CAPSUL:
a tool for computational homogenization of polycrystals

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SUMMARY

1. IMDEA Materials' suite of simulation tools

2. CAPSUL: a suite of computational homogenization tools
   - RVE generation
   - Crystal plasticity models
   - Levenberg-Marquardt optimization algorithm
   - Fatigue indicator parameters

3. Examples of applications
   - Virtual testing of extruded AZ31 Mg alloys
   - Virtual testing of wrought IN718 superalloy in fatigue

4. Conclusions

IMDEA MATERIALS' SUITE OF SIMULATION TOOLS

iRiS

Object oriented, general purpose, parallel code for computational mechanics in solid, fluid, and structural applications including finite element and meshless capabilities.

Muesli — a Material UnivErSal Library

An open source library of material models (solids & fluids) for general numerical methods of continuum mechanics problems, which can be easily integrated into commercial codes.

viPer

Computational micromechanics tool to predict ply properties of fiber-reinforced composites from the properties and spatial distribution of the phases and interfaces to carry out *in silico* ply design and optimization.

MMonCa — Modular Monte Carlo

An open source Kinetic Monte Carlo tool (coupled to a finite element code to include the effect of mechanical stresses and to an ion implant simulator) to simulate epitaxial growth and damage irradiation.

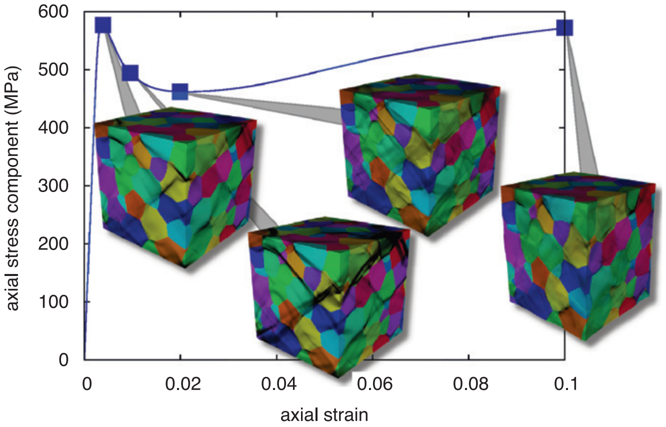
capsul — crystal plasticity simulation

Suite of homogenization tools for polycrystals within the framework of crystal plasticity.

http://www.materials.imdea.org/research/software

SINGLE CRYSTAL - POLYCRYSTAL HOMOGENIZATION

Virtual testing of polycrystalline materials can now be achieved by means of computational homogenization.



Key ingredients

Microstructural features: Grain size, shape and orientation distributions *easily* obtained by means of 2D and 3D characterization techniques (including serial sectioning, X-ray μtomography, 3D EBSD, X-ray diffraction, etc.)

Single crystal behavior: CRSS for each slip system and twinning (including latent and forest hardening) provided by

- Multiscale modelling
- Mechanical tests of single crystals
- Inverse problem: back up single crystal behavior from tests on polycrystals
    - Homogenization of polycrystals
    - Nanoindentation

CAPSUL

capsul
crystal plasticity simulation

- a suite of tools for computational homogenization of polycrystals

http://www.materials.imdea.org/CAPSUL

- A tool to generate RVE of the microstructure (grain size, shape and orientation distributions) using as input statistical data obtained from 2D microscopy images.

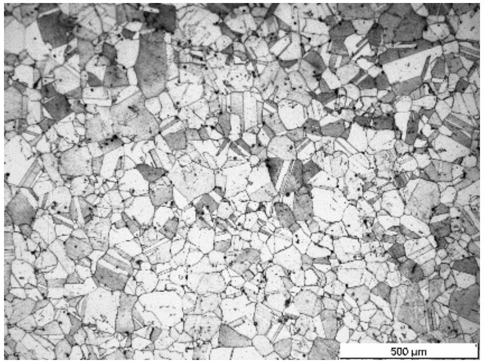
- A set of crystal plasticity constitutive models that take into account slip and twinning. Both monotonic and cyclic behavior can be considered by the combination of different laws for isotropic hardening, kinematic hardening and cyclic softening. The model is programmed as a UMAT subroutine for Abaqus.

- An inverse optimization tool to obtain the crystal plasticity model parameters from the result of a set of mechanical tests (both microtests on single crystals or macroscopic tests on polycrystals).

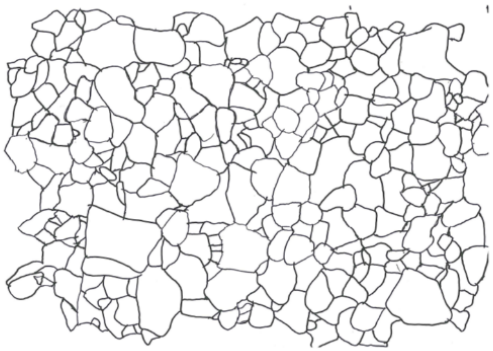
- A set of python scripts to generate cyclic loading conditions and to postprocess the results to obtain fatigue indicator parameters and other microfields.

RVE GENERATION

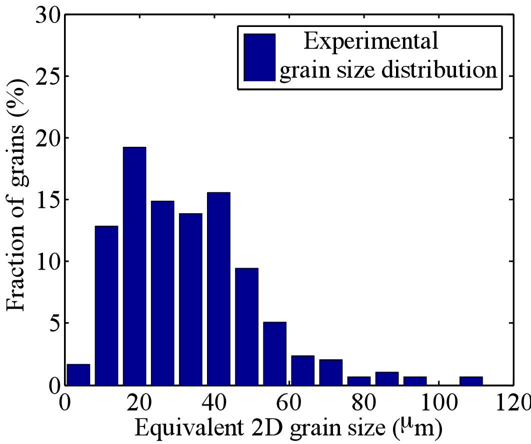
2D images of the microstructure



segmentation



2D grain size distribution



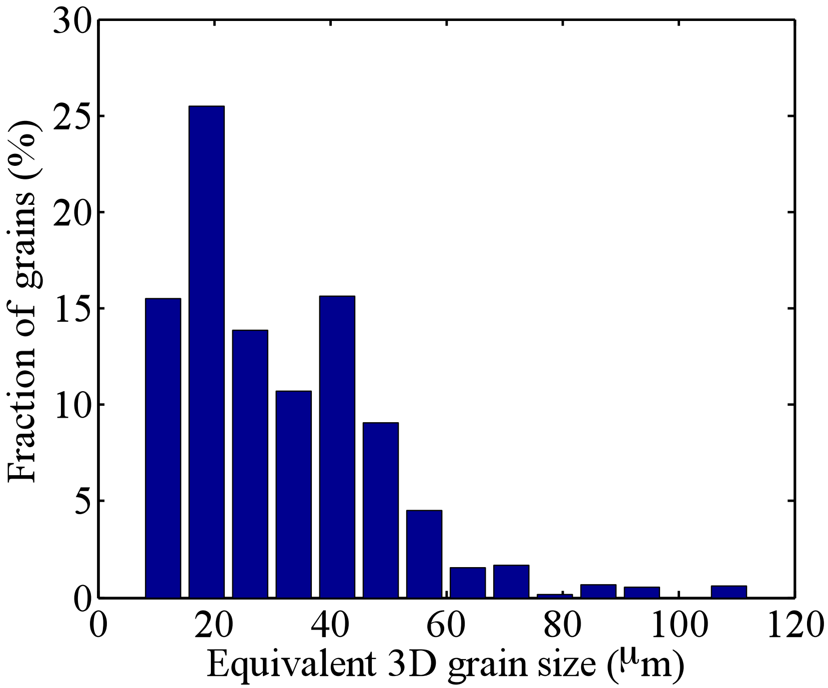
3D grain size distribution

The 2D equivalent radius distribution is transformed into a 3D distribution assuming:

- Spherical grains
- The probability p_i^j that the section of a sphere intercepted by a plane i is in the range given by $a \in [a_{i-1}, a_i]$

$$p_i^j = \frac{1}{\sqrt{A_j}}\left(\sqrt{A_j - a_{i-1}} - \sqrt{A_j - a_i}\right)$$

where A_j is the maximum section of the sphere



StripStar, Basel University

RVE GENERATION

The 3D RVE of the microstructure is an ensemble of N polyhedra (each one representing one grain) built from a Laguerre tessellation.

$$V(p_i) = \{d_L(p,p_i) < d_L(p,p_j), j \neq i\}$$

$$d_L(p,p_i) = [d_E(p,p_i)]^2 - r_i^2$$

with r_i distance to the p_i nearest neighbor.

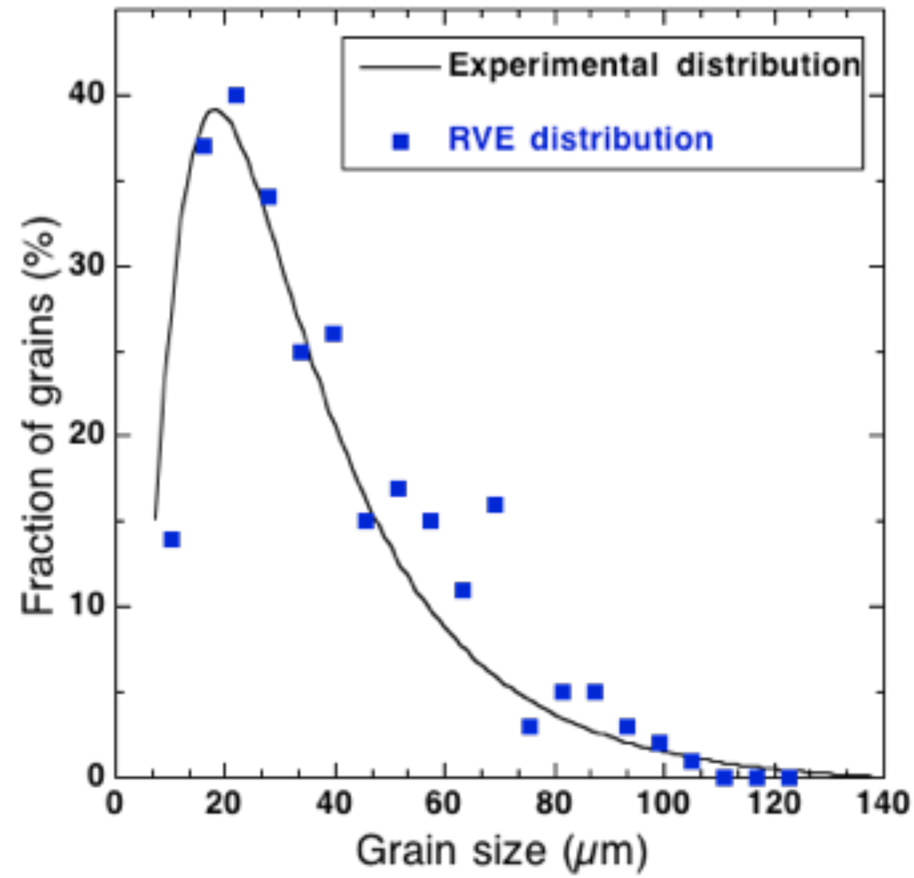
The set N of points for the tessellation, $O(\mathbf{p}), \mathbf{p} = p_i$ is obtained by minimizing the error function

$$O(\mathbf{p}) = \sum_{j=1}^{N} |PDF_{exp}(V_j) - PDF_{trial}(V_j)| \, \Delta V$$

