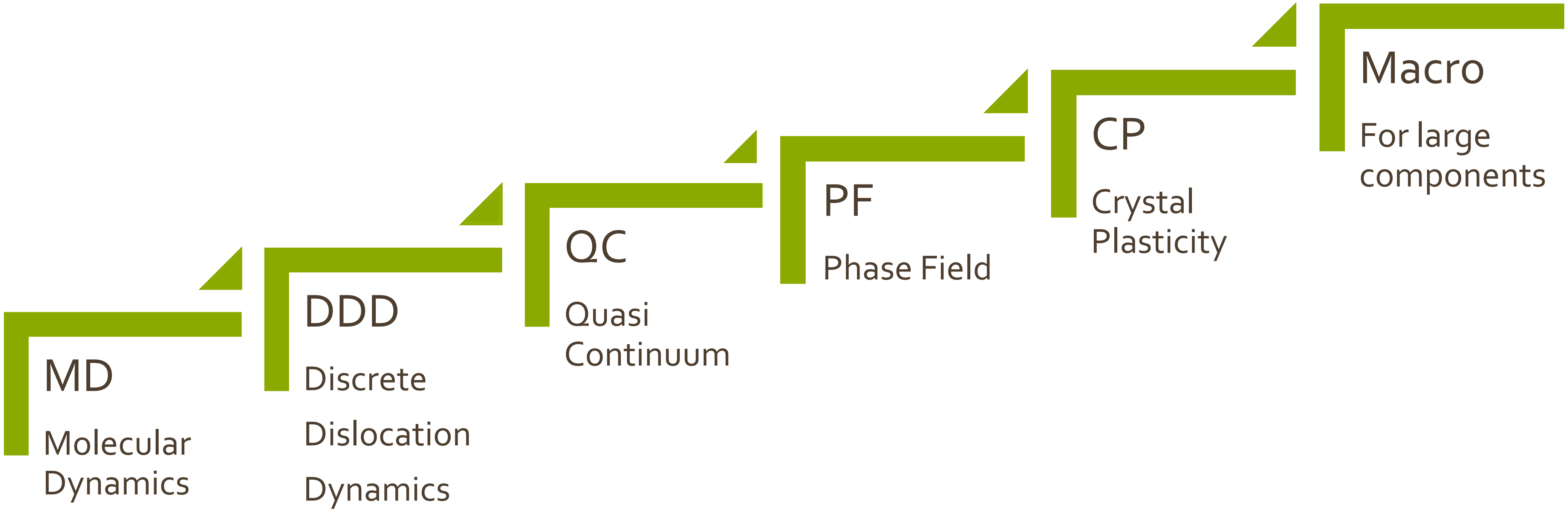
- Finite element method FEM
  - One element: Solid Shell
  - Mechanical constitutive laws
    - Deep Drawing
  - Thermo-mechanical analysis
    - Cooling of rolling mills
    - Continuous casting
  - Representative Volume Element (RVE) or in French VER

- Coupling solid FEM with … Computational Fluid Dynamics, Deep Learning
  - Additive Manufacturing

What are the **important phenomena** in your process ? What are their **scales**?

What is your access to software and to skilled scientists? Which time for training?

Which data are available?



MD
Molecular Dynamics

DDD
Discrete Dislocation Dynamics

QC
Quasi Continuum

PF
Phase Field

CP
Crystal Plasticity

Macro
For large components

MD - Molecular Dynamics

Basic principles

Particle (often individual atom) motion - computation

Forces on atoms: derivatives of analytic equations defining **potentials**

-Bimolecular (biology) –a few biomolecules, very large time
-Materials (engineer) → 10^9 atoms or coarse grains "meso scale",
& time µs or max s

Interests - Limits

LAMMPS open code

To compute for instance heat conductance,

stress –strain curve in single crystals

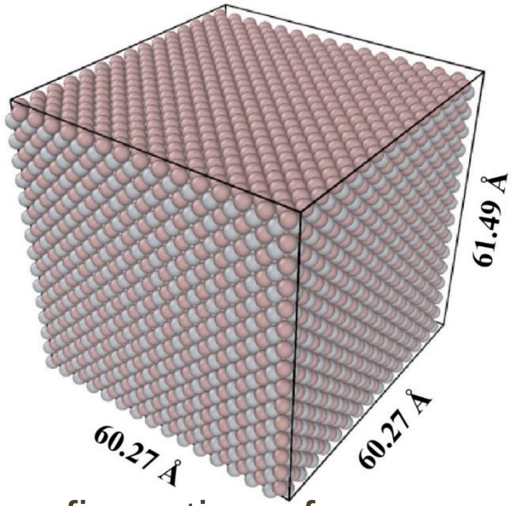
at different tps°

To observe GB effect of simple systems

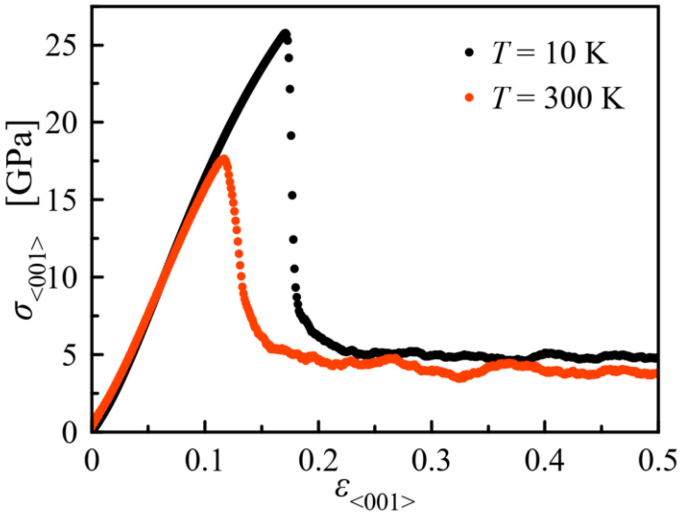
nm scale

Not for studying polycristalline materials
with porosities, precipitates…
or just one aspect at local scale,

Clear interest in material design
« 1st step of manufacturing process »



Initial configuration of TiAl alloy.
Gray balls =Ti atoms
Pink balls = Al atoms,



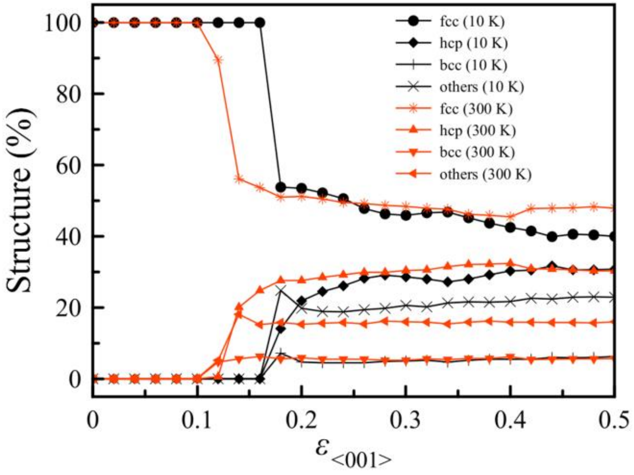
Uniaxial tensile loading of TiAl alloy in the <001> dir.

To predict of the **differential effect** in tension and compression known in TiAl

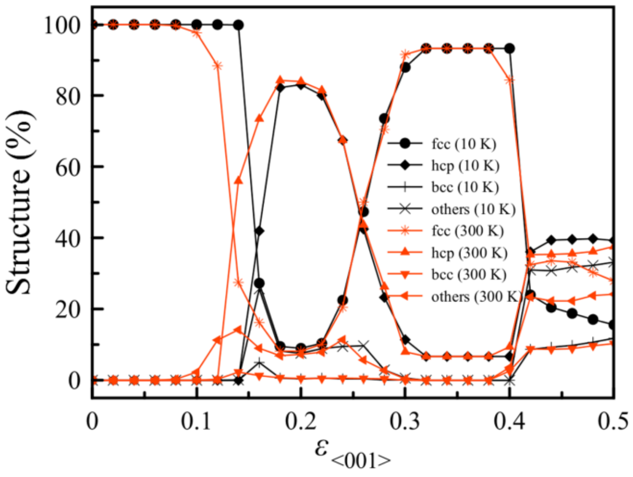
To relate it to phase changes
FCC → BCC and HCP at different moment and % according tension, compression, tp°

Experimental Young modulus: well predicted

Tension



Compression



Arifin, R. et al. *Metals 2021, 11, 1760*.

MD - Molecular Dynamics - References

LAMMPS -a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales **A. P. Thompson** et al. *Computer Physics Communications 271 (2022)* 108171 https://doi.org/10.1016/j.cpc.2021.108171

Principle, code feature

Structural Change of TiAl Alloy under Uniaxial Tension and Compression in the <001> Direction: A Molecular Dynamics Study **Arifin, R.** et al. *Metals 2021, 11, 1760*.https://doi.org/10.3390/met11111760

Stress differential effect phase change

Molecular Dynamics Simulations Correlating Mechanical Property Changes of Alumina with Atomic Voids under Triaxial Tension Loading. Modelling Chang, J et al. 2023, 4, 211–223. https://doi.org/10.3390/modelling4020012

Rupture of alumina

MEAM potentials for Al, Si, Mg, Cu, and Fe alloys B. Jelinek et al. arXiv:1107.0544 [cond-mat.mtrl-sci]

Potentials for Al,Si, Mg, Cu, Fe interactions

DDD -Discrete Dislocation Dynamics

Basic principles

forces on dislocations

-> dislocation stress field computed

-> dislocation movement integrated

-> contact reactions

2D OK to investigate

but 3DDD for quantitative simulations

Interests - Limits

To predict plastic material behavior

At mesoscopic scale (1 µm to 100 µm)

Increased complexity:

anisotropic elastic media

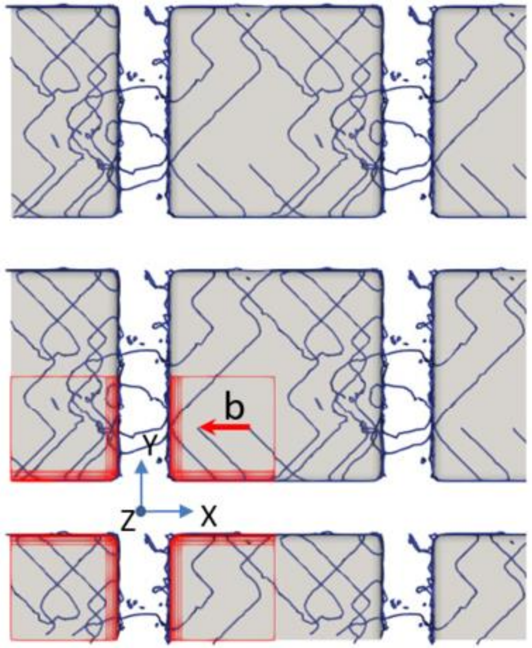
large strains, plastic distorsions

microstructure evolution

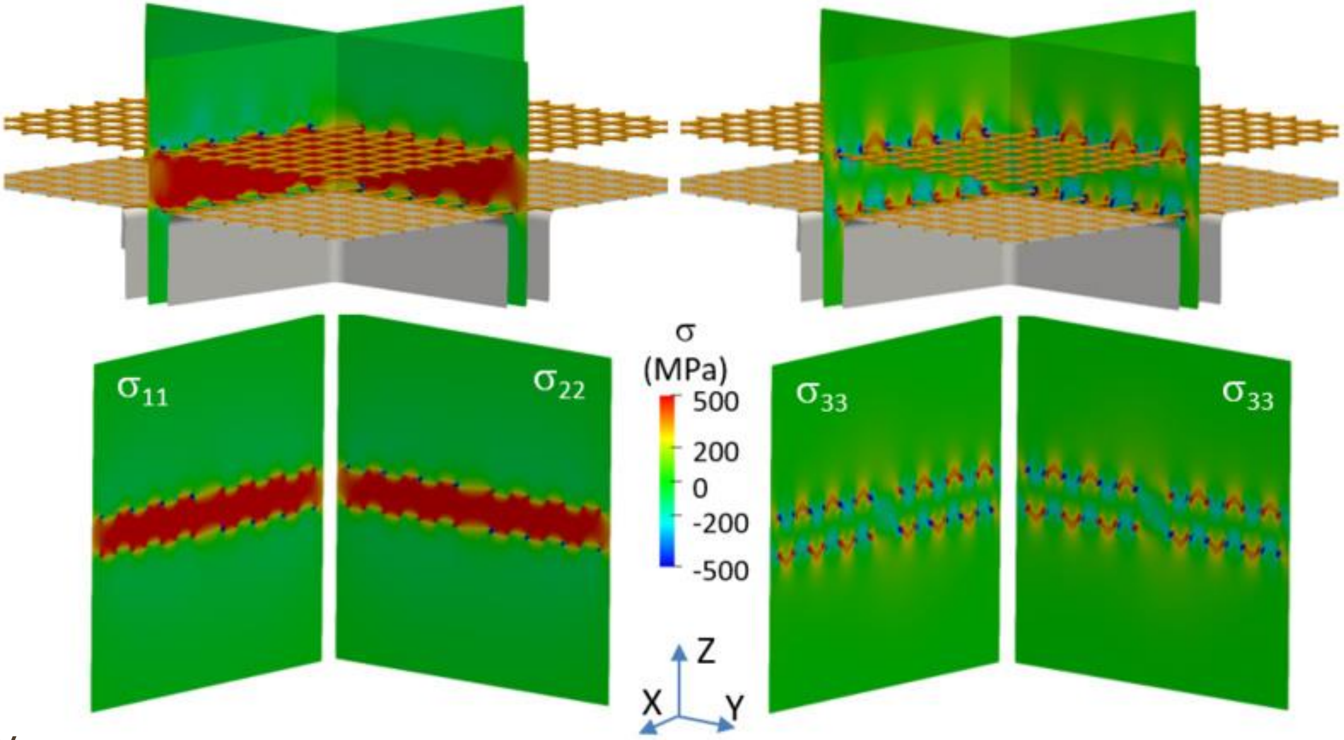
(-> coupling with Phase Field)

More about material property prediction than process modeling but of course linked.

DDD - Discrete Dislocation Dynamics - Creep



a)



b)

The 3 γ channels of the superalloys: not mechanically equivalent for the dislocation dynamics

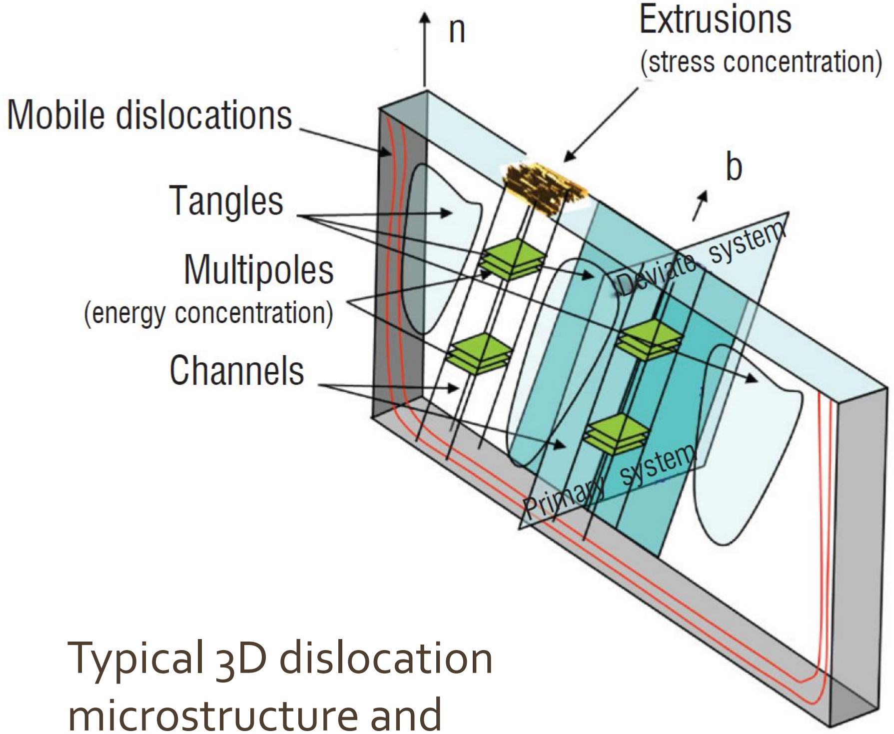
Ni based superalloys

Chang et al. IJP 2018

Dislocations induce a 2D plane stress elastic state
→ contraction along the loading direction

Results of 3D edge-screw model
TRIDIS

DDD - Discrete Dislocation Dynamics - Fatigue



Typical 3D dislocation microstructure and description of a single slip band

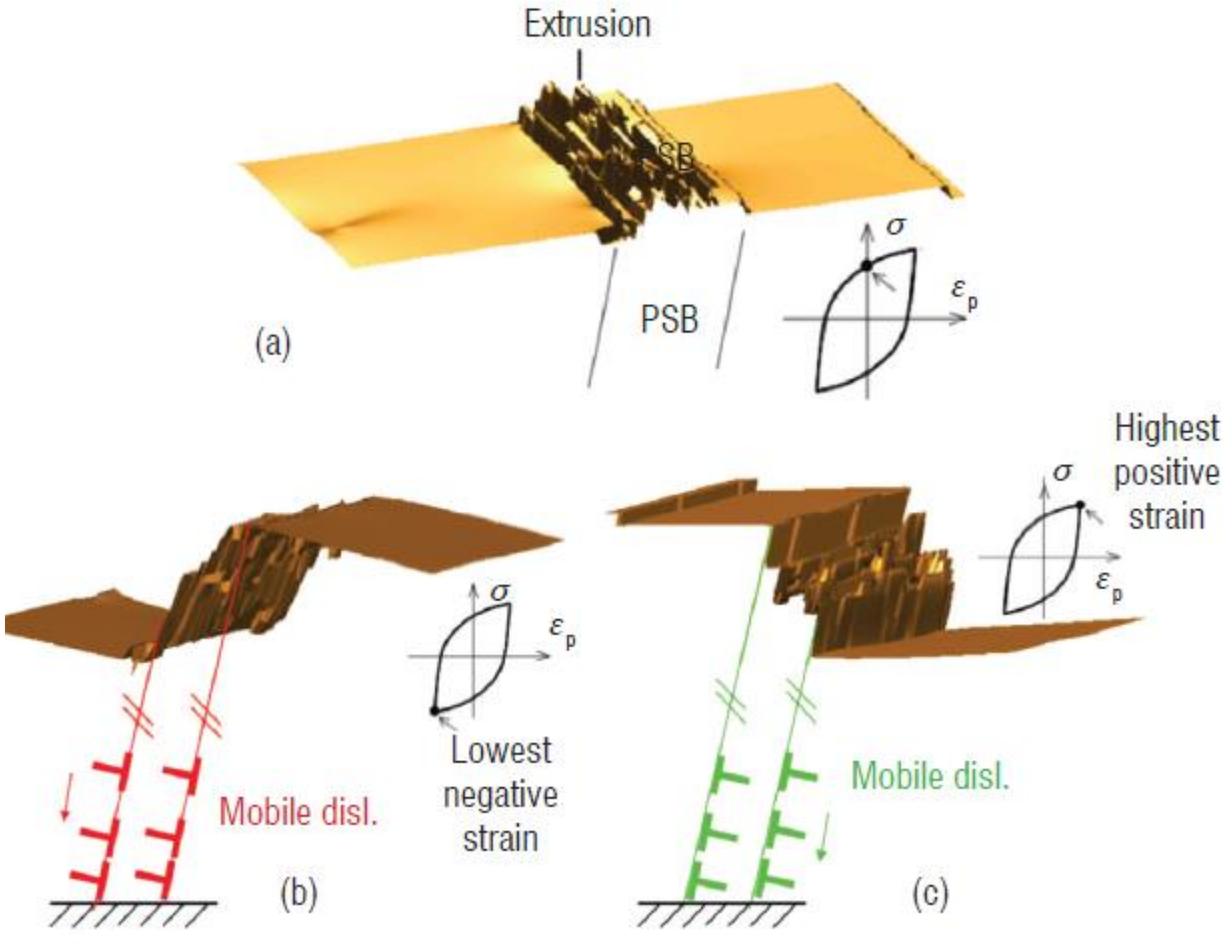
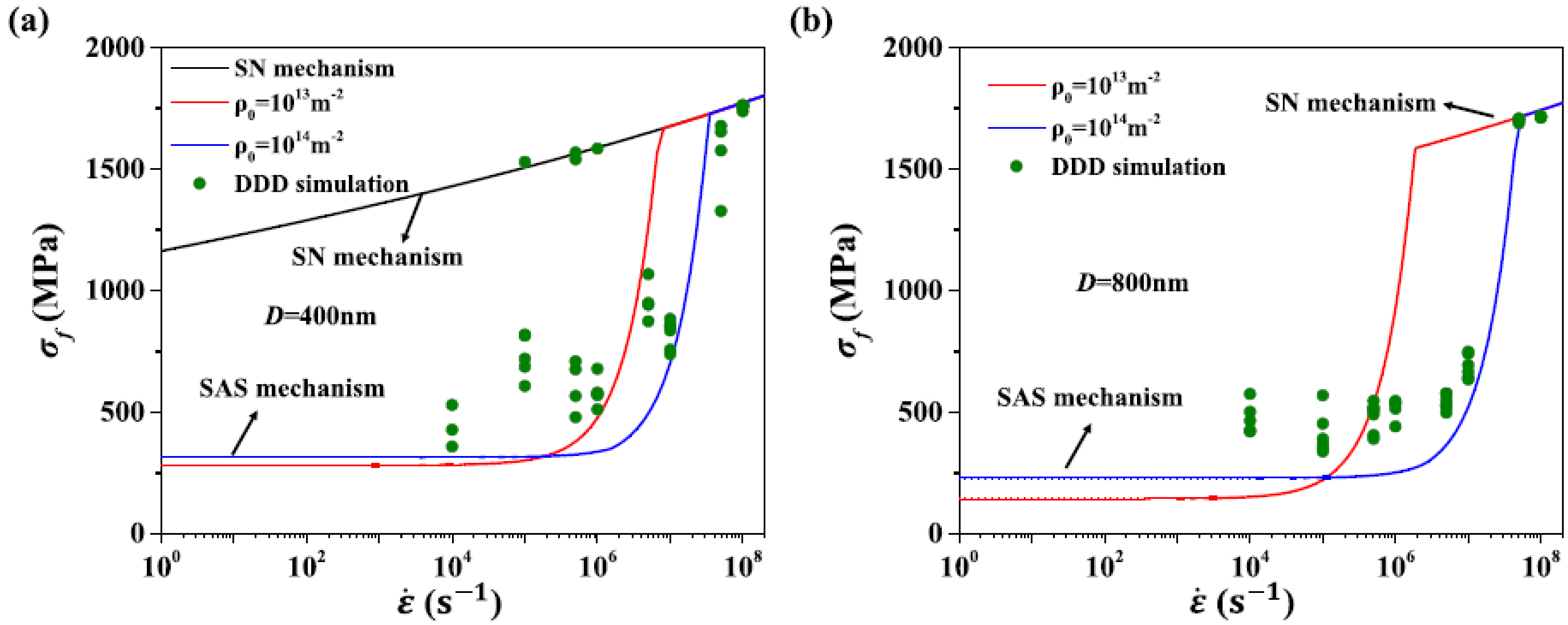


Figure 3 - Extrusion at the surface plotted for different instant of a given cycle

C. Déprés et al. *Aerospacelab Journal Issue 9 - June 2015*

DDD - Discrete Dislocation Dynamics - Stress- Strain Curve

J. Hu et al.
Sci Rep 9, 20422 (2019)



Prediction of micro Cu pillars behavior with different initial dislocation densities used to fit analytical models linked with mechanisms (curves)

For small pillars with diameter < 200 nm main plastic deformation mechanism = “surface nucleation” (SN)
For samples on the sub-micrometer scale, nucleation happens rather by so- called “single-arm sources” (SAS),
i.e. a dislocation segment which is pinned inside the sample that terminates on the sample surface.

DDD - Discrete Dislocation Dynamics - References

Discrete dislocation dynamics **F.Bioli et al.** *in Nickel Base Single Crystals Across Length Scales 2022 Elsevier*

https://doi.org/10.1016/B978-0-12-819357-0.00021-4

Principle, code feature, application Ni alloys

Influence of Excess Volumes Induced by Re and W on Dislocation Motion and Creep in Ni-Base Single Crystal Superalloys: A 3D Discrete Dislocation Dynamics Study **S. Gao et al.** *Metals 2019, 9, 637;*

https://www.mdpi.com/2075-4701/9/6/637

Creep application

3D Discrete Dislocation Dynamics Investigations of Fatigue Crack Initiation and Propagation-Life Prediction Methodologies for Materials and Structures **C. Déprés et al.** *Aerospacelab Journal Issue 9 - June 2015*

https://aerospacelab.onera.fr/sites/w3.onera.fr.aerospacelab/files/AL09-01_1.pdf

Fatigue application

Predicting the flow stress and dominant yielding mechanisms: analytical models based on discrete dislocation plasticity **J. Hu et al.** *Sci Rep 9, 20422 (2019).*

https://www.nature.com/articles/s41598-019-56252-x

Dominant yielding mechanisms single crystalline copper pillars

Dirk Raabe Research Unit website

https://www.dierk-raabe.com/ddd-discrete-dislocation-dynamics/

Course, video, indentation, large strain, BG penetration see many ref. Articles

QC- QuasiContinuum

Basic principles

Adaptive mesh « model » refinement :

Energy must be minimized but is computed

- by full atomistic modeling in regions of the problem
- by continuum assumptions elsewhere

Interest and drawbacks / process

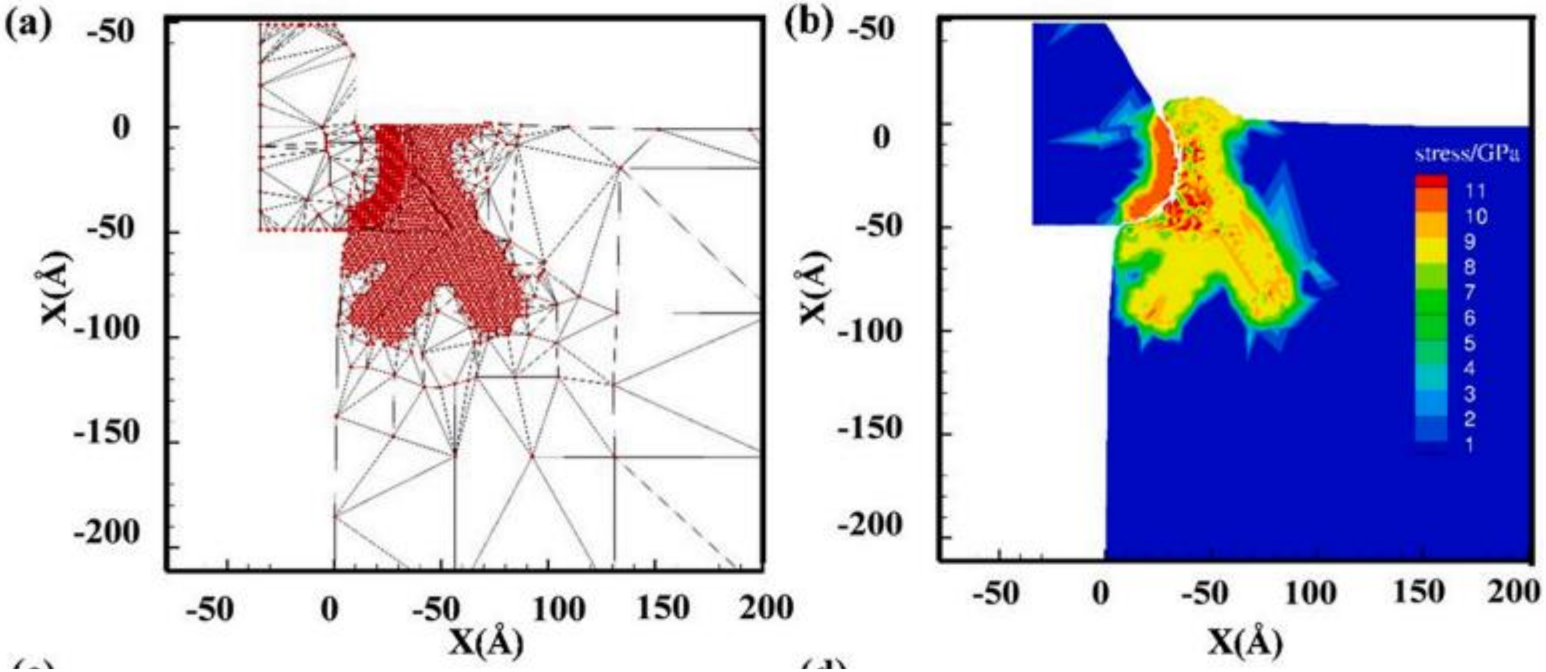
Methods to address larger problems

MEMS failure through fracture and fatigue processes

Cutting models in microforming-->

we arrive to « process modeling »

QC- QuasiContinuum - Applications - Nano cutting

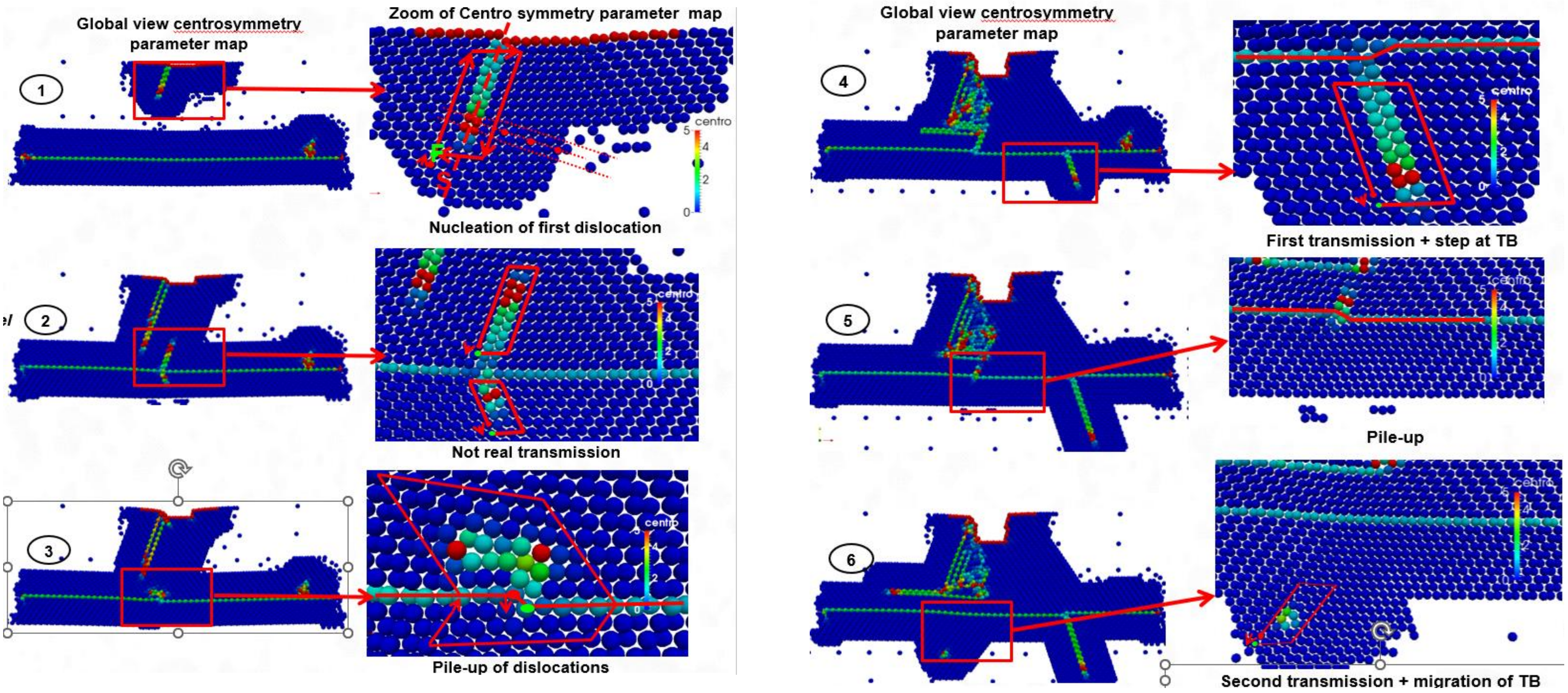


Optimized QC method
the material removal function is added,
Methods avoids unreasonable lattice excessive distortion, studies « large-area », deep dislocation slip.

→ Influence of the cutting depth, tool angle, rounded tool cutting edge radius
on the cutting force applied to a single-crystal copper workpiece

Yang et al. J Mat Processing 2021

QC- QuasiContinuum - Applications - Fundamental Science



Can a Dislocation cross a Coherent Twin Grain Boundary in cupper ? Tran Hoang Son et al ESAFORM 2017

QC- QuasiContinuum - References

The Quasicontinuum Method: Overview, applications and current directions **Miller, R.E., Tadmor, E.** *Journal of Computer-Aided Materials Design* **9**, 203–239 (2002). https://doi.org/10.1023/A:1026098010127

The Theory and Implementation of the Quasicontinuum Method. **Tadmor, E.B., Miller, R.E.** (2005). *In: Yip, S. (eds) Handbook of Materials Modeling. Springer, Dordrecht.* https://doi.org/10.1007/978-1-4020-3286-8_34

Principle, code feature

Free access to the code - tutorial - references see http://qcmethod.org/documentation

Open code feature + a community exchange platform

Multi-scale numerical analysis and experimental verification for nano-cutting **S. M. Yang, et al.** *Journal of Manufacturing Processes, 71, 260-268 (2021)*

https://doi.org/10.1016/j.jmapro.2021.09.030

Cutting application

PF - Phase Field

Basic principles

Thermodynamic approach

Phase η_i Liquid, Solid, Eutectic, Dendrite, Precipitate, Solid-Solution, Grain 1, Grain 2, … Grain n (microstructure related info)

Variable associated to each phase: concentration c_i , density,… (phase feature related info)

Smooth **interface between phases** with finite widths (solid-solid, solid-liquid …)

Computation of System Energy,

microstructure evolution is the result of energy minimization

Interests Limits

Generic method

Solidification, sintering, crack nucleation and propagation, phase transformation, …

Open source code available

Data base available Calphad

Many parameters, energy functions to find

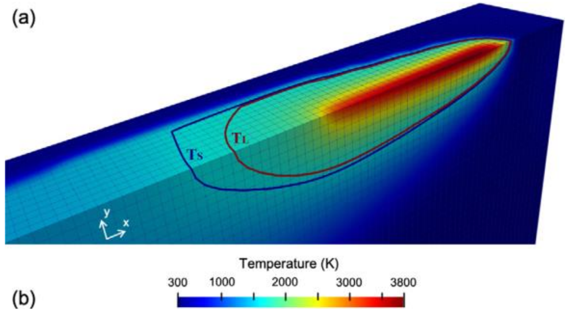
Request material scientist knowledge

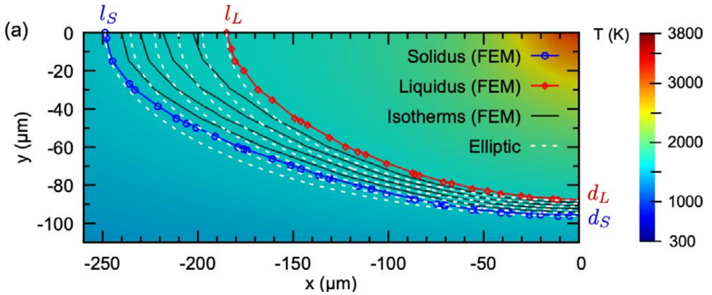
CPU can be very long

Nano to meso scale (grid nm², volume nm³)

The conserved fields like c_i evolve with time according to Cahn–Hilliard equation
The non-conserved fields (η_i) are governed by the Allen–Cahn equation

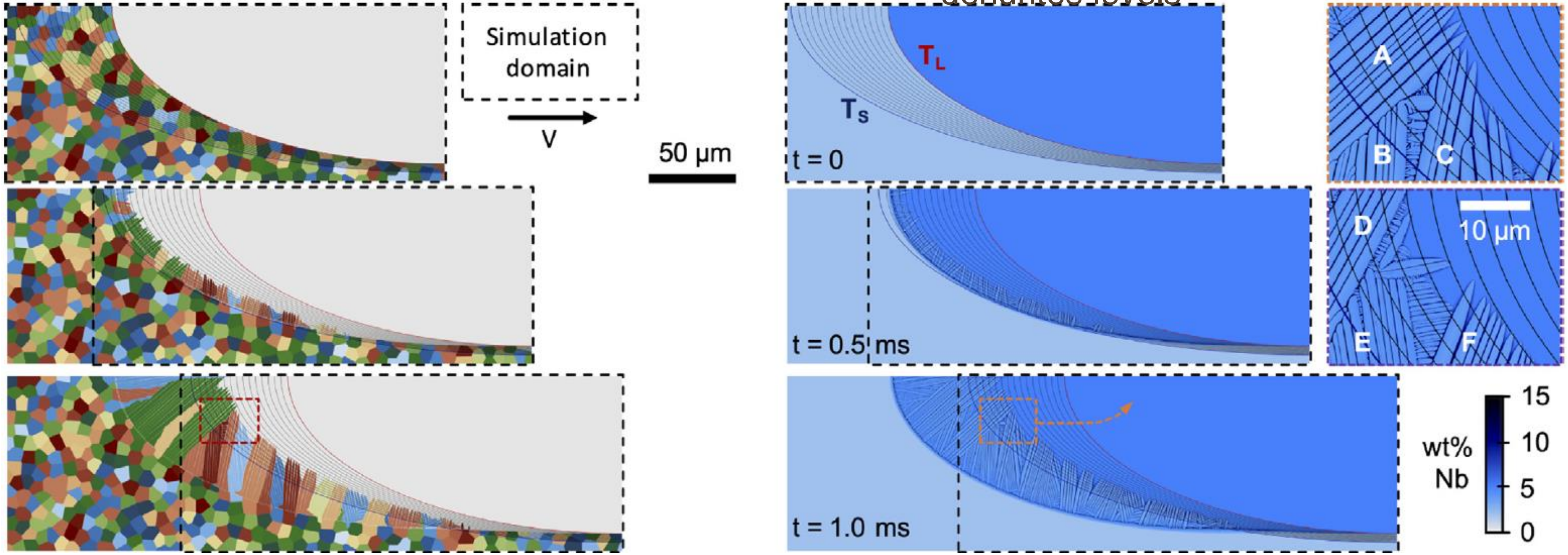
PF - Phase Field - Applications LPBF: FEM + PF





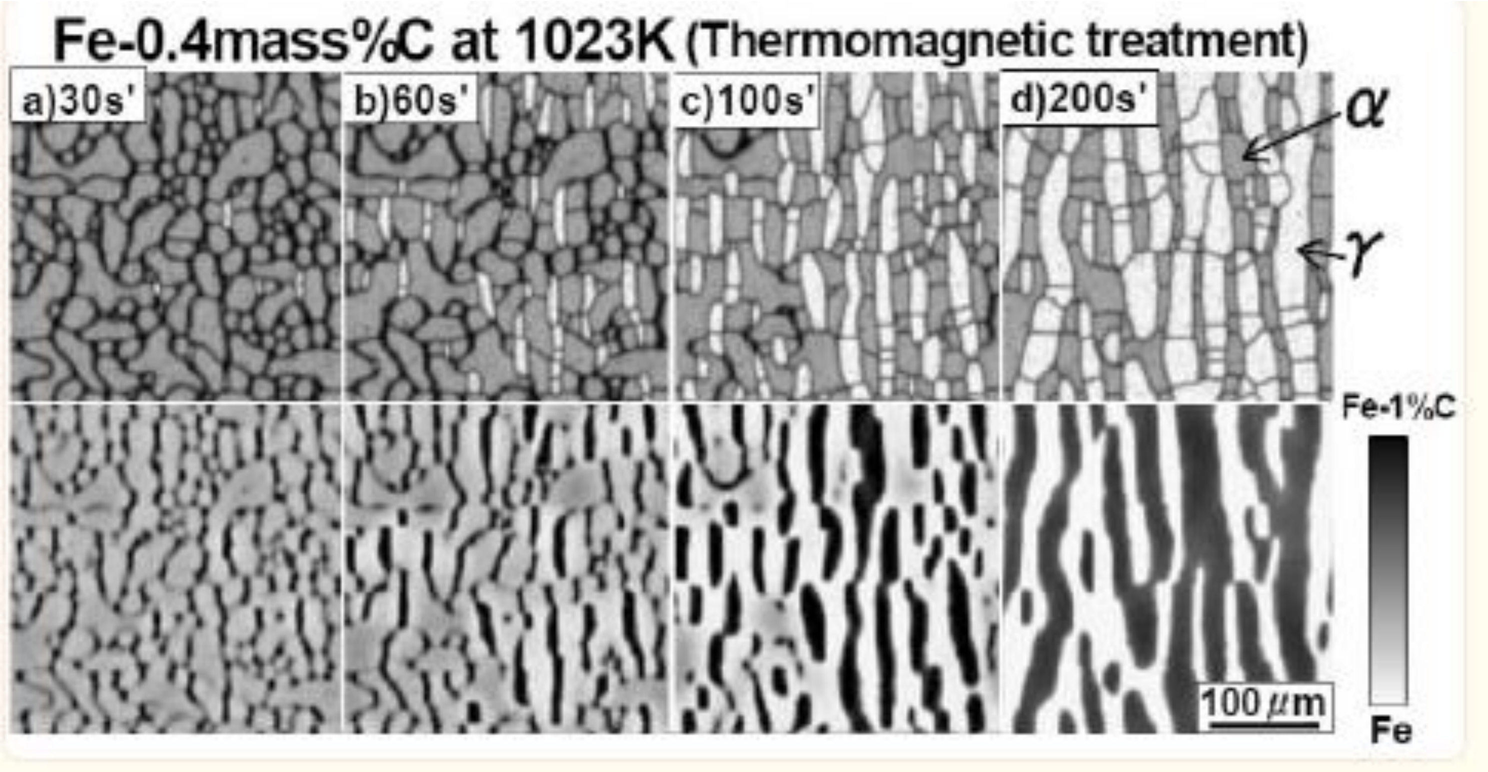
FEM thermal simulations of the material addition and fusion,
PF simulations of solidification in the melt pool.

