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Micromechanics using Spectral Method

Interface Decohesion in Polycrystals

L. Sharma, P. Shanthraj, M.Diehl, F. Roters, D. Raabe, R. Peerlings and M. Geers

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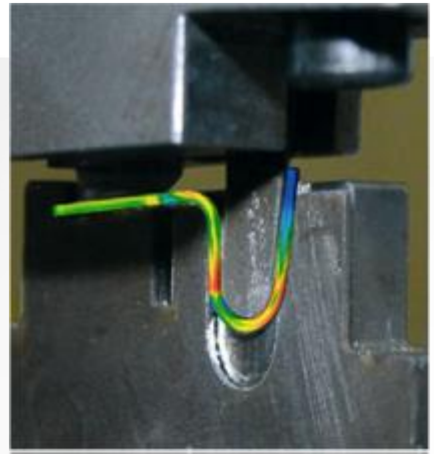
TATA STEEL

Outline

- Motivation
- **DAMASK**- material simulation kit
- The Spectral Solver
  - Basic scheme
  - Some applications
  - Demo: a very simple (1D) implementation using petsc4py
- Smeared damage mechanics
  - Interface decohesion in Polycrystals.
- Future Work

Motivation

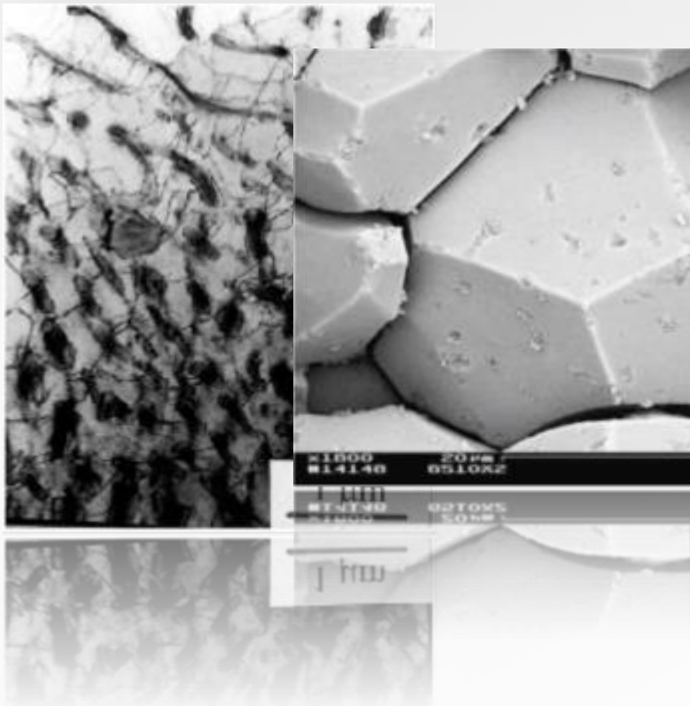





- strain localization
- damage initiation
- recrystallization nucleation
- ...

- tool design
- crashworthiness
- component properties
- ...