$$\Delta V = (V_{max} - V_{min})/N$$

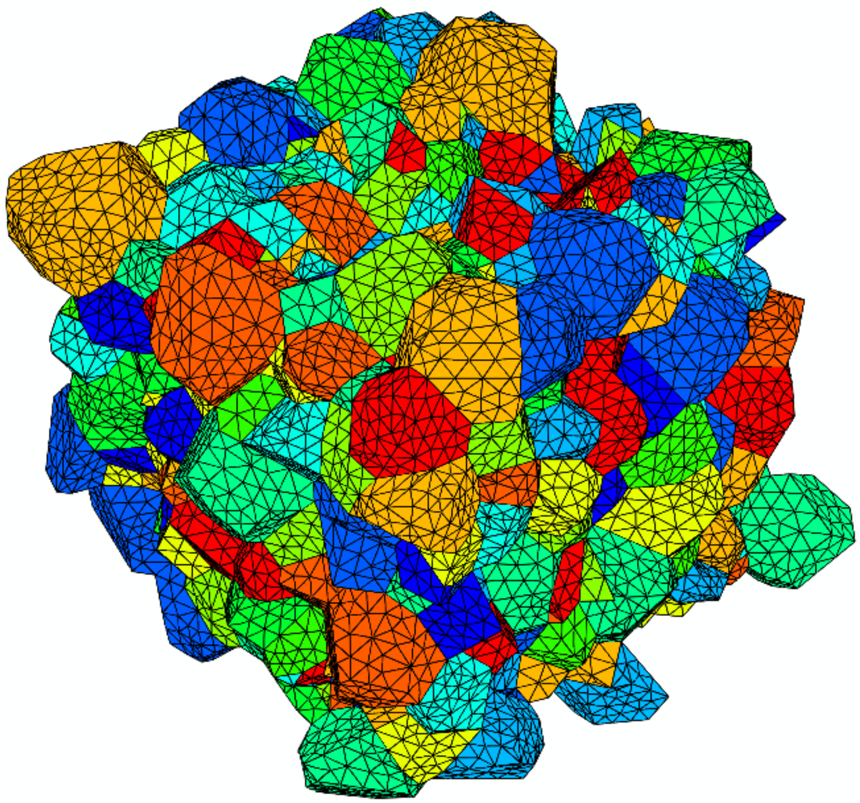
by means of the Monte Carlo method

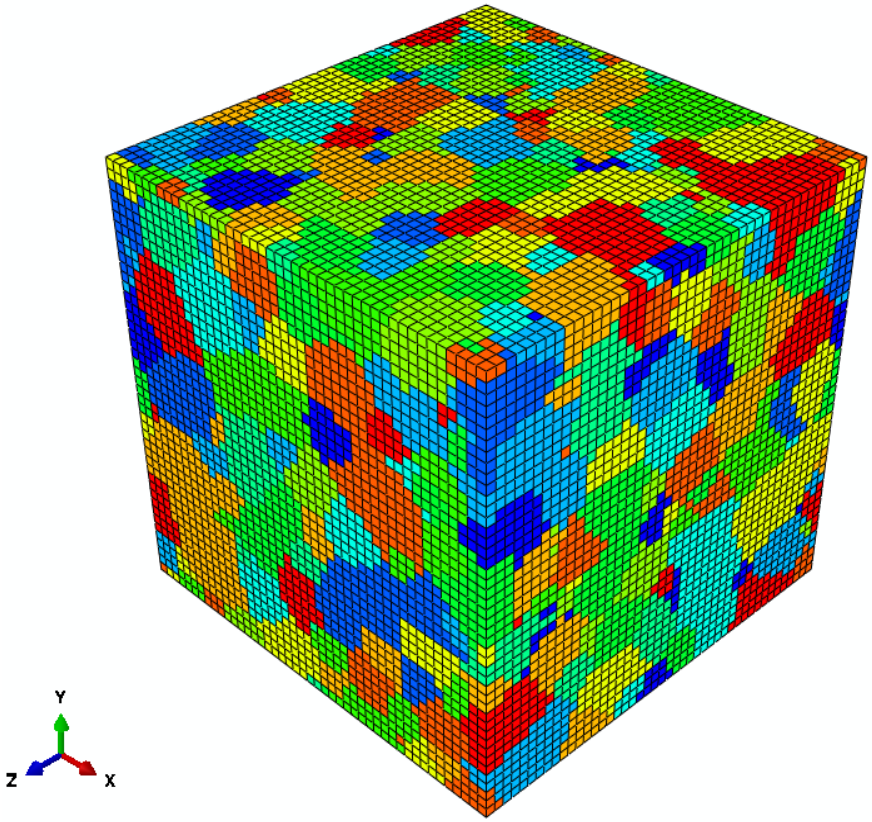
- PDF_{exp}: Experimental probability density function of the grain size ($[V_j, V_j + \Delta V]$)
- PDF_{trial}: Trial probability density function of the grain size ($[V_j, V_j + \Delta V]$)



RVE GENERATION

Periodic RVEs (including orientation distribution information obtained from textures measurements by X-ray diffraction) are automatically generated and meshed with *Gmesh* or *Dream3D* (voxel models).





CRYSTAL PLASTICITY MODEL

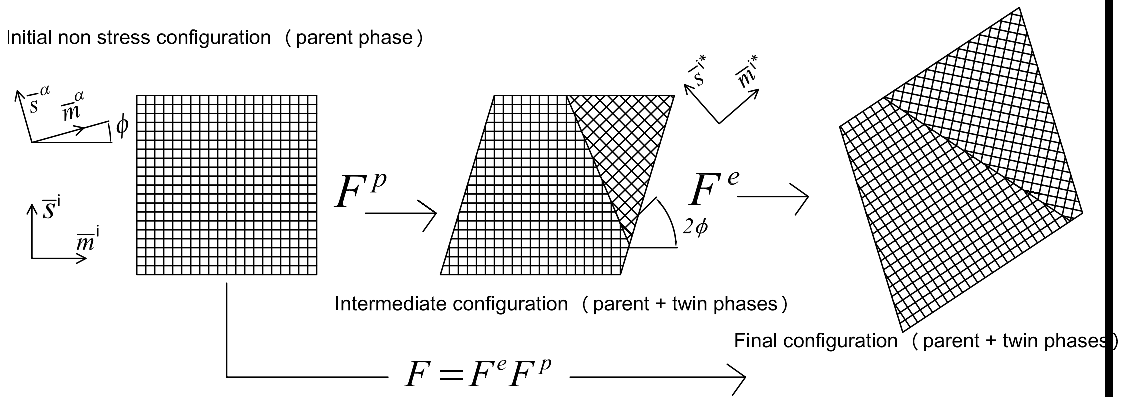
- A crystal plasticity model was implemented as a UMAT in Abaqus/Standard
- Multiplicative decomposition $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$; velocity gradient $\mathbf{L} = \mathbf{L}^e + \mathbf{F}^e\mathbf{L}^p\mathbf{F}^{e^{-1}}$
- Plastic deformation is accommodated by N_{sl} slip and N_{tw} twinning systems

$$\mathbf{L}^p = \mathbf{L}^p_{sl} + \mathbf{L}^p_{tw} + \mathbf{L}^p_{re-sl}$$

$$\mathbf{L}^p_{tw} = \sum_{\alpha=1}^{N_{tw}} \dot{f}^\alpha \gamma_{tw} \mathbf{s}^\alpha_{tw} \otimes \mathbf{m}^\alpha_{tw}$$

$$\mathbf{L}^p_{sl} = \left(1 - \sum_{\alpha=1}^{N_{tw}} f^\alpha\right) \sum_{i=1}^{N_{sl}} \dot{\gamma}^i \mathbf{s}^i_{sl} \otimes \mathbf{m}^i_{sl}$$

$$\mathbf{L}^p_{re-sl} = \sum_{\alpha=1}^{N_{tw}} f^\alpha \left(\sum_{i^*=1}^{N_{sl-tw}} \dot{\gamma}^{i^*} \mathbf{s}^{i^*}_{sl} \otimes \mathbf{m}^{i^*}_{sl} \right)$$



f^α volume fraction of twinned system α

S. R. Kalidindi, **J. Mech. Phys. Solids 46**, 267–271 and 273–290, 1998.

Phenomenological model: Monotonic deformation

- The crystal was assumed to behave as an elasto-viscoplastic solid.
- Plastic slip rate $\dot{\gamma}^i = \dot{\gamma}_0 \left(\frac{|\tau^i|}{\tau_c^i} \right)^{\frac{1}{m}} \mathrm{sign}(\tau^i)$ where $\tau^i = \mathbf{S} : (\mathbf{s}^i \otimes \mathbf{m}^i)$

  $\mathbf{s}^i$ slip direction

  $\mathbf{m}^i$ normal to the slip plane

- Twinning rate

$$\dot{f}^\alpha = \dot{f}_0 \left(\frac{\langle \tau^\alpha \rangle}{\tau_c^\alpha} \right)^{\frac{1}{m}} \quad \text{with} \quad \langle \tau \rangle = \begin{cases} \tau \text{ if } \tau \geq 0 \\ 0 \text{ if } \tau < 0 \end{cases} \quad \text{and} \quad \dot{f}^\alpha = 0 \quad \text{if} \quad \sum_{\alpha=1}^{N_{tw}} f^\alpha \geq 0.80$$

$$\tau^\alpha = \mathbf{S} : (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)$$