Inconel 718 grain texture via polycrystalline growth competition under at individual dendrites levels



Elah et al. Computational Material Science 2022

PF - Phase Field – Applications- Phase Transformation

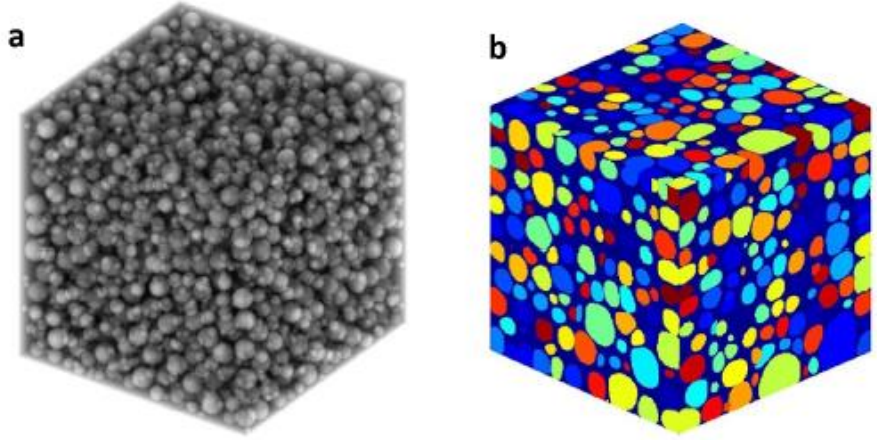


Phase-field modeling of microstructure evolutions in magnetic materials

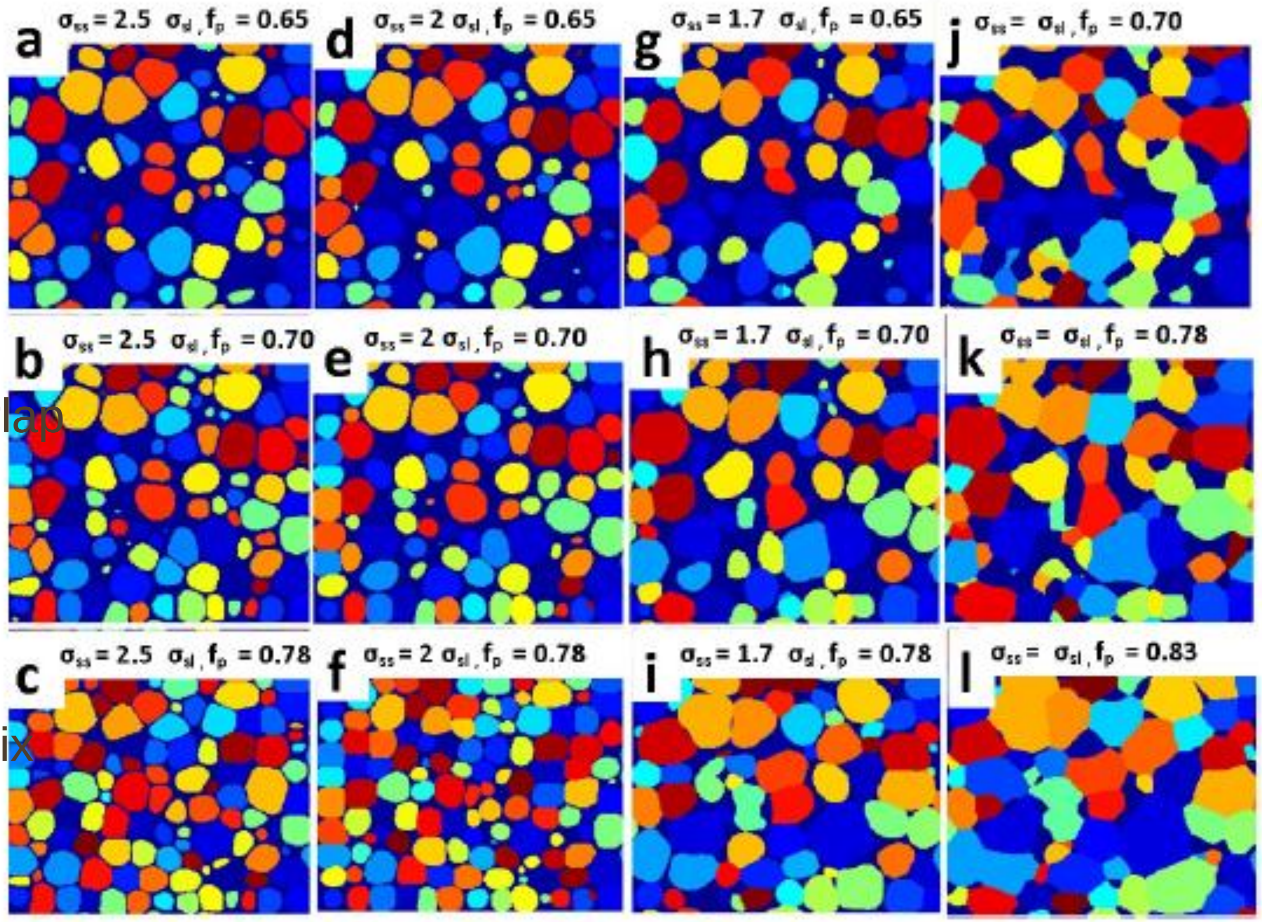
[Toshiyuki Koyama]

2D PF simulation of phase transformation and microstructure development in Fe-0.4 mass%C at 1023 K with external magnetic field along vertical direction

PF - Phase Field - Applications Sintering



5000 solid particles randomly placed without overlap



Liquid Sintering model
From fully connected grain structures with
liquid pockets at the grain junctions
to individual grains fully wetted by the liquid matrix

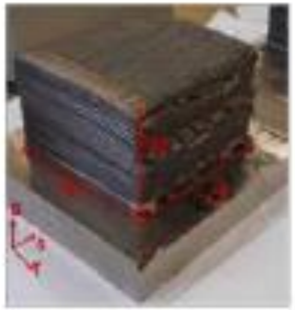
Simulations: sensitivity analysis
-solid-solid grain boundary energies/solid-liquid interface energies ratios [1 -2.5]
-particle volume fraction f_p and [0.65 -0.83]

Ravash, H. *et al.* Europ. J. Ceramic Soc. 2017

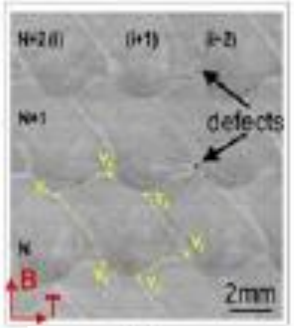
Ready to use different scales ?

Different experiments?

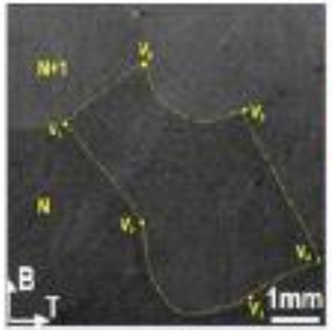
316L WAAM study



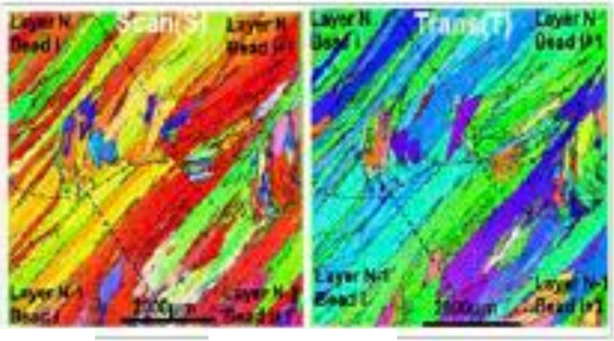
Dépôt



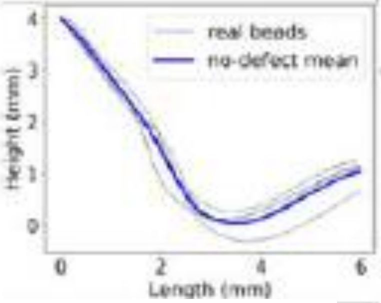
Optique



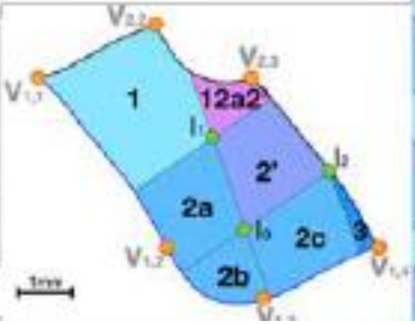
MEB Ferrite Austenite



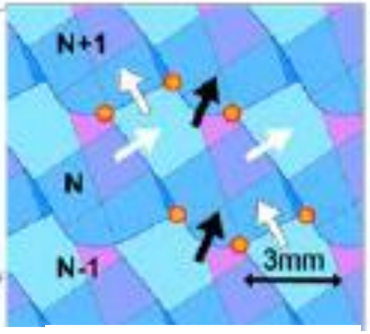
EBSD



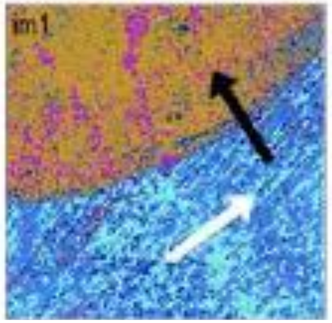
Modèle forme cordon



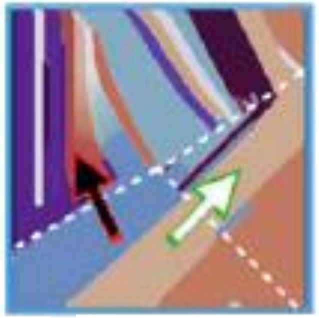
Zones orientation cristal.



Maillage 2D



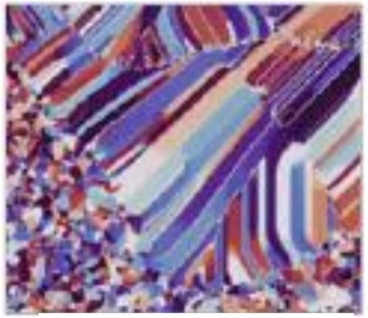
Identif. Interface



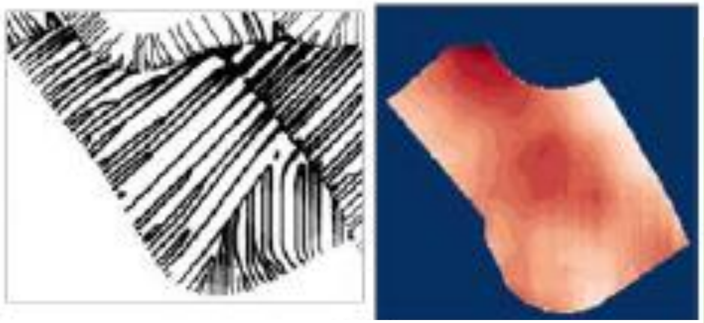
Résultat PF continuité

Résultat PF orientation

Résultat IA Ferrite % via image MEB



Maillage complet PF



Résultat PF Ferrite % Maillage complet

PhD A. Herbeaux
Saint Etienne
14/02/2023
Example of numerical & experimental work

PF - Phase Field - References

Phase-Field Methods in Material Science and Engineering **N. Provatas and K. Elder** Wiley-VCH ed 2010

ISBN: 978-3-527-40747-7

An introduction to phase-field modeling of microstructure evolution **Moelans N. et al.** Calphad - *Computer Coupling of Phase Diagrams and Thermochemistry 32 (2008)*

Principle, Introduction

https://doi.org/10.1016/j.calphad.2007.11.003

Multiscale simulation of powder-bed fusion processing of metallic alloys **S.M. Elahi et al.** *Computational Materials Science 209 (2022) 111383*

Process simulation LPBF FEM + PF

https://doi.org/10.1016/j.commatsci.2022.111383

Three-dimensional phase-field study of grain coarsening and grain shape accommodation in the final stage of liquid-phase sintering. **Ravash, H. al.** *Journal of the European Ceramic Society; 2017*

https://doi.org/10.1016/j.jeurceramsoc.2017.01.001

Process simulation sintering

Phase-field modeling of microstructure evolutions in magnetic materials **Toshiyuki Komaya** *Sci Technol Adv Mater*

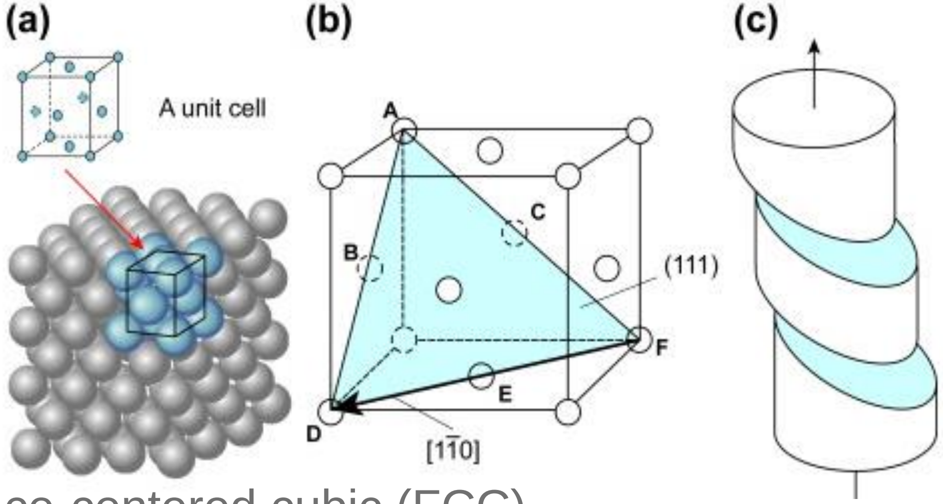
https://doi.org/10.1088/1468-6996/9/1/013006

Modeling Magnetic effect

CP - Crystal Plasticity

Basic principles

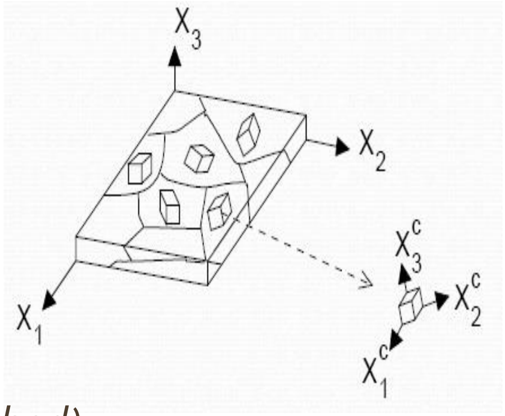
Dislocation slip computation in certain plane and direction due to a stress



(a) Face-centered cubic (FCC)
(b) a particular slip system (111)[1$\bar{1}$0] ;
(c) effect of single slip in a single crystal.

Slip Systems activated?
Notion of Critical Resolved Shear Stress reached
Or Viscoplasticity (easier)
Texture evolution due to crystal rotation under stress

Texture



Interests Limits

Implemented in FEM (Finite Element Method)

Multiple commercial and academic softwares

either CPFEM (Material Science) or with a different Homogenization schemes → process models

Multiscale approach FE^2 and other ones → process models

Implemented FFT Fast Fourrier Transformation

for cubic volume, periodic boundary conditions

→ material science

Open source software DAMASK (coupling FEM and FFT)

→ also adapted to handle process models

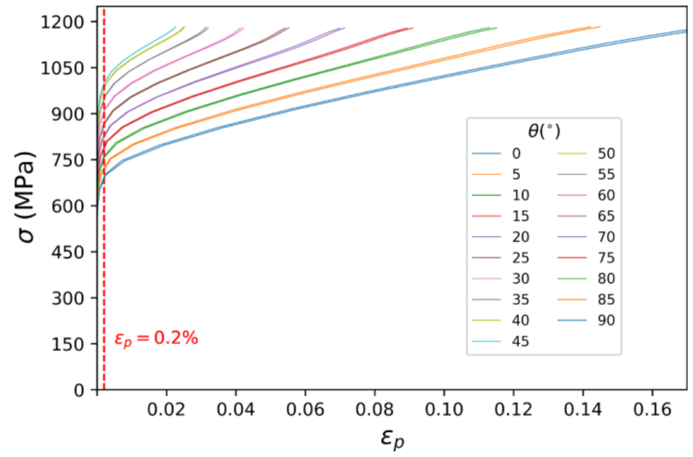
CP adapted for single and for polycrystals

CP applied for Metals but also Ice, …

Focused on Large strain - Large deformation but linked with Elasticity

CP - Crystal Plasticity – Applications - FEM

Representative Volume Element (RVE) synthetic microstructure.



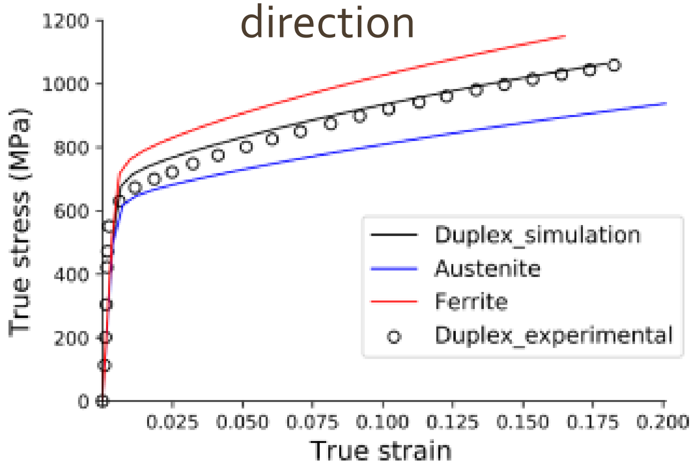
Abaqus mesh:
Austenite grains =Green,
Ferrite ones = White

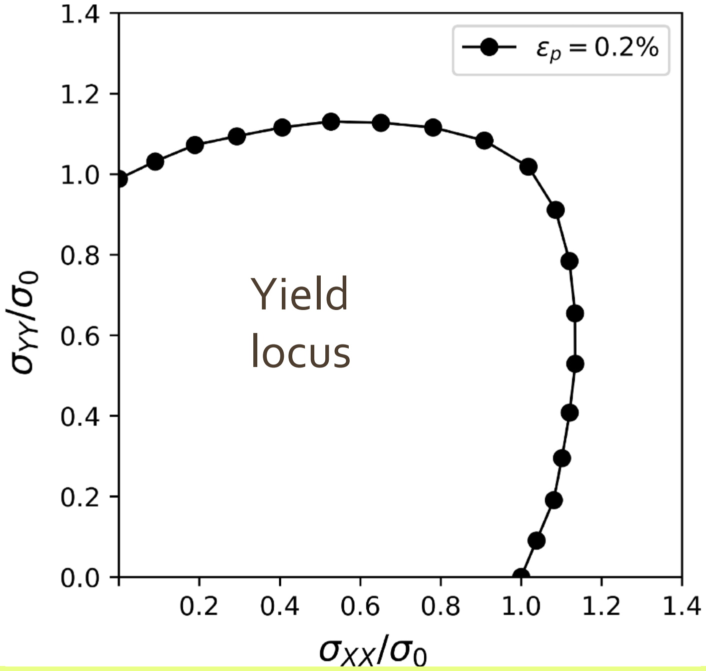
What is called CPFEM

The homogenisation is done by the RVE itself

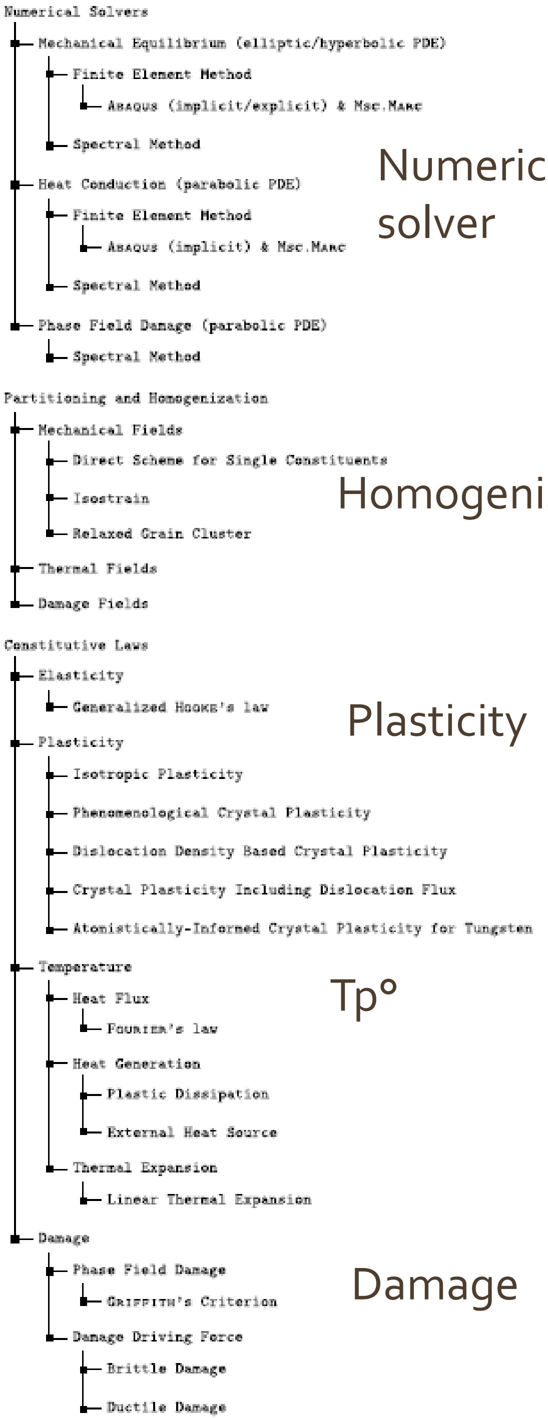
No assumption of total or partial equality in macro strain and micro strain
No loop on set of crystals f or self consistent approach

Tensile curve in a reference direction





CP - Crystal Plasticity – Applications - FFT



- Numerical Solvers
  - Mechanical Equilibrium (elliptic/hyperbolic PDE)
    - Finite Element Method
      - Abaqus (implicit/explicit) & Msc.Marc
    - Spectral Method
  - Heat Conduction (parabolic PDE)
    - Finite Element Method
      - Abaqus (implicit) & Msc.Marc
    - Spectral Method
  - Phase Field Damage (parabolic PDE)
    - Spectral Method
- Partitioning and Homogenization
  - Mechanical Fields
    - Direct Scheme for Single Constituents
    - Isostrain
    - Relaxed Grain Cluster
  - Thermal Fields
  - Damage Fields
- Constitutive Laws
  - Elasticity
    - Generalized Hooke's law
  - Plasticity
    - Isotropic Plasticity
    - Phenomenological Crystal Plasticity
    - Dislocation Density Based Crystal Plasticity
    - Crystal Plasticity Including Dislocation Flux
    - Atomistically-Informed Crystal Plasticity for Tungsten
  - Temperature
    - Heat Flux
      - Fourier's law
    - Heat Generation
      - Plastic Dissipation
      - External Heat Source
    - Thermal Expansion
      - Linear Thermal Expansion
  - Damage
    - Phase Field Damage
      - Griffith's Criterion
    - Damage Driving Force
      - Brittle Damage
      - Ductile Damage

Numerical solver

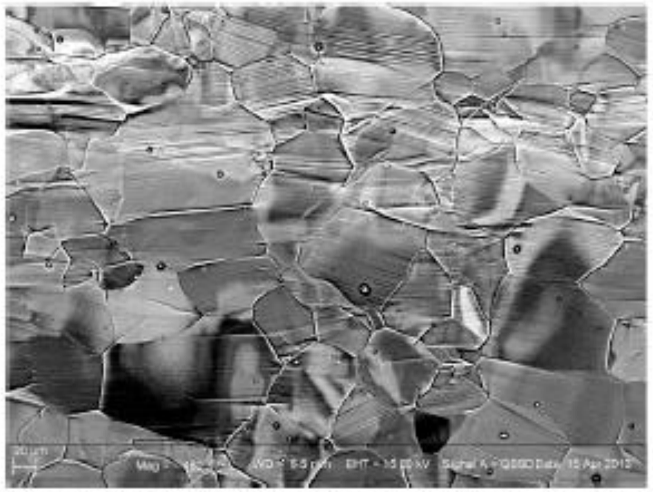
Homogenisation

Plasticity

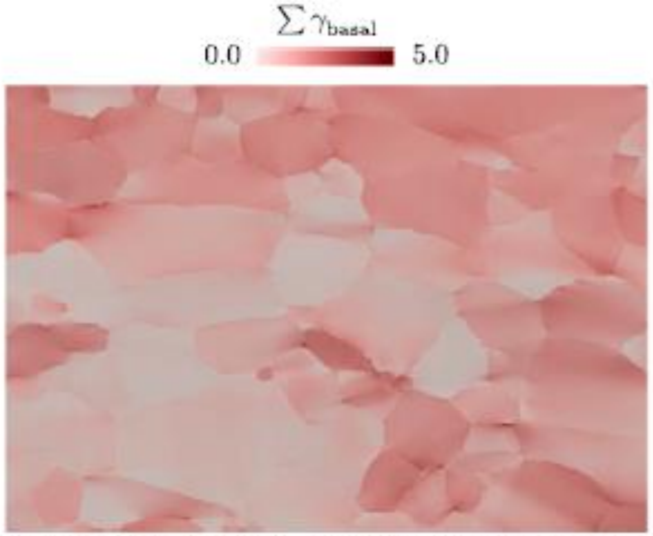
Tp°

Damage

DAMASK Flowchart



(a) Experimental result obtained by Electron Channeling Contrast Imaging (ECCI).



(b) Results of the Crystal Plasticity (CP) simulations: Magnitude of shear on all basal slip systems.

Tp° dependent activation of twinning induced plasticity (TWIP) and transformation induced plasticity (TRIP) in high-Manganese steel (Fe-22Mn-0.6C)

RVE with FFT 100 grains + tensile experiments + different data bases (austenite, HCP phases) including thermodynamic ones

→identification of TRIP/TWIP models
Results = Twin fraction, Martensite %, stress-strain curves predictions
This type of constitutive law can then be used in a thermomechanical process.

CP - Crystal Plasticity - References

Modeling in Crystal Plasticity: From Theory to Application **Weiling Wang, Wei Wen**, Encyclopedia of Materials: Metals and Alloys *2022*

https://doi.org/10.1016/B978-0-12-819726-4.00058-2

Modelling the plastic anisotropy of metals**. Habraken, A**. *Archives of Computational Methods in Engineering, 11, 3-96 (2004)*.

https://doi.org/10.1007/BF02736210

Principle, Introduction

Analysis of ESAFORM 2021 cup drawing benchmark of an Al alloy, critical factors for accuracy and efficiency of FE simulations. **Habraken et al**. *Int. J. Mat. For.*, 15 (5), 61.

https://doi.org/ 10.1007/s12289-022-01672-w

Homogenization for polycrystal

Multi-scale material modelling to predict the material anisotropy of multiphase steels **Ravi S.K. et al.** Computational Materials Science; 2019

https://doi.org/10.1016/j.commatsci.2019.01.028

Application in Deep Drawing

DAMASK – The Düsseldorf Advanced Material Simulation Kit for modeling multi-physics crystal plasticity, thermal, and damage phenomena from the single crystal up to the component scale **F. Roters et al.** *Computational Materials Science 158 (2019) 420–478*

https://doi.org/10.1016/j.commatsci.2018.04.030

Multi physic software linking FEM and FFT

https://damask.mpie.de/

What are the **important phenomena** in your process ? What are their **scales**?

What is your access to software and to skilled scientists? Which time for training?

Which data are available?

MD
Molecular Dynamics

DDD
Discrete Dislocation Dynamics

QC
Quasi Continuum

PF
Phase Field

CP
Crystal Plasticity

Macro
For large components

Artificial Intelligence ? Can be applied at any scales!!!

- Used to help to identify your models (post treatment of images, process data by multiple sensors, digitalize curves…)
- Trained by your complex constitutive laws → able to replace it?
- Trained on the "process parameters-final properties" link (measured or computed)

A. Tongne HDR-ENIT Tarbes ENIT, Chap 2, good introduction 8/2/2024

Contents

✓A survey of scales and methods

- Finite element method FEM
  - One element: Solid Shell
  - Mechanical constitutive laws (multi scale ?)
    - Deep Drawing
  - Thermo-mechanical analysis
    - Cooling of rolling mills
    - Continuous casting
- Representative Volume Element (RVE) or in French VER
- Coupling solid FEM with … Computational Fluid Dynamics, Deep Learning
  - Additive Manufacturing

Very Basic FEM Flowchart

Many choices if generic FE softwares

1. Analysis

Thermal, **M**echanical, **M**etallurgical, **Scale** Macro or Micro

2. Level of coupling

Total, partial coupling or staggered (meeting points, different or similar meshes)

3. Boundary conditions
4. Mesh density, type of element and of constitutive laws
5. Solver
6. Iterative loop on equilibrium, energy balance, …
7. Results to plot and **check**

Less choices if customized FE softwares

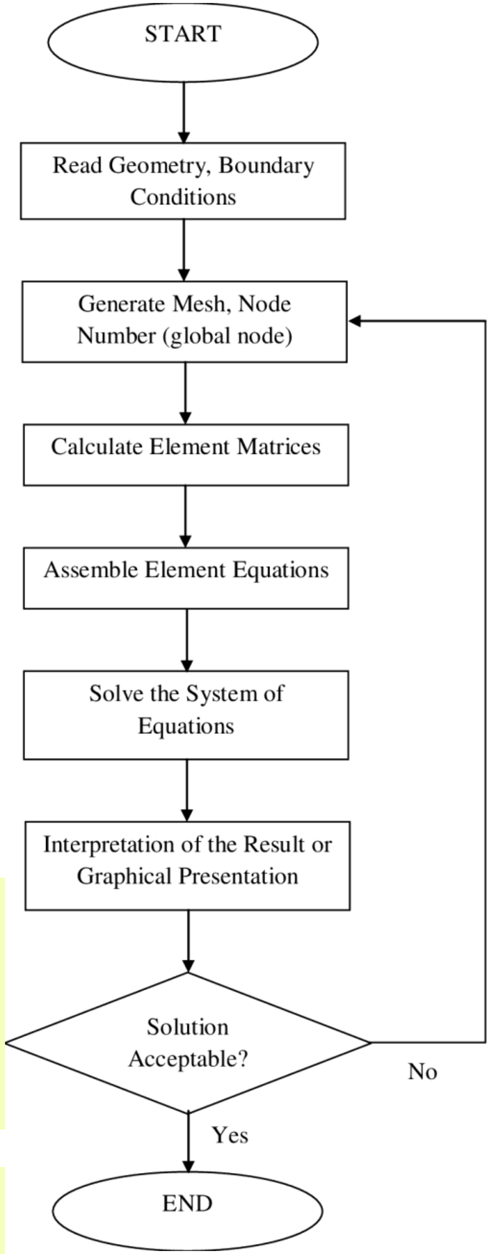
Still Researches with FEM ?

Element

Constitutive laws

Efficient computer sciences (solvers, coupling, pre and post processing…)

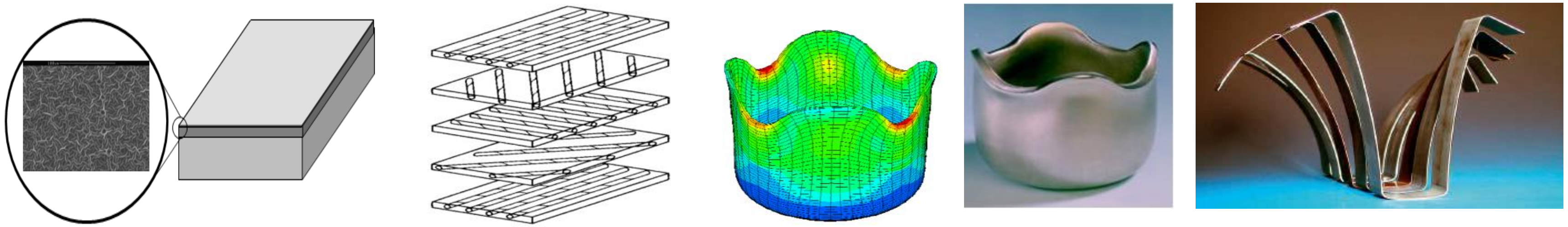
Alternatives: Meshless, Coupled Eulerian Lagrangian, Arbitrary Lagrangian Eulerian, Particle-FEM: PFEM, Artificial Intelligence (big family)

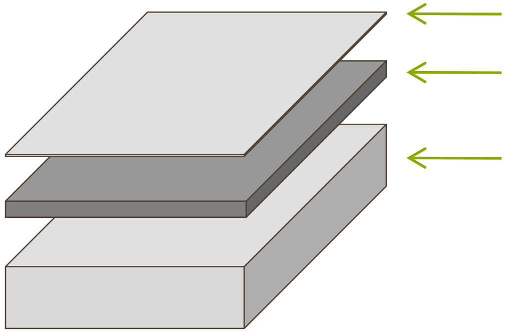


FEM - A solid shell element… Why?

Applications:

- Thin structures
- Multilayer materials: Coating , composite …
- Sheet metal forming, anisotropy, springback ...
- Composites





Aluminum film (t=50nm)

Polymer layer (t=5μm)

Steel sheet (t=0.27mm)

x 100

x 54

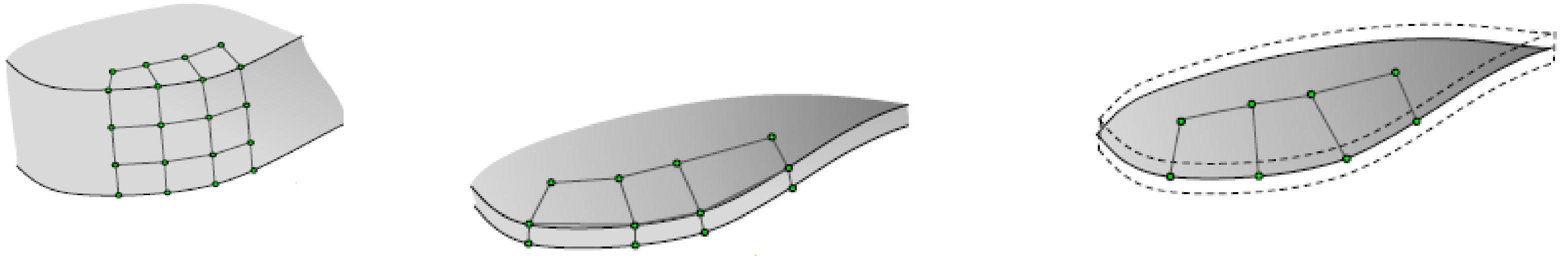
large incompatibilities between layer thicknesses

Poor behaviour
of thin **Bulk element**
with plane size/ thickness > 10

Thickness, Through Thickness
behavior in **Shell elements** ~~OK~~

Crystal Plasticity
= 3D constitutive law

FEM - A solid shell element… What is it ?



Solid

Solid-Shell

3 DOFs per node:
3 Displacements

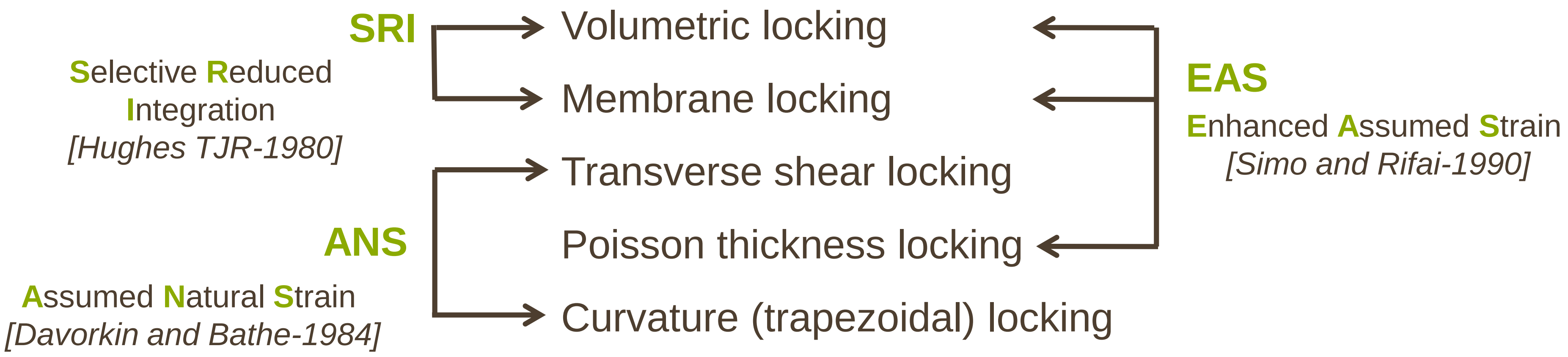
Shell
6 DOFs per node:
3 Displacements
3 Rotations

Due to their geometry, thin bulk solids have plenty of lockings → special features of Solid Shell Solid Shell

❖Volumetric locking:
❖Membrane locking
❖Transverse shear locking
❖Poisson thickness locking
❖ Curvature thickness (Trapezoidal) locking

FEM - A solid shell element…Features

- Some remedies for locking pathologies



SRI

Selective **R**educed **I**ntegration
[Hughes TJR-1980]

ANS

Assumed **N**atural **S**train
[Davorkin and Bathe-1984]

Volumetric locking

Membrane locking

Transverse shear locking

Poisson thickness locking

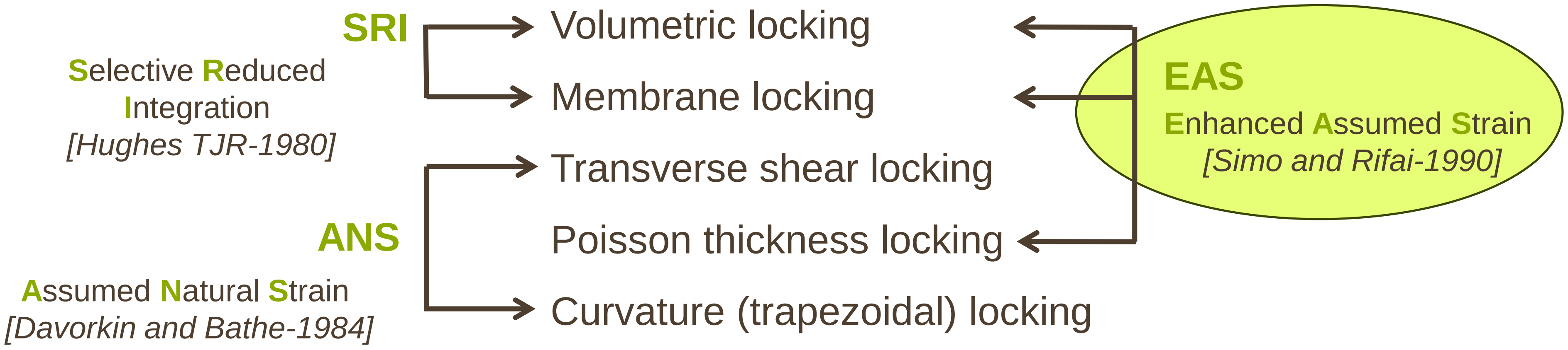
Curvature (trapezoidal) locking

EAS

Enhanced **A**ssumed **S**train
[Simo and Rifai-1990]

FEM - A solid shell element…Features

- Some remedies for locking pathologies



SRI

Selective **R**educed **I**ntegration
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Assumed **N**atural **S**train
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Volumetric locking

Membrane locking

Transverse shear locking

Poisson thickness locking

Curvature (trapezoidal) locking

EAS

Enhanced **A**ssumed **S**train
[Simo and Rifai-1990]

FEM - A solid shell element… One variational principle choice

- The Hu-Washizu variational principle (3 unknown fields) :

Mech work equilibrium

$$\int_{\mathscr{B}} \nabla^s \underline{\eta}.\underline{\sigma} dv - G_{ext}(\underline{\eta}) = 0$$

Strain field OK ?

$$\int_{\mathscr{B}} \underline{\tau}.\left[\nabla^s \underline{\eta} - \underline{\varepsilon}\right] dv = 0$$

Stress Field OK?

$$\int_{\mathscr{B}} \underline{\gamma}.[-\underline{\sigma} + \underline{\sigma}^m(\underline{x},\underline{q},\underline{\varepsilon})] dv = 0$$

$$\left.\right\} \text{for all variations} \begin{bmatrix} \underline{\eta} \\ \underline{\gamma} \\ \underline{\tau} \end{bmatrix} \text{of the} \left\{\begin{array}{c} \text{displacement} \\ \text{strain} \\ \text{stress} \end{array}\right\} \text{fields} \begin{bmatrix} \underline{u} \\ \underline{\varepsilon} \\ \underline{\sigma} \end{bmatrix}$$

∇^s	the symmetric gradient
$G_{ext}(\underline{\eta})$	the virtual work of the external loading
$\underline{\sigma}^m(\underline{x},\underline{q},\underline{\varepsilon})$	the stress computed by the constitutive law

FEM A solid shell element… EAS modes

Or Enhanced Assumed Strain field:

$$\underline{\varepsilon} = \underline{\varepsilon}^{com} + \underline{\varepsilon}$$

Enhanced part of the strain field

Compatible part of the strain field

$$= \underline{\underline{G}}(\xi,\eta,\zeta).\underline{\alpha}$$

$$= \frac{j_0}{j(r,s,t)}.\underline{\underline{F}}_0^{-T}.\underline{\underline{M}}(\xi,\eta,\zeta).\underline{\alpha}$$

$$= \nabla^s \underline{u} = \underline{\underline{B}}(\xi,\eta,\zeta).\underline{U}$$

Displacement DOF's (24)

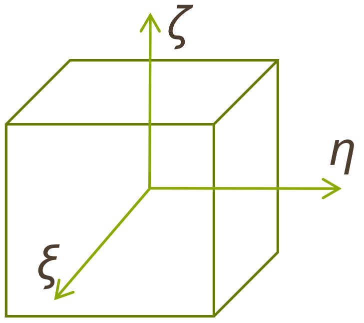
Classical B-matrix

$\underline{\alpha}$ **EAS DOF's (user defined)**

$$\left.\begin{matrix}\underline{\underline{G}}(\xi,\eta,\zeta)\\ \underline{\underline{M}}(\xi,\eta,\zeta)\end{matrix}\right\}\text{EAS modes}$$

$\underline{\underline{F}}_0^{-T}$ transformation matrix from ξ, η, ζ to x, y, z coordinates

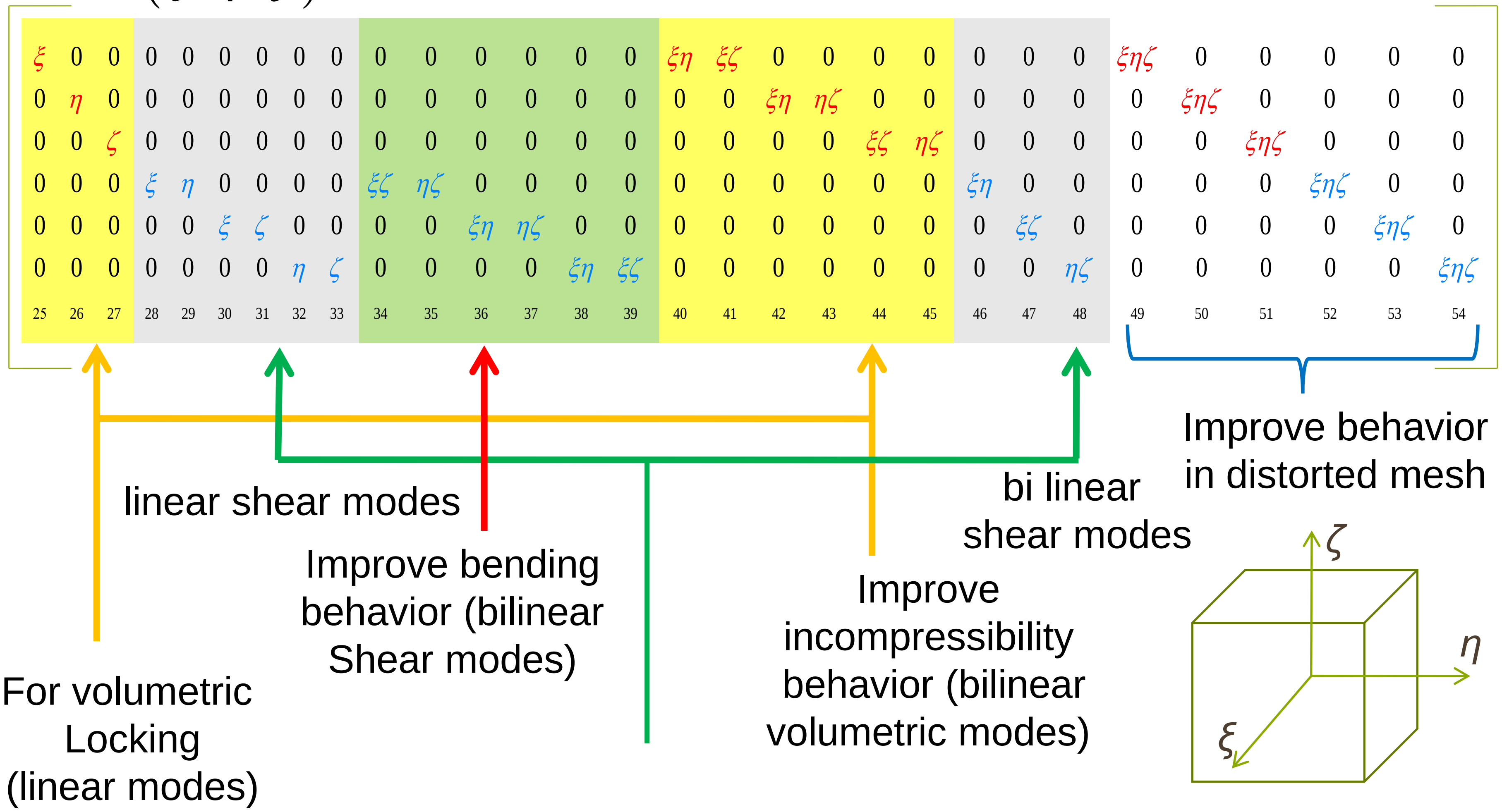
j Jacobian determinant



ξ, η, ζ : intrinsic coordinates (∈ [-1,1])

Possible choices of EAS (Enhanced Assumed Strain modes)

→ New EAS DOF's (user defined)
Solved at the element level



$$\underline{M}(\xi,\eta,\zeta)=\left[\begin{array}{cccccccccccccccccccccccccccccc}
\xi & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\eta & \xi\zeta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\eta\zeta & 0 & 0 & 0 & 0 & 0 \\
0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\eta & \eta\zeta & 0 & 0 & 0 & 0 & 0 & 0 & \xi\eta\zeta & 0 & 0 & 0 & 0 \\
0 & 0 & \zeta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\zeta & \eta\zeta & 0 & 0 & 0 & 0 & 0 & \xi\eta\zeta & 0 & 0 & 0 \\
0 & 0 & 0 & \xi & \eta & 0 & 0 & 0 & 0 & \xi\zeta & \eta\zeta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\eta & 0 & 0 & 0 & 0 & 0 & \xi\eta\zeta & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \xi & \zeta & 0 & 0 & 0 & 0 & \xi\eta & \eta\zeta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\zeta & 0 & 0 & 0 & 0 & 0 & \xi\eta\zeta & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \eta & \zeta & 0 & 0 & 0 & 0 & \xi\eta & \xi\zeta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \eta\zeta & 0 & 0 & 0 & 0 & 0 & \xi\eta\zeta \\
25 & 26 & 27 & 28 & 29 & 30 & 31 & 32 & 33 & 34 & 35 & 36 & 37 & 38 & 39 & 40 & 41 & 42 & 43 & 44 & 45 & 46 & 47 & 48 & 49 & 50 & 51 & 52 & 53 & 54
\end{array}\right]$$