Motivation



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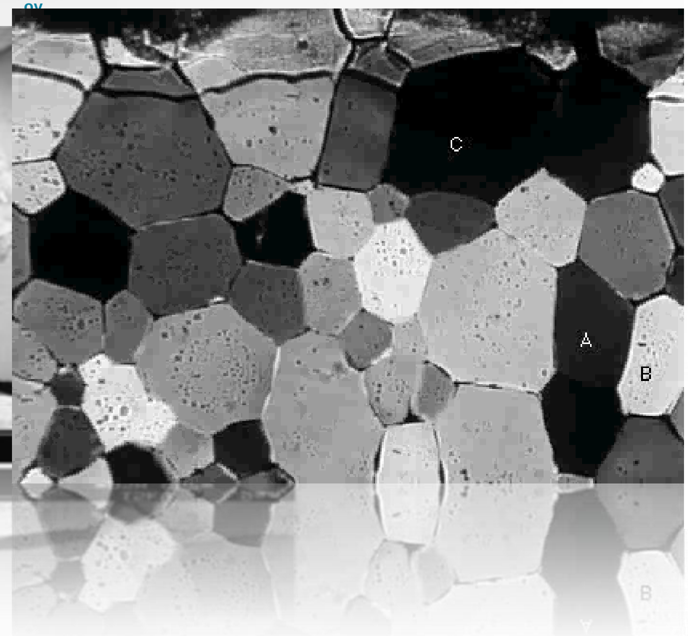
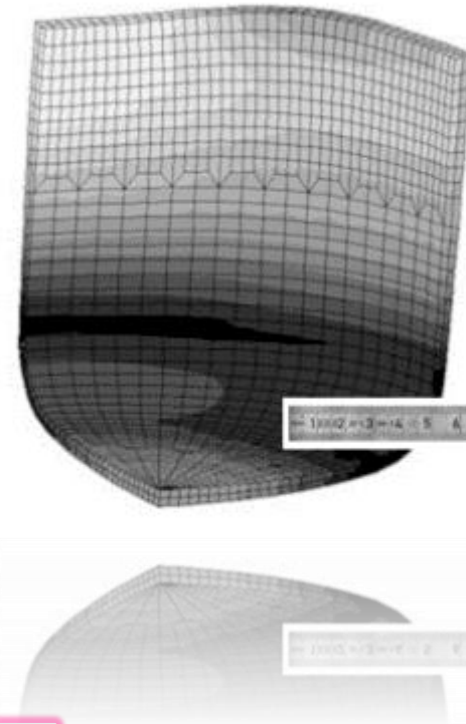




Crystal Plasticity is always a multi-scale problem !