- Evolution of the shear strength

slip
$$\dot{\tau}_c^i = q_{sl-sl} \sum_{j=1}^{N_{sl}} h_{0j} \left(1 - \frac{\tau^j}{\tau_{sat}^j} \right)^{a_{sl}} |\dot{\gamma}^j| + q_{tw-sl} \sum_{\beta=1}^{N_{tw}} h_{0tw} \left(1 - \frac{\tau^\beta}{\tau_{sat}^{tw}} \right)^{a_{tw}} |\dot{\gamma}^\beta|$$

twinning
$$\dot{\tau}_c^\alpha = q_{tw-tw} \sum_{\beta=1}^{N_{tw}} h_{0tw} \left(1 - \frac{\tau^\beta}{\tau_{sat}^{tw}} \right)^{a_{tw}} \dot{f}^\alpha \gamma_{tw}$$

re-slip
$$\dot{\tau}_c^{i*} = q_{sl-sl} \sum_{j=1}^{N_{re-sl}} h_{0j} \left(1 - \frac{\tau^j}{\tau_{sat}^j} \right)^{a_{sl}} |\dot{\gamma}^j|$$

V. Herrera-Solaz, J. LLorca, E. Dogan, I. Karaman, J. Segurado. **International Journal of Plasticity, 57,** 1-15, 2014.

Phenomenological model for cyclic deformation

- The crystal was assumed to behave as an elasto-viscoplastic solid.

- The phenomenological model can account for the different cyclic deformation mechanisms, such as Bauschinger effect, cyclic softening/hardening and mean stress relaxation/ratcheting.

- Plastic slip rate in the slip system i is given by $\dot{\gamma}^i = \dot{\gamma}_0 \left(\frac{|\tau^i - \chi^i|}{\tau_c^i} \right)^{\frac{1}{m}} \text{sign}(\tau^i - \chi^i)$

- The slip resistance has three contributions: $\tau_c^i = \tau_0 + \tau_{is}^i + \tau_{cs}$

- Isotropic hardening: $\dot{\tau}_{is}^i = \sum_j q_{ij} h_0 \,\text{sech}^2 \left| \frac{h_0 \Gamma}{\tau_s - \tau_0} \right| \qquad \Gamma = \sum_i \int_0^t |\dot{\gamma}^i| \text{d}t$

- Cyclic softening:

$$\tau_{cs}(\Gamma_c) = -(\tau_{\Delta s} + h_2 \Gamma_c)\left(1 - \exp^{-\frac{h_1 \Gamma_c}{\tau_{\Delta s}}}\right) \qquad \Gamma_c = \sum_i \left(\int_0^t |\dot{\gamma}^i| dt - \left| \int_0^t \dot{\gamma}^i \text{d}t \right| \right)$$

The backstress χ^α is introduced to include kinematic hardening

$$\dot{\chi}^i = c\dot{\gamma}^i - d\chi^i |\dot{\gamma}^i| \left(\frac{|\chi^i|}{(c/d)} \right)^{mk}$$

N. Ohno, J.-D. Wang. **International Journal of Plasticity, 9,** 375-390, 1983.

Physically-based model

- The model is based on the Orowan equation $\dot{\gamma}^i = \rho_m^i b^i v^i$

where ρ_m stands for the mobile dislocation density, b^i the Burgers vector and

$$v^i = \begin{cases} 0 & \text{if} \quad \tau_{ef}^i \leq 0 \\ \bar{l}\omega \exp\left\{ -\frac{\Delta F}{kT}\left(1 - \left[\frac{\tau_{ef}^i}{s_t^i}\right]^p\right)^q \right\} \text{sign}(\tau^i) & \text{if} \quad 0 < \tau_{ef}^i \end{cases}$$

and $\bar{l}$ is the average distance between barriers, ω the attempt frequency and ΔF the activation free energy.

- $\tau_{ef} = |\tau^i| - s_a^i$ where s_a^i is the athermal contribution to the slip resistance

s_a^t is the thermal contribution to the slip resistance

D. Rodríguez-Galan, I. Sabirov, J. Segurado. **International Journal of Plasticity, 70,** 191-205, 2015.

LEVENBERG-MARQUARDT METHOD

- Parametrization of the phenomenological constitutive models from experimental data is critical for the accuracy. This task is carried out using the Levenberg-Marquardt algorithm, well suited for non-linear problems.

- Levenberg-Marquardt method:

$$O(\boldsymbol{\beta}) = \sum_{i=1}^{n} |y_i - f(x_i,\ \boldsymbol{\beta})| = \|\mathbf{y} - \mathbf{f}(\boldsymbol{\beta})\|$$

- (x_i, y_i) are experimental data (i.e. stress-strain curves in different orientations)
- $(x_i, f(x_i; \boldsymbol{\beta}))$ are the model predictions for a set of parameters $\boldsymbol{\beta}$

- Objective: find the set of parameters $\boldsymbol{\beta}$ that minimizes $O(\boldsymbol{\beta})$

- Assuming a small perturbation $\boldsymbol{\delta}$ of the model parameters and linearizing:

$$\mathbf{f}(\boldsymbol{\beta} + \boldsymbol{\delta}) \approx \mathbf{f}(\boldsymbol{\beta}) + \mathbf{J}\boldsymbol{\delta} \qquad J_{ij} = \frac{\partial f(x_i, \boldsymbol{\beta})}{\partial \beta_j} \qquad O(\boldsymbol{\beta} + \boldsymbol{\delta}) \approx \|\mathbf{y} - \mathbf{f}(\boldsymbol{\beta}) - \mathbf{J}\boldsymbol{\delta}\|$$

- Levenberg and Marquardt minimized $O(\boldsymbol{\beta})$ by adding a dumping factor λ to the expression of steepest descent, leading to the following linear set of equations:

$$(\mathbf{J}^T\mathbf{J} + \lambda\,\mathrm{diag}(\mathbf{J}^T\mathbf{J}))\boldsymbol{\delta} = \mathbf{J}^T[\mathbf{y} - \mathbf{f}(\boldsymbol{\beta})]$$

whose solution $\boldsymbol{\delta}$ provides the new set of parameters that minimizes O.

FATIGUE LIFE PREDICTION

- Fatigue life is assumed to be controlled by crack initiation.
- Crack initiation is associated with the development of persistent slip bands in grains favorably oriented for slip. The crack propagates within the slip band.