Improve behavior in distorted mesh

linear shear modes

bi linear shear modes

Improve bending behavior (bilinear Shear modes)

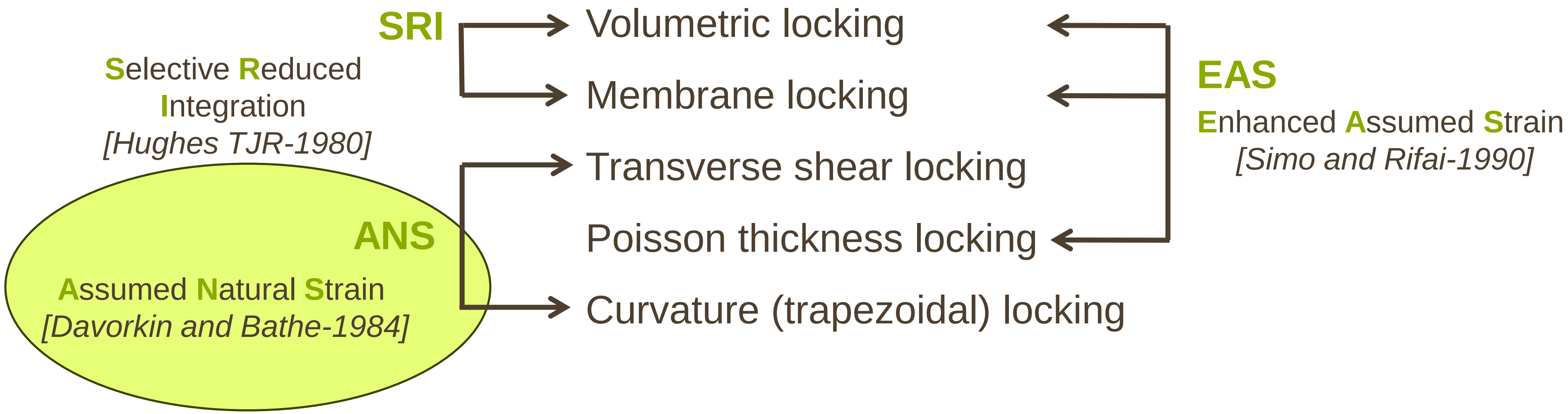
Improve incompressibility behavior (bilinear volumetric modes)

For volumetric Locking (linear modes)

How many to add? From 3 to 30 modes

FEM A solid shell element…Features

- Some remedies for locking pathologies



SRI

Selective **R**educed **I**ntegration
[Hughes TJR-1980]

ANS

Assumed **N**atural **S**train
[Davorkin and Bathe-1984]

Volumetric locking

Membrane locking

Transverse shear locking

Poisson thickness locking

Curvature (trapezoidal) locking

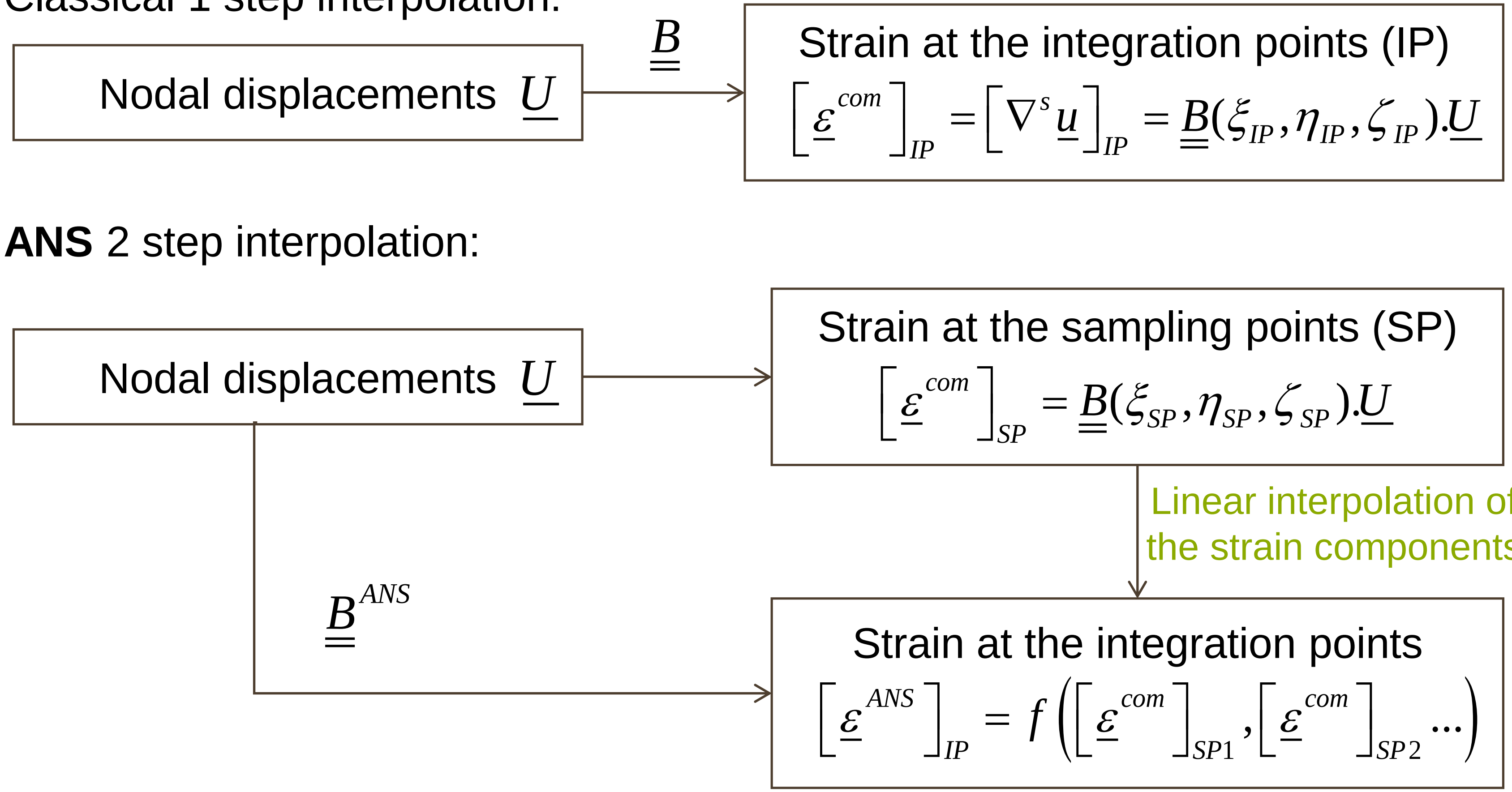
EAS

Enhanced **A**ssumed **S**train
[Simo and Rifai-1990]

FEM A solid shell element…ANS (Assumed Natural Strain)

Principle :

Classical 1 step interpolation:



Nodal displacements $\underline{U}$ $\xrightarrow{\underline{\underline{B}}}$

Strain at the integration points (IP)

$$\left[\underline{\varepsilon}^{com}\right]_{IP} = \left[\nabla^{s}\underline{u}\right]_{IP} = \underline{\underline{B}}(\xi_{IP},\eta_{IP},\zeta_{IP}).\underline{U}$$

ANS 2 step interpolation:

Nodal displacements $\underline{U}$

Strain at the sampling points (SP)

$$\left[\underline{\varepsilon}^{com}\right]_{SP} = \underline{\underline{B}}(\xi_{SP},\eta_{SP},\zeta_{SP}).\underline{U}$$

Linear interpolation of the strain components

$\underline{\underline{B}}^{ANS}$

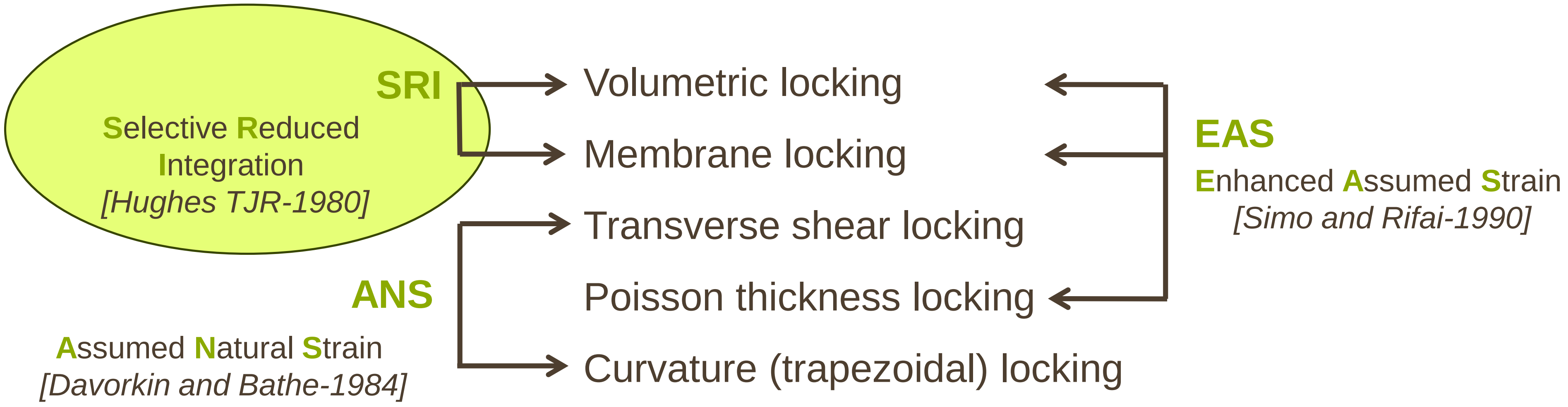
Strain at the integration points

$$\left[\underline{\varepsilon}^{ANS}\right]_{IP} = f\left(\left[\underline{\varepsilon}^{com}\right]_{SP1},\left[\underline{\varepsilon}^{com}\right]_{SP2}\ldots\right)$$

Many choices possible

FEM A solid shell element…Features

- Some remedies for locking pathologies



SRI

Selective **R**educed Integration
[Hughes TJR-1980]

ANS

Assumed **N**atural **S**train
[Davorkin and Bathe-1984]

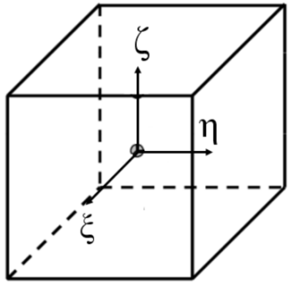
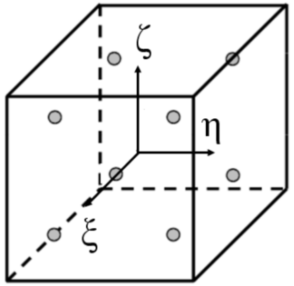
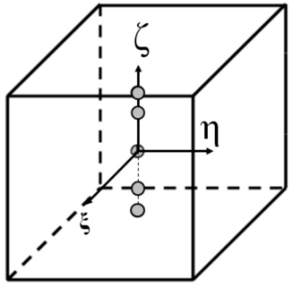
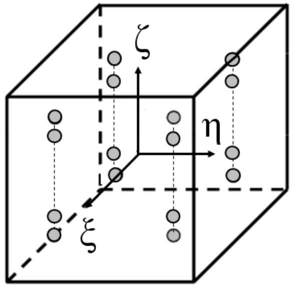
Volumetric locking
Membrane locking
Transverse shear locking
Poisson thickness locking
Curvature (trapezoidal) locking

EAS

Enhanced **A**ssumed **S**train
[Simo and Rifai-1990]

FEM A solid shell element…SRI Selective Reduced Integration

Comparative study considering 6 integration points through thickness

	Reduced integration scheme	Full integration scheme
Classical	 6 layers => 28 nodes => 6 IP **84 DOF’s**	 3 layers => 16 nodes => 24 IP **48 DOF’s**
Arbitrary number of IP over the thickness	 1 layer => 8 nodes => 6 IP **24 DOF’s**	 1 layer => 8 nodes => 24 IP **24 DOF’s**

FEM A solid shell element… Intensive parametric study

- **Conclusion ?** Effect of Material Behavior:

→ Linear elastic
2 IP over the element thickness OK
(linear through-thickness stress distribution)

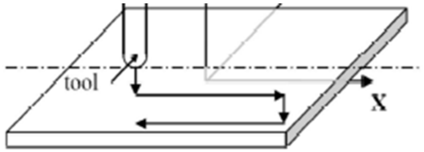
→ Non linear behavior

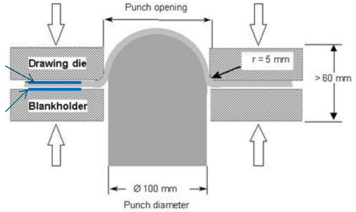
>5 IP over the element thickness to provide accurate results
(non-linear through-thickness stress distribution)

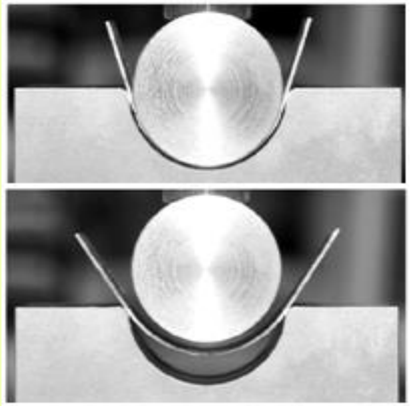
- ‘Solid tests’
- ‘Shell tests’
- ‘Beam test’
- ‘Sheet Metal Forming and coating’

Different choices of EAS and ANS are optimal

5 patch tests
1 incompressibility test
7 Membranne + Bending elastic linear tests
4 Non linear tests





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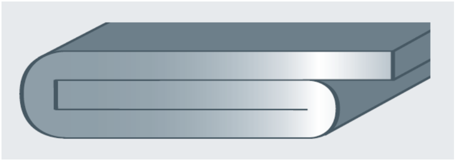

1T

FEM A solid shell References

A reduced integration solid-shell finite element based on the EAS and the ANS concept-Large deformation problems**, M. Schwarze, S. Reese** *Int. J. for Num. Methods in Eng.*, 85 (2011), 289-329

A new one-point quadrature enhanced assumed strain (EAS) solid-shell element with multiple integration points along thickness: Part I - geometrically linear applications, **R. J. Alves de Sousa et al.** *Int. J. for Num. Methods in Eng.,* 62 (2005), 952-977

A new one-point quadrature enhanced assumed strain (EAS) solid-shell element with multiple integration points along thickness - Part II: Nonlinear applications, **R. J. Alves de Sousa et al.** *Int. J. for Num. Methods in Eng.,* 67 (2006), 160-188

W. Van Paepegem, A. M. Habraken, J. Degrieck: A mixed solid-shell element for the analysis of laminated composites**, K. Rah et al.** *Int. J. for Num. Methods in Eng., 89 (2012), 805-828*

On the comparison of two solid-shell formulations based on in-plane reduced and full integration schemes in linear and non-linear applications, **A. B. Bettaieb et al.** *Finite Elements in Analysis and Design, 107 (2015), 44-59*

Different variants: Variational Principle, EAS, SRI, ANS

Comparison between de Souza and Bettaieb approach

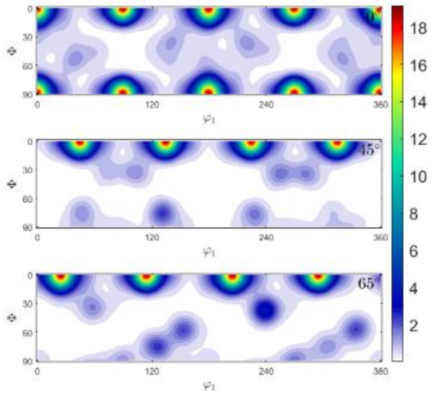
Contents

- ✓ A survey of scales and methods
- Finite element method FEM
  - ✓ One element: Solid Shell
  - Mechanical constitutive laws (multi scale ?)
    - Deep Drawing
  - Thermo-mechanical analysis
    - Cooling of rolling mills
    - Continuous casting
- Representative Volume Element (RVE) or in French VER
- Coupling solid FEM with … Computational Fluid Dynamics, Deep Learning
  - Additive Manufacturing

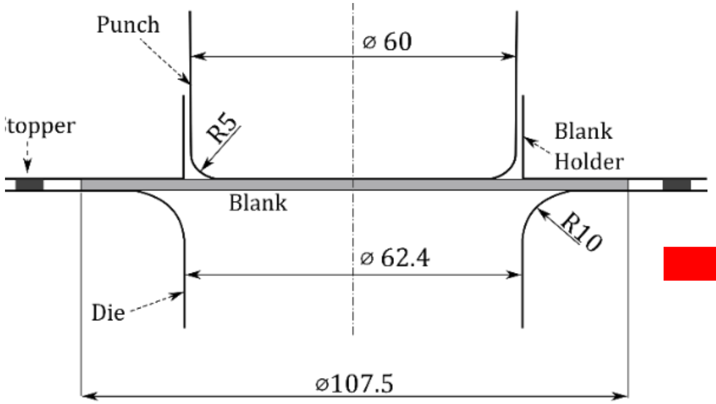
Experiment and FEM Simu. of AA6016 Cup Drawing Test

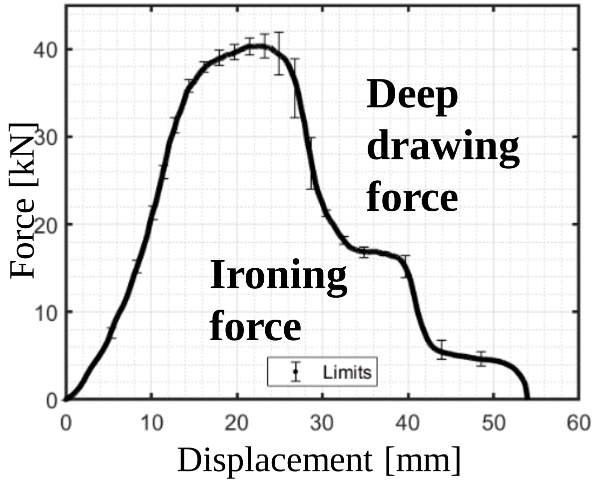
Cup drawing of a circular blank (Φ =107.5mm) of AA 6016 sheet

ESAFORM Benchmark 2021

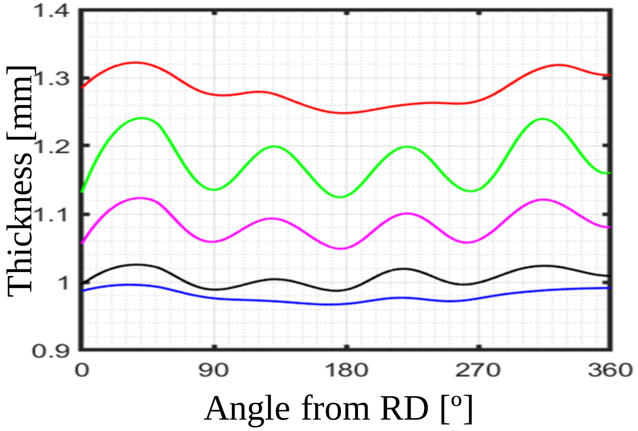


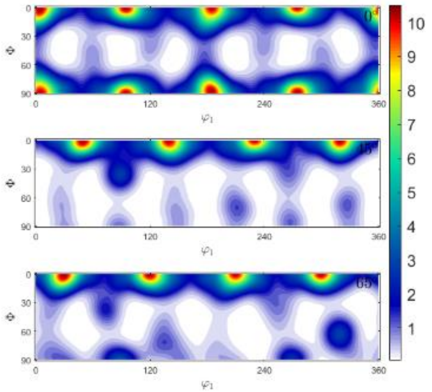
Initial texture





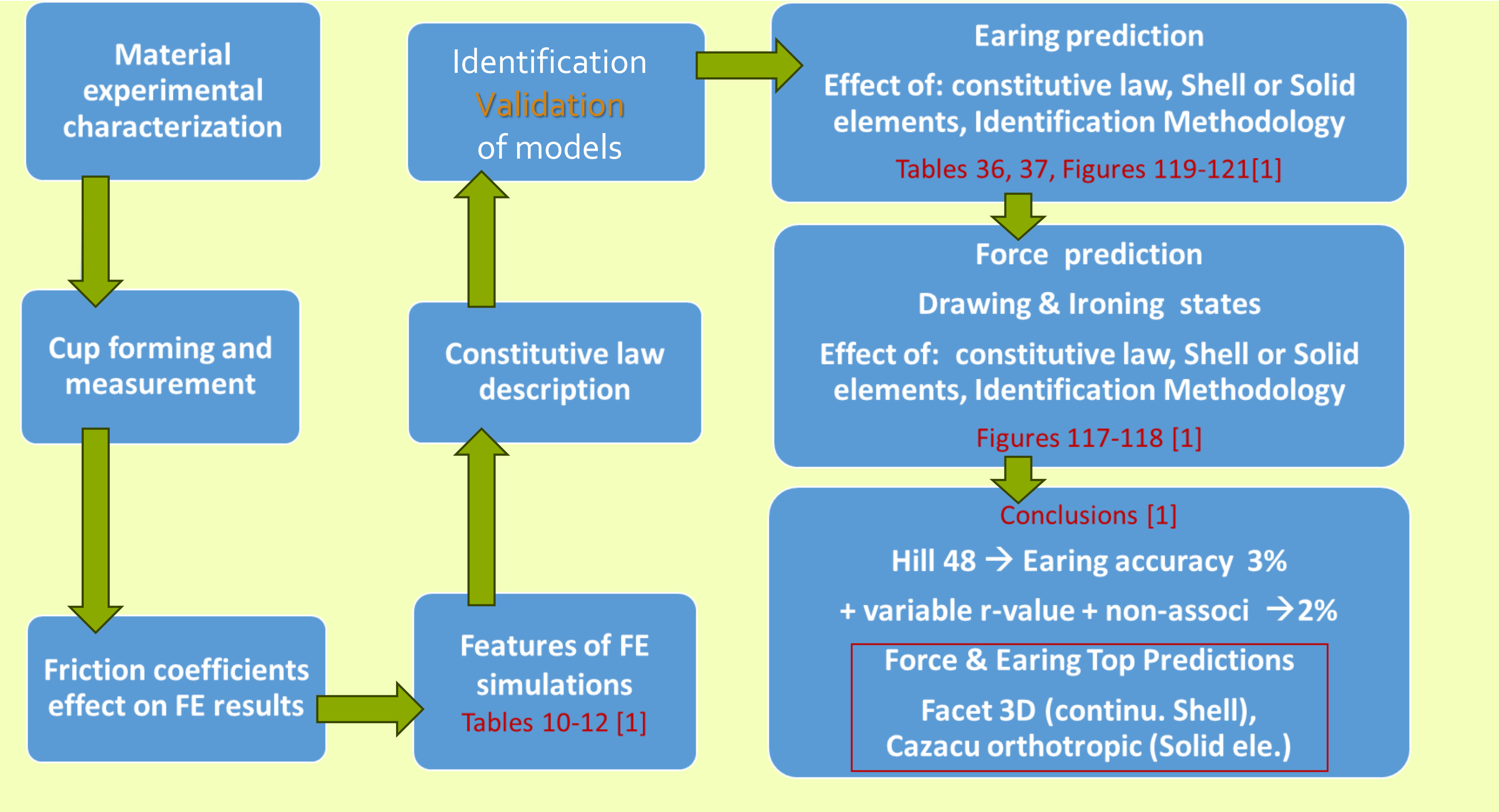
At different heights from cup bottom





Texture mid wall

FEM - Content of a collaborative work of 13 teams



Material experimental characterization

Cup forming and measurement

Friction coefficients effect on FE results

Features of FE simulations
Tables 10-12 [1]

Constitutive law description

Identification
Validation
of models

Earing prediction

Effect of: constitutive law, Shell or Solid elements, Identification Methodology

Tables 36, 37, Figures 119-121[1]

Force prediction

Drawing & Ironing states

Effect of: constitutive law, Shell or Solid elements, Identification Methodology

Figures 117-118 [1]

Conclusions [1]

Hill 48 → Earing accuracy 3%

+ variable r-value + non-associ →2%

Force & Earing Top Predictions

Facet 3D (continu. Shell),
Cazacu orthotropic (Solid ele.)

Int. J. Material Forming Habraken et al. 2022 (40 authors)

FEM Codes, elements, contact / constitutive laws/ identification

FE Code
ABAQUS (explicit & implicit), DD3IMP, Lagamine, MARC, LS-DYNA, PAMSTAMP

F Element
Different types of Shell and Solid elements and refinements

Contact model
Penalty, Surface to Surface,..., Large range of constant friction coefficients

Experimental data
Texture; Tensile tests; Monotonic and reverse shear tests; bi-axial tests

Crystal plasticity laws used for identification of phenomenological models
Facet 3D & ALAMEL, DAMASK, Full Taylor Model, Visco-Plastic Self-Consistent (VPSC)

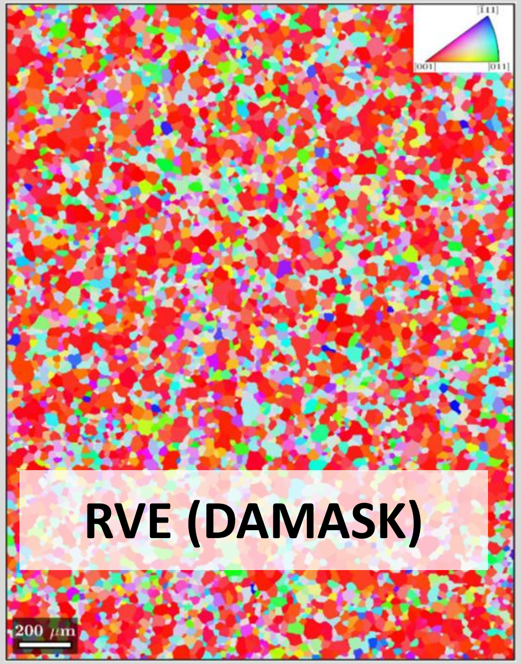
Analytical yield laws
2D and 3D yield laws of Barlat and Cazacu (Yld89, Yld2000-2D, CB2001, Yld2004–18p, CPB06); Cazacu single crystal; associated & non associated Hill'48; Cazacu orthotropic (Caz2018-Orth), 4th and 6th polynomial models (HomPol4 & 6)

Polycrystalline Models (CP-FEM)
Minty, Cazacu Polycrystal

Hardening model - Isotropic: Voce, Swift; - Kinematic: Armstrong Frederick

FEM Multiscale : different ways to exploit Crystal plasticity

Texture input → Homogenization procedure for Crystal Plasticity models



+

Crystal data set:
from 250
(Caz2018polycrys)
to 10.000 grains
(ALAMEL)

Homogenization Approach

Full Taylor assumption
$\varepsilon^{Macro} = \varepsilon^{Micro}$
(**Minty, Cazacu polycrystal**)

$\varepsilon^{Macro} = \varepsilon^{Applied\ on\ RVE}$
(**DAMASK** spectral method)

Relaxed Taylor assumption
& cluster of grains
(**ALAMEL**)

Self Consistent approach,
(**VPSC**)

Constitutive law

Data set used for Identification:

Texture

+

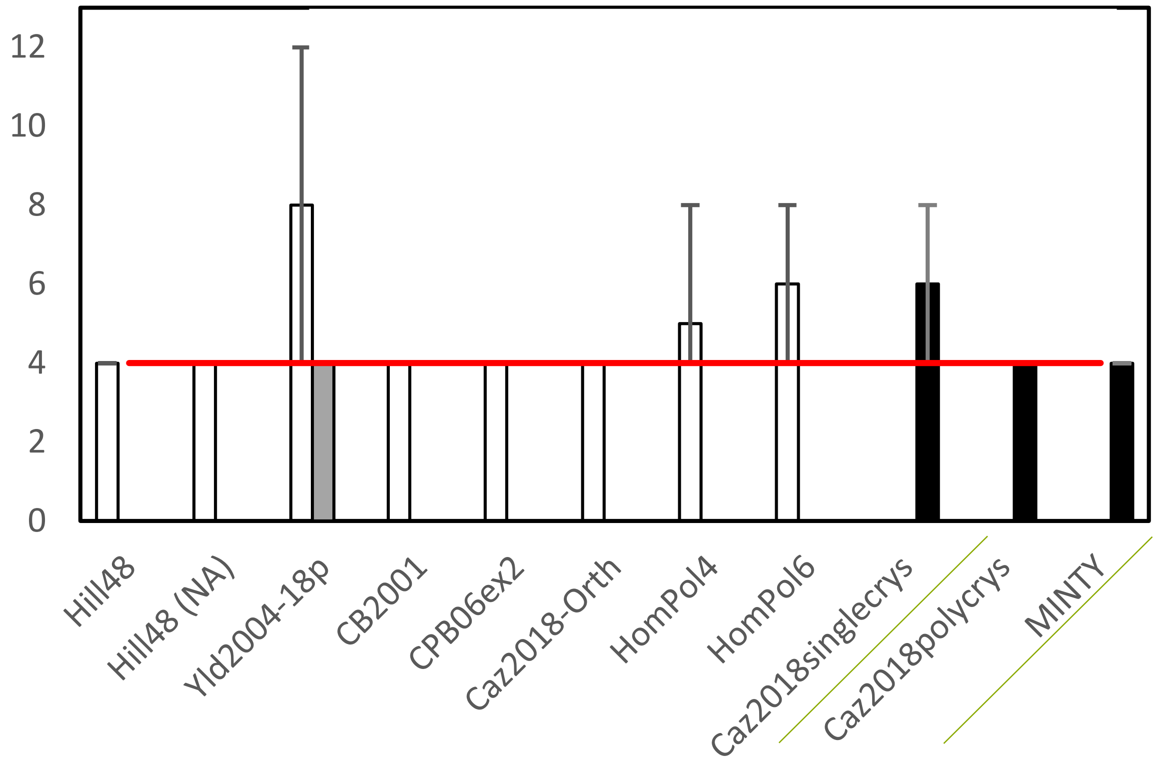
- 7 exp. r- values and yield stresses for Cazacu polycrystal, and VPSC.
- 1 tensile curve in RD (Minty, ALAMEL, DAMASK)
- Facet 3D identified by virtual tensile tests with ALAMEL

FEM predictions Number of ears

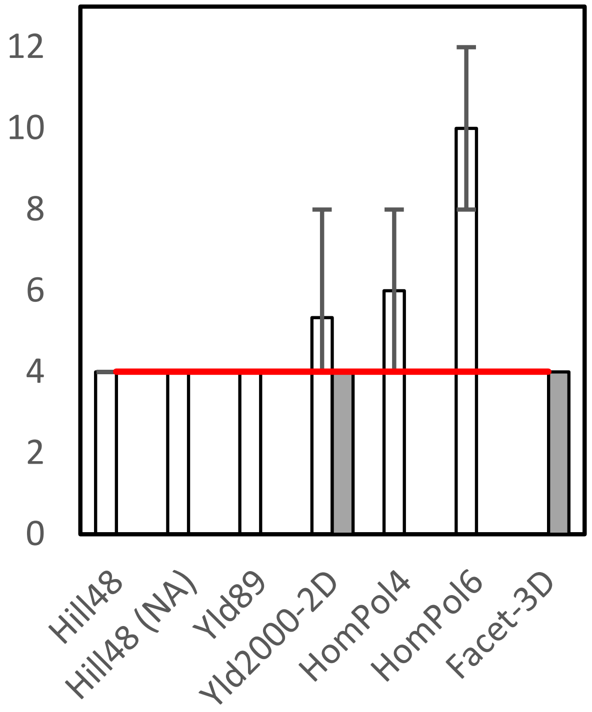
Indentification method of the constitutive law

- □ Based on physical tests
- ▨ Based on physical tests + Virtual ones
- ■ Constitutive law based on crystal plasticity
- 🟥 Experimental drawing force

Most 3-D orthotropic yield functions → 4 ears, as in experiments



Solid and Solid -Shell elements + use of yield locus except Caz2018polycrys and Minty (set of representative crystals)



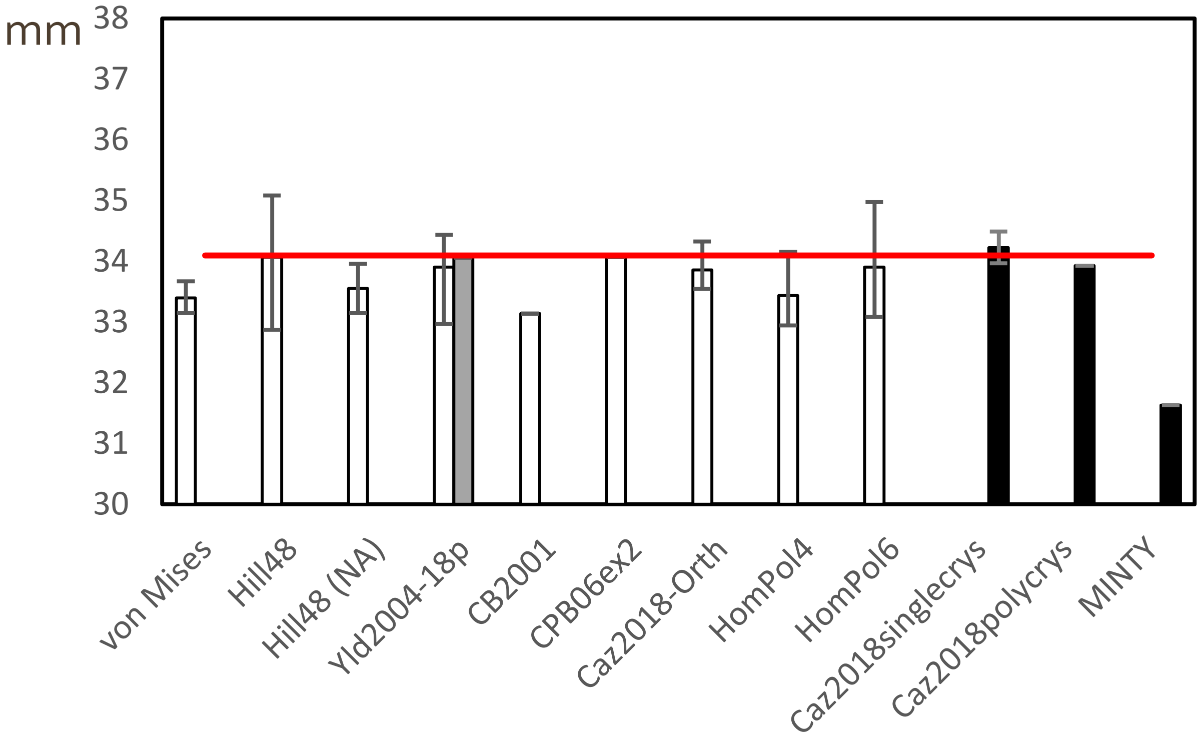
Shell elements
Use of Yield locus

Average cup height **OK**

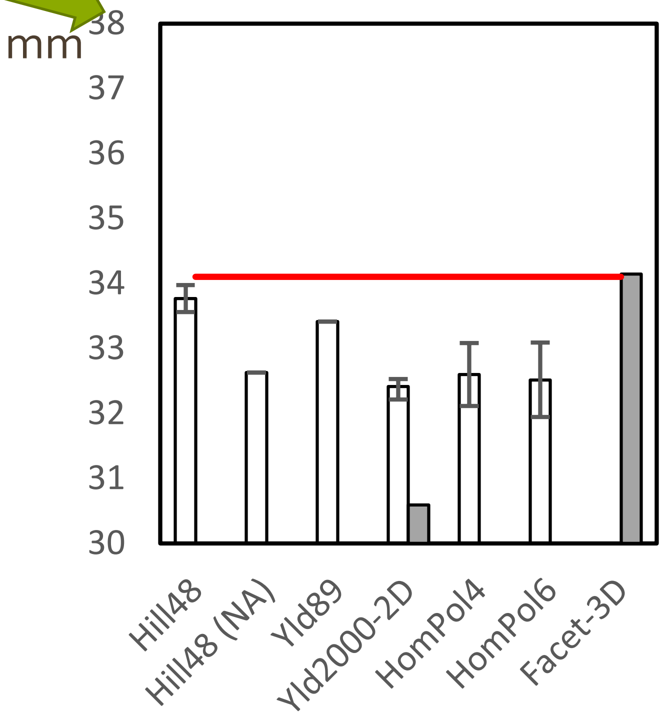
Indentification method of the constitutive law

□ Based on physical tests
▒ Based on physical tests + Virtual ones
■ Constitutive law based on crystal plasticity
— Experimental drawing force

- **von Mises** isotropic yield criterion for reference
- 2D orthotropic yield functions
 Yld89, Yld2000-2D, HomPol4 and HomPol6
 → tend to underestimate
 particularly when combined with shell elements.



Solid and Solid -Shell elements + use of yield locus
except Caz2018polycrys and Minty (set of representative crystals)



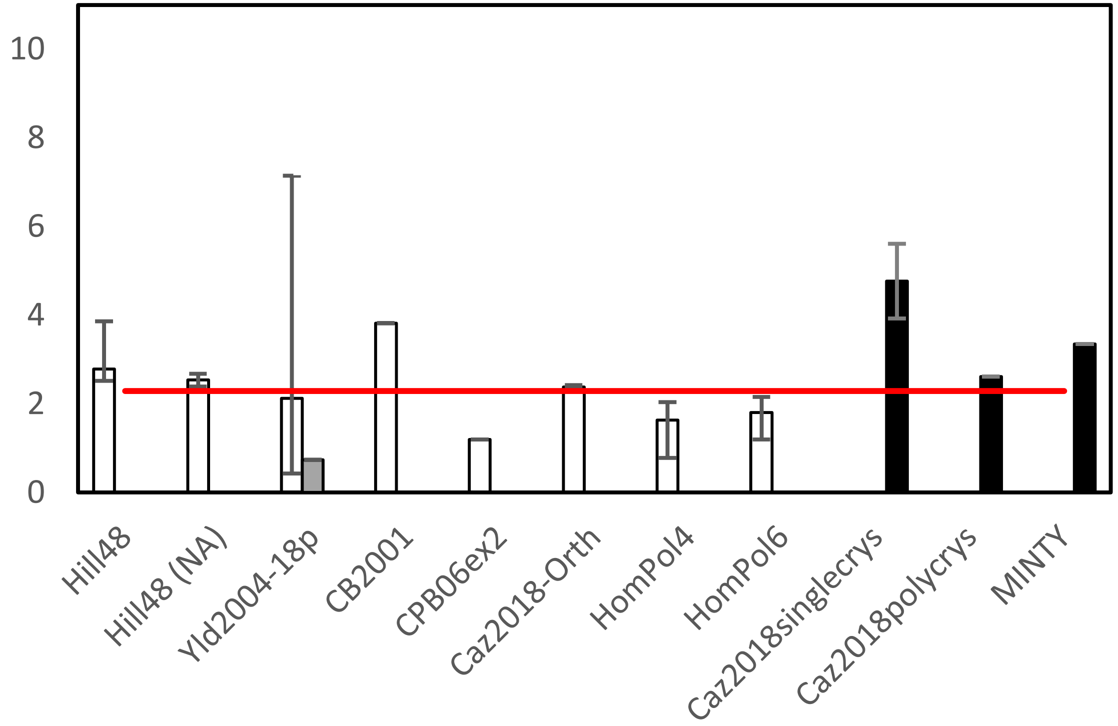
Shell elements
Use of Yield locus

Indentification method of the constitutive law

□ Based on physical tests
▨ Based on physical tests + Virtual ones
■ Constitutive law based on crystal plasticity
— Experimental drawing force

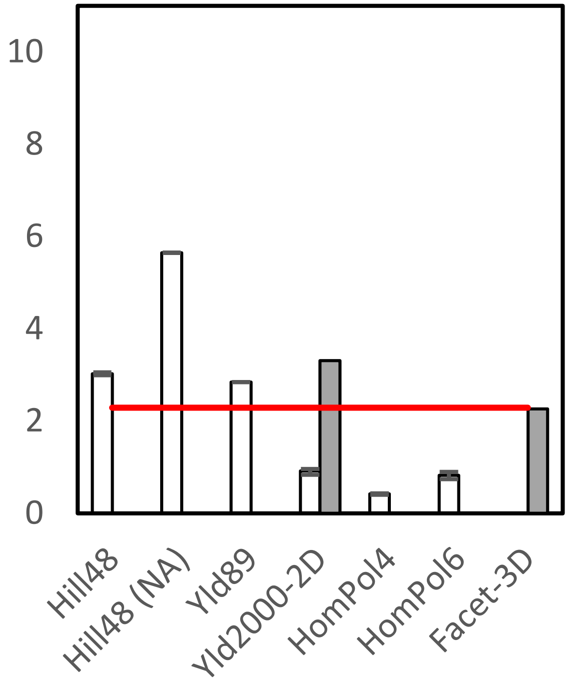
Average amplitude of the earing profile

Texture variability is important → Single crystal not accurate



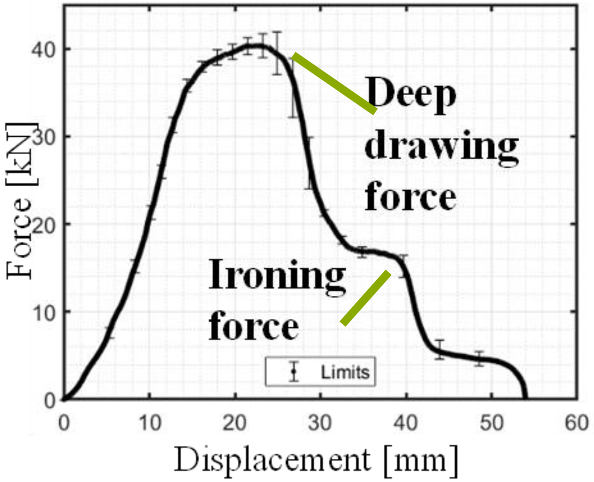
Solid-Shell elements (use of yield locus) except Caz2018polycrys

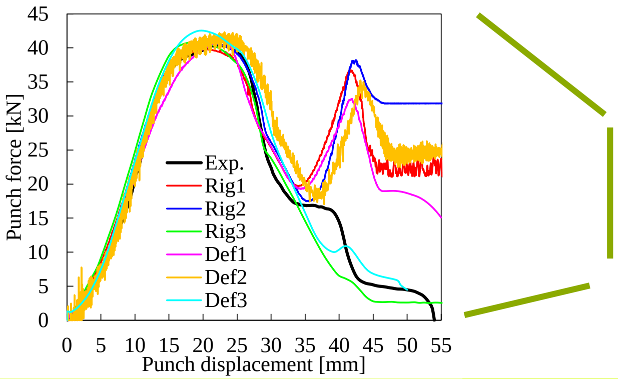
Hill Non Associative seems less accurate for this result.



Shell elements
Use of Yield locus

Force predictions





1st peak : quite well predict by all models with the adjustment of the friction coefficient

a reasonable physical range :
Solid or Solid- shell models → μ=0.01 up-to μ=0.100
Shell models → μ=0.07 or higher values

2nd Peak : most FE predictions too high
worst for shell elements
except - for ABAQUS + S4R element (Ugent)
- for ABAQUS + SC8R element (KUL)

Further analysis with deformable tools:
negligible impact on deep drawing peak
slight impact on 2nd peak
but inverse according solid or solid shell elements

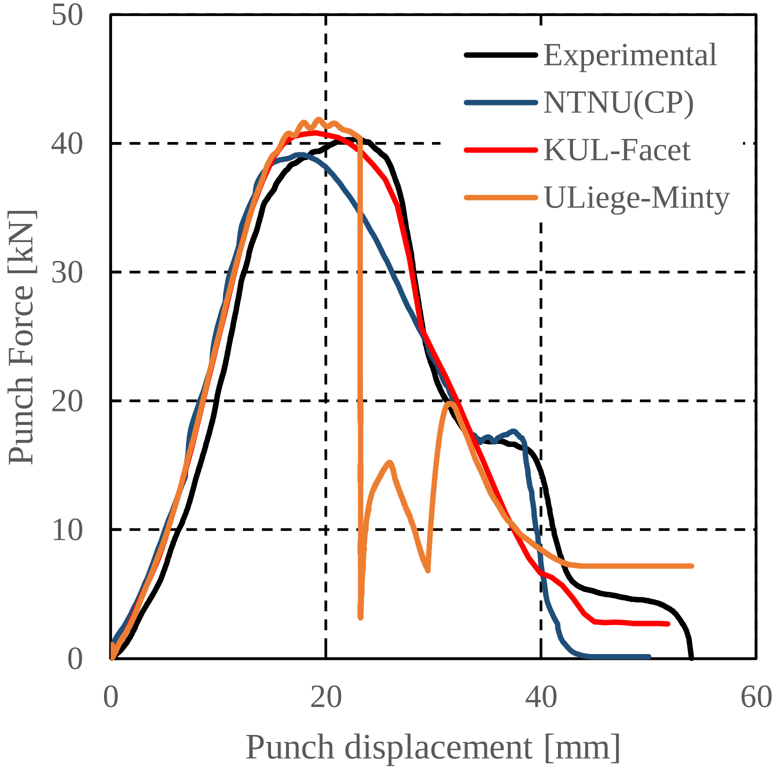
Force predictions - 3 interesting configurations (ironing peak)

Yld2004-18p -ABAQUS implicit – solid element from **NTU,**
an identification based on 7 virtual tensile tests (Damask -FFT, 7509 grains in RVE + physical RD tensile test).