Motivation

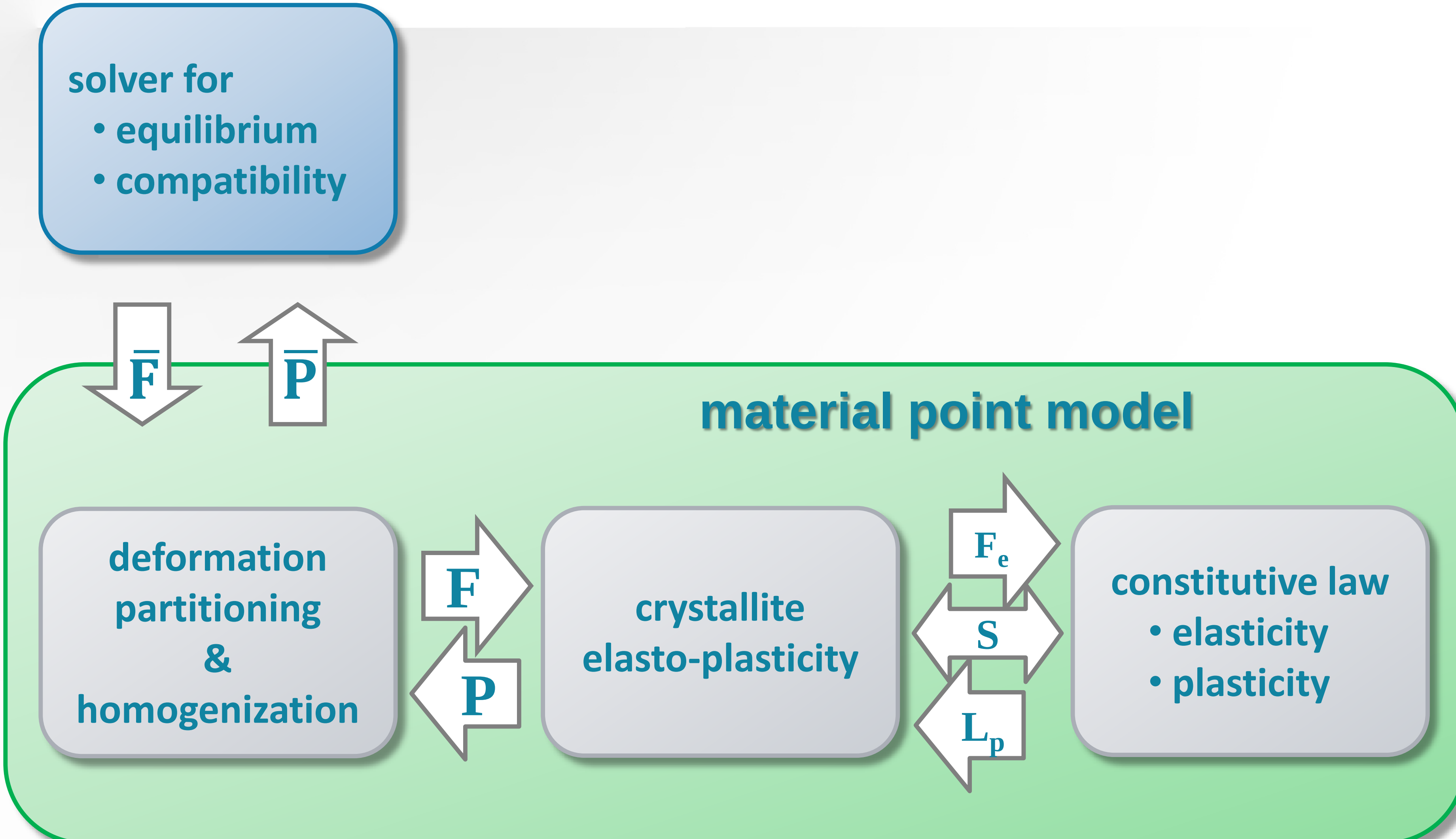
simulation requirements

- arbitrary mechanical boundary value problems
- continuum mechanics
- accounting for crystal plasticity

→

Crystal Plasticity
Finite Elemente Method
(CPFEM)
Or
Crystal Plasticity
Spectral Method
(CPFFT)

CPFEM/CPFFT strategy



The spectral solver

A little history

- Use spectral method instead of FEM
- Solution based on FFT
- Much faster than FEM
- Small strain framework
- Elastic material law

ELSEVIER

Comput. Methods Appl. Mech. Engrg. 157 (1998) 69–94

Computer methods in applied mechanics and engineering

A numerical method for computing the overall response of nonlinear composites with complex microstructure

H. Moulinec, P. Suquet*

L.M.A./C.N.R.S., 31 Chemin Joseph Aiguier, 13402 Marseille, Cedex 20, France

Received 28 May 1996; revised 1 May 1997

Abstract

The local and overall responses of nonlinear composites are classically investigated by the Finite Element Method. We propose an alternate method based on Fourier series which avoids meshing and which makes direct use of microstructure images. It is based on the exact expression of the Green function of a linear elastic and homogeneous comparison material. First, the case of elastic nonhomogeneous constituents is considered and an iterative procedure is proposed to solve the Lippman–Schwinger equation which naturally arises in the

- Extended to viscoplastic materials

Pergamon

Acta mater. 49 (2001) 2723–2737

Acta MATERIALIA

www.elsevier.com/locate/actamat

N-SITE MODELING OF A 3D VISCOPLASTIC POLYCRYSTAL USING FAST FOURIER TRANSFORM

R. A. LEBENSOHN

Instituto de Fisica Rosario (UNR-CONICET), 27 de Febrero 210 Bis, 2000 Rosario, Argentina

(*Received 7 November 2000; received in revised form 18 April 2001; accepted 18 April 2001*)

Abstract—We present a formulation to compute the local response of elastic and viscoplastic anisotropic 3D polycrystals based on the Fast Fourier Transform (FFT) algorithm. This formulation is conceived for periodic heterogeneous microstructures and also for materials with random spatial distribution of heterogeneities. The approach is of the *n*-site kind, provides an exact solution of the equilibrium equation and has better numerical performance than small-scale FEM. The viscoplastic FFT formulation combined with an ad-hoc microstructure updating scheme is used to predict local states, morphology and texture evolution of ideal f.c.c. polycrystals. The model predicts strain localization, intragranular misorientation and subgrain formation and overall textures which are smoother than those obtained with classical 1-site schemes, in better agreement with experiments.