Accumulated plastic strain

$$FIP_p = \frac{2}{3}\int_0^t \left|(\mathbf{L}_p : \mathbf{L}_p)^{1/2}\right| \mathrm{d}t$$

Plastic energy dissipated

$$FIP_w^i = \int_0^t \tau^i \dot{\gamma}^i \mathrm{d}t$$

Fatemi-Socie

$$FIP_{FS} = \frac{\gamma^i}{2}\left(1 + K' \frac{\sigma^i_{n,max}}{\sigma_y}\right)$$

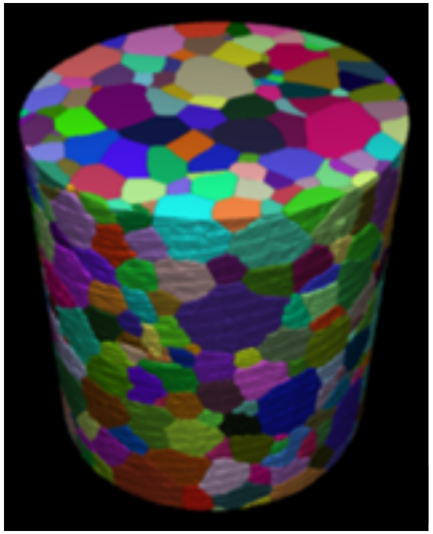
- The fatigue life is related to the range of the FIP, ΔFIP, in one fatigue cycle (averaged on a microstructural feature: grain, slip band, etc.)

$$N\ \Delta FIP = FIP_c$$

- This approach can take into the effect of microstructural features (grain size distribution, texture, etc.), defects (surface roughness, inlcusions, notches) as well as multiaxial stress states on the fatigue life.

VIRTUAL TESTING OF Mg ALLOYS

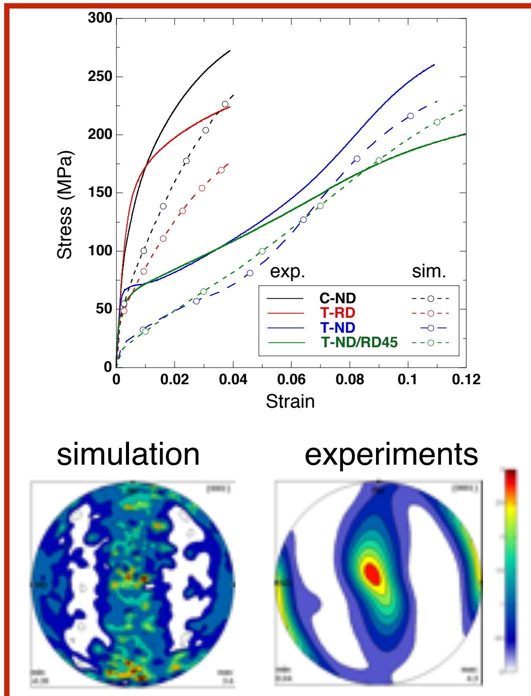
RVE microstructure:
grain size, shape, texture