FACET-3D – ABAQUS explicit - continuum shell from **KUL**,
an identification based on 200 virtual tests relying on
10 000 grains + ALAMEL crystal plasticity model

MINTY – Lagamine implicit - solid element from **ULiege,**
an interpolation yield locus approach based on 1000 crystals
+ simple Full Taylor plasticity approach;
(however the start of the ironing stage is not correctly predicted).

crystal plasticity computations to complement physical tests in the identification of the yield functions seems to improve the prediction of the ironing force.



Messages from EXACT ESAFORM Benchmark 2021

- Same set of experiments for the material parameter identification,

Trained scientists using **Hill48 model** (≠ codes, meshes, element types) → similar predicted earing profiles.

Simple Hill48 model lead to robust predictions of the earing profile.

- For the identification of the parameters: **particular relevance was given** by the participants **to the description of the anisotropy of the Lankford coefficients**, (known strong impact on the earing profile).

- **The identification methodology is a key point to generate reliable results.**

The choice of a representative set of crystals,
The analysis of Lankford coefficient evolution or not
Complex yield locus need of a larger training than applying simple analytical formula to identify Hill48 model.
This identification work request skilled scientists.

- **The need of pre-validation checks :**

is the model able to predict stress anisotropy and Lankford coefficient

Messages from EXACT ESAFORM Benchmark 2021

- Six types of data.

☐ Tensile flow stress anisotropy,
☐ r-value anisotropy,
☐ yield locus (biaxial tests),
☐ earing profile,
☐ force evolution in cup forming
☐ monotonic and reverse shear tests are available.

none of the models could accurately describe the complete picture.

- Yield stress anisotropy under uniaxial loadings not well predicted, particularly the one at 45°, by most of the models (including the ones based on crystal plasticity).

Not critical for the correct prediction of the earing profile relevant for other processes

- Barlat model 2004-18parameters: yield locus quite sensitive

it can be quite accurate
however implementation by different teams
for the same set of parameters generate different results

Macro and Multiscale FEM references in sheet forming

Benchmark ESAFORM 2021 Raw data
https://zenodo.org/records/6874577
Description ↘


Analysis of ESAFORM 2021 cup drawing benchmark of an Al alloy, critical factors for accuracy and efficiency of FE simulations

A.M. Habraken, T.A. Aksen,J.L. Alves, R.L. Amaral, E. Betaieb, N. Chandola, L. Corallo, D.J. Cruz, L. Duchêne, B. Engel,·E. Esener, M. Firat, P. Frohn-Sörensen, J. Galán-López, H. Ghiabakloo, L.A.I. Kestens, J. Lian, R. Lingam, W. Liu, J. Ma, L.F. Menezes, T. Nguyen-Minh, S.S. Miranda, D.M. Neto, A.F.G. Pereira, P.A. Prates, J. Reuter, B. Revil-Baudard, C. Rojas-Ulloa, B. Sener, F. Shen, A. Van Bael, P. Verleysen,·F. Barlat, O. Cazacu, T. Kuwabara, A. Lopes, M.C. Oliveira, A.D. Santos, G. Vincze,

Int J Mater Form **15**, 61 (2022).
https://doi.org/10.1007/s12289-022-01672-w

Cazacu O, Revil-Baudard B, Chandola N (2019)
Plasticity damage couplings: from single crystal to polycrystalline materials. *Springer, Berlin Heidelberg*

Yield locus functions + Polycrystal Multiscale Crystal Plasticity (CP) (small set of grains but high accuracy) → OK for forming process

Van Houtte P, Gawad J, Eyckens P, Van Bael B, Samaey G, Roose D (2011)
A full-field strategy to take texture-induced anisotropy into account during FE simulations of metal forming processes. *JOM 63(11):37–43.*
https:// doi. org/ 10. 1007/ s11837- 011- 0189-9

Update yield locus shape due to CP relying on 1000 grains in FE simu but efficient CPU computation

Galan J, Verleysen P, Lebensohn RA (2014)
An improved algorithm for the polycrystal viscoplastic self-consistent model and its integration with implicit finite element schemes. *Model Simul Mater Sci Eng 22(5):055023.*

Efficient VPSC code ready to collaborate, share

ESAFORM grant of 15000€ enhances true collaboration. It aims to study any related problem to material forming. Deliverables :
-oral presentation of the conf.
-an IJMF paper
Spirit of understanding, transparancy of methods experiments to reach results. No competition
Application each 3rd Sept
(4 pages, 3 institutions, within organizing committee
3 ESAFORM members)

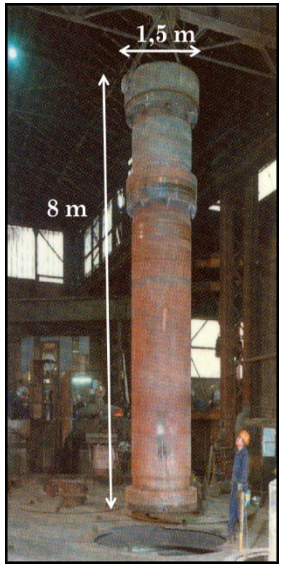
Contents

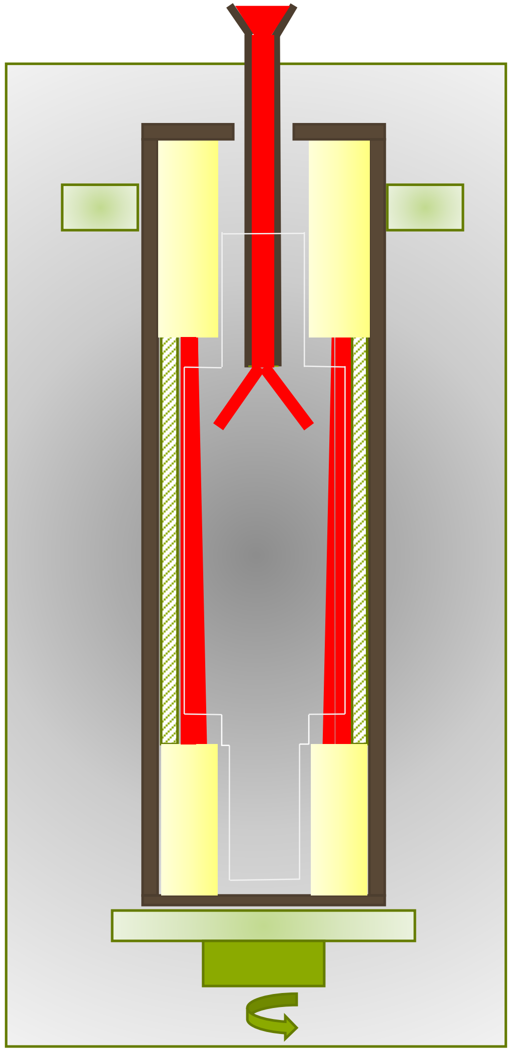
✓ A survey of scales and methods

- Finite element method FEM
  - ✓ One element: Solid Shell
  - ✓ Mechanical constitutive laws (multi scale ?)
    - ✓ Deep Drawing
  - Thermo-mechanical analysis
    - Cooling of rolling mills
    - Continuous casting
- Representative Volume Element (RVE) or in French VER
- Coupling solid FEM with … Computational Fluid Dynamics, Deep Learning
  - Additive Manufacturing

FEM Thermo-Mechanical –Metallurgic Simulations

Vertical spin casting process



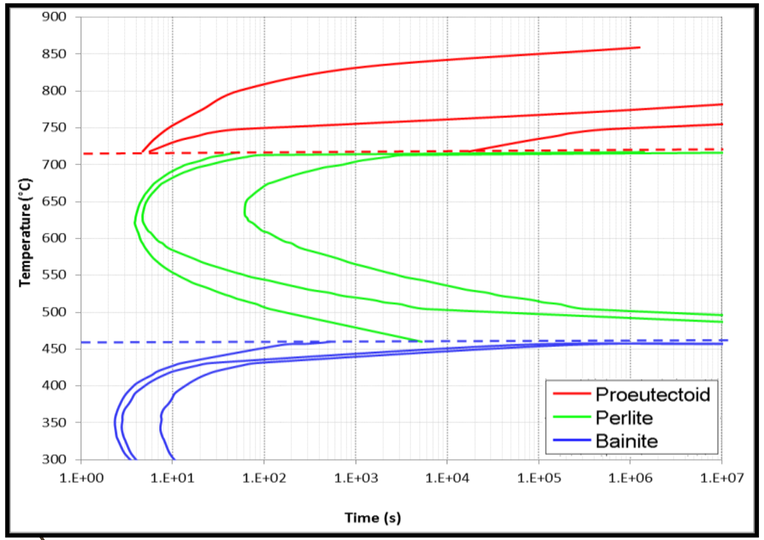


Transformations during cooling

- by diffusion (ferrite, pearlite, bainite)

- TTT diagram
- Additivity rule
- Sheil’s sum (nucleation)
- JMAK law

(Johnson-Mehl-Avrami-Kolmogorov)



- Displacive Martensitic transformation

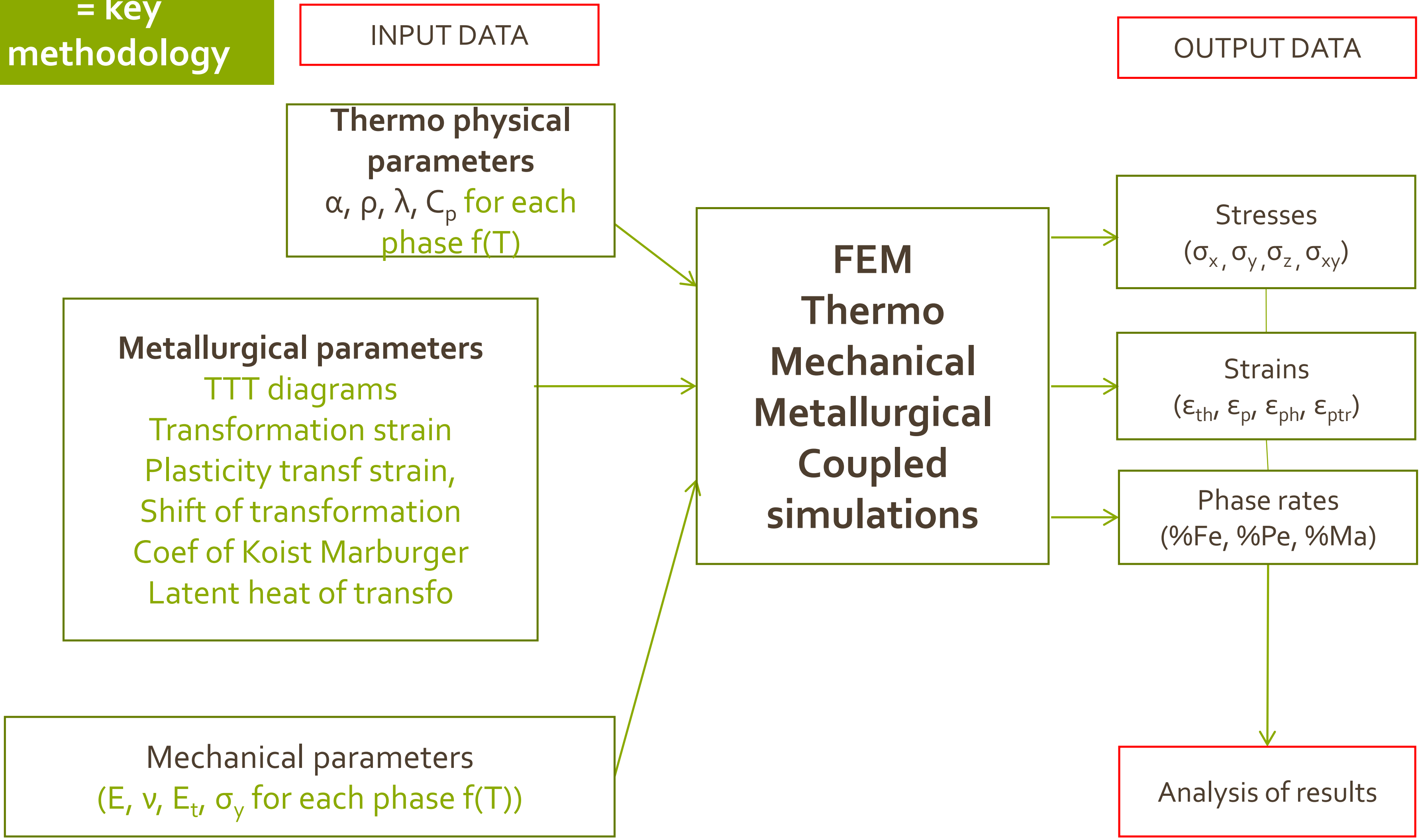
Koistinen Marburger’s law

$$y_i = y_{i,\gamma}(1 - \exp(-A_M(M_s - T))$$

High wear resistance in shell: High Chromium Steel Alloy
High toughness in core : Spherical Graphite Iron

Challenge:
high amount of data
+
Average values
(heterogeneous material) :
High Chromium Steel Alloy
12 to 15% carbides
strong variation in C contents in the matrix
→ scattering in Ms tp°, etc

Inverse model
= key
methodology



INPUT DATA

Thermo physical parameters
α, ρ, λ, C_p for each phase f(T)

Metallurgical parameters
TTT diagrams
Transformation strain
Plasticity transf strain,
Shift of transformation
Coef of Koist Marburger
Latent heat of transfo

Mechanical parameters
(E, ν, E_t, σ_y for each phase f(T))

FEM Thermo Mechanical Metallurgical Coupled simulations

OUTPUT DATA

Stresses
(σ_x, σ_y, σ_z, σ_{xy})

Strains
(ε_{th}, ε_p, ε_{ph}, ε_{ptr})

Phase rates
(%Fe, %Pe, %Ma)

Analysis of results

TTT diagrams recovered from literature CCT

Heat transfer during cooling recovered from surface tp° measurement

Thermo Physical properties + latent heat : measured

Phase transformation strain recovered from dilatometric tests

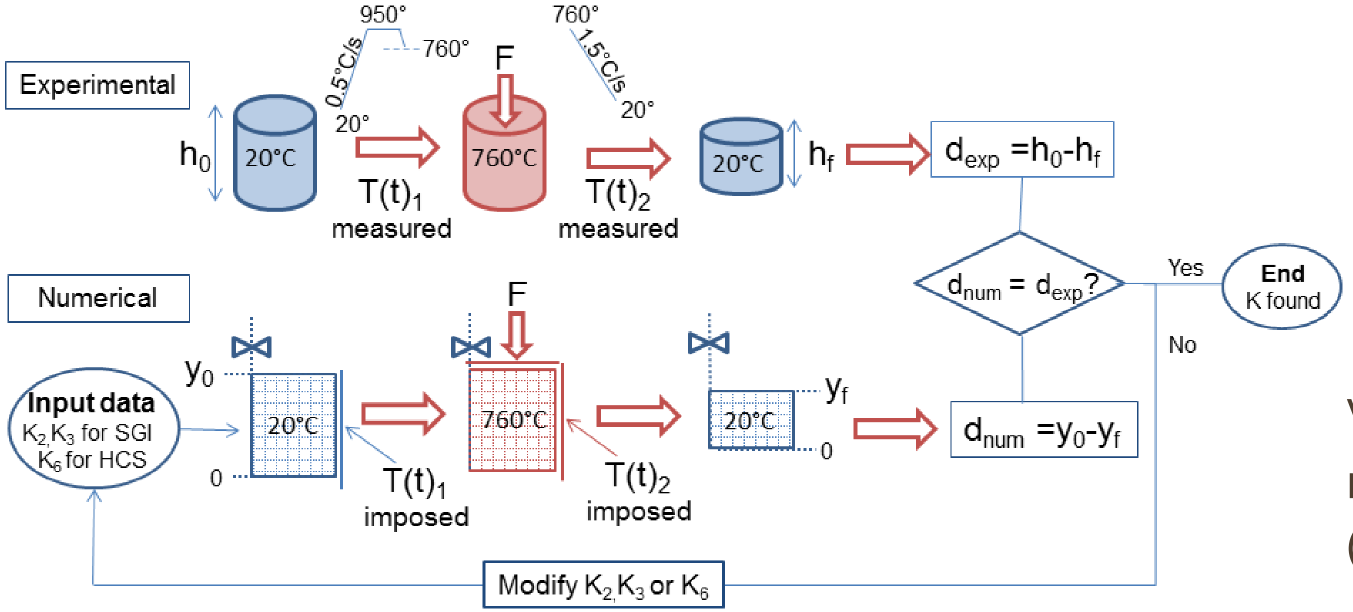
Compression tests on samples with known % Fe Ba Ms

Tests at different tp° but 1 strain rate –>EP model and not EVP

Induced Plasticity Transformation = a strain additional to the phase transformation strain that appears if a stress is present during transformation

Experiment

Compress the sample during cooling and phase transformation

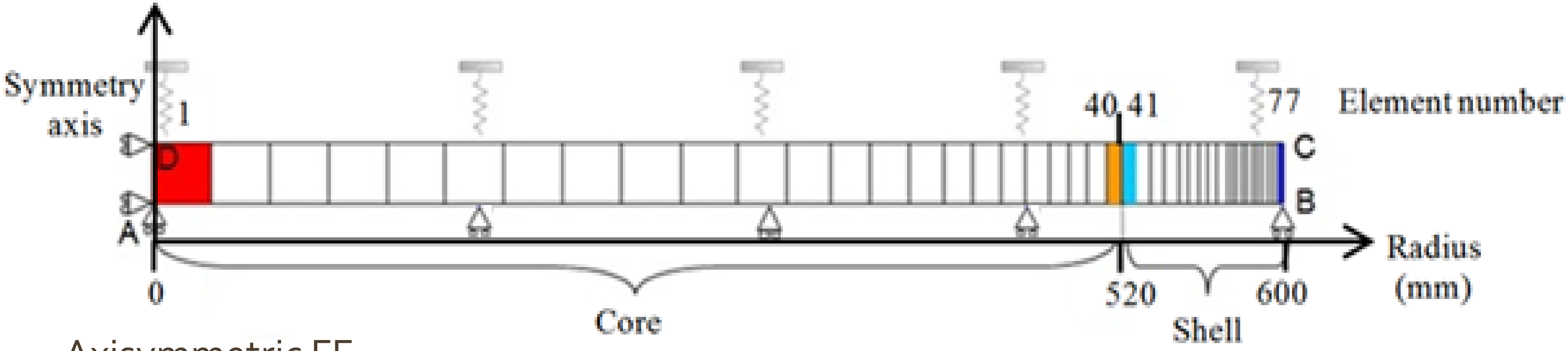


Values not easy to measure (large scattering)

$\bar{\varepsilon}_{pt} = K_2(\bar{\sigma} - \sigma_s)y_{Fe}$	11 x10^{-10} Pa	k_2	ferrite
$\bar{\varepsilon}_{pt} = K_3(\bar{\sigma} - \sigma_s)y_{Pe}$	11 x10^{-10} Pa	k_3	pearlite
$\bar{\varepsilon}_{pt} = K_6\bar{\sigma}(2 - y_M)y_M$	0.60x10^{-10} Pa	k_6	martensite

Within range of literature values

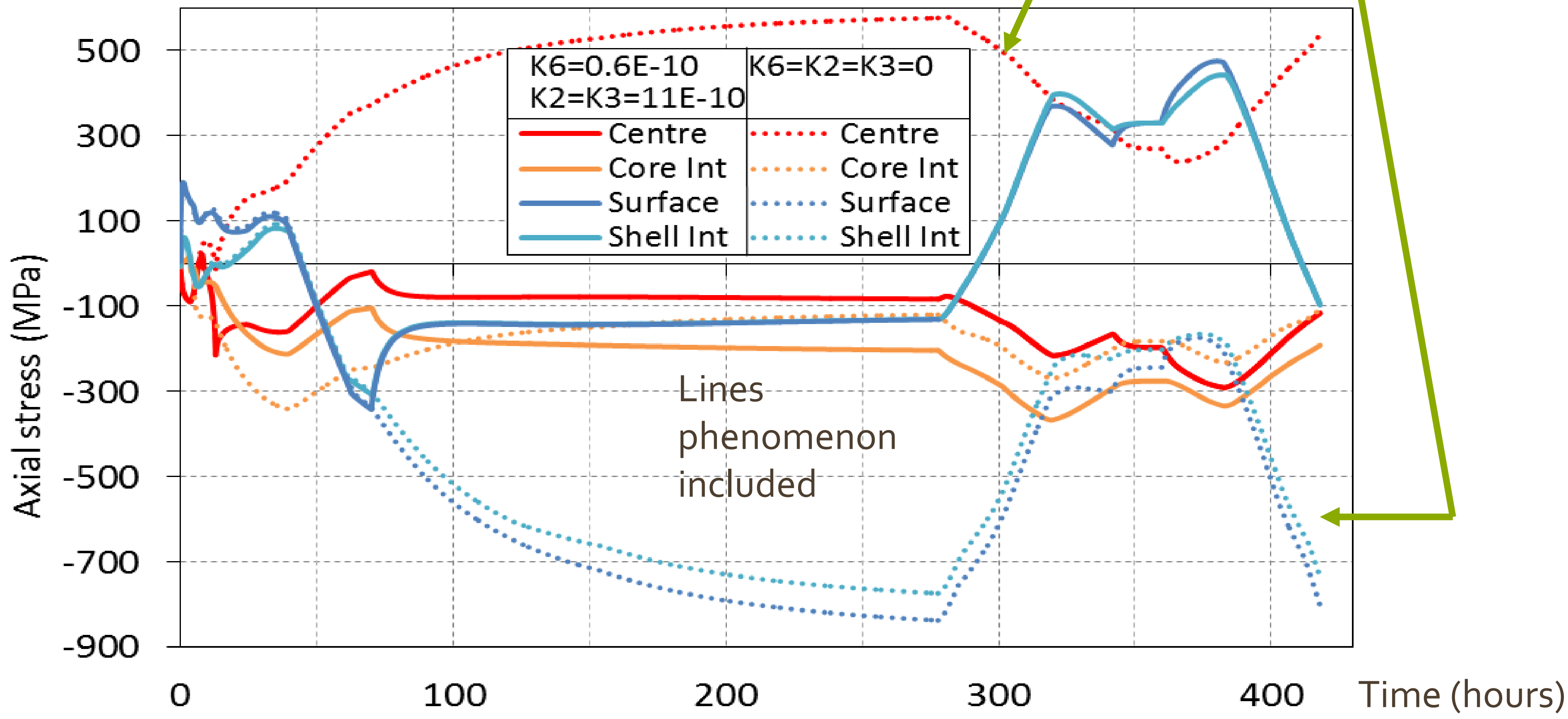
FE stress vs time



Axisymmetric FE simulation

Stress history in different locations

Strong sensitivity
to plasticity
transformation
parameters
(**Accuracy ??**)



Lines phenomenon included

Dot = results if neglected plasticity transformation

K_2 = ferrite transformation K_3 = ferrite transformation K_6= martensite transformation

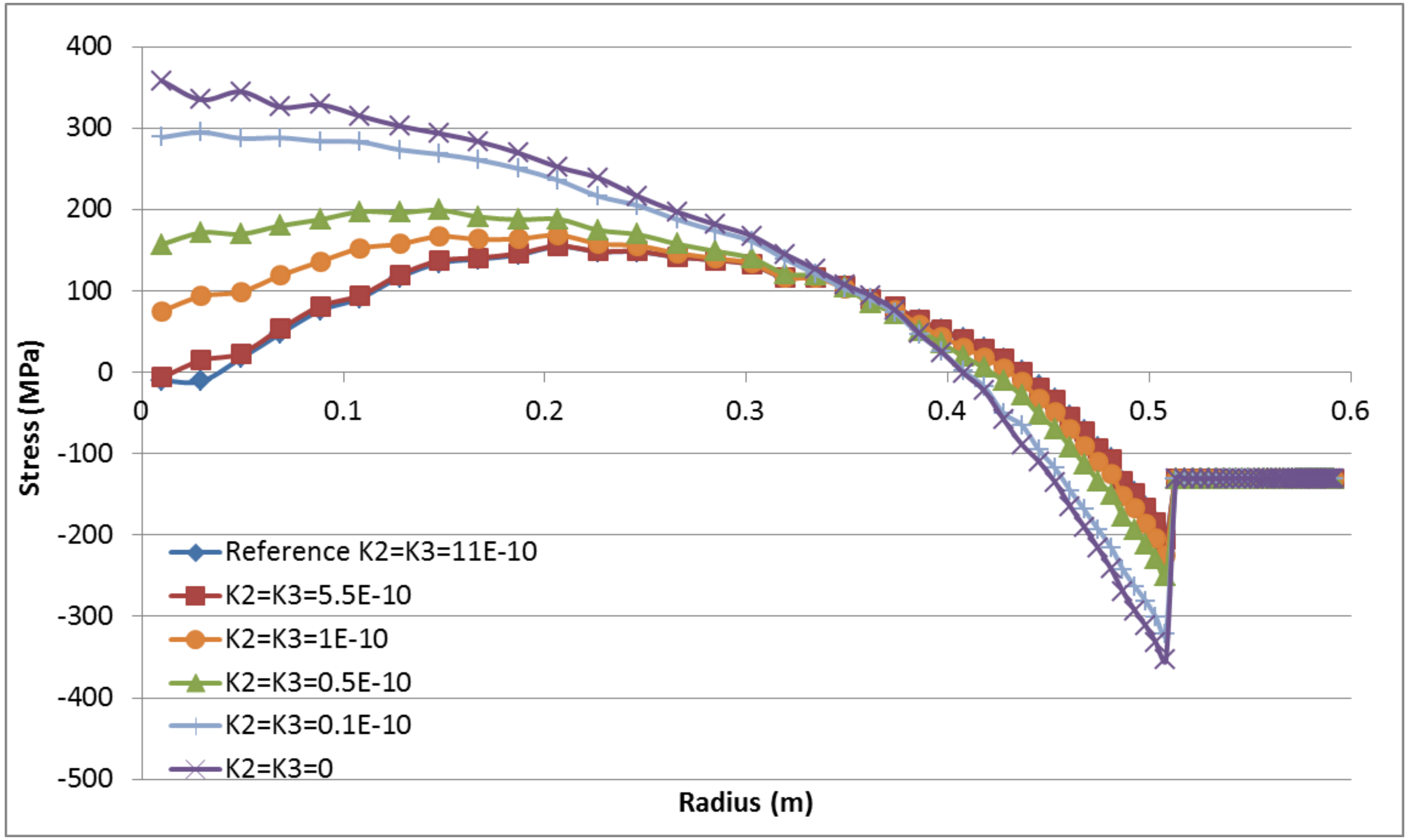
Effect of “Induced Plasticity Transformation” coefficients

FE stress vsradius

Spherical Graphite Iron: Ferrite and Pearlite transformations under stress generate “induced plastic strain”

→ Modify shape of core residual stresses

not of shell stress



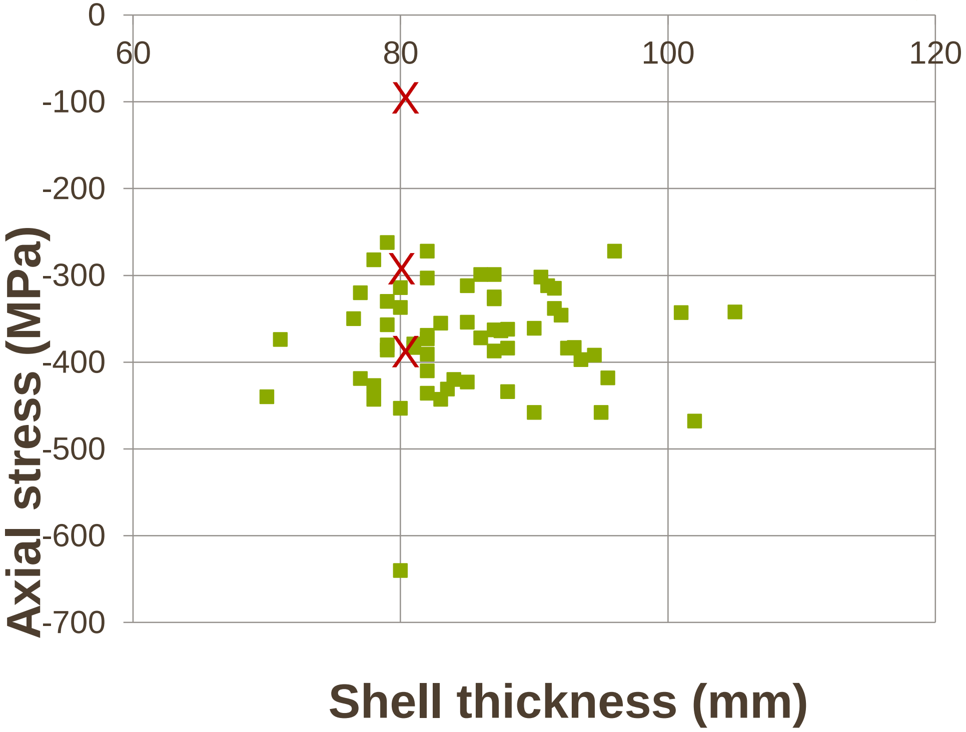
Constant k_6 value

Residual axial stress measurements // simulations

X FE = predictions

with different K6

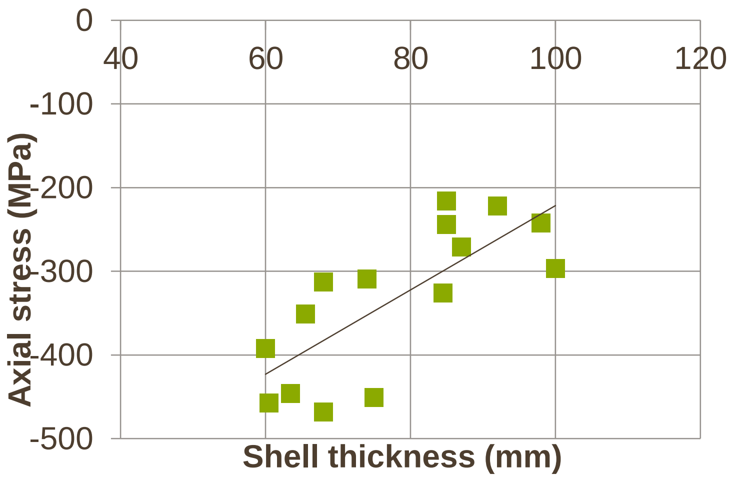
Reference case roll of 1.2 m diameter



🟩 measurements

Diameter roll of 1.2 m:
no clear effect of shell thickness

For smaller diameter rolls
(0.95 to 1 m):
stress ↑
if shell thickness ↑



Thermo Mechanica Metallurgical FE simulations - References

Phase Transformations and Crack Initiation in a High-Chromium Cast Steel Under Hot Compression Tests. **Tchuindjang J. et al.** (2015). *Journal of Materials Engineering and Performance, 24* https://doi.org/10.1007/s11665-015-1464-7

Experiments, Simulation for Rolling Mill case

FE modeling of the cooling and tempering steps of bimetallic rolling mill rolls. **Neira Torres et al.** (June 2017). *International Journal of Material Forming, Volume 10,* (Issue 3), 2017 https://doi.org/10.1007/s12289-015-1277-0

A New Concept for Modeling Phase Transformations in Ti6Al4V Alloy Manufactured by Directed Energy Deposition. **Tchuindjang J. et al.** (2021) *Materials, 14* (11),

About JMAK, KM models for LPBF and TA6V alloy

Modelling of austenite transformation along arbitrary cooling paths **Pohjonen A. et al. ,** 2018, *Computational Materials Science, Volume 150,* https://doi.org/10.1016/j.commatsci.2018.03.052

Variant of JMAK model

Coupling kinetic Monte Carlo and finite element methods to model the strain path sensitivity of the isothermal stress-assisted martensite nucleation in TRIP-assisted steels **Cluff et al.** (2021) *Mechanics of materials, (154)* https://doi.org/10.1016/j.mechmat.2020.103707

The model TRIP behavior needs a phase transfo model : thermodynamic and crystallography approach implemented through Monte Carlo kinetic computation and RVE FEM

Contents

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- Representative Volume Element (RVE) or in French VER
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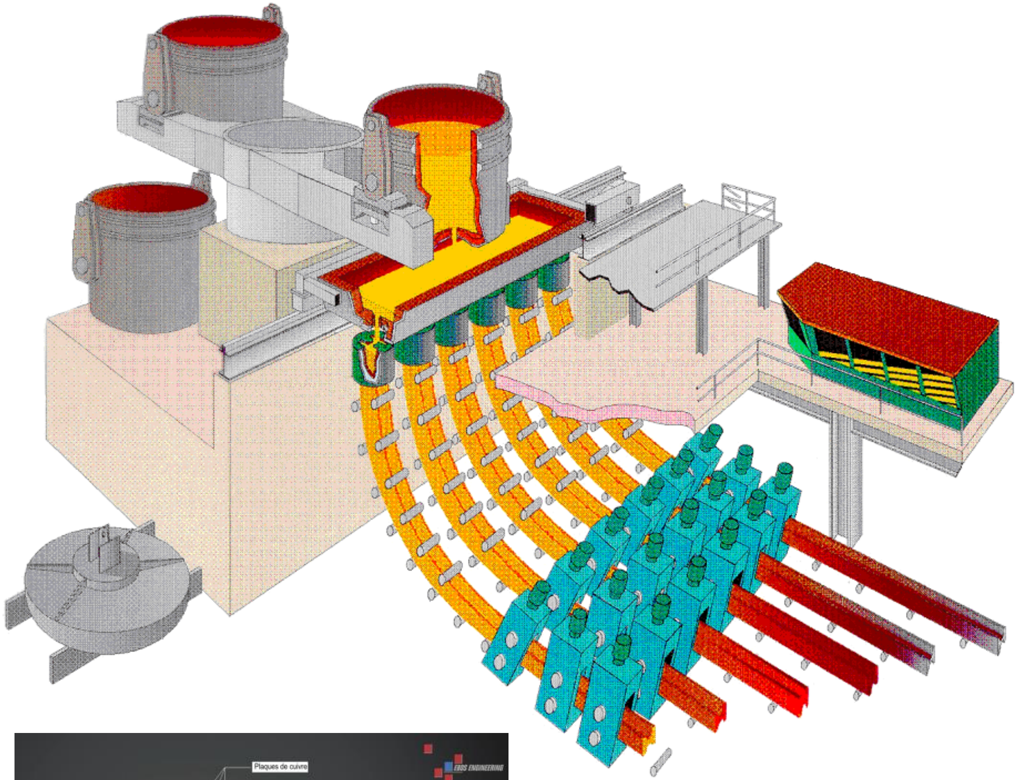
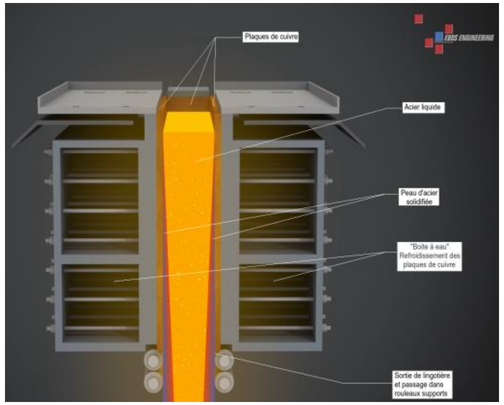
  - Additive Manufacturing

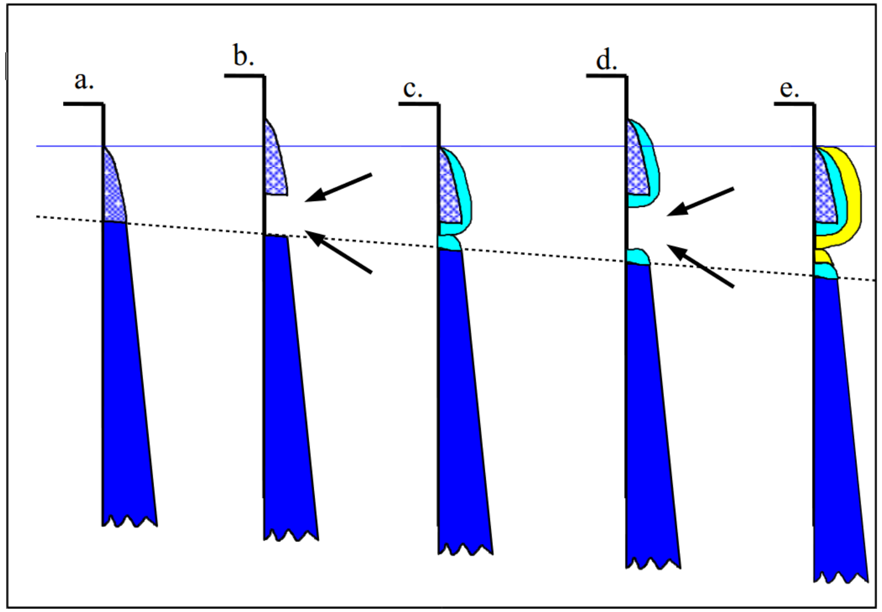
Continuous casting



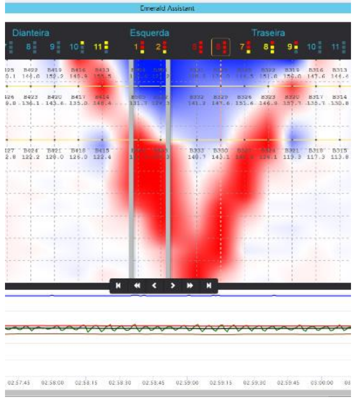


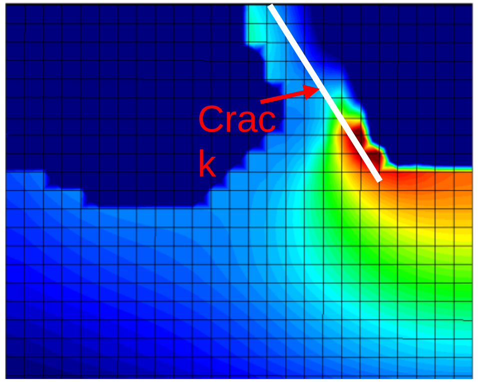
What is the issue ?

Breakthrough prevention



EBDS Engineering observation // FE prediction





Principal Strain

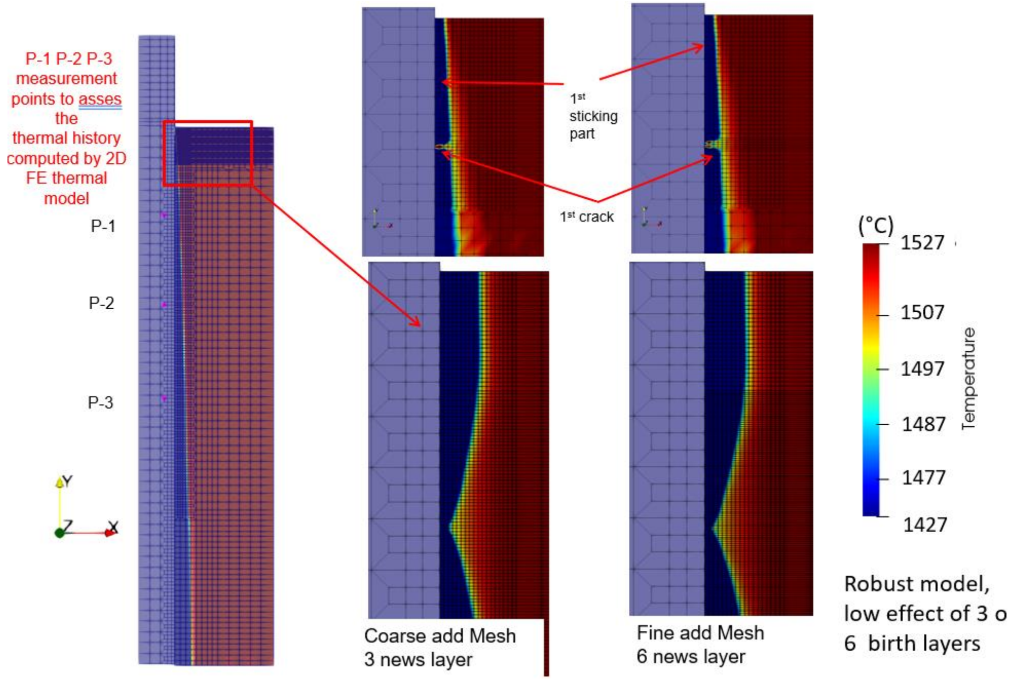
Thermal signature of a crack propagating within the mold

Solid FEM analysis well chained…

Continuous casting

Methodology ?

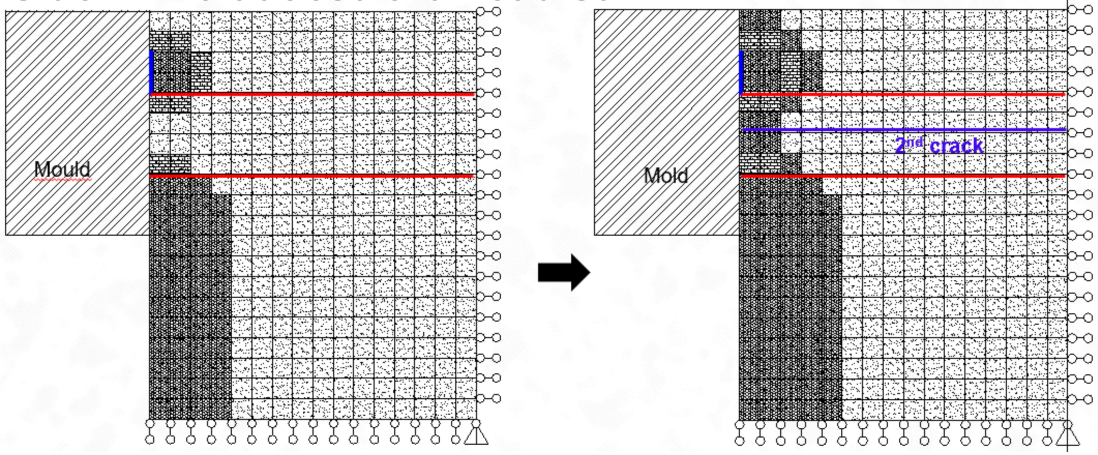
Breakthrough Model



Robust model, low effect of 3 o 6 birth layers

Crack 1 introduced than cooled

Later Crack 2



2D FE global thermal analysis - coarse mesh → thermal macro field

specific feature : "switch" on of new element for new fluid

On going simulation to reach stationary state (no eulerian approach, lagrangian one)

2D FE local thermal analysis – refined mesh

-projection of stationary Tp° field as initial state

-introduction of a crack:

- A mesh part sticked to the mold "upper mesh"
- A "lower mesh" part go down
- *Between: a* few layers of FE at liquid tp° fill the gap "crack layers"

→ Crack 1

- Time of cooling Crack 1 is solidified (strand compression)
- Oscillation goes on (strand tensile) a new crack appears

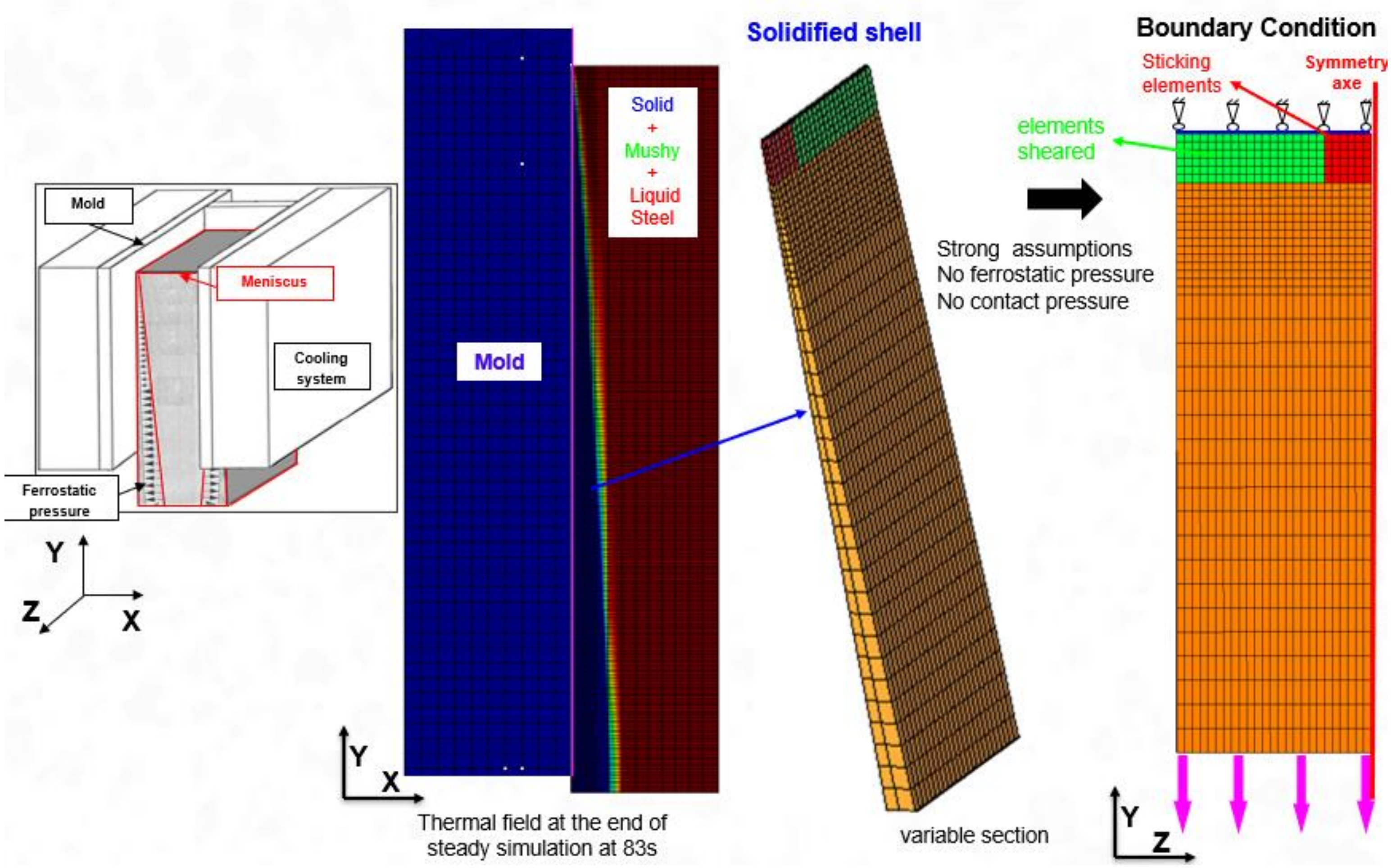
→ Thermal field follows the crack propagation as new cracks are inserted based on *relative mould-strand velocity*

Model validated by the trends known in industry

Tran H. S. et al. Procedia Manufacturing 50 2020

Continuous casting

Methodology ?