Keywords: Theory & modeling; Polycrystal; Mechanical properties (plastic); Texture; Microstructure

1. INTRODUCTION

This paper is concerned with the determination of local states of heterogeneous materials. Due to the development of new characterization techniques which allow the investigation of the materials proper-

degrees of freedom required by such FEM calculations limit the complexity and the size of the microstructures that can be investigated by these methods. On the other hand, the prediction of intracrystalline states using homogenization techniques requires n-

- Large strain formulation
- Coupled with DAMASK

Spectral method

Static equilibrium:

$$\mathrm{div}(\boldsymbol{\sigma}) = 0$$

Material law:

$$\boldsymbol{\sigma} = \boldsymbol{C}\boldsymbol{\varepsilon}$$

Split strain:

$$\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}$$

Introduce reference medium:

Stiffness $\bar{\boldsymbol{C}}$

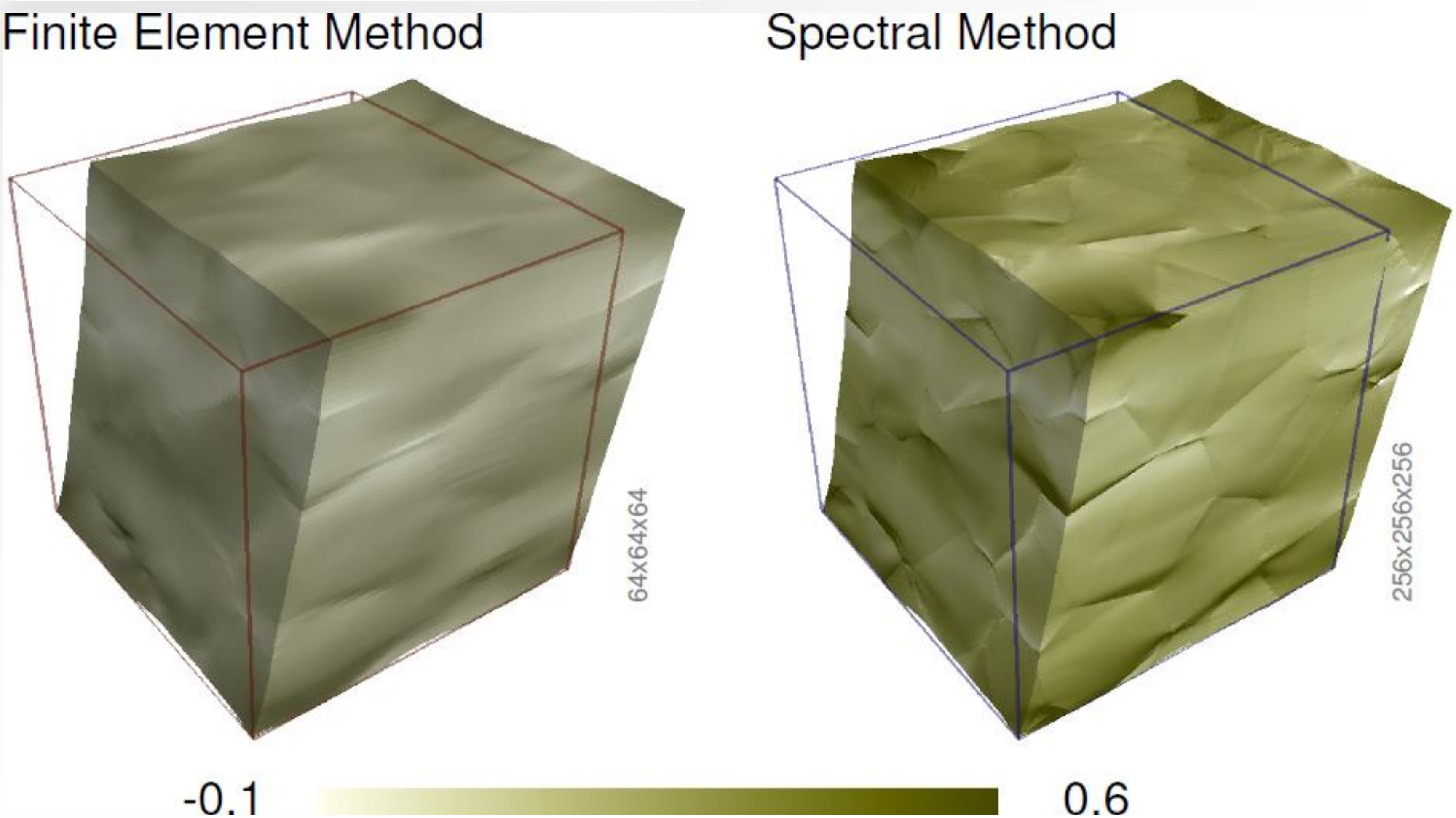
$$\boldsymbol{\varepsilon}^{m+1} = \boldsymbol{\varepsilon}^{m} - \boldsymbol{\Gamma} * \boldsymbol{\sigma}^{m}$$