Single crystal
plasticity model

Numerical simulation
(FEM; FFT) of mechanical tests

Comparison with
experiments



Error
minimization

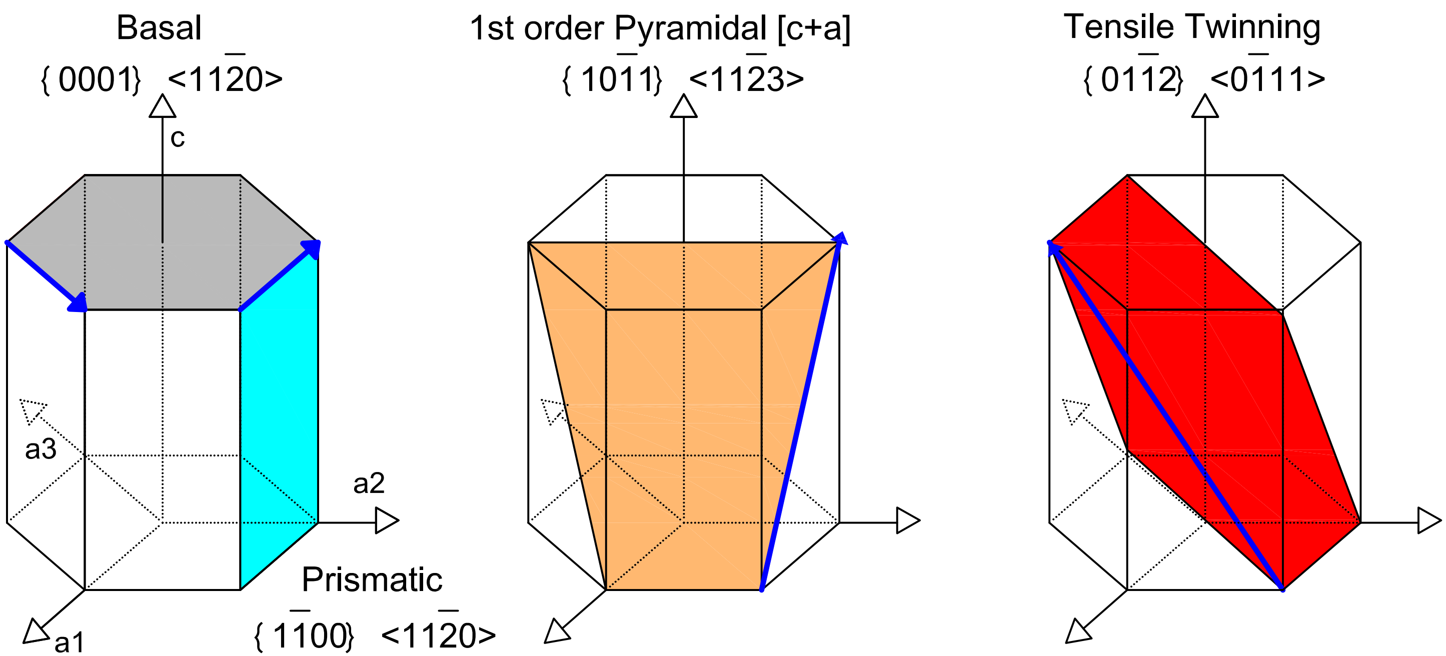
single crystal
properties

Error objective
function

V. Herrera-Solaz, J. LLorca, E. Dogan, I. Karaman, J. Segurado. **International Journal of Plasticity, 57,** 1-15, 2014.

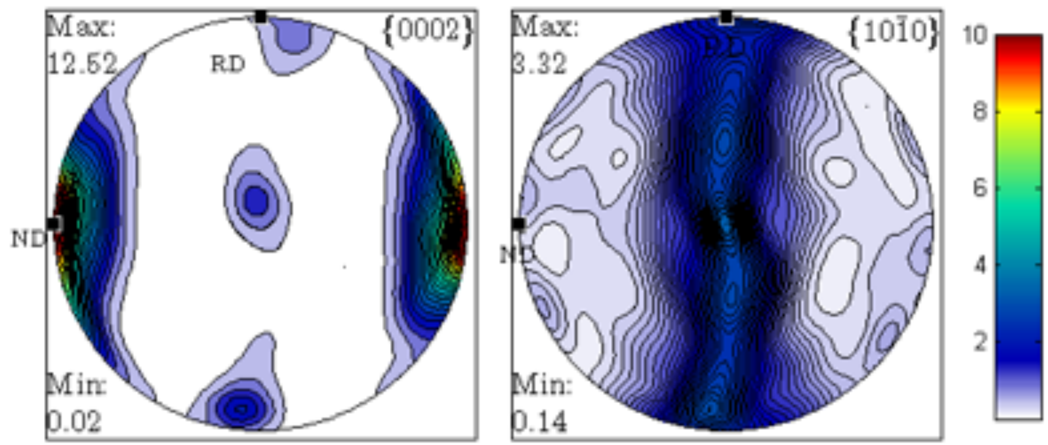
Mg DEFORMATION MECHANISMS

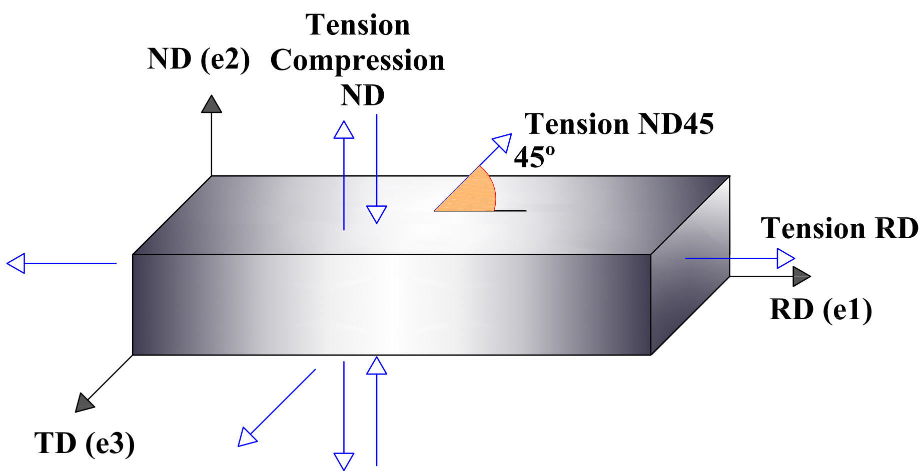
- Basal <a>, prismatic <a> and pyramidal <c+a> slip
- Tensile twinning

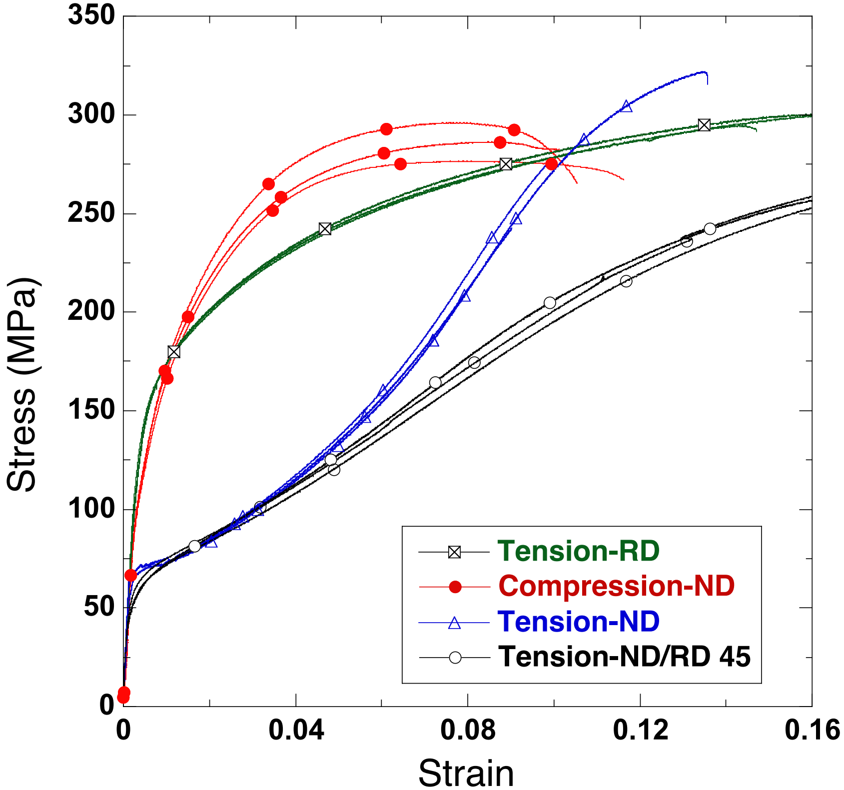


APPLICATION to AZ31 Mg ALLOY

- AZ31 Mg alloy processed by hot rolling (25.4 mm thickness)
- Average grain size (25 μm)
- Typical rolling texture
- Tensile and compression tests along different directions.



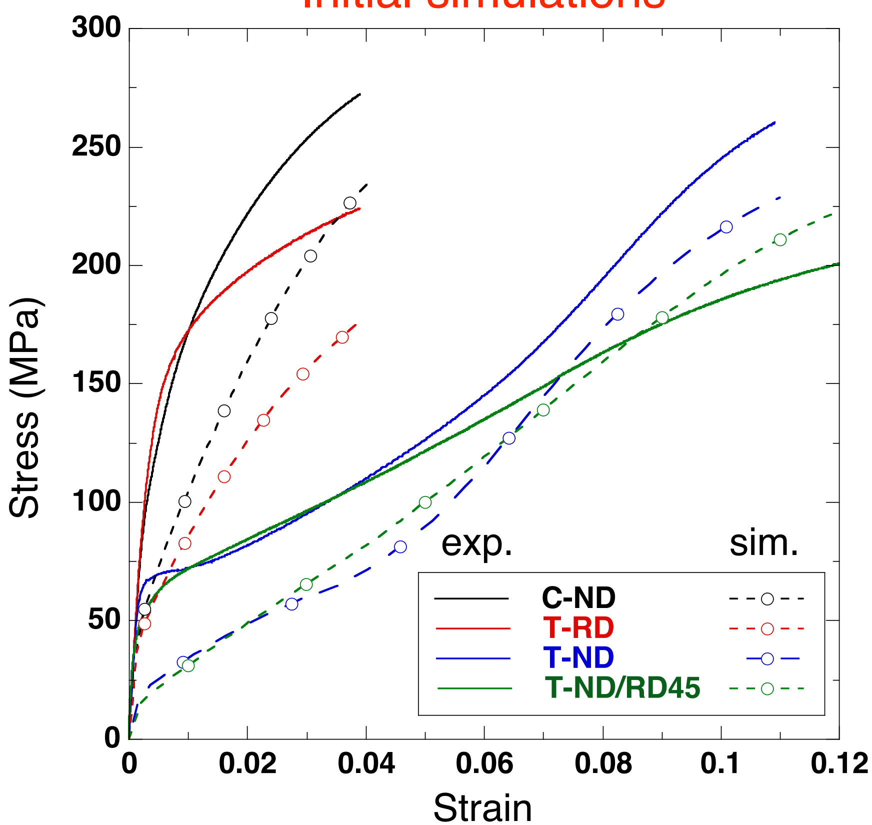




DETERMINATION of AZ31 SINGLE CRYSTAL PROPERTIES

- Parameters to be determined: initial strength, τ_0 , saturation strength, τ_s , initial hardening modulus, h_0, for basal, prismatic, pyramidal c+a slip and extension twining
- Fixed parameters:
  - elastic constants of Mg single crystal
  - Latent hardening parameters $q_{sl-sl} = 1.0 \quad q_{sl-tw} = 2.0$
  - Hardening exponents $a_{sl} = 0.6 \quad a_{tw} = 1.0$
  - Strain rate sensitivity exponent $m = 0.1$