Tran H. S. et al. Procedia Manufacturing (ESAFORM and Metal Forming 2020)

Breakthrough Model

3D FE thermo mechanical analysis based on the 2D thermal defining boundary conditions

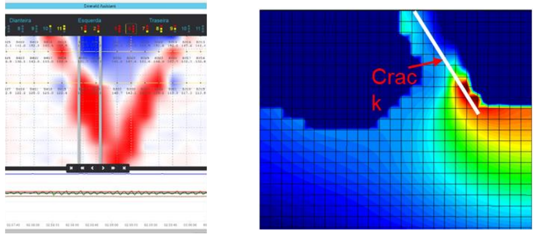
Constitutive model of mushy zone based on Schwartz PhD (Uliege 2011)

Crack criterion ??
Just Principal strain "rate"

→ effect of casting speed
→ steel grade

Crack angle and speed // Experiments
Model for trends

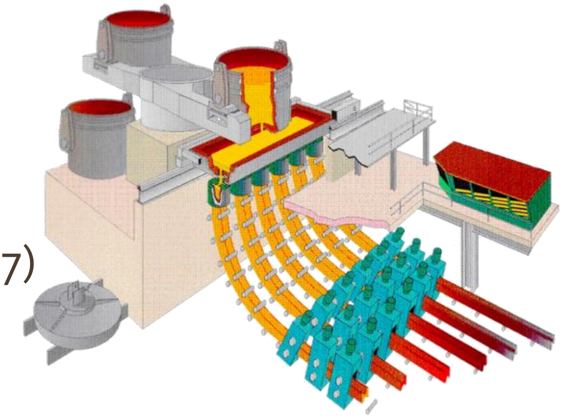
EBDS Engineering observation // FE prediction



Principal Strain

Continuous casting

What is the issue ? **Transversal Cracks in Unbending zone**



Methodology ? **1st Get Stress and Tp° histories**

2.5 D FEM Correct Mechanical Field (Stress history)

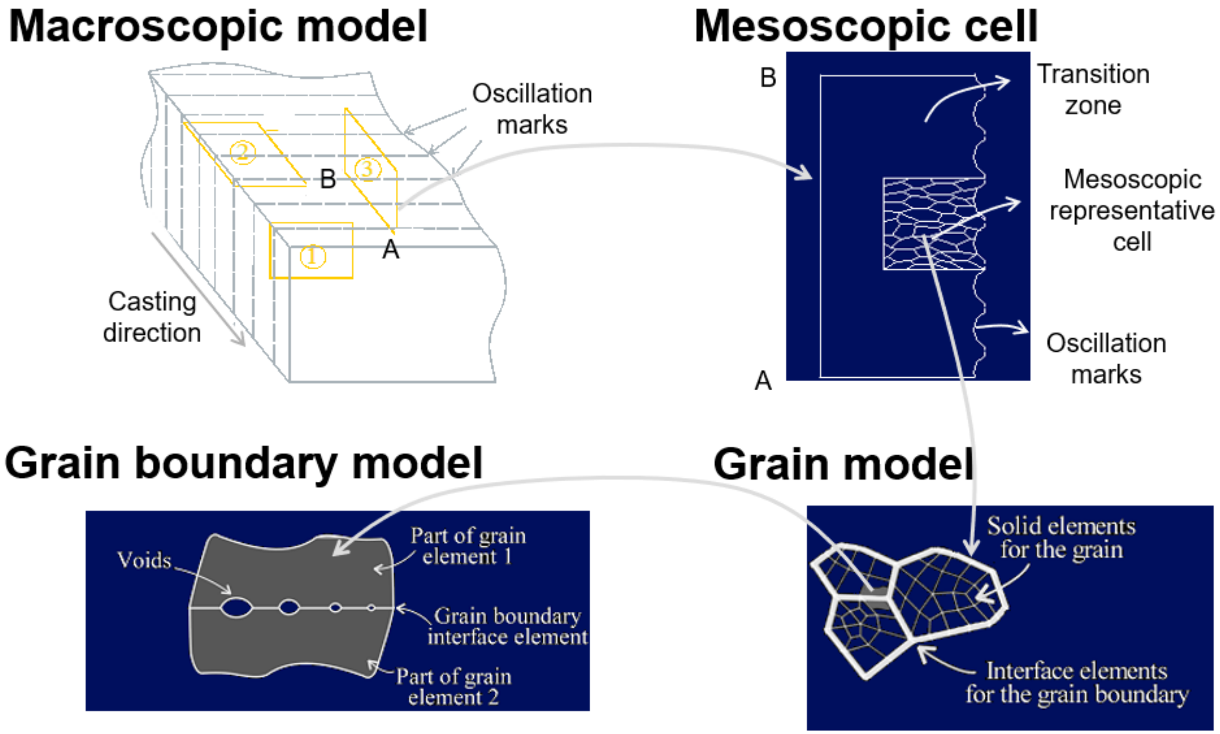
Generalized plane strain FE with interaction with bulging measurement

Pascon et al Computer Methods in Applied Mechanics & Engineering (2007)

3D FEM Coupled or staggered codes but often difficult to get the whole history

2ndChange of scale

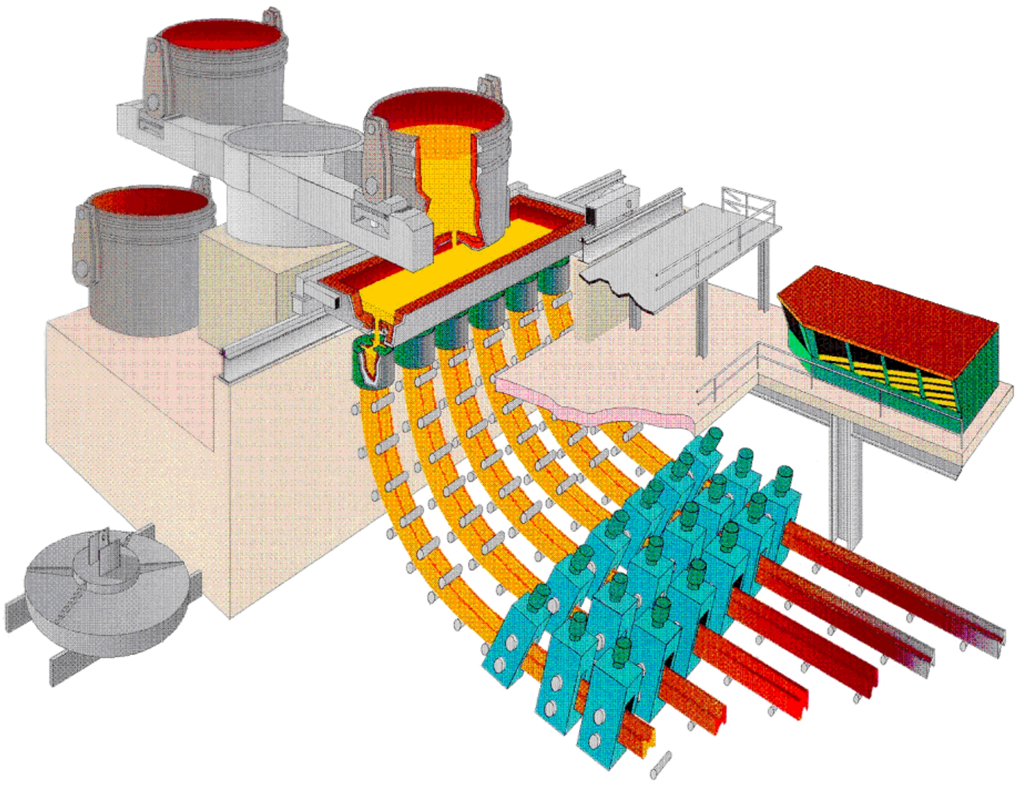
Tp° and Stress are applied at the level of oscillation marks

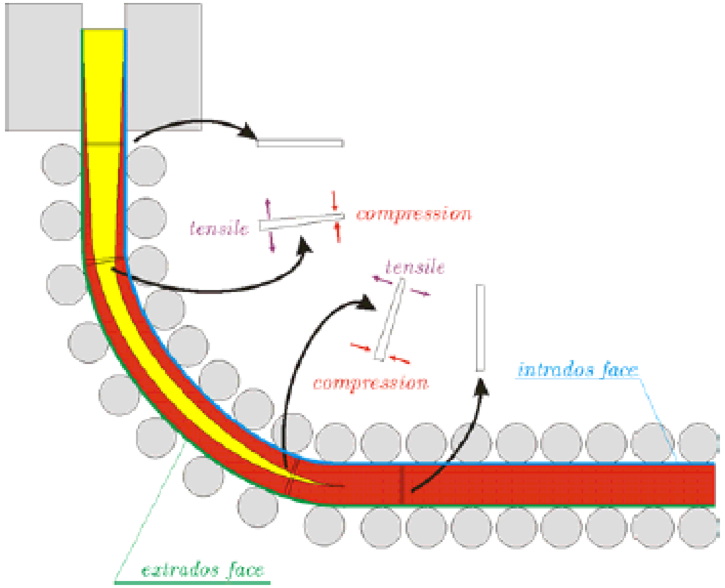


Continuous casting

Methodology ?

1st Get Tp° and Stress histories

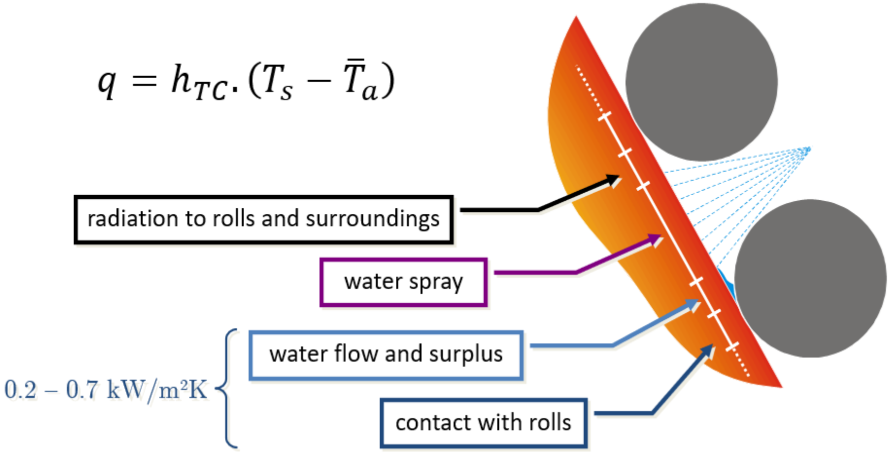




1. Correct Thermal Field

Heat exchange in secondary cooling

$$q = h_{TC}.(T_s - \bar{T}_a)$$



radiation to rolls and surroundings

water spray

water flow and surplus

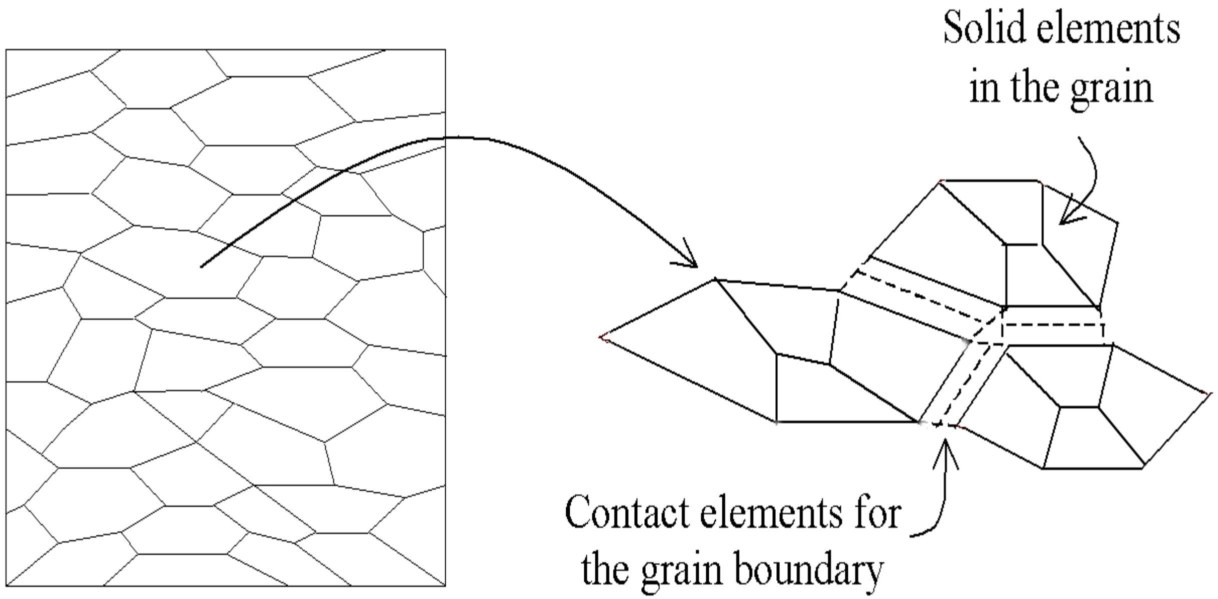
contact with rolls

0.2 – 0.7 kW/m²K

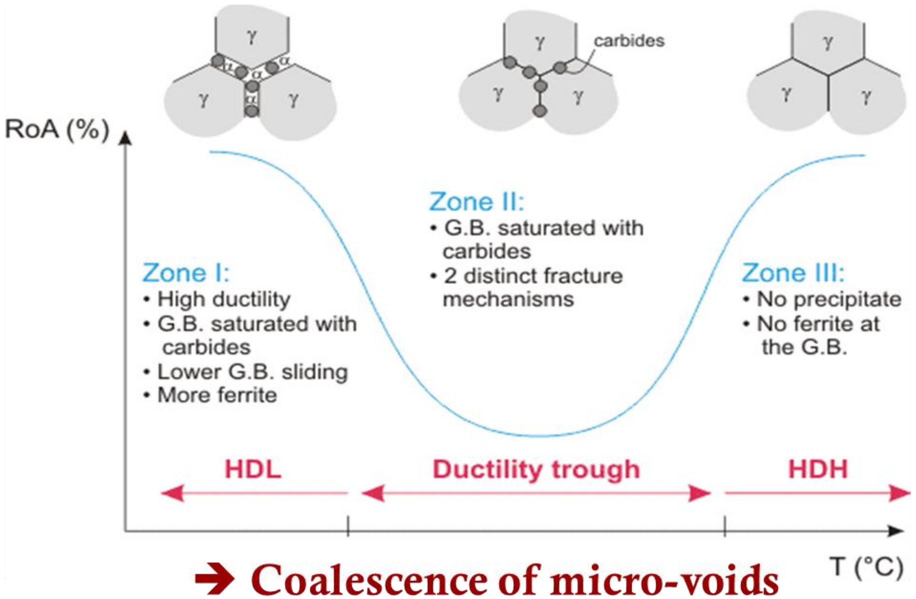
2. Staggered analysis

Tp° → Meca → Tp° ….2.5D FE simulation for a plane going through the whole process

3. Change the scale → Mesoscopic Model



Ductility curve



→ Coalescence of micro-voids

→ GB sliding

- **Grains** : quadratic elements with a **Norton-Hoff constitutive law**

$$\bar{\sigma} = \bar{\varepsilon}^{p_4} . \exp\left(-p_1 \bar{\varepsilon}\right) . p_2 . \sqrt{3} . \left(\sqrt{3} . \dot{\bar{\varepsilon}}\right)^{p_3}$$

- **Grain boundaries** : interface elements with a damage constitutive law

4 Peritectic steel grades

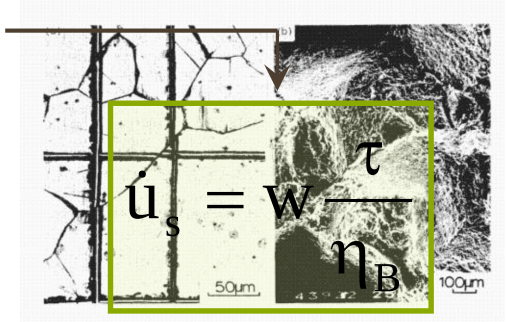
	V (ppm)	Nb (ppm)
Grade A	1	161
Grade B	60	139
Grade C	**550**	**565**

+Grade D : 0 V, **Nb** 370
Carbone between grades C & D

Damage law (Onck, van der Giessen 99)

✓Grain boundary sliding (Ashby)

w = thickness of the grain boundary
η_B = viscosity parameter
τ = shear at previous step



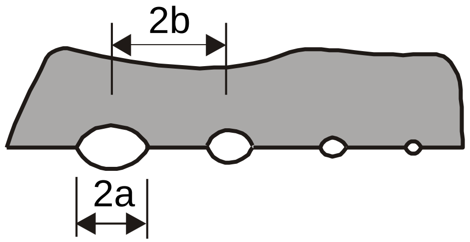
$$\dot{u}_s = w\frac{\tau}{\eta_B}$$

Suzuki, 1984

✓Grain boundary cavitation

2l

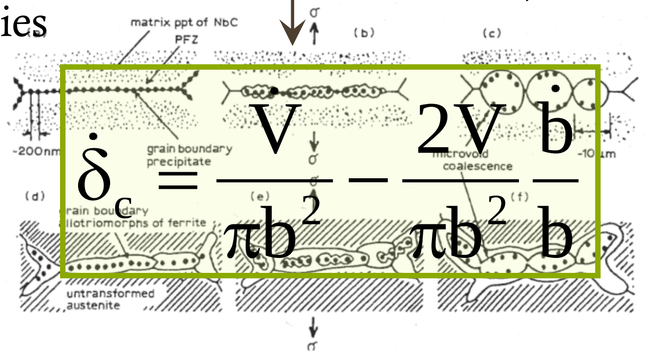
wo cavities



✓**Damage**

a/b = threshold

Mintz, 1991



$$\dot{\delta}_c = \frac{\dot{V}}{\pi b^2} - \frac{2V}{\pi b^2}\frac{\dot{b}}{b}$$

with

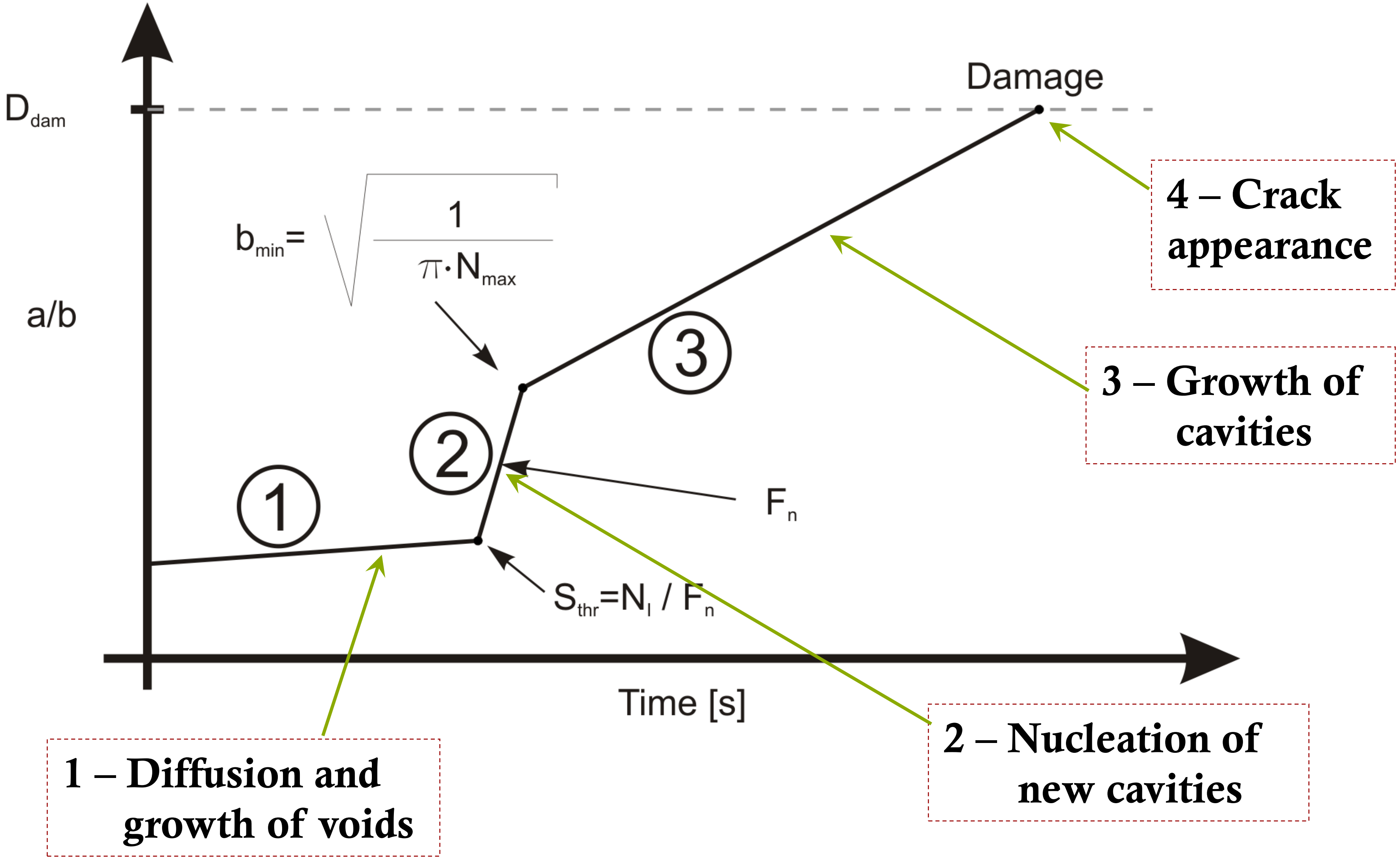
$$\begin{cases} \dot{V} = f(\dot{\varepsilon}, \sigma_n, \sigma_m, \sigma_e, n, D, a, h) = \dot{V}_1 + \dot{V}_2 & \text{growth} \\ \dot{b} = f(\dot{\varepsilon}, \sigma_n) & \text{nucleation} \end{cases}$$

by diffusion by creep

Damage curve

a void size
b void spacing
at Grain Boundary

F_n Nucleation parameter
N Cavity density
I initial, maximal



4 – Crack appearance

3 – Growth of cavities

2 – Nucleation of new cavities

1 – Diffusion and growth of voids

N_I depends on Temperature

Damage law data (14)

Identification thanks to
- Norton Hoff law
- Metallography
- Crack tests
- Literature

6 param. to extract from micrography
but
4 not obtained

d	Mean grain size	Grain boundary sliding
$\dot{\varepsilon}_e^C/\dot{\varepsilon}_B$	Viscosity parameter	
$n(T)$	Creep exponent	
$B(T)$	Creep parameter	
b_o	Initial cavities distance	Nucleation of cavities
$\sum_0(T)$	Normalisation stress	
F_n	Nucleation parameter	
N_I	Initial density of cavities	
N_{max}	Maximum density of cavities	
Ψ	Cavity angle or litterature	
a_o	Initial size of the cavities	Cavity growth by diffusion and creep
$D_{b0}\delta_0$	Diffusion parameter in the grain boundary	
Ω	Atomic volume	
Q_b	Activation energy of diffusion in boundary	
$\left(\frac{a}{b}\right)_{crit}$	Rupture criteria	

4 param by inverse modeling of tensile notch tests or compression test with accoustic emission

14 → 6 → 4 parameters to determine

Results of this code chaining and limits

- **Physic based does not mean easy identification … Inverse model required**
  - **need of** compression tests *with acoustic emission analysis* **or** tensile notched tests
  - + micrography + literature
- **Chemical composition effect on damage**: OK
- **Reliable results only for a realistic continuous casting stress and tp° histories**
  - 3 successes: thermal discontinuities were taken into account
  - 1 failure: tp° history received was "smoothed"
- **Oscillation marks effect**, a **process defect effect** (misalignment of 1 pair of rolls…)

  → **Process defects and grade effects can be analysed**

Continuous Casting CC - References

Pascon, F., & Habraken, A. (2007). Finite element study of the effect of some local defects on the risk of transverse cracking in continuous casting of steel slabs. *Computer Methods in Ap. Mech. And Eng., 196*, https://doi.org/10.1016/j.cma.2006.07.017

Generalized Plane strain 2D FE to model CC

Castagne, S., Talamona, D., Habraken, A. (2007). A damage constitutive law for steel elevated temperature.
Identification of the parameters. *International Journal of Material Processing*, (1), 23-43.
https://hdl.handle.net/2268/19624

Schwartz, R., Castagne, S., & Habraken, A. (2007). Numerical study to identify the material parameters of a
damage model. *Computer Methods in Materials Science, 7* (2), 237-242
https://hdl.handle.net/2268/16210

Implementation and identification of Onck damage model for hot tp°
Onck, P., van des Giessen, E., 1999, J. Mech. Phys. Solids, 47(1), 99-139

Uliege PHDs are now available on ORBI (Castagne can be sent on request but paper)
Pascon https://orbi.uliege.be/handle/2268/25500
Schwartz https://hdl.handle.net/2268/97124

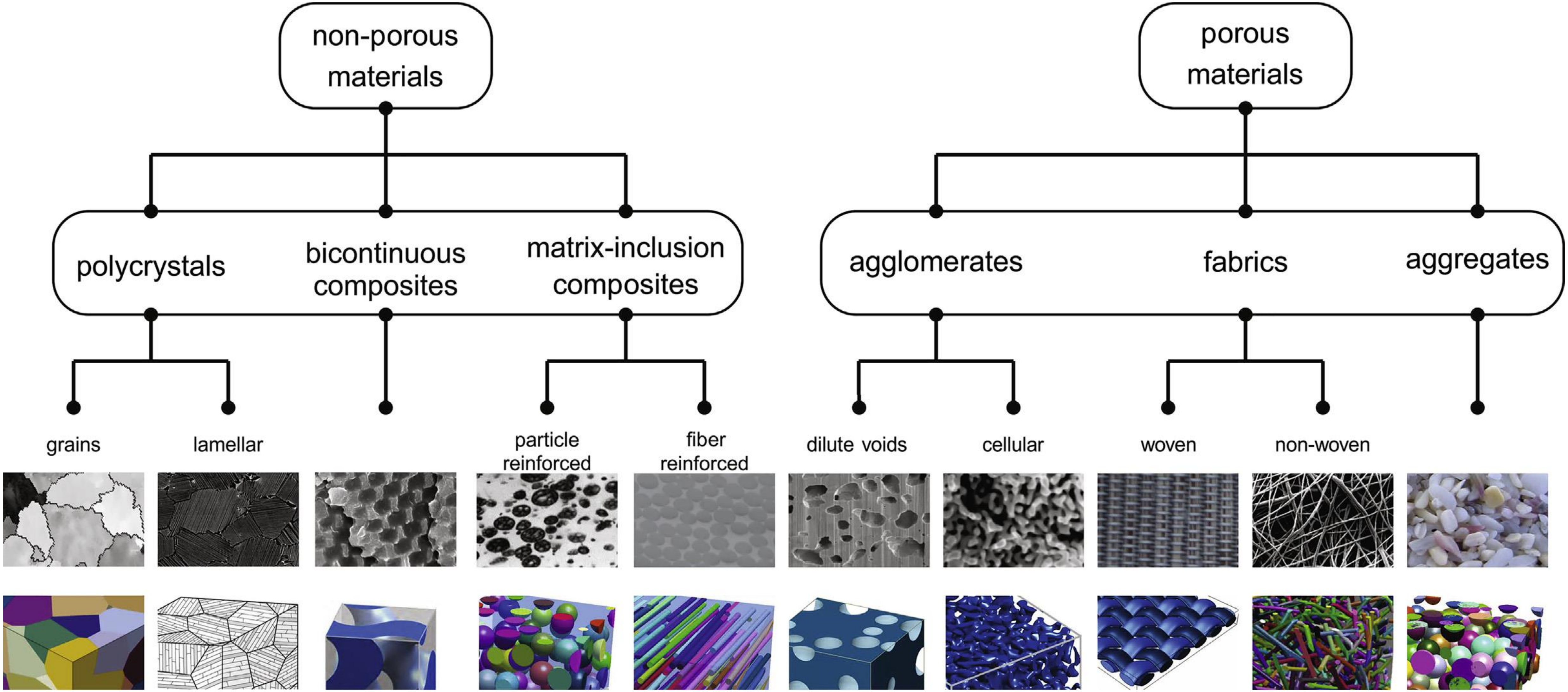
J. K. Brimacombe and K. Sorimachi. Crack formation in the continuous casting of steel. Met trans B, **1977.**

Reference about CC → issues and solutions based on practice and studies

Contents

- ✓A survey of scales and methods
- Finite element method FEM
  - ✓ One element: Solid Shell
  - ✓ Mechanical constitutive laws (multi scale ?)
    - ✓Deep Drawing
  - ✓Thermo-mechanical analysis
    - ✓Cooling of rolling mills
    - ✓Continuous casting
- Representative Volume Element (RVE) or in French VER
- Coupling solid FEM with … Computational Fluid Dynamics, Deep Learning
  - Additive Manufacturing

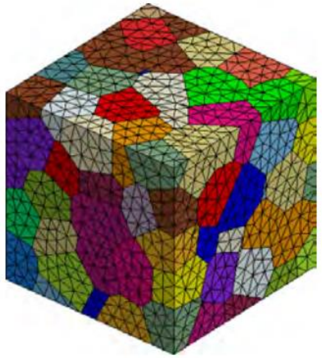
Representative Volume Element --> a generic practice



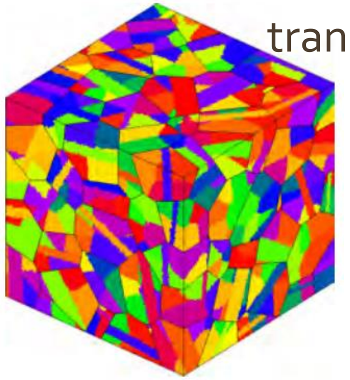
Bargmann et al. Review Progress in Materials Science 96 (2018)

Representative Volume Element --> use ?

- To understand, to model behaviour, to identify 'phenomenologic laws'
  - → static stress stain curves, anisotropy, elastic, plastic, viscoplastic behaviour
  - → rupture, shear band, void nucleation growth propagation (static or fatigue)
  - → creep, any damage ...



Parent austenite grains

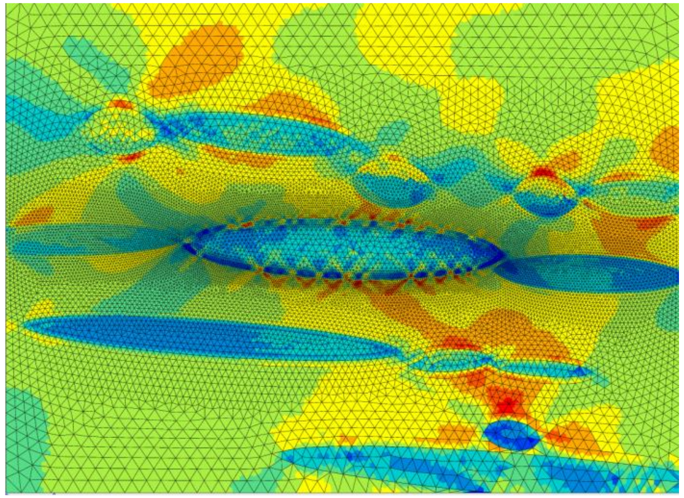


After Bainite transformation

Crystal PL.
→ local stress & strain fields,
→ inputs of cleavage models

16MND5
N. Osipov et al. *Matériaux 2006*

FE CALCULATIONS OF PLUMES WITH VIRTUAL ANGLES
PhD Kuzmenkov 2012 Ecole des Mines **Ti6242**



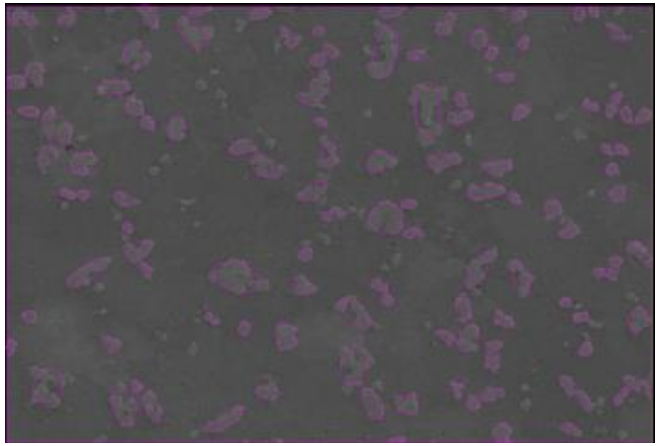
- To replace constitutive law in FE²

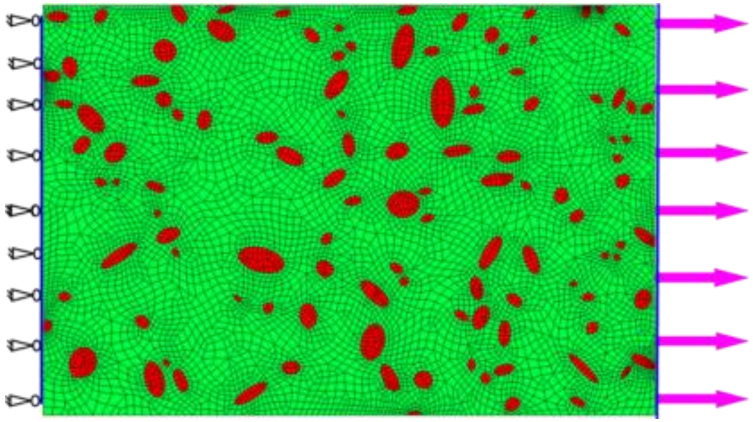
- Surrogate model within Artificial Intelligence → training of ANN, RNN, FFNN,.... **Today**

Validation of a large RVE by tensile test

Exp. Microstr.
Zhao et al.
MSEA 2019

AlSi10Mg

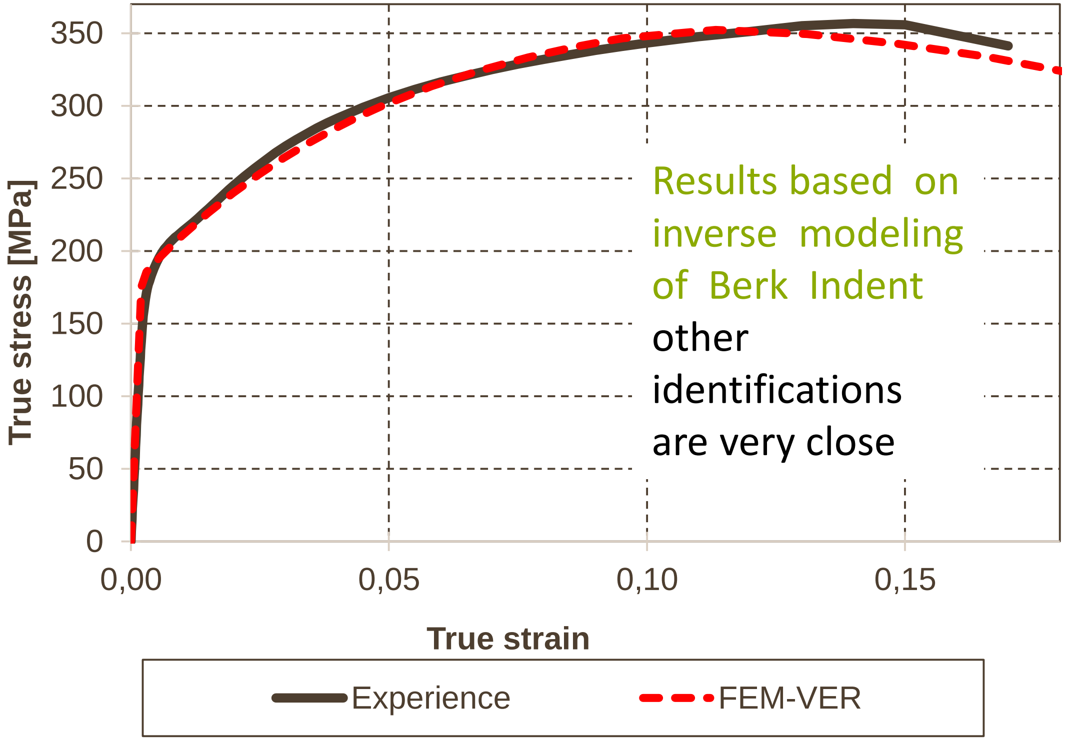




No specific boundary Conditions
A single Layer of 3D element

Si stays elastic

H.S. Tran, C. Bouffioux et al. Materials and Design 2022

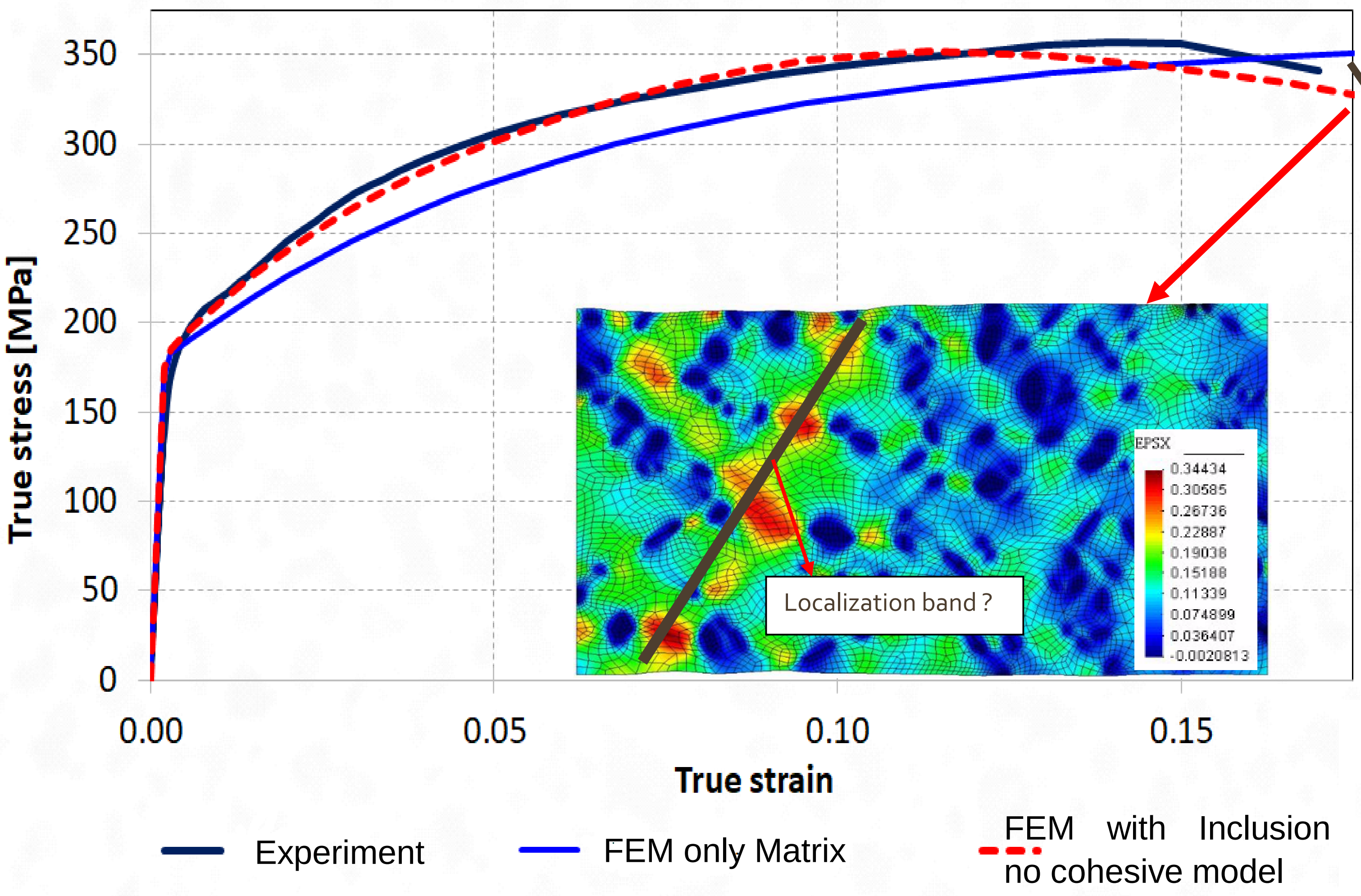


Results based on inverse modeling of Berk Indent
other identifications are very close

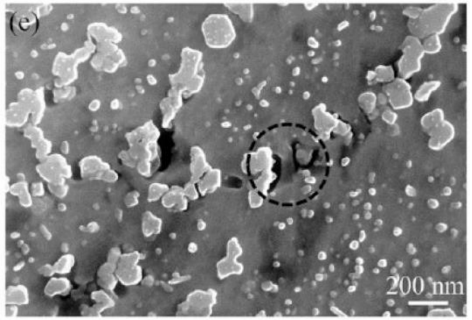
σy of Solid solution of Al Si ??