FFT

$$\boldsymbol{\varepsilon}^{m+1} = \boldsymbol{\varepsilon}^{m} - \mathcal{F}^{-1}\left(\hat{\boldsymbol{\Gamma}}: \hat{\boldsymbol{\sigma}}^{m}\right)$$

with $\hat{\Gamma}_{ijkl} = k_j k_l \bar{N}_{ik}$ and $\bar{N}_{ik} = \left[k_l k_j \bar{C}_{ijkl}\right]^{-1}$

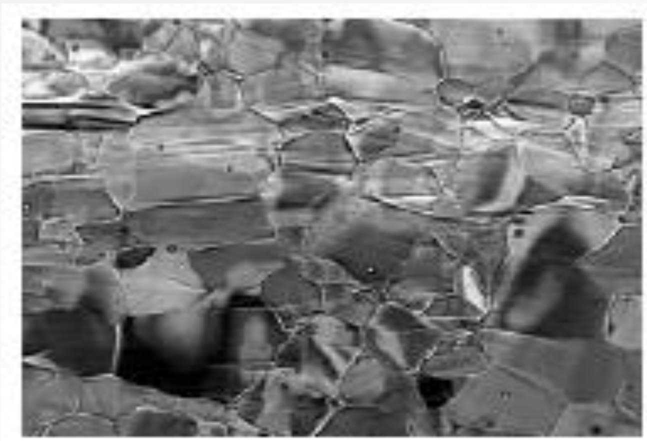
Comparion FEM vs FFT



P. Eisenlohr., M. Diehl, R. A. Lebensohn, F. Roters: International Journal of Plasticity (2013), 37 - 53

Experimental-Numerical

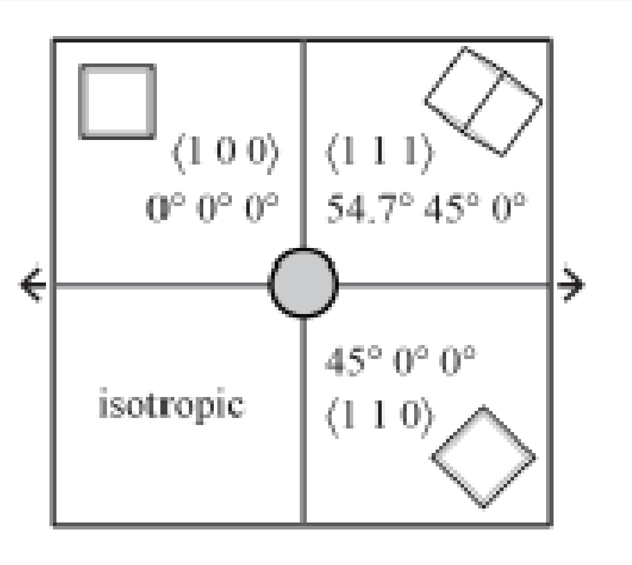
Example: Basal slip in Magnesium

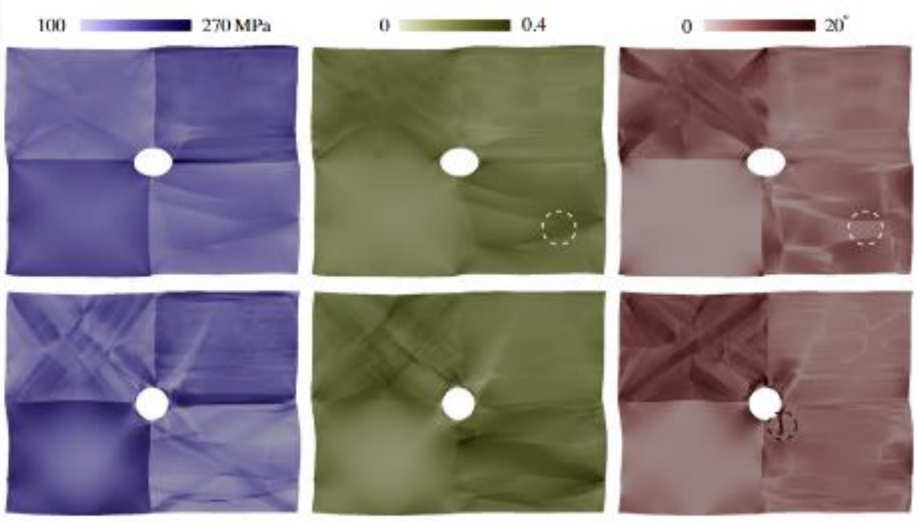