Initial simulations

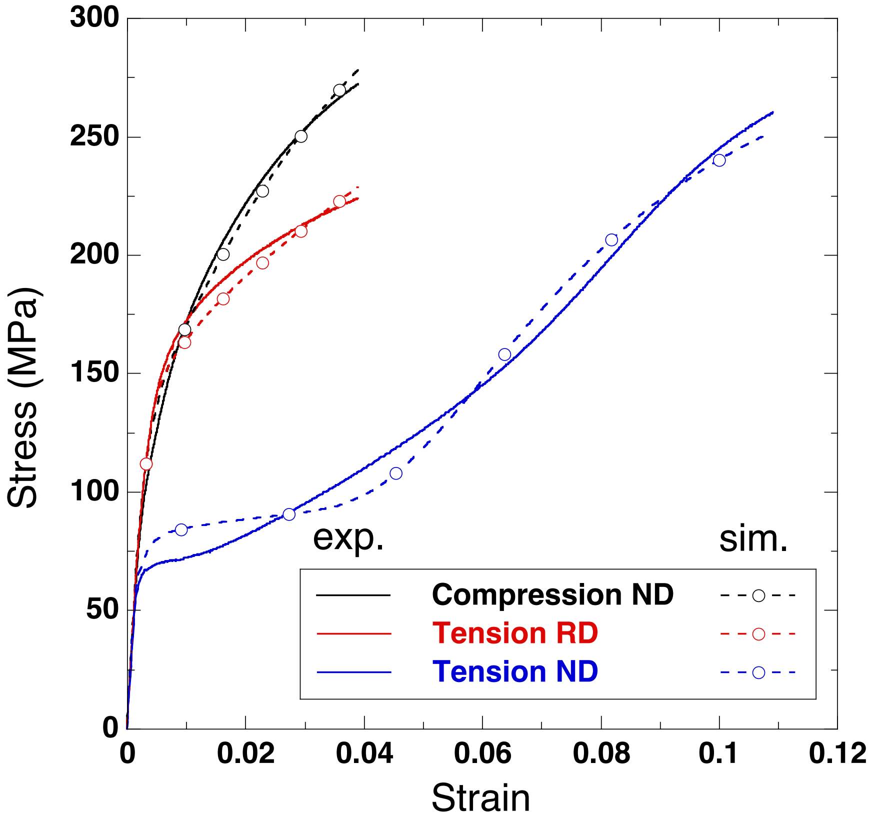


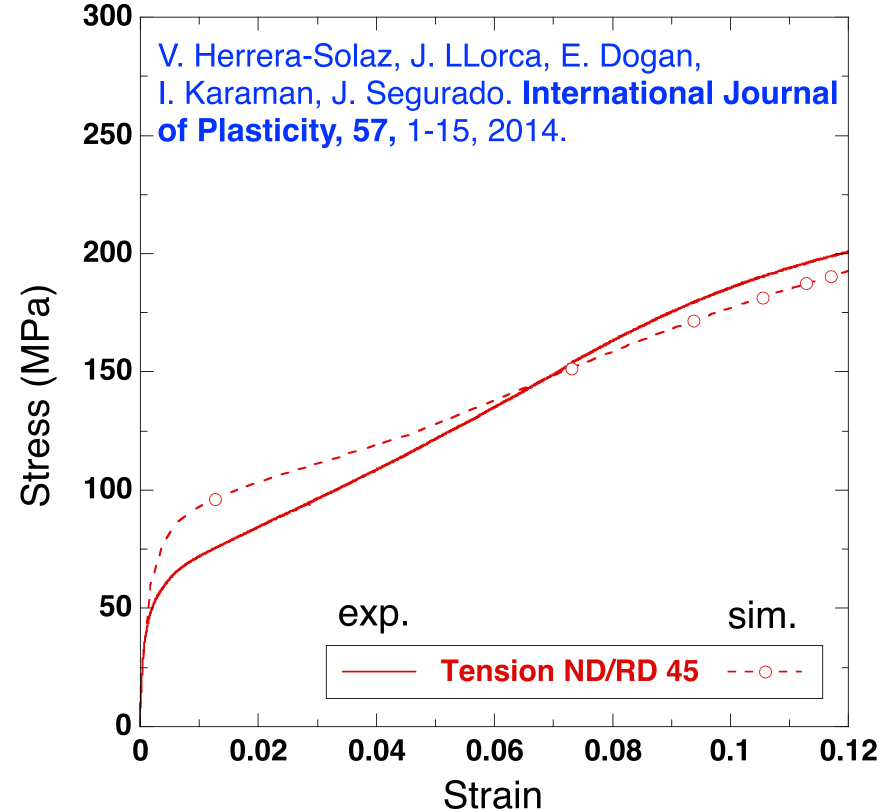
Input single crystal parameters

(pure Mg, values in MPa)

Parameter	Deformation mode	initial values
τ_0	Basal	1.75
	Prismatic	25
	Pyramidal c+a	40
	Twinning	3.5
τ_s	Basal	40
	Prismatic	85
	Pyramidal c+a	150
	Twinning	20
h_0	Basal	20
	Prismatic	1500
	Pyramidal c+a	3000
	Twinning	100