- Nanoindentadion Bucaille, Exp approach 3 indents (Dedry 2021 ESAFORM)
- Inverse modelling - Berkovich indent - care about particle interactions
- Analytical formula + DL Borlaf master thesis 2023

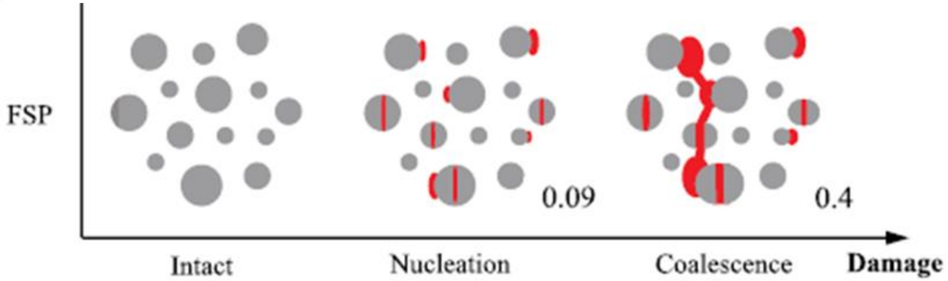
Validation of large RVE by tensile test



H.S. Tran, C. Bouffioux et al. Materials and Design 2022



ductile failure with damage nucleation sites
= mainly particle-matrix decohesion
(Zhao et al. MSEA 2019)

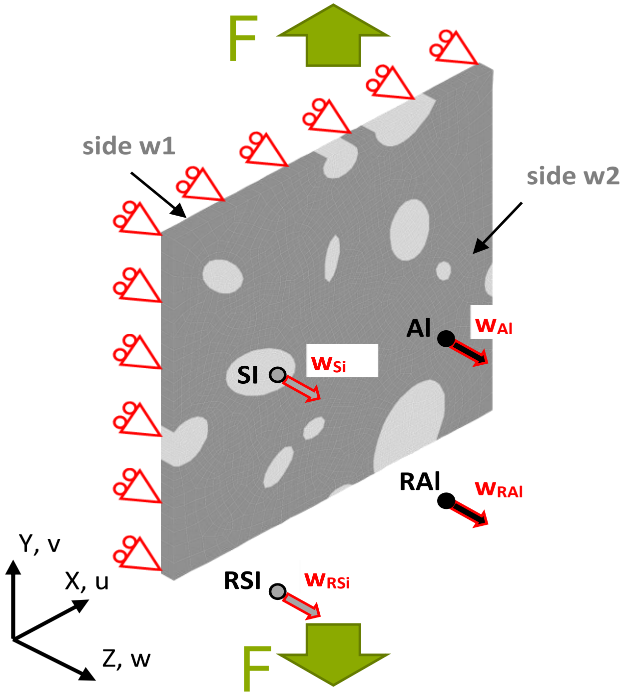


→ **Need of cohesive elements to capture real rupture mechanism, current RVE OK until 0.08 strain**

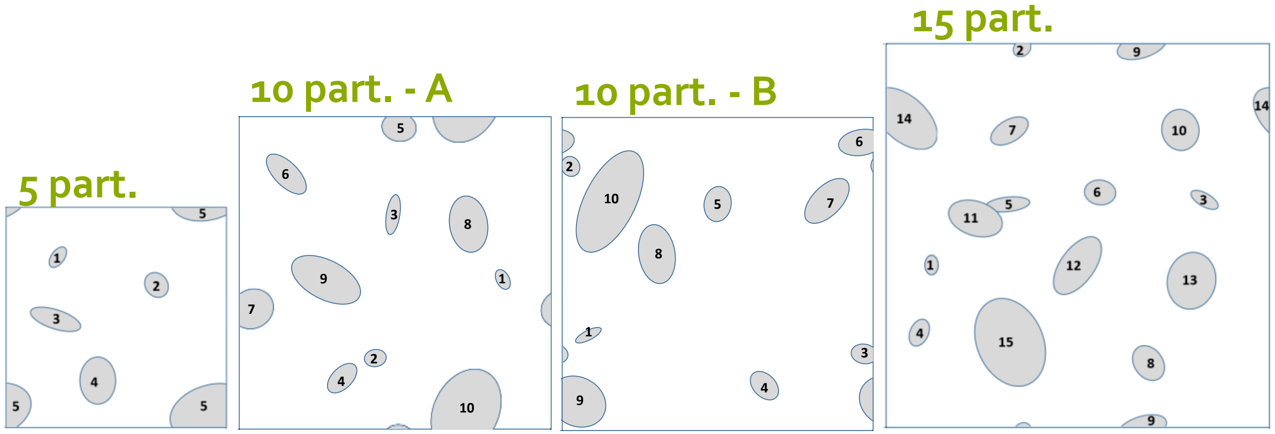
Small 2.5D RVE - Details

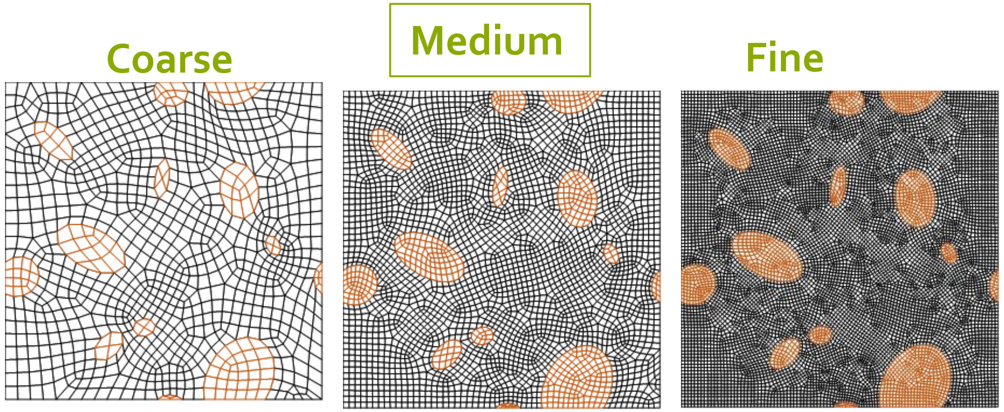
2D or 3D ? → 2.5D

- Particles: statistically representative
- Out-of-plane stiffness adjustment
- Same behavior: num. & exp.
  - → Representative size: 10 particles
  - → Optimum mesh density: Medium
  - → Out-of-plane stiffness adjustment

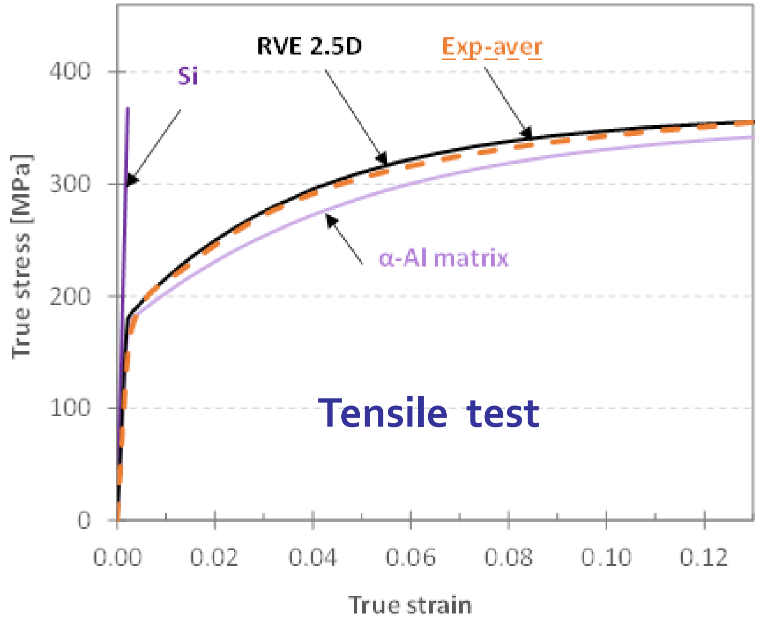


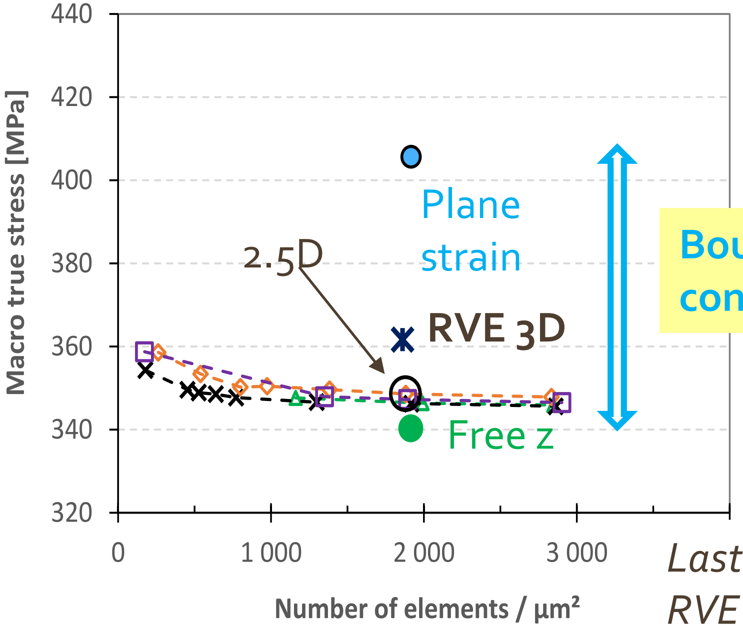
- Target: representativity of a macro tensile test in Y dir.
- Macro level : $\varepsilon_{XX} \approx \varepsilon_{ZZ}$ isotropic material
- Local level: ε_{ZZ} identical for all particles
- Interface: Cohesive elements
- Bouffioux et al. ESAFORM 2022



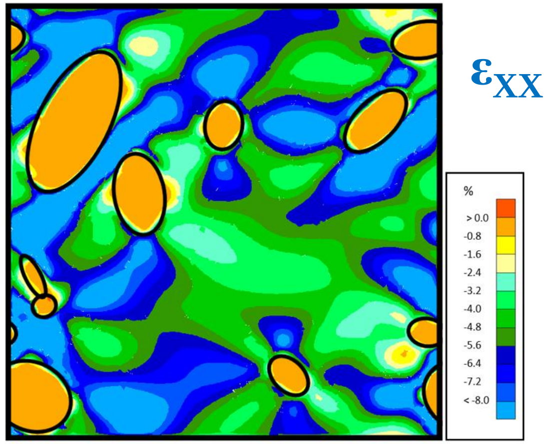


Smaller RVE with periodic boundary





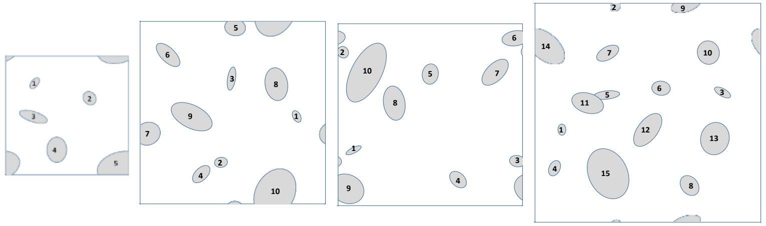
Boundary condition effect



Last result tuning ↓
RVE 3D and 2.5D differences

Comparison of all simulations

△ Small ✕ Medium-A ◇ Medium-B ☐ Large



Poor macro stress effect between Free Z, 2.5 D, 3D RVE

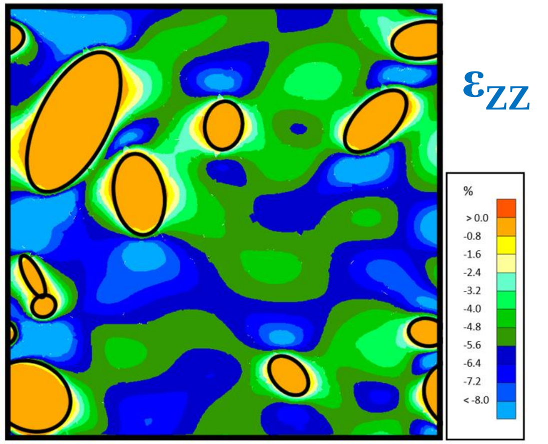
Exp between 2.5D and 3D RVE

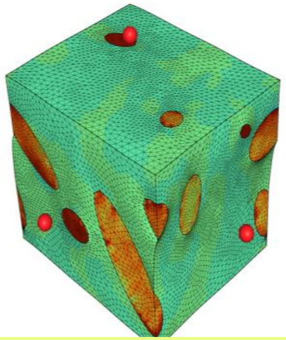
RVE plane strain too stiff

Effect on local stress ?

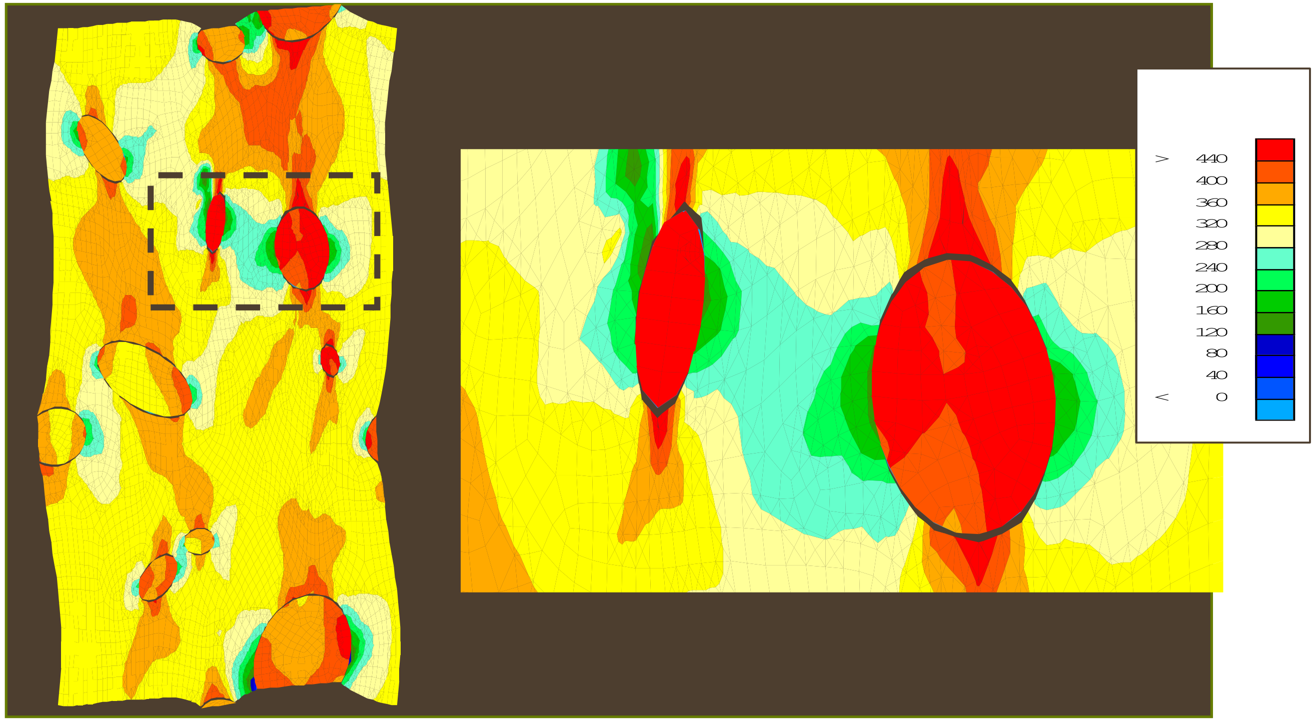
2.5D // 3D RVE (in average) –

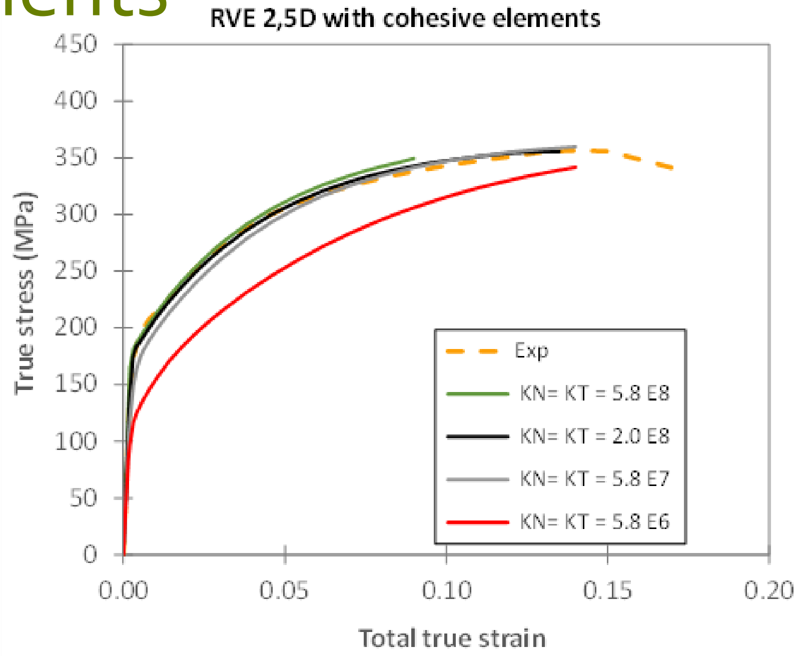
Absolute max values depend on particle distribution

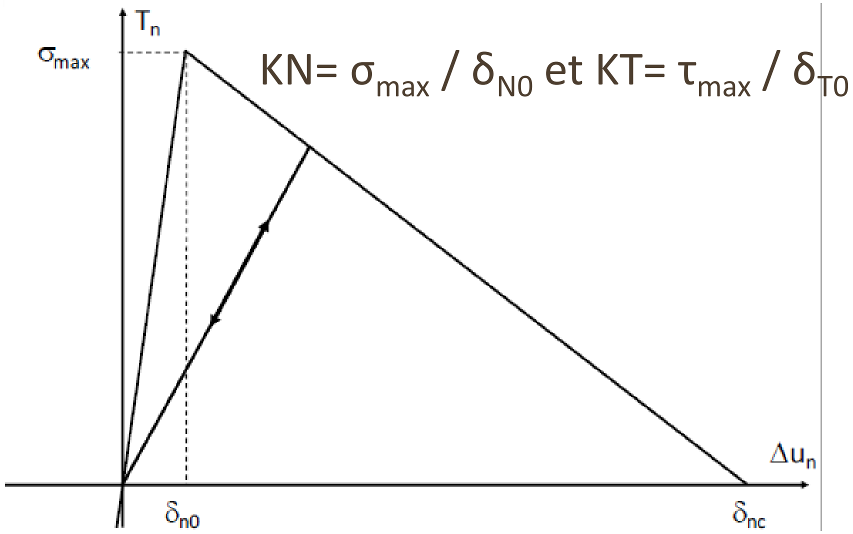




Validation of **small 2.5D RVE** with Periodic Boundary conditions & cohesive elements







KN= $\sigma_{max} / \delta_{N0}$ et KT= τ_{max} / δ_{T0}

Stress in tensile direction [MPa] at macro strain of 10 %.

Displacement x 10 to enhance decohesion.

Indentified set of parameters

same strength in tensile and shear decohesion → tensile decohesion first

Representative Volume Element references

Generation of 3D representative volume elements for heterogeneous materials: A review **S. Bargmann et al.** Progress in Materials Science 96 (2018)
https://doi.org/10.1016/j.pmatsci.2018.02.003

About RVE FE mesh generation

FE² Computations with Deep Neural Networks: Algorithmic Structure, Data Generation, and Implementation **Eivazi H.** 2023 *Mathematical and Computational Applications*

https://doi.org/10.3390/mca28040091

Concept Equations Academic example

Déc 2007 : **Nikolay Osipov** PhD Génération et calcul de microstructures bainitiques, approche locale intragranulaire de la rupture Paris Ecole Centrale - not open?
→ First steps Numerical generation and study of synthetic bainitic microstructures *Matériaux 2006*, Dijon, France.
⟨hal-00144530⟩

Déc 2009: **Thibault Herbland** PhD Une méthode de correction élastoplastique pour le calcul en fatigue des zones de concentration de contraintes sous chargement cyclique multiaxial non proportionnel
https://pastel.hal.science/tel-0047999

Cailletaux's RVE use to study phenomena

Juin 2012 **K Kuzmenkov** PhD Etude de l'effet du temps de maintien sur le comportement et la rupture (effet Dwell) de l'alliage base Ti6242

See also **Forest S.** and so many....

Contents

- ✓A survey of scales and methods
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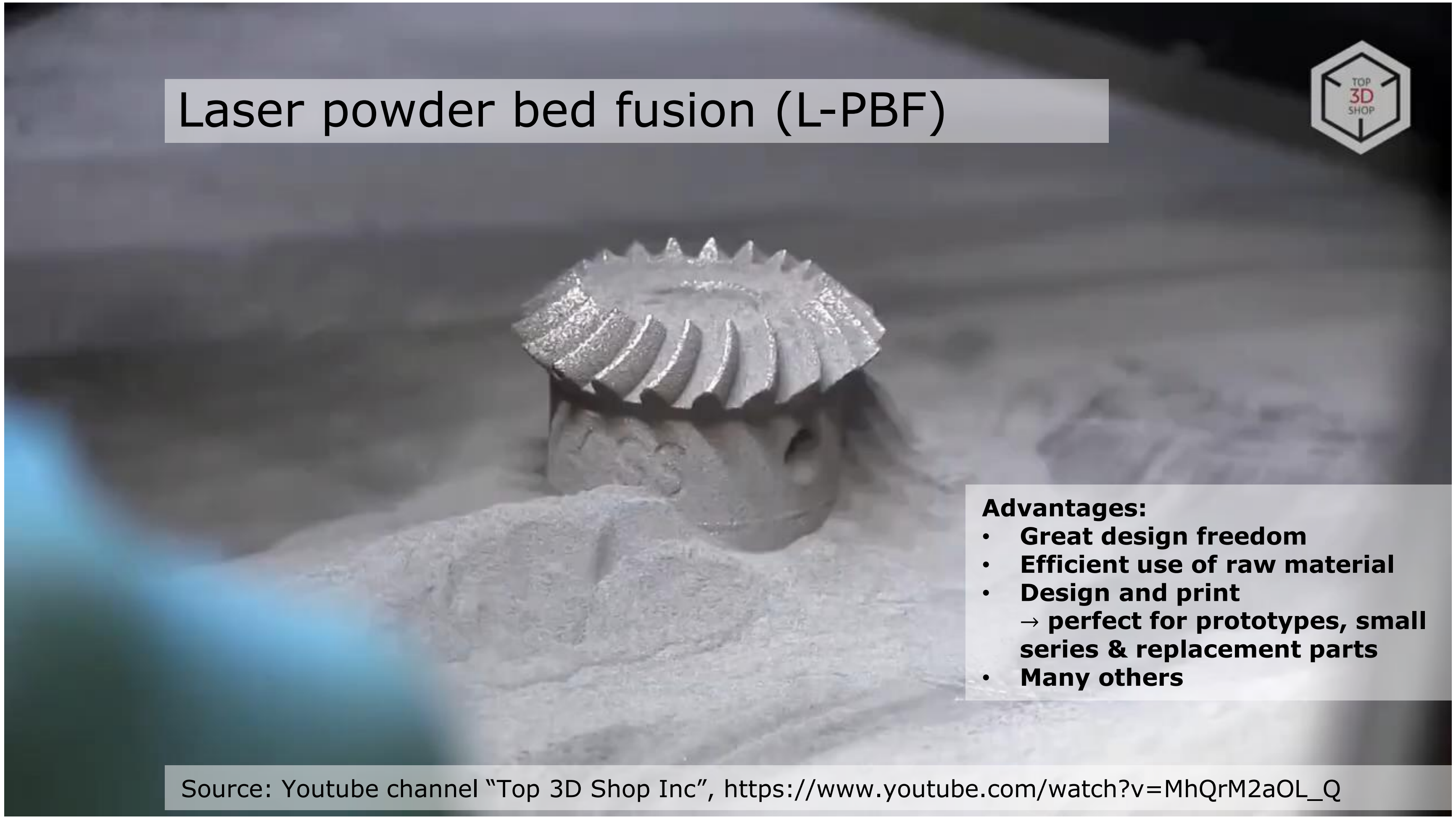
- Coupling solid FEM with … Computational Fluid Dynamics, Deep Learning
  - Additive Manufacturing

Additive Manufacturing



Laser powder bed fusion (L-PBF)

Advantages:
- **Great design freedom**
- **Efficient use of raw material**
- **Design and print**
  → perfect for prototypes, small series & replacement parts
- **Many others**

Source: Youtube channel "Top 3D Shop Inc", https://www.youtube.com/watch?v=MhQrM2aOL_Q

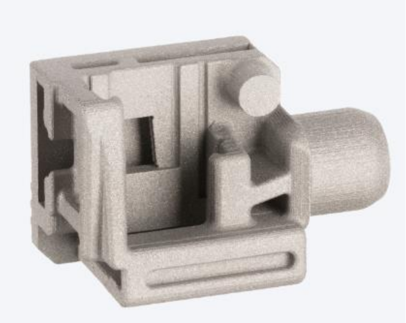
Time > 9 min (end advertisement but before good introduction to L-PBF)

Courtesy of
Dr. B.J. Bobach

PhD 2023
under
J.P. Ponthot
supervision
Uliege

PhD Oct 2023

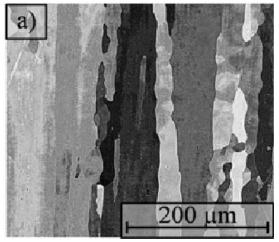
Typical length scales → a choice

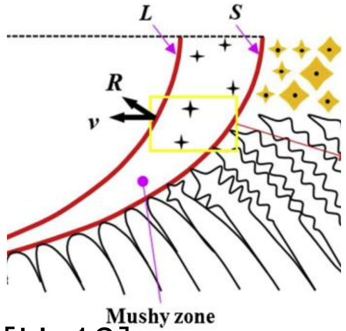


Micro-scale

Resolves grain structure

- Anisotropic grain growth (e.g. dendrites, columnar grains)
- Anisotropic material behavior





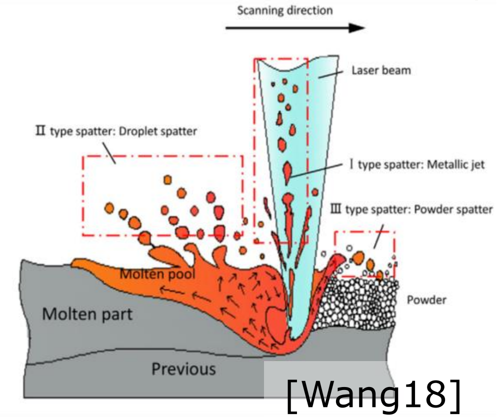
[Liu19]

[Kör14]

Meso-scale

Resolves melt pool

- Heat source interaction
- Melt front advancement
- Convective flow
- Localized residual stresses
- Powder effects, spatter
- Keyhole formation

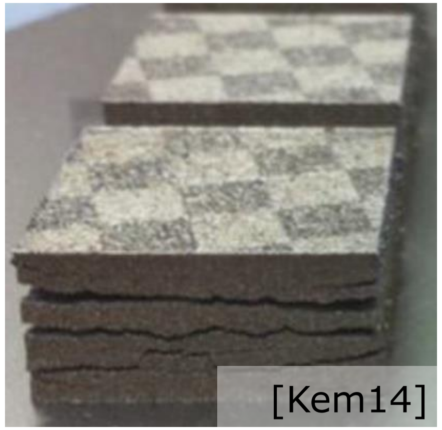


[Wang18]

Macro-scale

Resolves whole part

- Whole process
- Thermal history
- Overall residual stress
- Part distortion



[Kem14]

[Liu19] P. Liu et al., Insight into the mechanisms of columnar to equiaxed grain transition during metallic additive manufacturing, Additive Manufacturing 26,2019,
[Kör14] C. Körner et al., 2014, Tailoring the grain structure of IN718 during selective electron beam melting. MATEC Web of Conferences.
[Wang18] D. Wang et al.,Mechanisms and characteristics of spatter generation in SLM processing and its effect on the properties," Materials & Design, vol. 137, pp. 33–37,Jan. 2018,
[Kem14] K. Kempen et al. ‚SLM of Crack-Free High Density M2 High Speed Steel Parts by Baseplate Preheating", Journal of Manufacturing Science and Engineering, vol. 136, p. 131-139, 2014.

Which model type ? Goal = Part quality (with low porosity)

→Computational Fluid Dynamics

(Meso-scale)

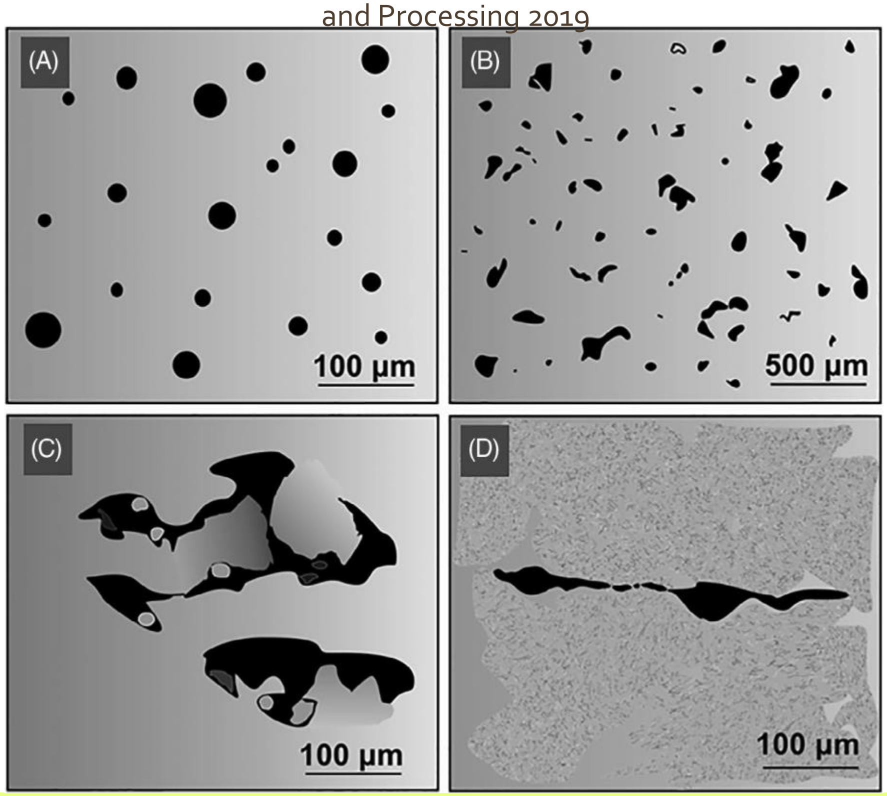
First what is porosity origin….

(A) Entrapped gas porosity (Keyhole);

(B) Incomplete melting-induced porosity;

(C) Lack of fusion with unmelted particles inside large irregular pores

A. Sola A Nouri Wiley Advanced manufacturing and Processing 2019



→Solid Finite Element

(D) Cracks

→Either accurate finite element thermo-mechanical analysis

→Or inherent or eigen-strain-method

+ contour method (calibration)

→OrAnalytical formulae if very simple shape….

→Or

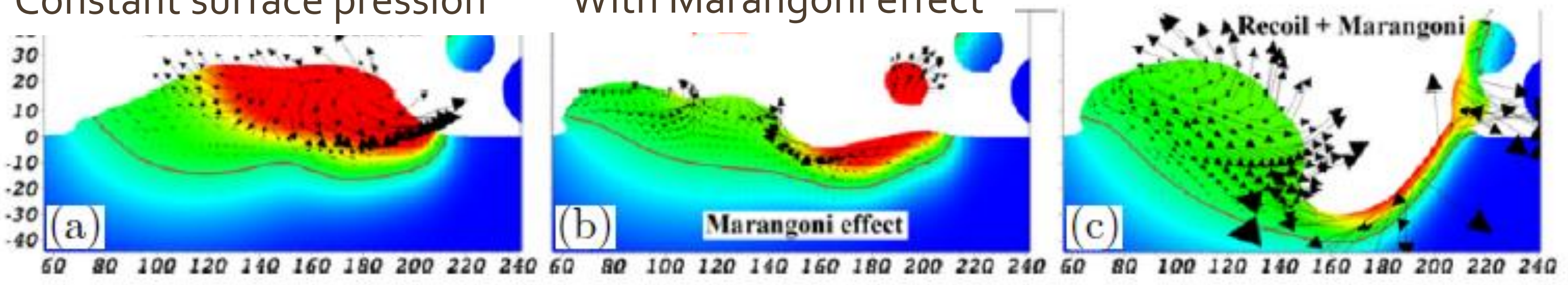
(Macro-scale)

Not a simplified CFD code
Surface tension, Marangoni, recoil pressure

Constant surface pression

With Marangoni effect

+ Recoil pressure effect



400K 🟥

293K 🟦

Predictions
Temperature field
+ fluid free surface

S. A. Khairallah, A. T. Anderson, A. Rubenchik, and W. E. King. Laser powder-bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones. *Acta Materialia*, 108:36–45, 2016.

→ convection-related terms (Marangoni)

→ recoil pressure

Essential features in a CFD model for AM

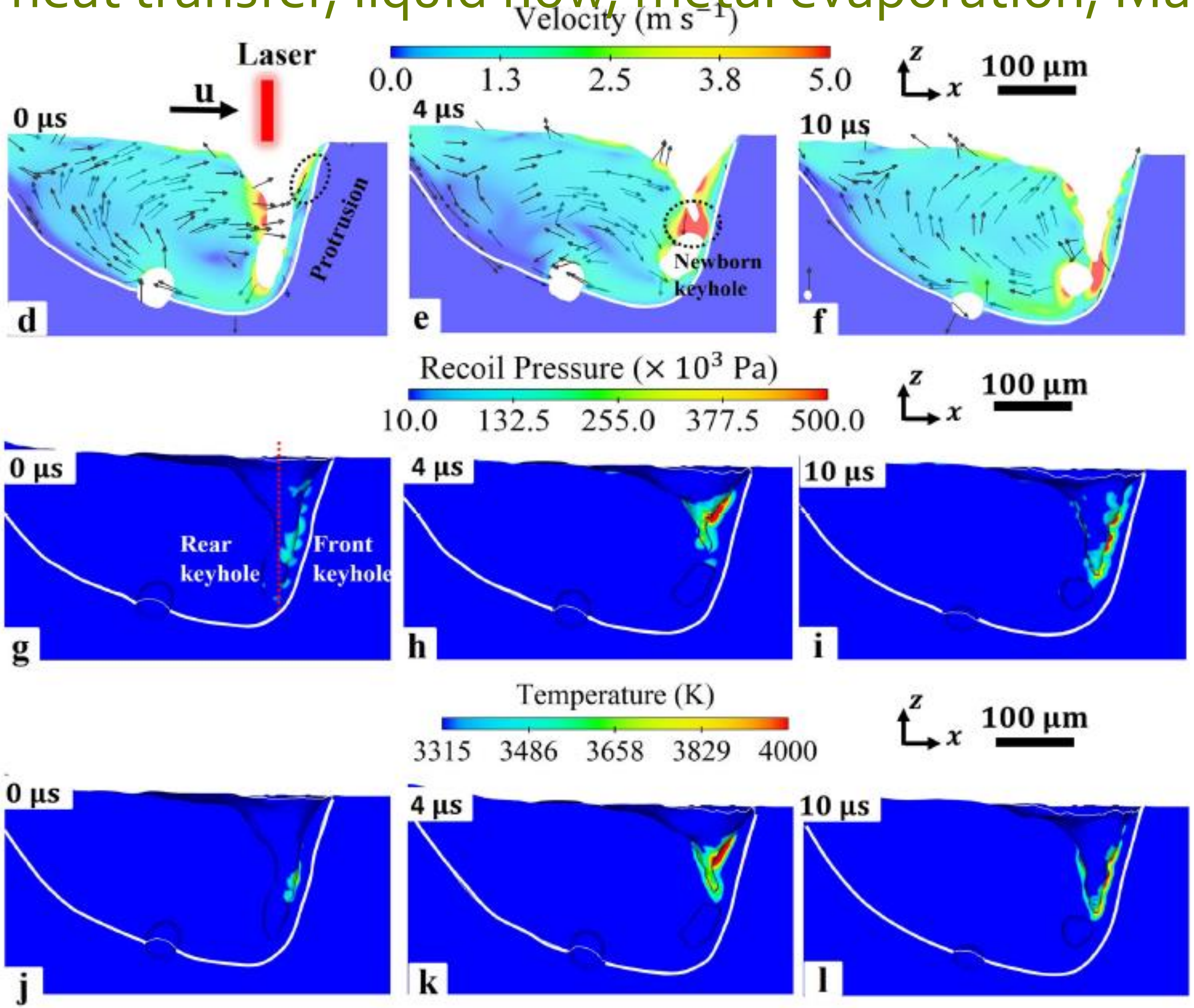
CFD model with heat transfer, liquid flow, metal evaporation, Marangoni effect, Darcy’s law

Wang et al. Computational Materials (2022)

Velocity

Recoil Pressure

Temperature



Which model type ? Goal = Microstructure prediction

1. Accurate Finite Element Thermo (Mechanical) analysis
2. Post processing or coupled analysis (Tp° Field + Metallurgy)

→phenomenological based Johnson-Mehl-Avrami-Komlogorov or Koistingen-Marburger models…

Macro-scale

→Phase Field models (micro scale - thermodynamic laws)

→Cellular Automata approach (CAFE)

→Deep learning approaches (DL Deep Learning & its acronyms)

Micro-scale

Real challenge: lack of data and knowledge

-high temperature cooling rate and heating rate

-multiple cycles (remelting or just heating + cooling) → strong out of equilibrium microstructures

-complexity: phases, morphology, distribution, heterogeneity

FE variants for Additive Manufacturing

- FEM models with birth elements

⚠

or Approach with all elements there and property variation ?

2nd choice less accurate: COMSOL has both and it can be checked.

- Thermal model associated to liquid within solid FE elements?

Assumption about thermal properties within melt pool

→"Marangoni effect" : multiplying real conductivity

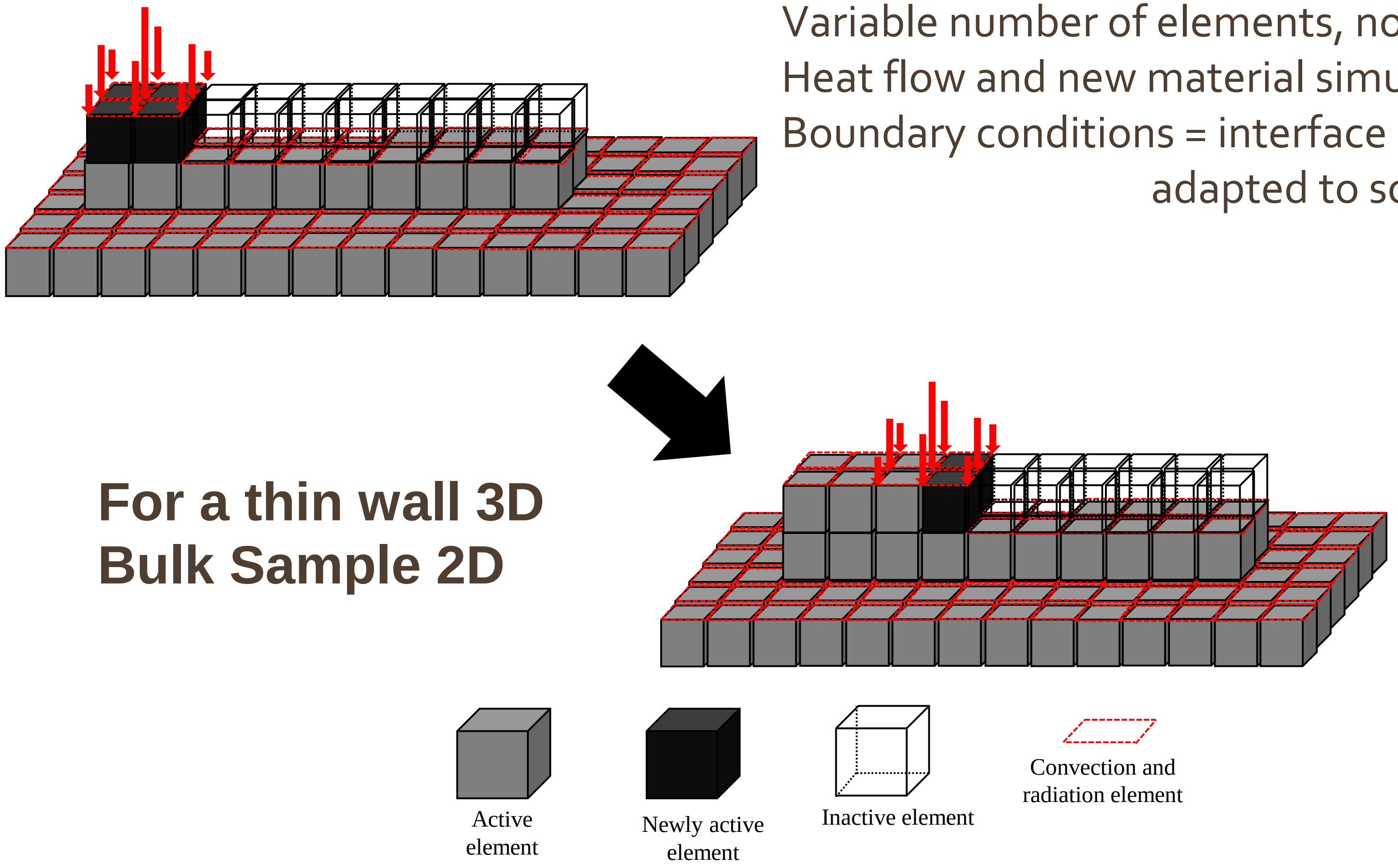
- Rheological model?