F. Wang, S. Sandloebes, M. Diehl, L. Sharma, F. Roters, D. Raabe:Acta Materialia 80 (2014) 77-93

Mesoscale mechanics

- High Resolution Crystal plasticity enabled through robust spectral solvers

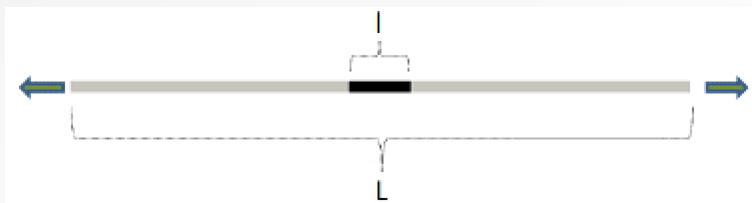




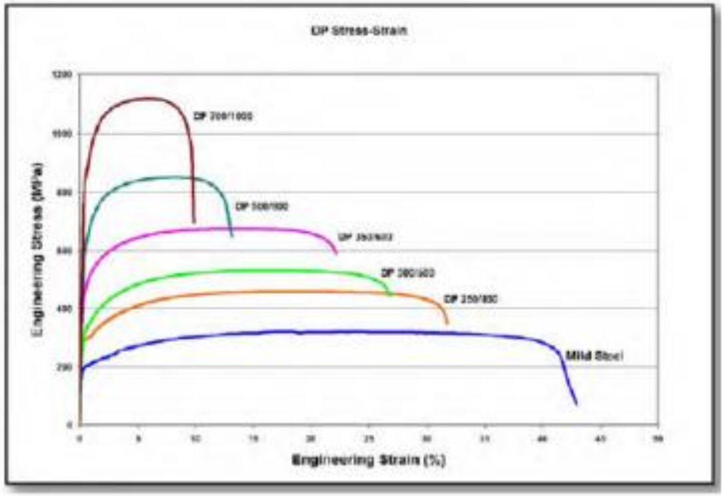
(a) Equivalent stress σ_{vM} (b) Equivalent strain ε_{vM} (c) Rotation angle between initial and current grain orientation

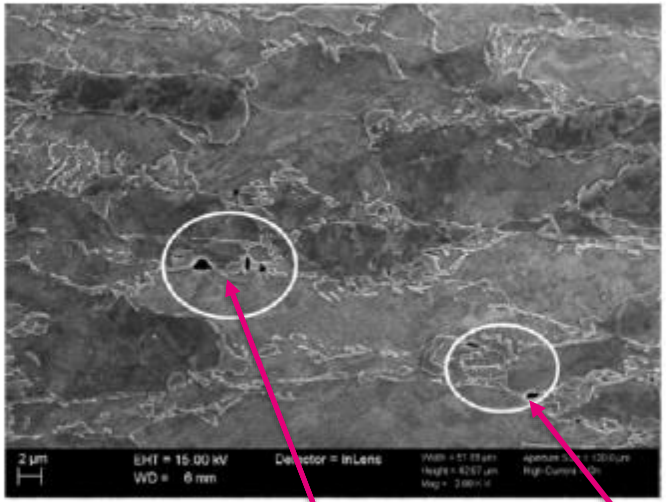
Shanthraj et al. [IJP, 2015]

Demo (1D elasticity + spectral method using petsc4py)



Interface decohesion (formability limiter)





Role of the Interfaces
Surrounding Microstructure

?