PREDICTIONS WITH OPTIMIZED PARAMETERS





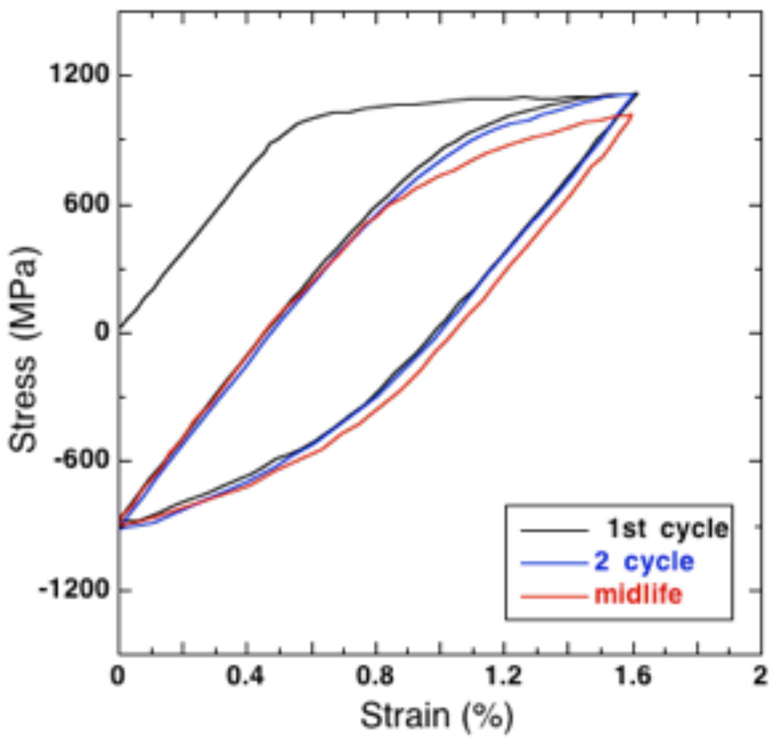
ROBUSTNESS and UNIQUENESS

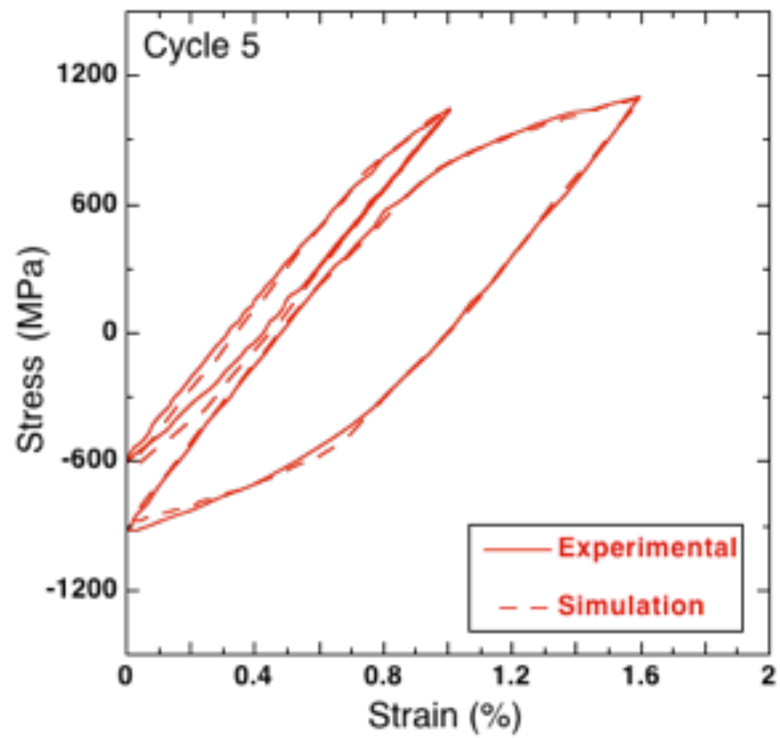
- The input has to provide information for all the deformation mechanisms (minimum two stress-strain curves, better three and, in the future, texture).
- The results obtained have been shown to be independent of the initial values of the CRSS for each system.

V. Herrera-Solaz, J. Segurado, J. LLorca. **European Journal of Mechanics A/Solids, 53**, 220-228, 2015.

FATIGUE OF WROUGHT IN718

- Wrought IN718 subjected to fatigue at 400ºC. Average grain size ≈ 12 μm.
- The alloy subjected to cyclic deformation undergoes isotropic hardening, Bauschinger effect, cycles softening, mean stress relaxation and ratcheting.
- Cyclic deformation is simulated by means of the simulation of an RVE of the microstructure. The parameters of the phenomenological cyclic fatigue model are calibrated using the Levenberg-Marquardt method from the experimental cyclic stress-strain curves.





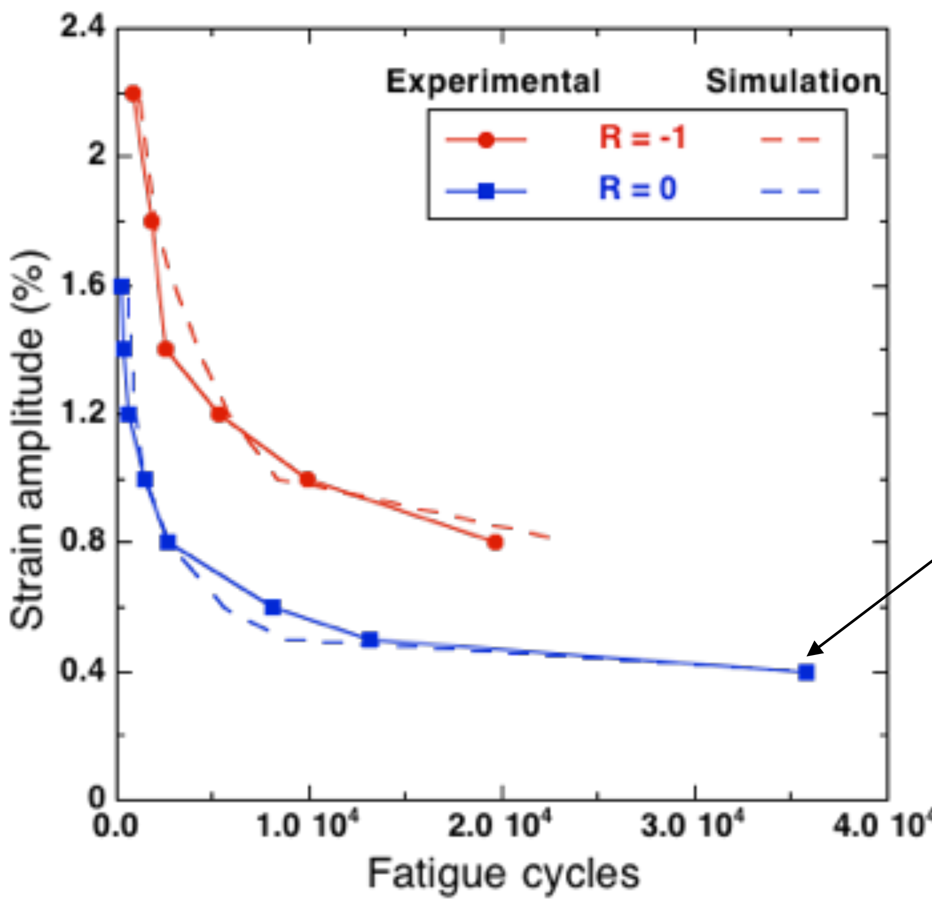
D. Gustafsson; J. J. Moverare; K. Simonsson; S. Sjöström. **J. Eng. Gas Turbines Power., 133,** 094501, 2011.

FATIGUE LIFE PREDICTION

Fatigue life predictions for R= 0 and R=-1 were carried out using

$$N \, \Delta FIP_w^i = FIP_c$$

where the FIP was averaged in all the slip systems in each grain.



$$FIP_c = \frac{N}{\Delta FIP_w^i}$$

CONCLUSIONS

- CAPSUL is a suite of tools for crystal plasticity homogenization of polycrystals which can be used to take into account the effect of the microstructure on the mechanical properties of polycrystals.

- It includes tools to built a realistic RVE of the microstructure from easily available experimental data (2D sections of the microstructure, X-ray diffraction textures) and a robust inverse homogenization strategy (based on the Levenberg-Marquardt method) to obtain the single crystal properties from experimental data (micropillar compression of single crystals, monotonic and cyclic polycrystal tests, etc.)

- Current capabilities are focussed in the prediction of monotonic and cyclic deformation as well as fatigue life. Further developments will include creep and thermo-mechanical fatigue.

ACKNOWLEDGEMENTS

- MAGMAN project (*Analysis of the microstructural evolution and mechanical behavior of Mg-Mn-rare earth alloys*)

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