⚠

Elasticity → Elasto Visco Plasticity with metallurgy…

Experimental calibration is strongly different

Element birth technique



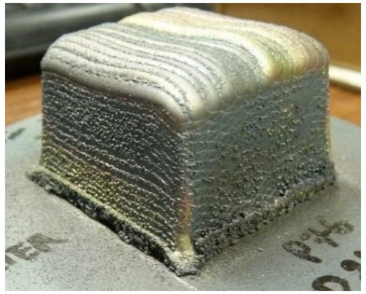
Variable number of elements, node, DOF
Heat flow and new material simulated by 2 to 9 elements
Boundary conditions = interface elements
adapted to solid element

For a thin wall 3D
Bulk Sample 2D

Element size defined
by laser beam size !
→Direct mesh
convergence
→Mesh variable
density by GMSH

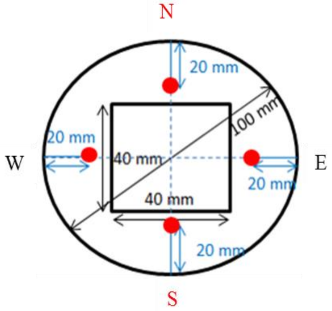
Convection-radiation elem. on vertical planes of the clad not drawn

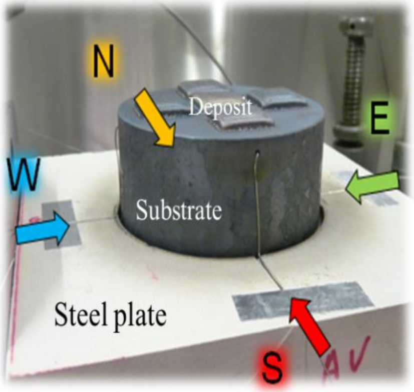
Bulk sample M4 high speed steel



40 x 40 x 27.5 mm
(874 tracks)

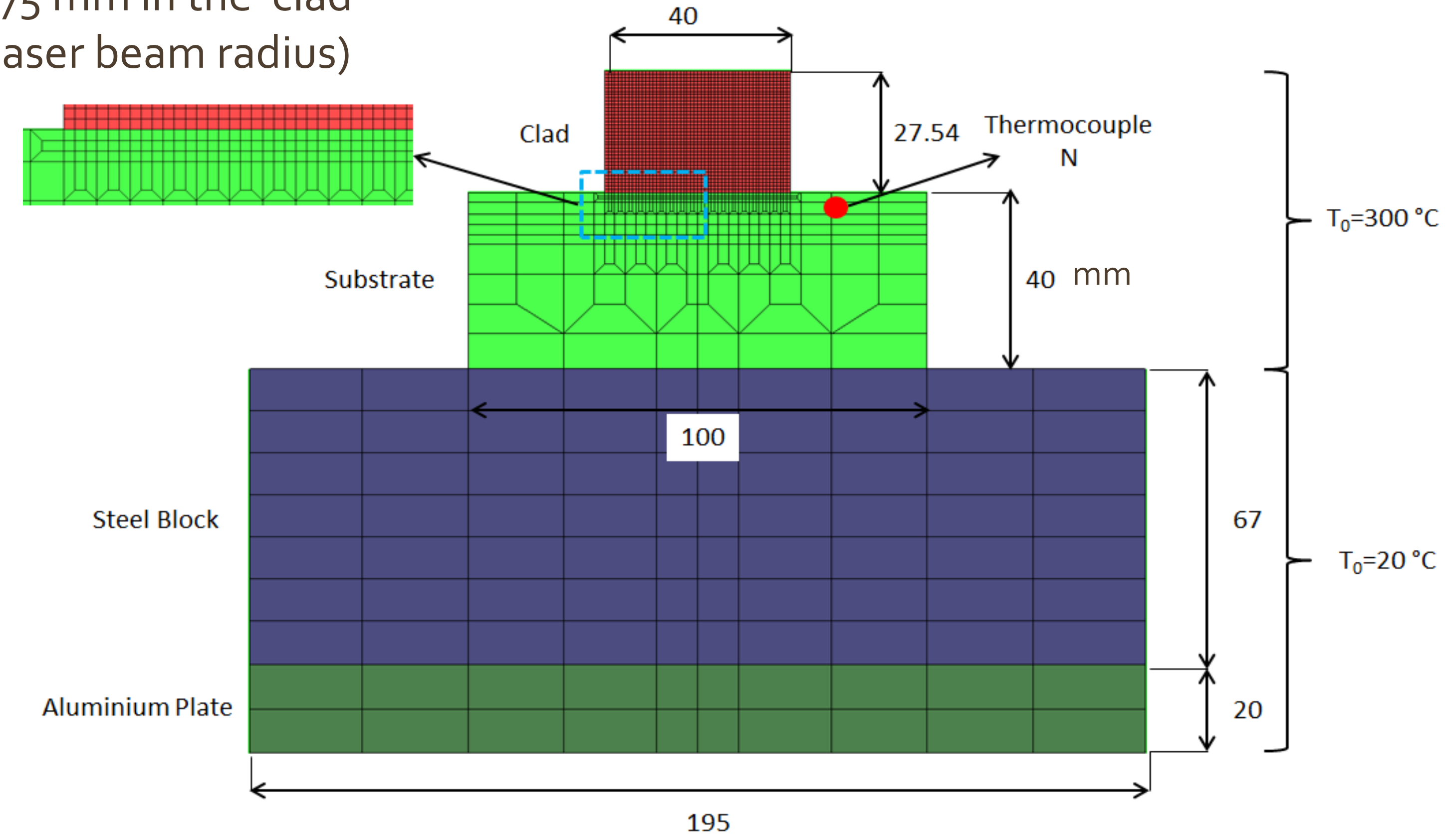
4 Thermocouples Tp(time)





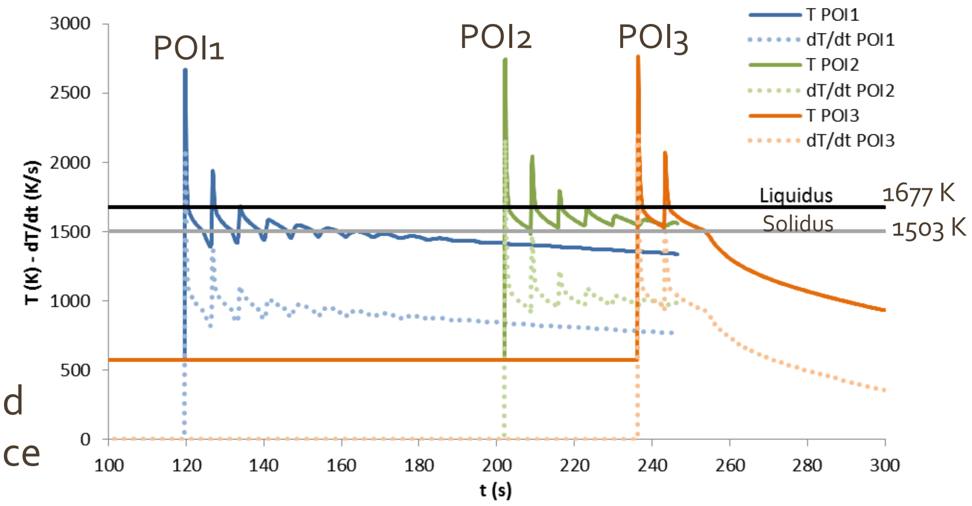
2D FE Mesh

Mesh element size
0.75 mm in the clad
(Laser beam radius)

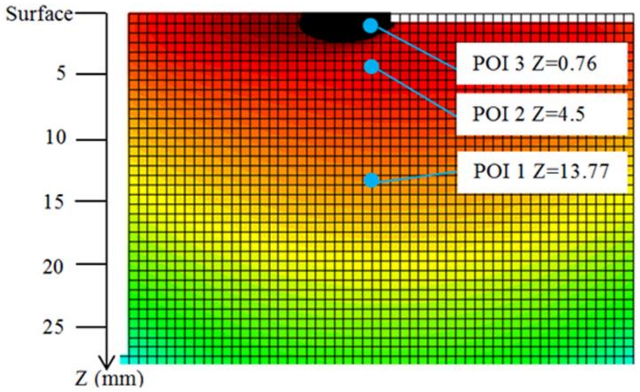


Simple thermal model
It needs good identification
to reach good results

FE Tp field & history in the clad (constant laser power)

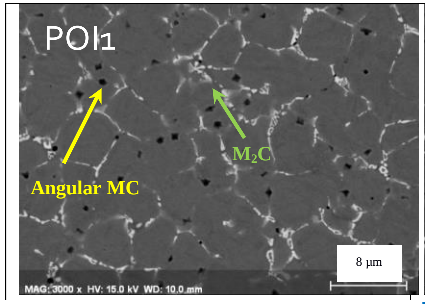


substrate
pre-heated
in a furnace

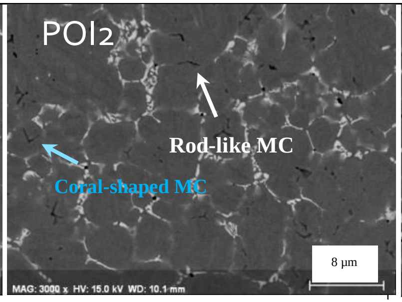


Jardin et al Materials Letters 2019

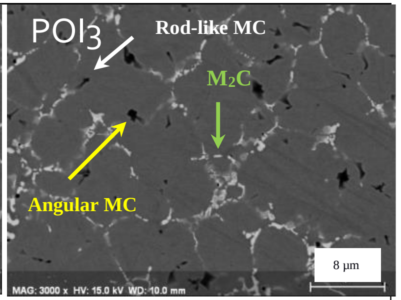
- -Number of full partial remelting
- -Tp° Level between solidus & liquidus
- - Superheating temperature



star-like MC
lamellar eutectic M_2C
intercellular carbides



coral-shaped **intra**cellular MC,
intercellular eutectic M_2C
and refined cells due
to multiple melting



coarse angular MC
eutectic M_2C within
intercellular zones
larger cell

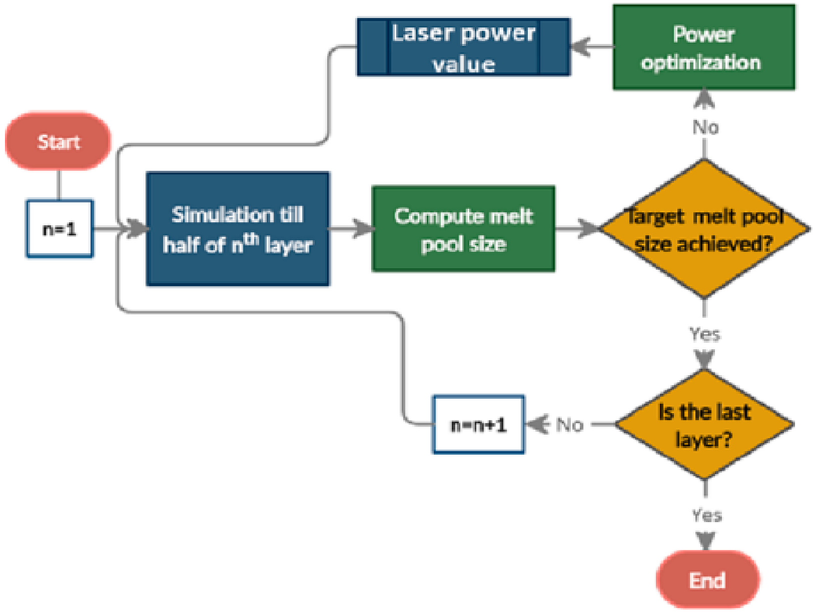
Validations :

1. **Thermocouples**
2. **Melt pool size of last layer**
3. **Microstructure**

Laser power optimization to ↗ microstructure homogeneity

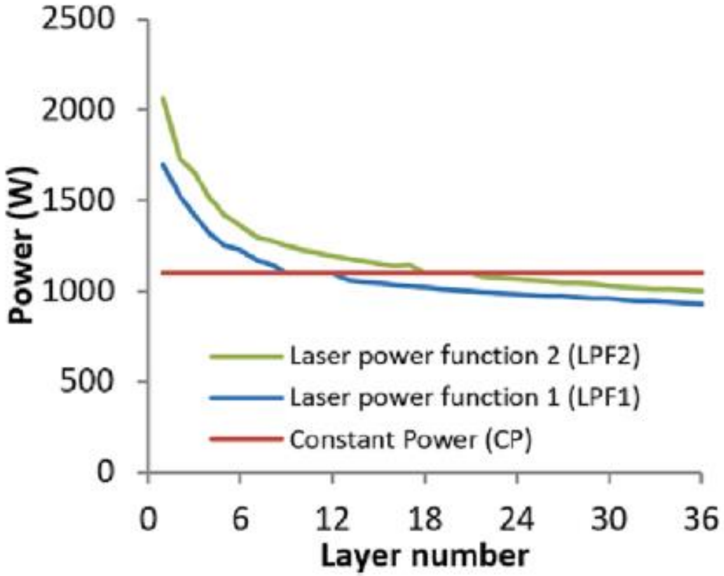
1st METHOD

Netwton Raphson algorithm such that melt pool = ct value
Two different constant values → Laser Power Functions LPF1 and LPF2



Melt pool size target:

LPF 1 → 1.4 mm depth, 4.4 mm length
LPF 2 → 1.8 mm 5.7 mm



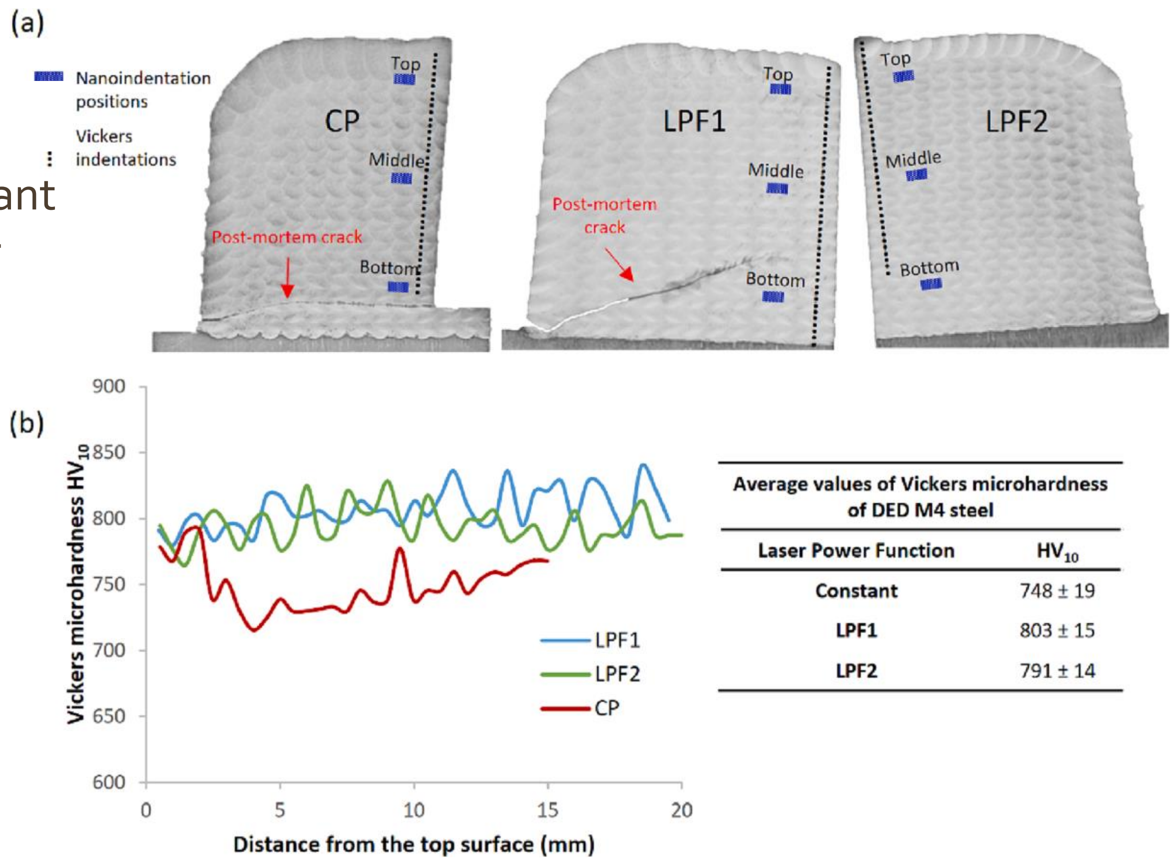
Jardin et al. Optic & Laser technology 2023

Hardness measurements confirm homogeneity

.... Vickers measurements

Laser Power Function LPF

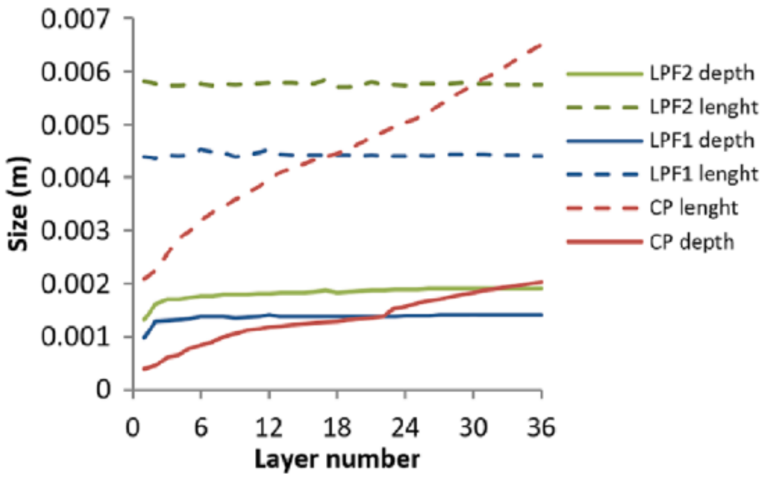
CP
Constant
power



Average values of Vickers microhardness of DED M4 steel

Laser Power Function	HV_{10}
Constant	748 ± 19
LPF1	803 ± 15
LPF2	791 ± 14

Predicted melt pool depth & length



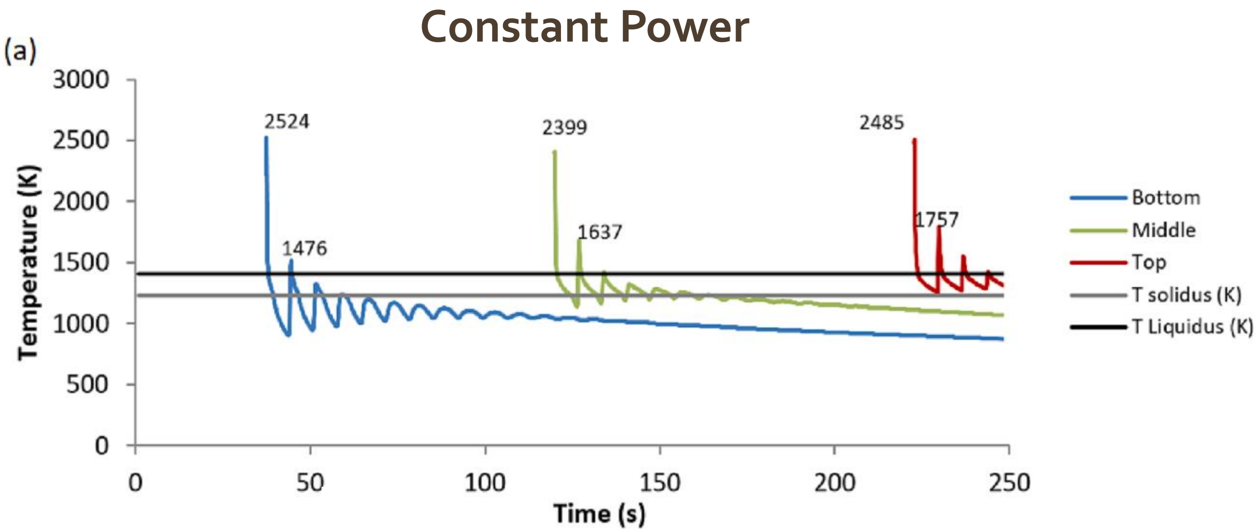
Jardin Optic & Laser technology 2023

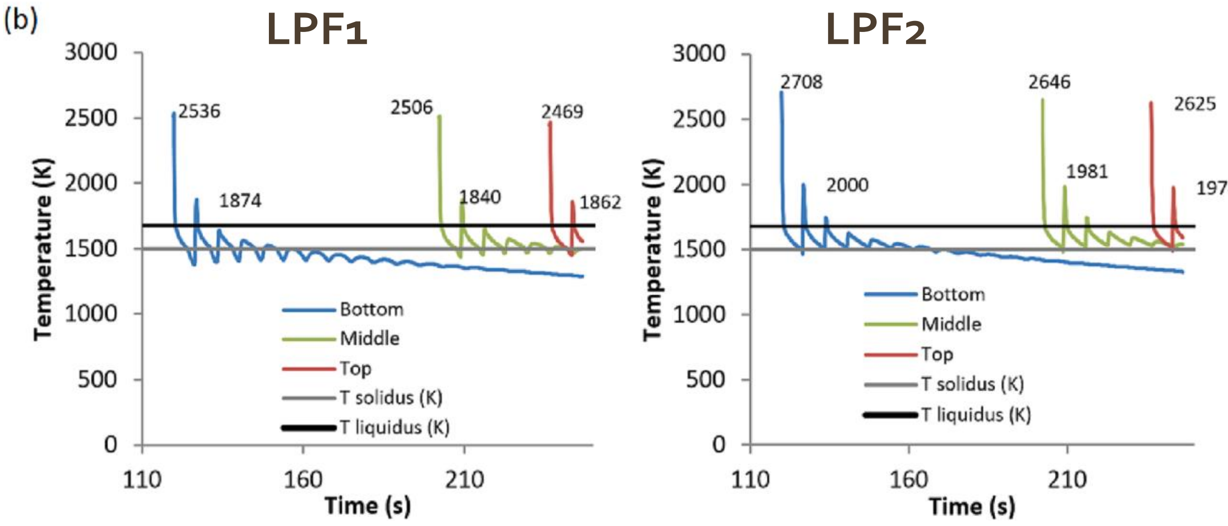
Constant target depth = assumption for constant tp° history

→ homogeneous microstructure

LPF 1 → 1.4 mm depth, 4.4 mm length
LPF 2 → 1.8 mm 5.7 mm

Tp history analysis





LPF2
Higher homogeneity
Higher in situ annealing Tp°

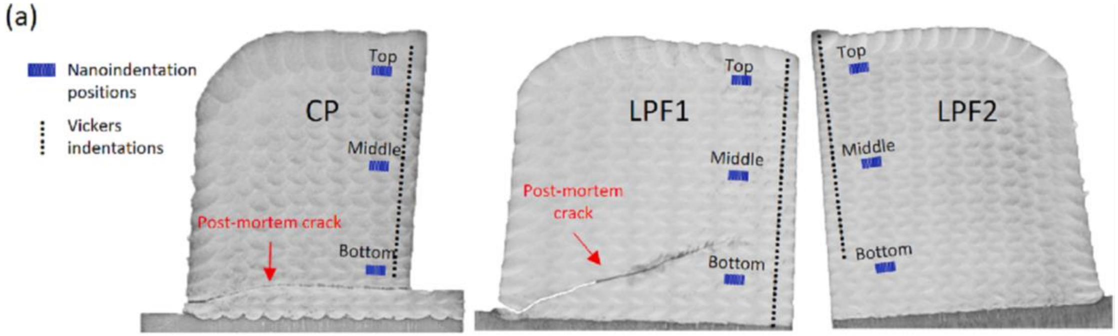
Average max peak Tp°
LPF2 : 2569 K
LPF1: 2505 K
CP : 2469 K

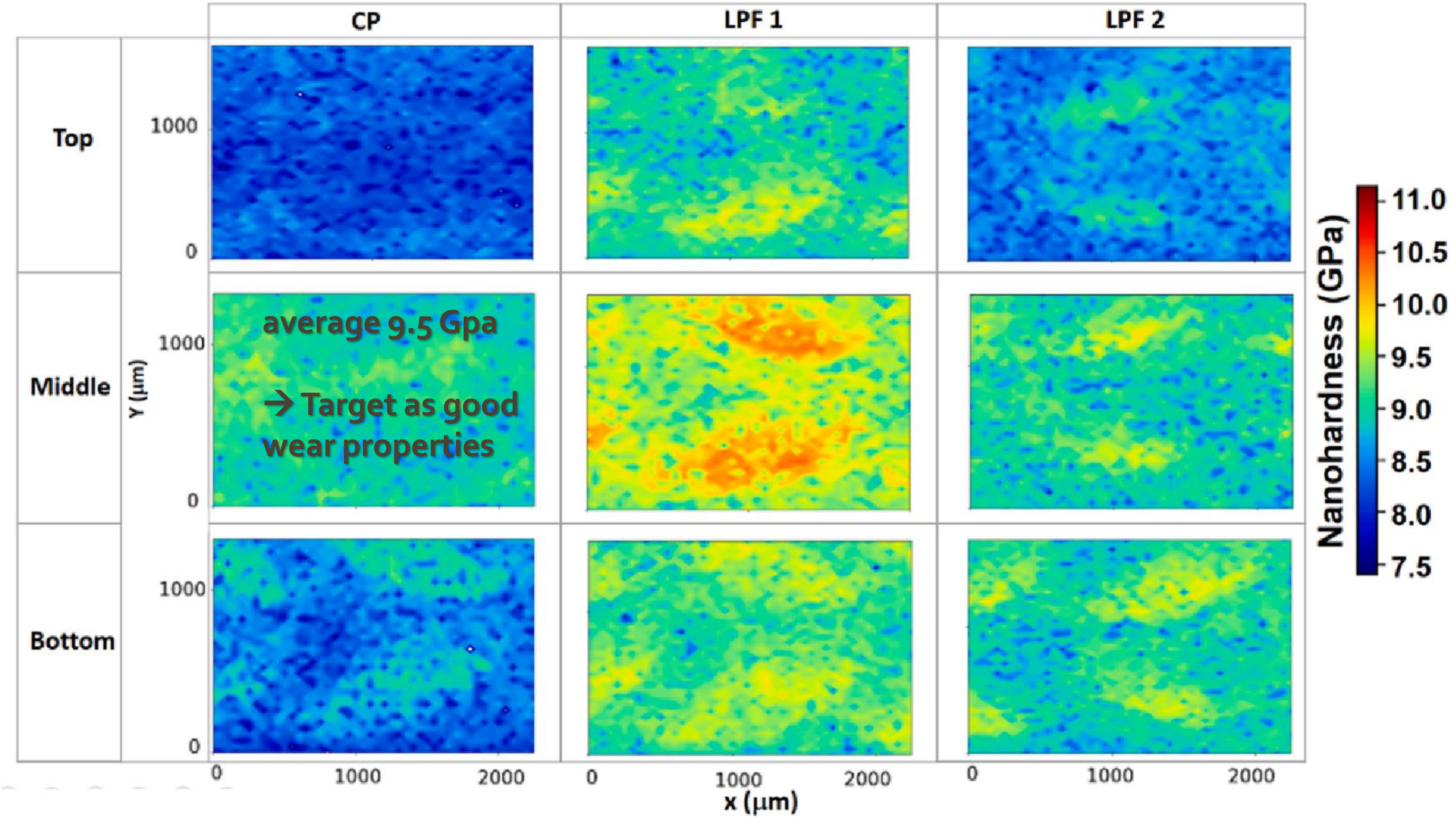
Higher accumulation of heat
→slower cooling process
→more homogenous microstructure
→lower residual stresses

→No crack in LPF2 sample at cutting.

Jardin Optic & Laser technology 2023

Nano indentation maps
Confirm homogeneity





average 9.5 Gpa

→ Target as good wear properties

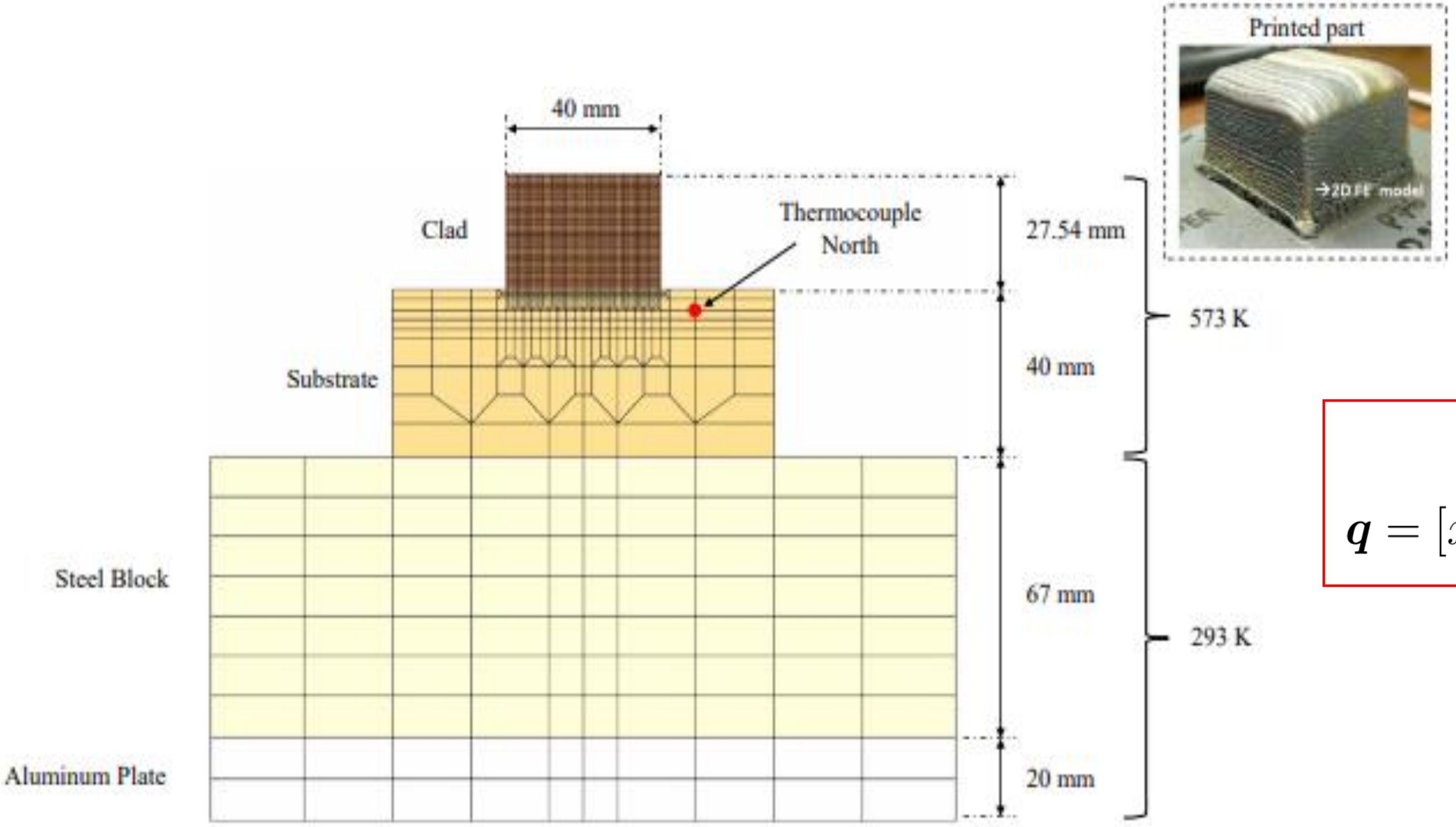
Homogeneity of LPF2 confirmed
+
Interest level of hardness reached

= optimum

For prediction heterogeneity : melt pool events
→ CFD needed

2nd METHOD

Feed Forward Neural Network (FFNN) replaces FE



Input $\boldsymbol{q}$

Output T

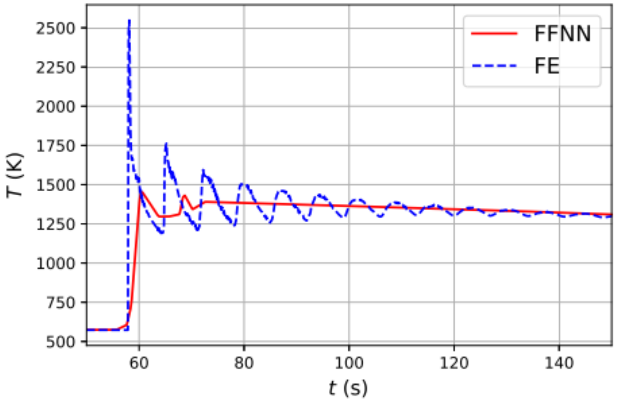
$$T = T(\boldsymbol{q}),$$
$$\boldsymbol{q} = [x,\ y,\ z,\ t,\ m_1,\ \ldots, m_\mu,\ p_1,\ \ldots, p_\nu]$$

Position, Time | Material properties | Process parameters

T.Q.D Pham Journal of Intelligent Manufacturing 2022

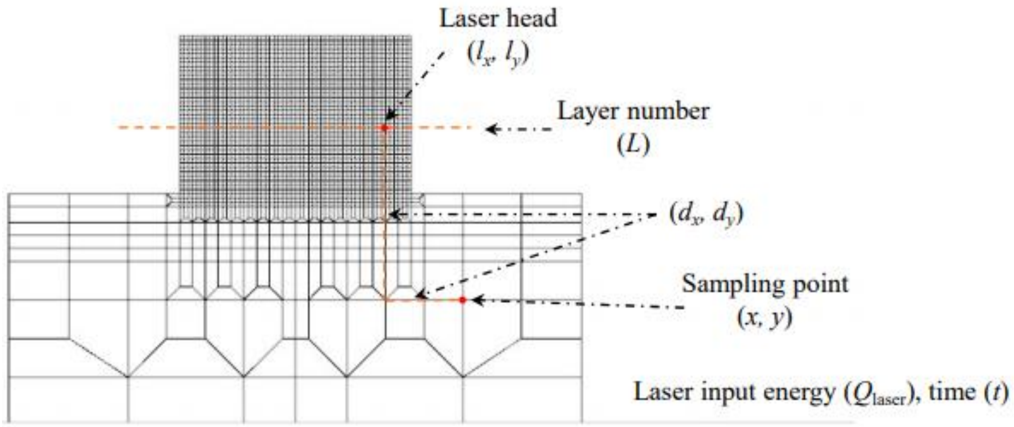
Feature selection q in the FFNN

Using only the $(x, y, t, Q_{\text{laser}})$



Integrate

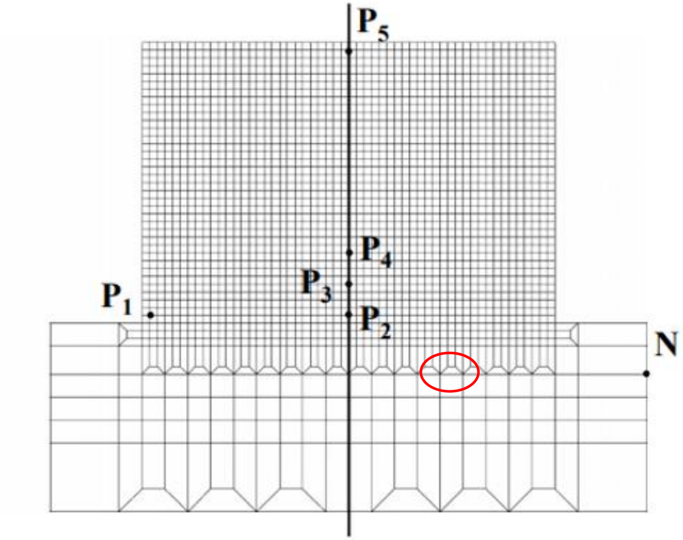
physics

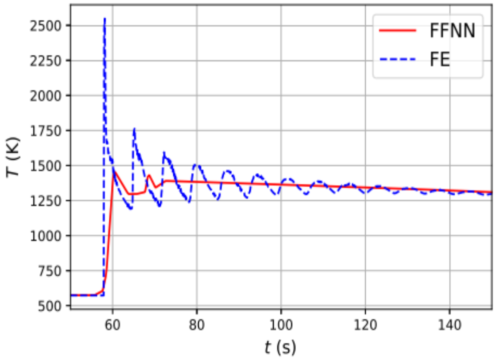


Model	Base model (BM)	Intermediate model (IM)	Full model (FM)
Input features	$x, y, t, Q_{\text{laser}}$	$x, y, t, l_x, l_y, Q_{\text{laser}}$	$x, y, t, l_x, l_y, d_x, d_y, L, Q_{\text{laser}}$
Number of input features	4	6	9
R^2	0.798	0.968	0.994

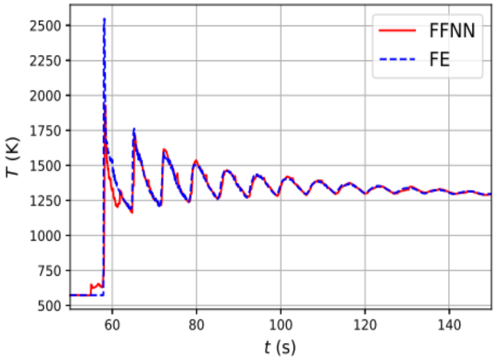
T.Q.D Pham Journal of Intelligent Manufacturing 2022

FFNN Result analysis Tp° at Point 2

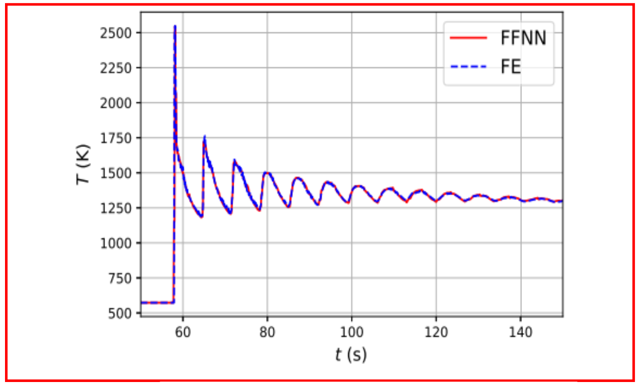




Base model (4)



Intermediate model (6)



Full model (9)

➡ **Integrating physics to the DL model to capture cycles and peaks**

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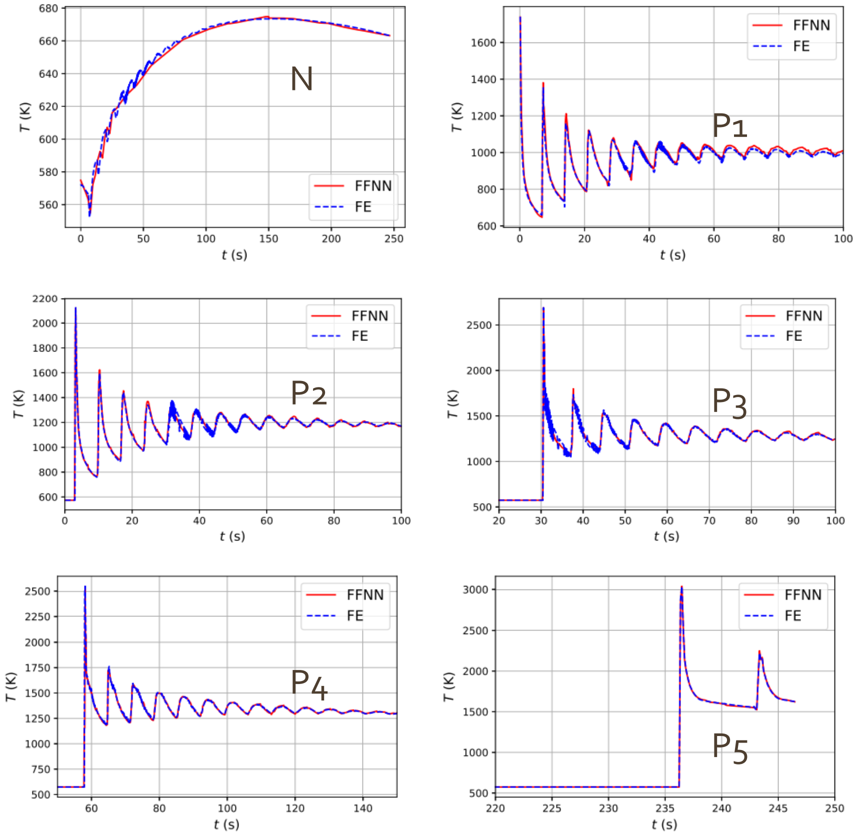
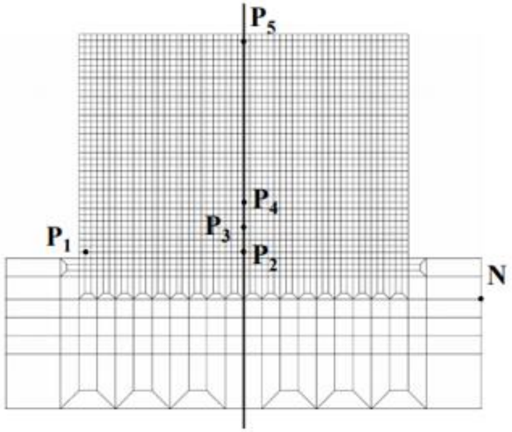
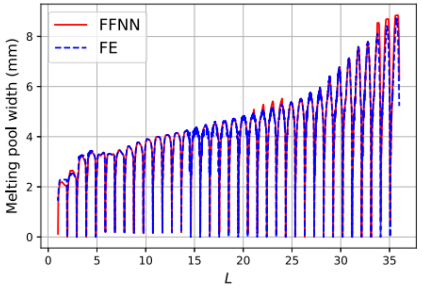
FFNN Result analysis Tp° + Melt pool size

Tp° history T(t)

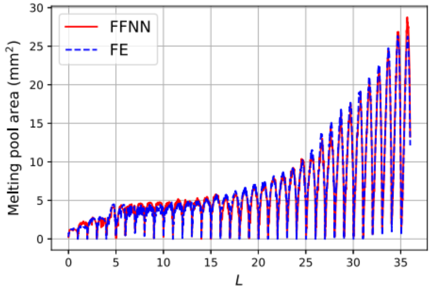




Melting pool sizes



Melt pool width

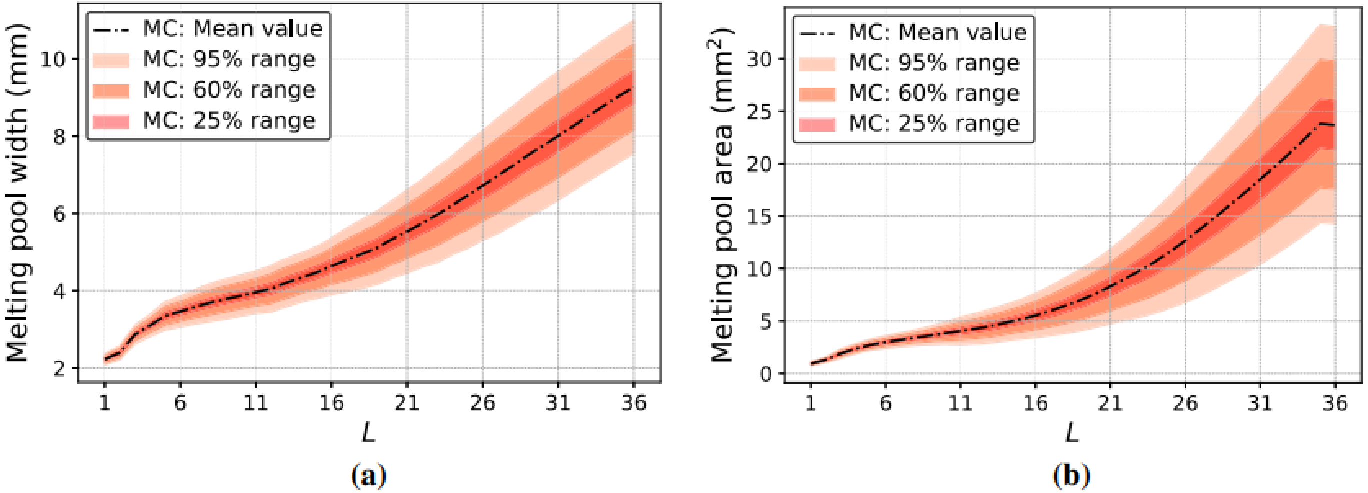


Melt pool area

For each layer

FFNN Result analysis

Extreme sensitivity of the melt pool to the uncertainty of Q_{laser}



Computational cost

	Running FE simulations for creating training dataset	Training time	Single temperature field evaluation	1000 temperature fields evaluation
FE (h)	2.4	–	35→25 min	600
FFNN (h)	–	0.5	0.0033 (or 12 s)	3.3

Please do not tell

-use good parallel code
-use better PC
....
Just observe in same conditions
the CPU reduction

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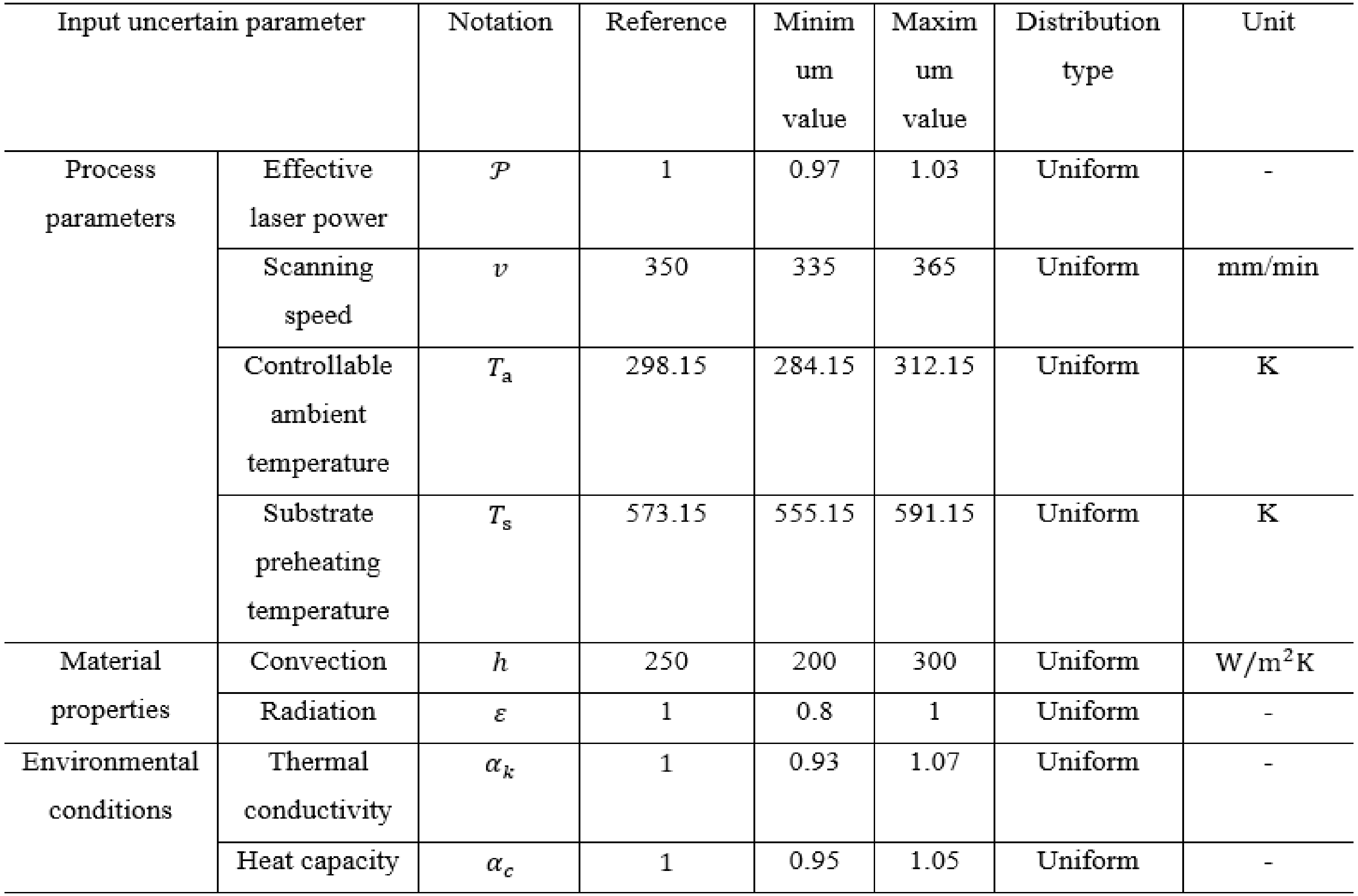
Parameter uncertainty based on literature review & domain knowledge



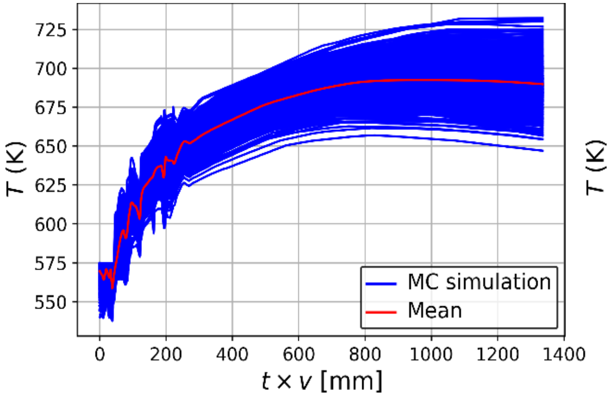
Input uncertain parameter		Notation	Reference	Minimum value	Maximum value	Distribution type	Unit
Process parameters	Effective laser power	$\mathcal{P}$	1	0.97	1.03	Uniform	-
	Scanning speed	v	350	335	365	Uniform	mm/min
	Controllable ambient temperature	T_a	298.15	284.15	312.15	Uniform	K
	Substrate preheating temperature	T_s	573.15	555.15	591.15	Uniform	K
Material properties	Convection	h	250	200	300	Uniform	W/m^2K
	Radiation	ε	1	0.8	1	Uniform	-
Environmental conditions	Thermal conductivity	α_k	1	0.93	1.07	Uniform	-
	Heat capacity	α_c	1	0.95	1.05	Uniform	-

T.Q.D Pham Probabilistic-Engineering-Mechanics 2022

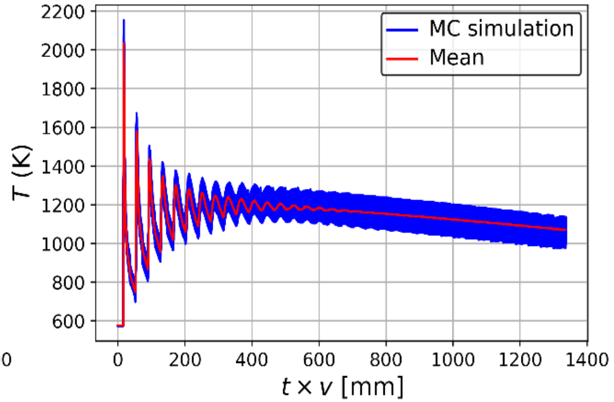
Propagation of uncertainty on Tp°

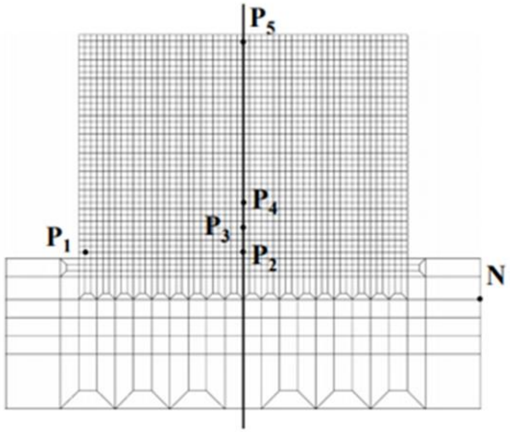
Monte Carlo simulations to explore the space

N

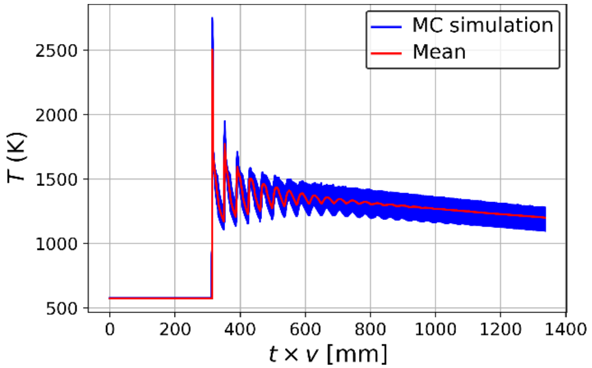


P1

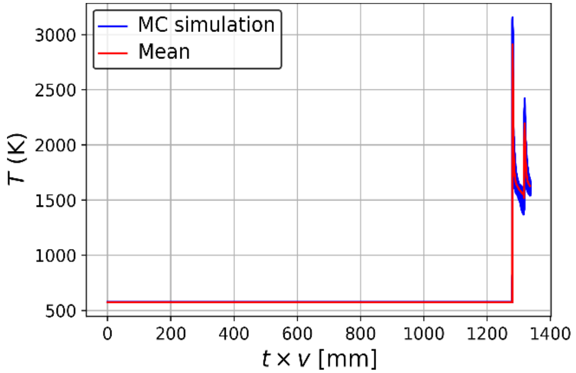




P2



P4

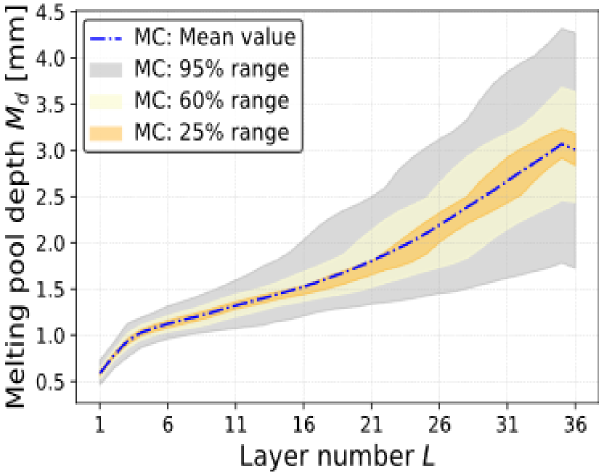


→ details in:

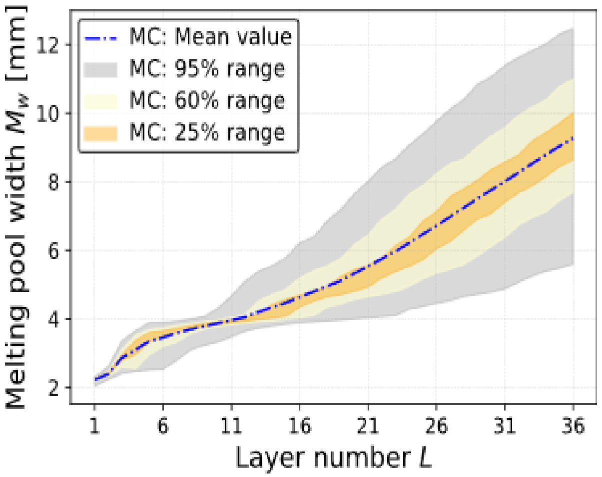
Characterization, propagation, and sensitivity analysis of uncertainties in the DED process using a DL surrogate model

Thinh Quy Duc Pham, et al. *Probabilistic-Engineering-Mechanics*, 2022

Uncertainty on melt pool size + CPU time



Depth

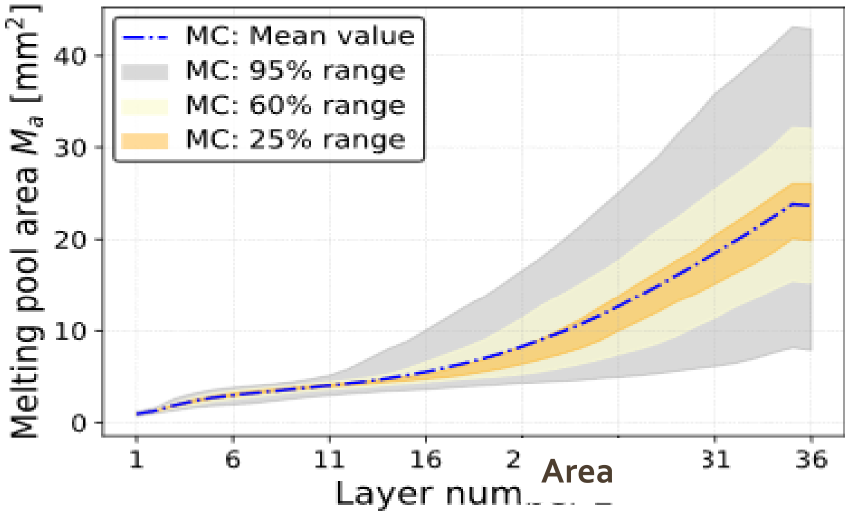


Width

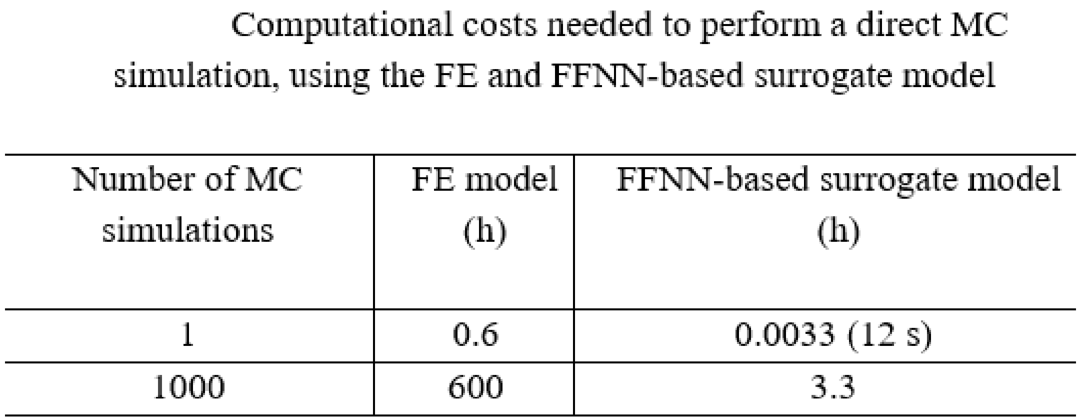
→Steady melting pool during DED process… a challenge !

Need optimal laser power

+ minimum uncertainty



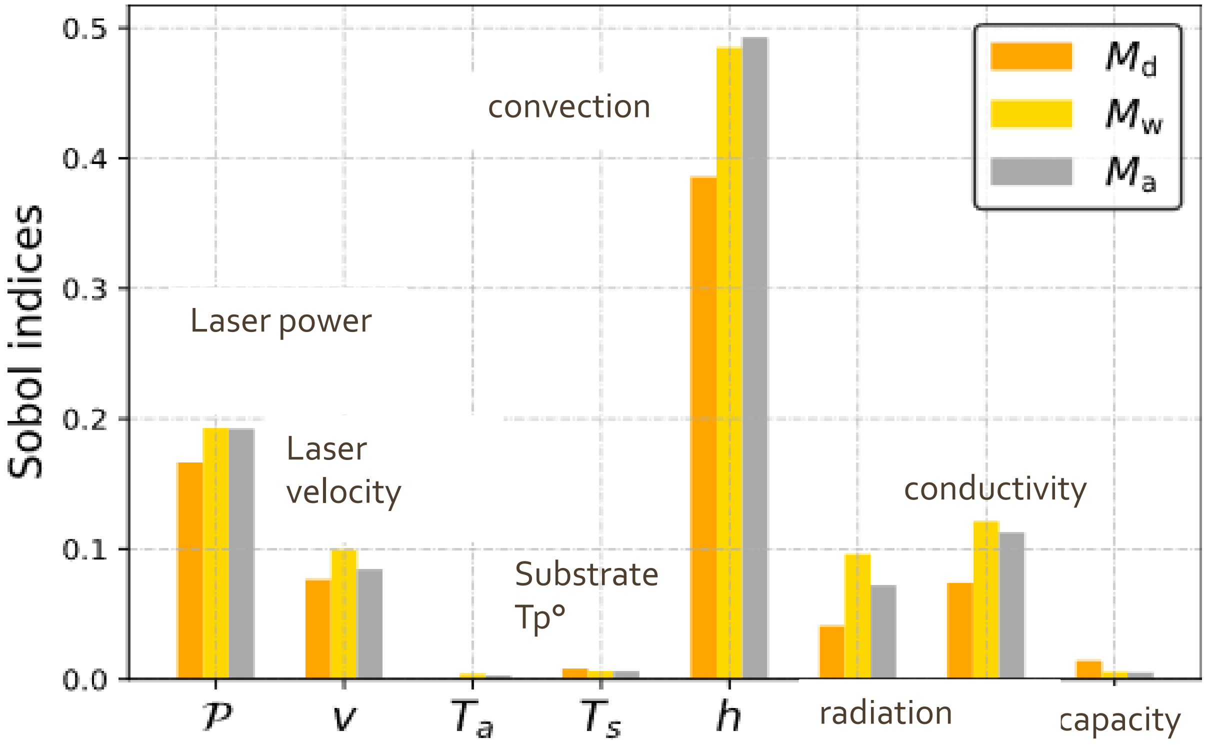
Area


Computational costs needed to perform a direct MC simulation, using the FE and FFNN-based surrogate model

Number of MC simulations	FE model (h)	FFNN-based surrogate model (h)
1	0.6	0.0033 (12 s)
1000	600	3.3

T.Q.D Pham Probabilistic-Engineering-Mechanics 2022

Conclusions about uncertainty study



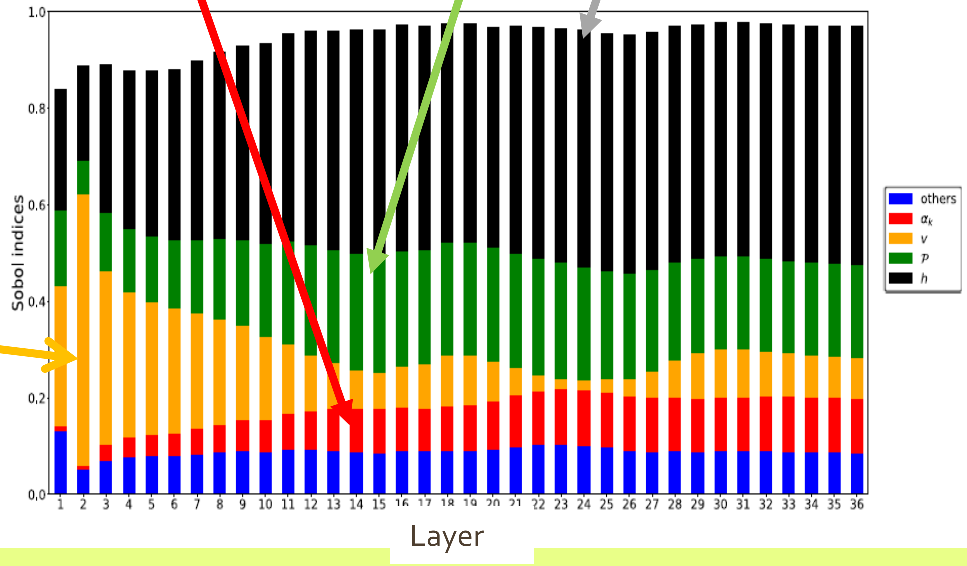
Melt pool size M_d M_w M_a

→ Microstructure

→ Product properties

Mostly modified due to Uncertainties on

- -Convection h
- -Laser power P
- - Laser velocity
- -Thermal conductivity



Need of stable input material properties & boundary conditions in industry

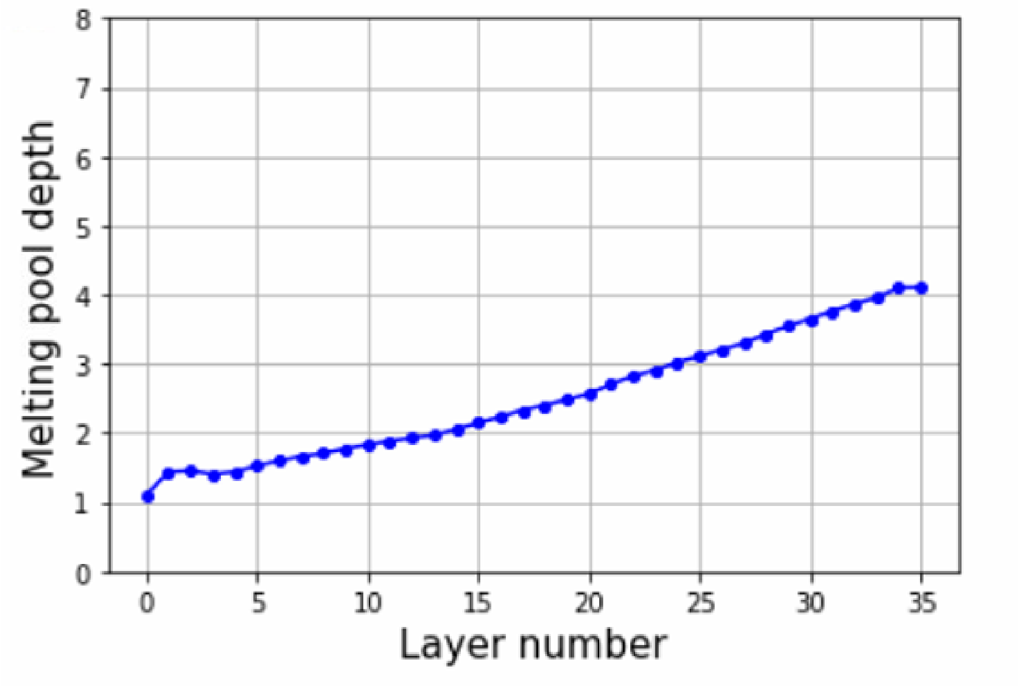
Material values input in model have a high impact

T.Q.D Pham Probabilistic-Engineering-Mechanics 2022

Remind: constant laser power
→ non constant Melt pool depth

Const power

$P = 1100\ \mathrm{W}$



⇒ Need to consider the laser power varying with layer number

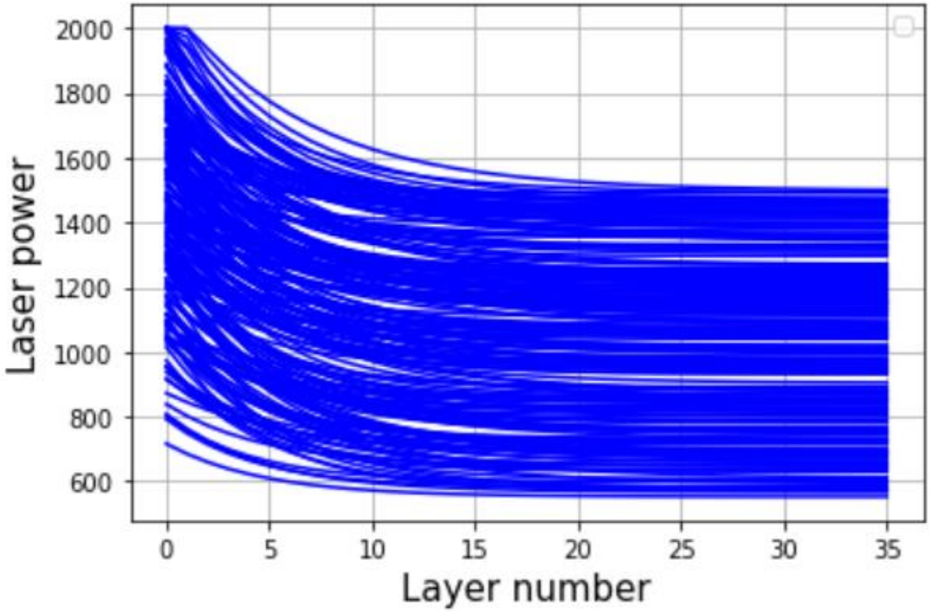
⇒ More homogeneous melt pool and microstructure

Laser power varying with layer number

Choice of a function $f(x) = a \times e^{-kx} + b$

$a \in [200,800], b \in [550,1500], k \in [0.15,0.25]$

Its coefficients
a, b, k
also called
$\alpha_1\ \alpha_2\ \alpha_3$
= the unkowns



If laser power value < 578 W, there will be no melting pool since the tp° is smaller than the melting temperature

→ Space not explored

T.Q.D Pham Journal of Manufacturing Processes 2023

Optimal P(layers) under Minimal Energy

Objective function (step 5) :

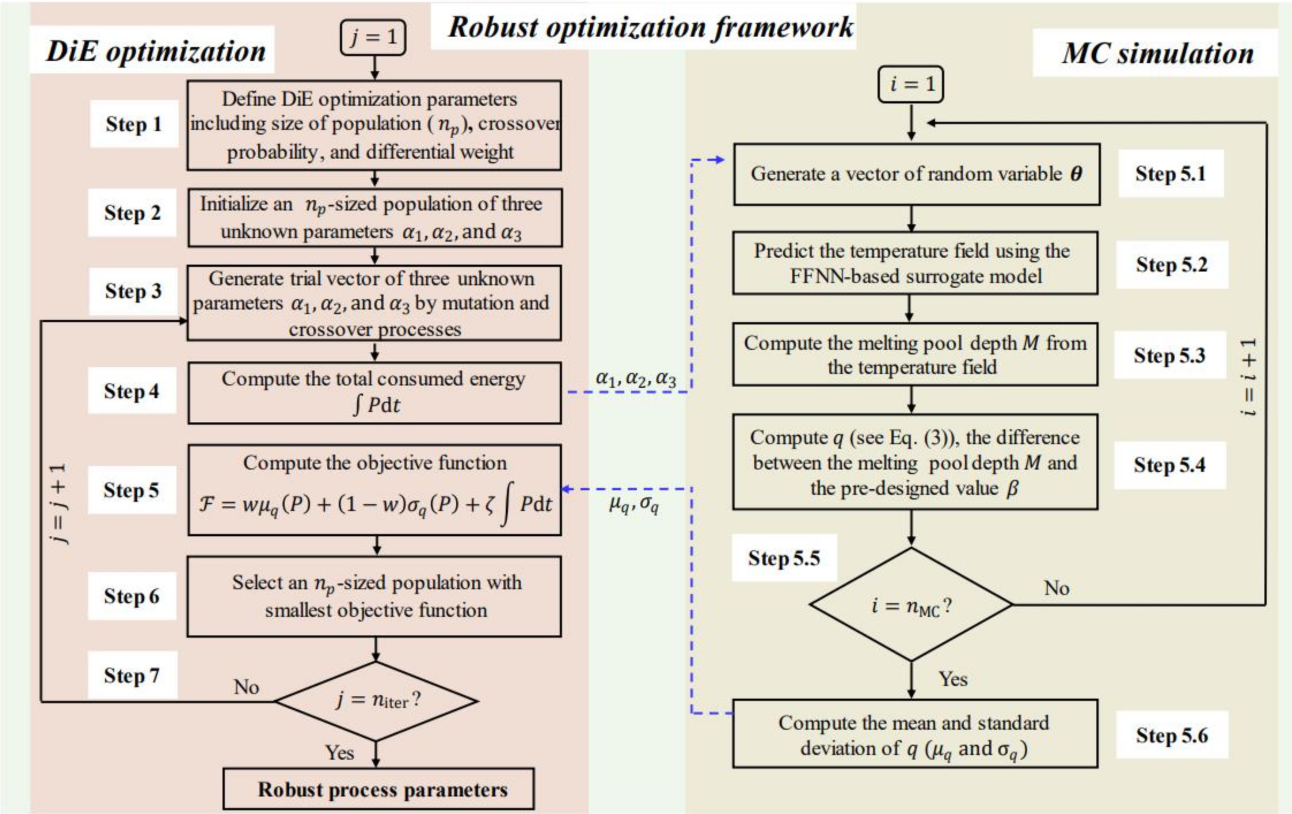
Mean μ_q
& Standard deviation σ_q
of the difference
(computed melt pool size-user defined value)
+
Process Energy

(w weight and ζ scale factors)

DiE:

Price KV. *Differential evolution, intelligent systems reference library* 2013.

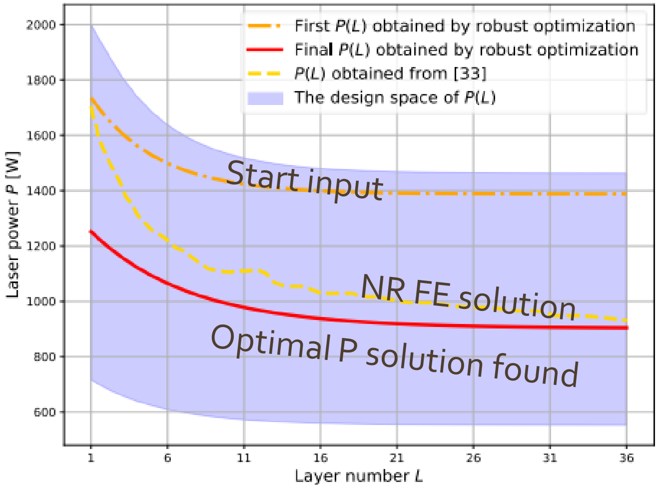
& Frame inspiration:
Bilal M *Eng Appl Artif Intel* 2020
Opara *Evol Comput* 2019



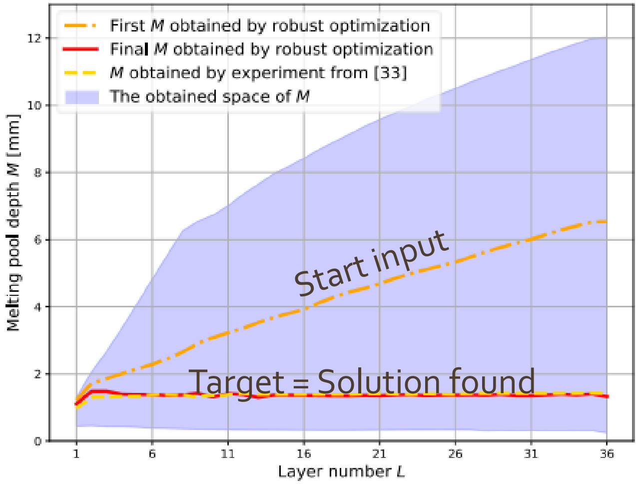
Differential Evolution (DiE)
Monte Carlo Simulations (MC)

T.Q.D Pham Journal of Manufacturing Processes 2023

Robust Results



Power Laser function versus layers



Melt pool depth versus layers

$$f(x) = a \times e^{-kx} + b$$

$$a \in [200{,}800], b \in [550{,}1500],$$
$$k \in [0.15{,}0.25]$$

→ **Found:**

$$a = 407.1,$$

$$b = 910.16, k = 0.1498$$

FE solution: Newton Raphson optimization without energy constraint

Jardin *Optic & Laser technology* 2023

DL solution: Robust optimization - uncertainty & energy constraint added

T.Q.D Pham *Journal of Manufacturing Processes* 2023

Contents

✓A survey of scales and methods

- Finite element method FEM
  - ✓ one element: Solid Shell
  - ✓ mechanical constitutive laws (multi scale ?)
    - ✓Deep Drawing
  - ✓thermo-mechanical analysis
    - ✓Cooling of rolling mills
    - ✓Continuous casting

✓Representative Volume Elemen RVE) or in French VER

✓Coupling solid FEM with … Computational Fluid Dynamics, Deep Learning
  - ✓Additive Manufacturing

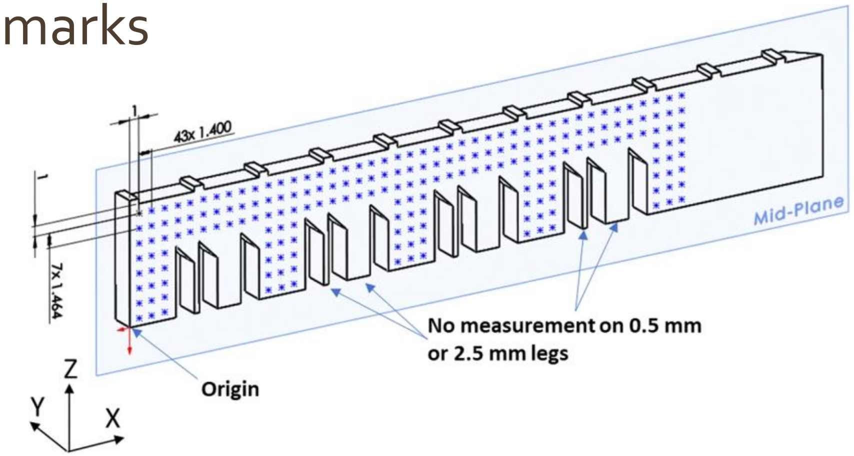
If interest in the last examples
R. Jardin
PhD defense March 24
T.Q.D. Pham
PhD defense April 24

TO END … Selection of infos and PhDs giving interesting ideas for AM

Models evolve! Check benchmarks and data provided

- https://**www.nist.gov**/ambench/types-benchmarks

Yang, Y., Allen, M., London, T. *et al.* Residual Strain Predictions for a Powder Bed Fusion Inconel 625 Single Cantilever Part. *Integr Mater Manuf Innov* **8,** 294–304 (2019). https://doi.org/10.1007/s40192-019-00144-5



- Airbus, Apworks, Siemens … have reliable eigen strain method to design their pieces

I. Setien, M. Chiumenti, S. van der Veen, M. San Sebastian, F. Garciandía and A. Echeverría,

Empirical methodology to determine inherent strains in additive manufacturing, *Computers and Mathematics with Applications*, (**2018**)

Principle of inherent (eigen) strain method

-Identify a strain field

-Compute the associate stress field (elastic or an elastoplastic model)

to recover internal stress field able to generate the part distortion

In industry calibration is done by experiments :

cut in a simple AM part (cube) and measure displacement

If your cube is representative OK ….

What if large complex shape…

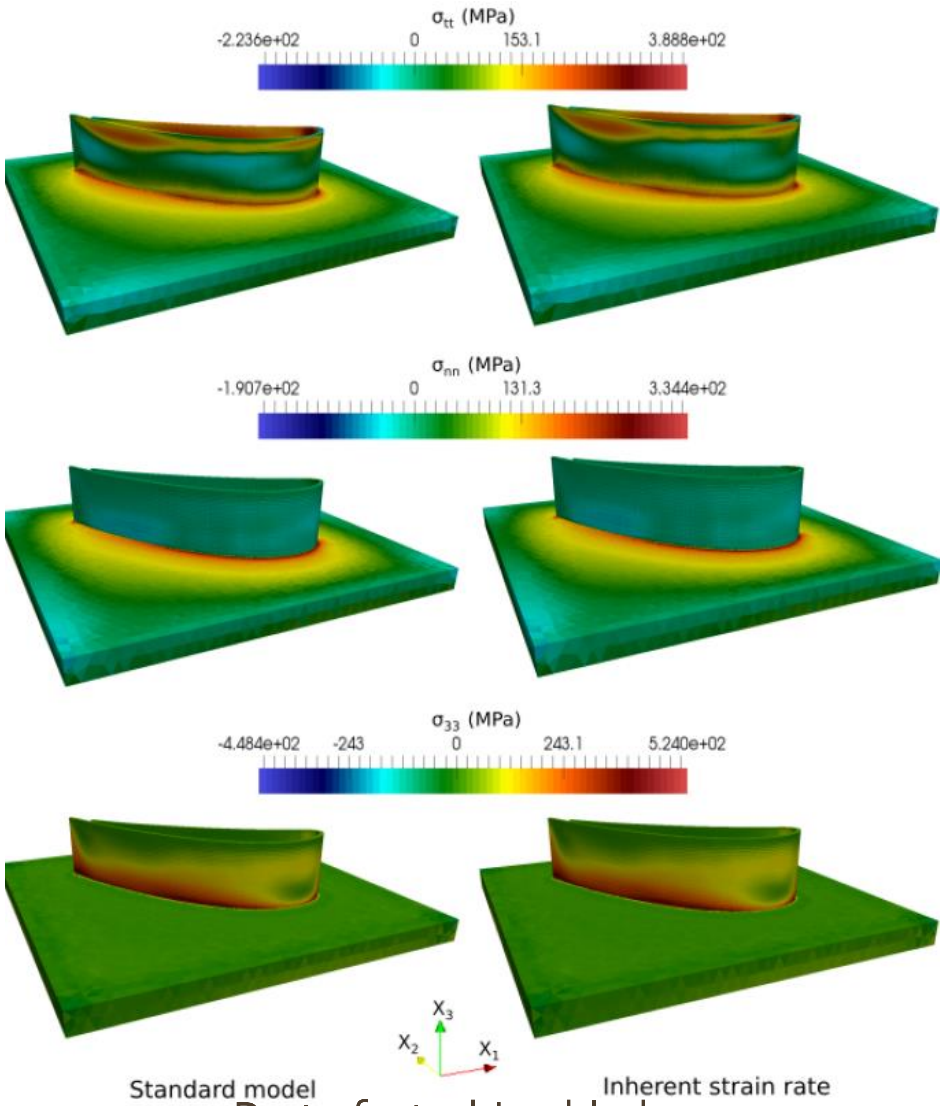
OK for distortion however customers not happy: calibration is time consuming.
Your specific case, not always in the data base (related to LPBF and TA6V, 316L, Incoloy……)

Nothing invented… methodology already use by Eshelby 1957 Proceedings of the Royal Society of London Series A –Mathematical and Physical Sciences 241 (1226), 376–396.

PhD Keumo Tematio DED 316L Thick curve wall - CEMEF 2023

- **Theoretical approach applying the large strain formalism to the monitoring of Inactive/Active thermal and mechanical elements and their interface to control the mesh distortion**

- The inherent strain fields can be:
  - **computed on the first layers** and exploited on the last layers : OK for linear thin wall but not for curvilinear ones
  - **computed on the whole simulation**, it gave better results …but rely on a total simulation that we want to avoid…
  - **computed based on the plastic strain rate close to the laser**: OK for curvilinear wall but requires also a total model of the laser path (larger steps) but still long CPU (reduction factor 5)

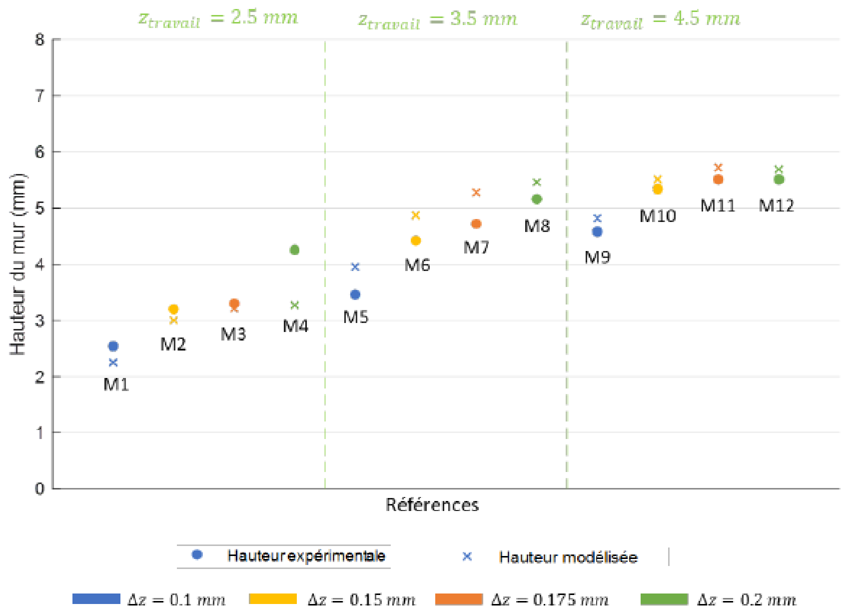


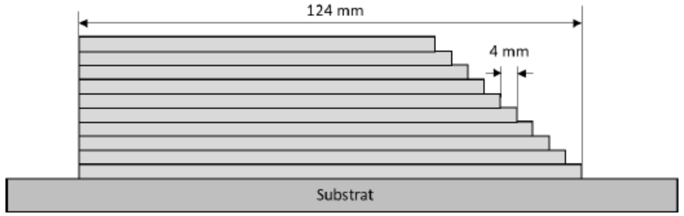
Part of a turbine blade

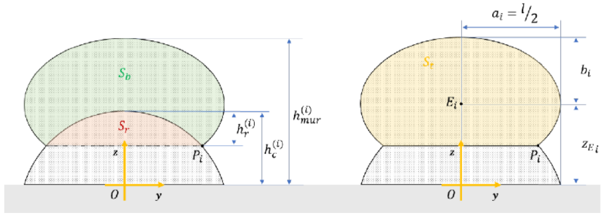
PhD Leroy Dubief - DED 316L - Université de Bordeaux 2023

- **Analytic** model providing the **shape of the clad for different process parameters**

(initial working distance and z-increment) & position within the wall, good accuracy







Many physical ingredients and experimental validations
Code shared in Annex.

PhD Leroy Dubief - DED 316L - Université de Bordeaux 2023

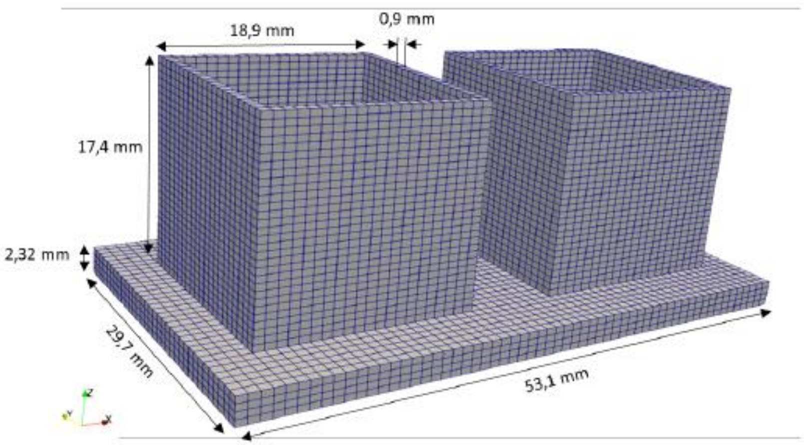
FE coupled with a proper orthogonal decomposition (POD)

It exploits the thermal behavior induced by the repetitive nature of the process.

POD = thermal field expressed as a linear addition of thermal modes

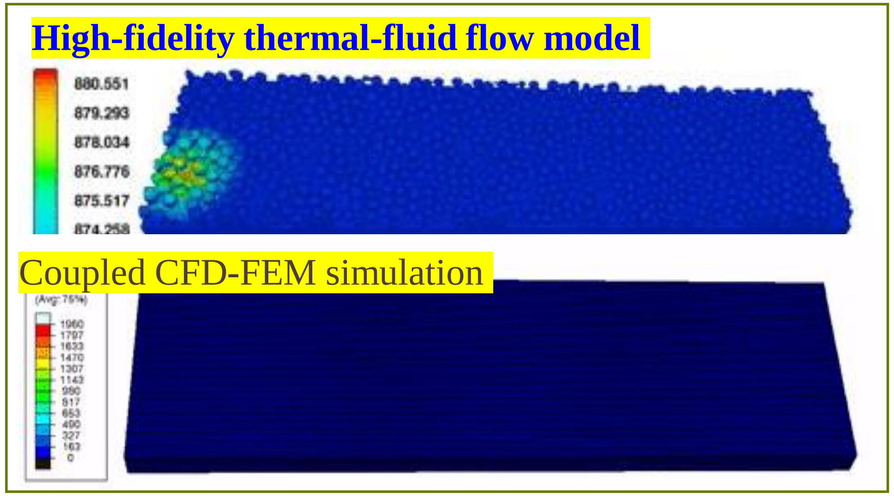
A specific enrichement of the POD is linked to the FE results

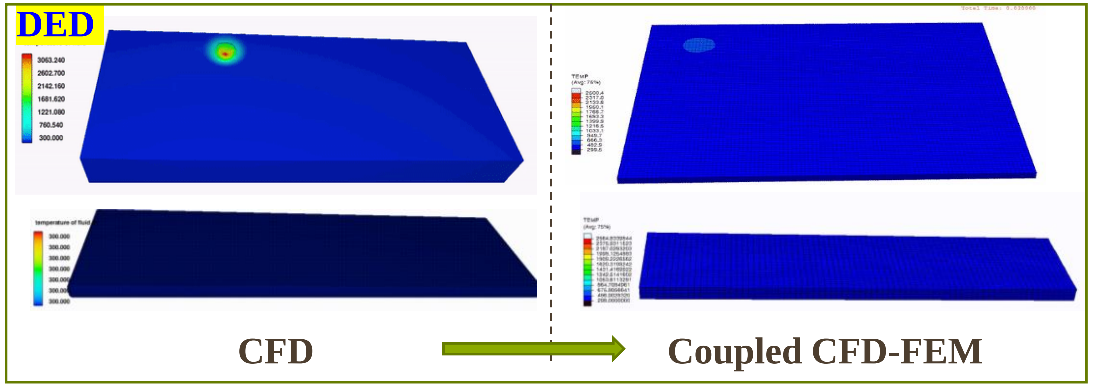
Code able to model 'complex' manufacturing

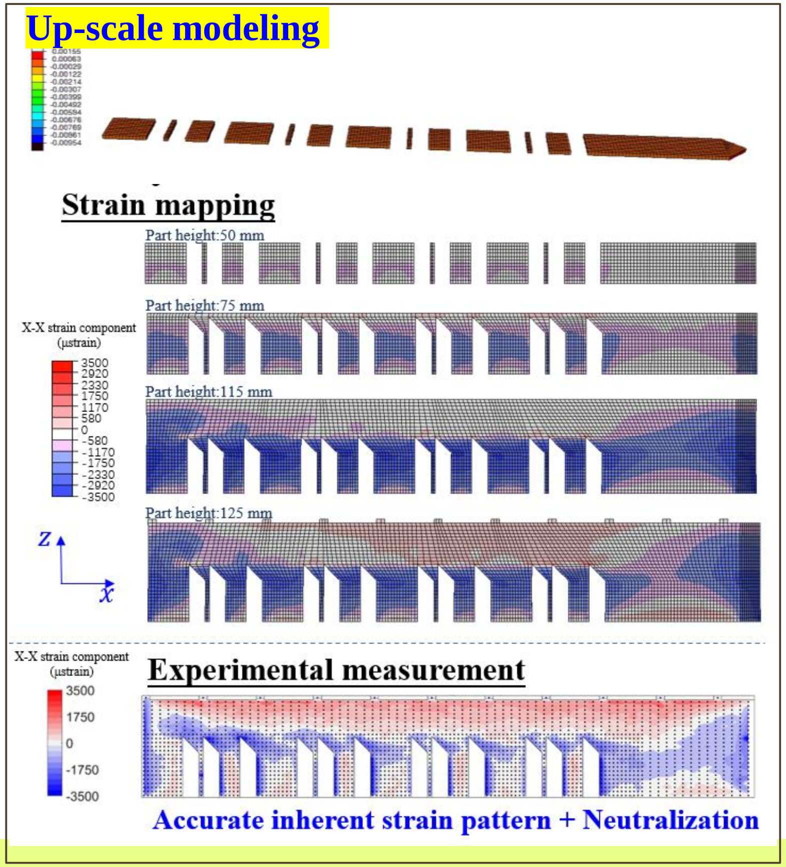


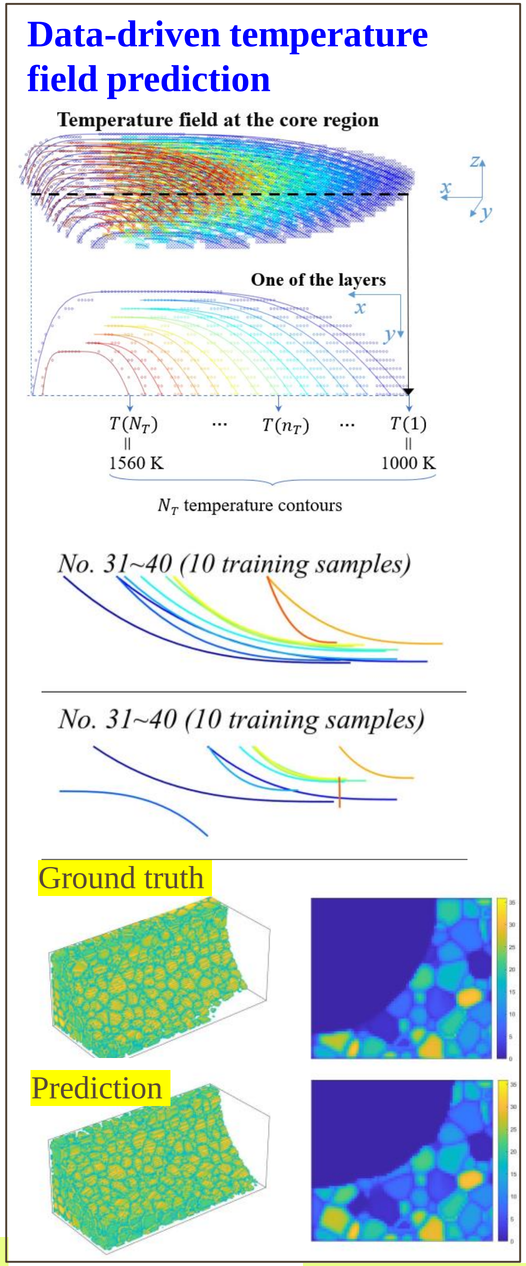
Experimental validation
However still simple FE model
(constant properties)

PhD of Fan Chen Nat. Univ. Singapore 2022









Post doc scientist
currently in LIÈGE université

PFEM: PhD of B.J. Bobach University of Liege oct 2023

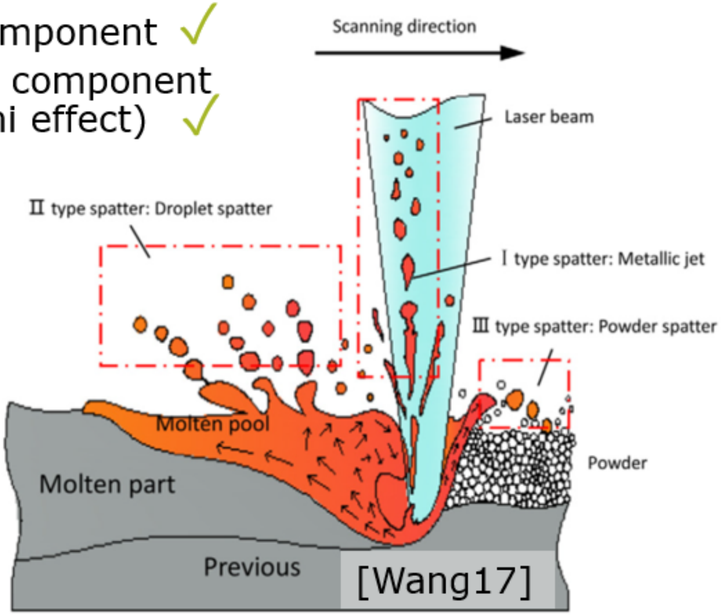
Particle Finite Element Method = Classic FEM + Particle behavior

- Relatively young method , 1st publication by Idelsohn et al. 2004
- Review paper by Cremonesi et al. 2020, 1st PhD in Uliege Marco Lucio Cerquaglia

- Fluid dynamics ✓
- Solid mechanics
  - Elastic ✓ +....
  - Elasto-visco-plastic
- Powder model
  - Continuum powder
  - Solid spheres
- Heat transfer ✓
- Heat source model
  - Laser beam
    - Volume heat source ✓
    - Surface heat flux ✓
    - Ray tracing
  - Electron beam
  - Electric arc
  - etc.
- Thermal expansion ✓

- Phase transition
  - solid↔fluid ✓
  - fluid↔gas
    - Recoil pressure
    - Evaporative cooling
- Surface tension
  - Normal component ✓
  - Tangential component (Marangoni effect) ✓

Don't forget:
2D → 3D



[Wang17]

Constant remeshing
Liquid boundary surface identified
Phase change efficient
Constitutive law unified between solid and liquid
...

Still work to do but close to AM now

Merci de votre attention

Bon choix d'échelles, de couplages, de modèles

Si questions, n'hésitez pas

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