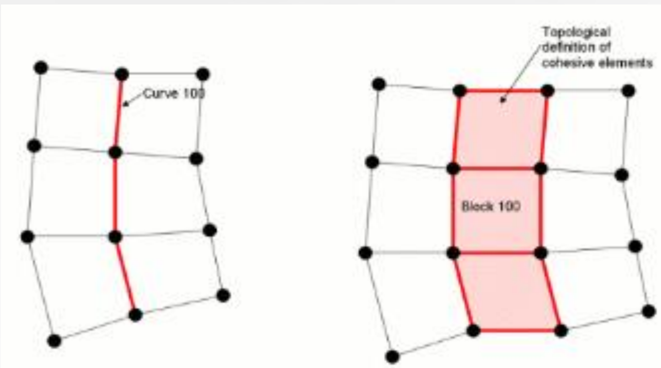
Void
Growth/Propagation

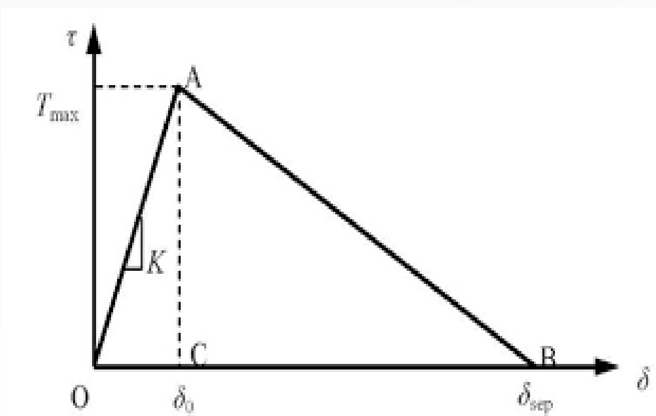
Void
Initiation

Computational tool to model
Interface decohesion

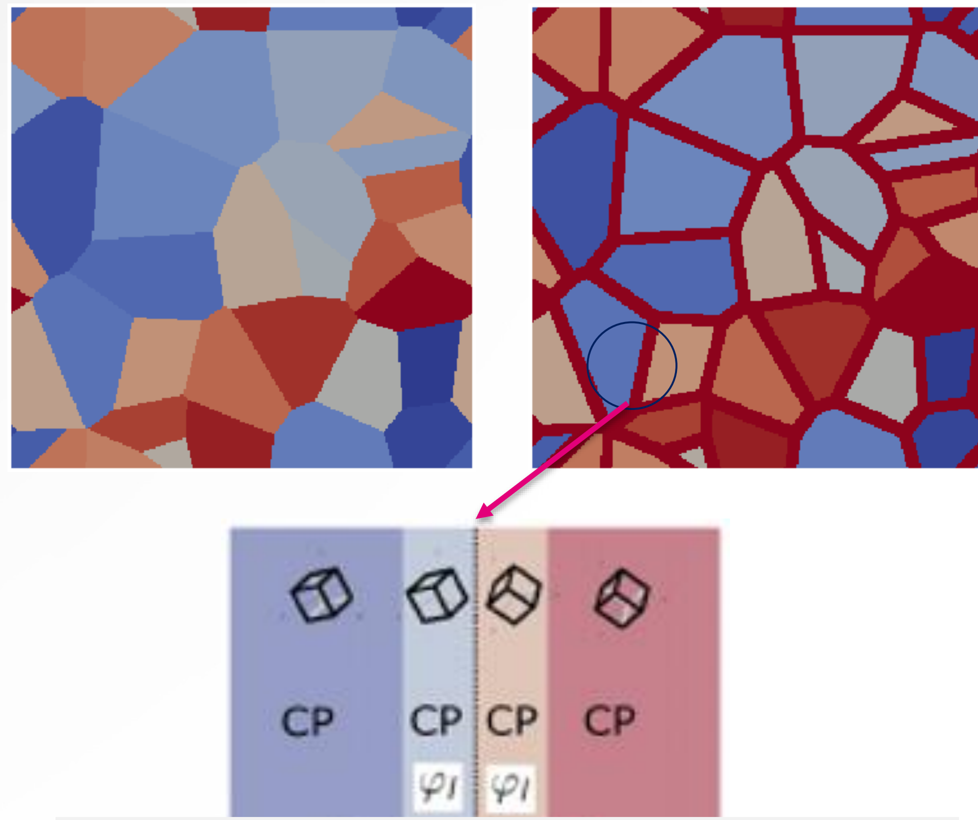
Interface modeling of polycrystals

Interface elements



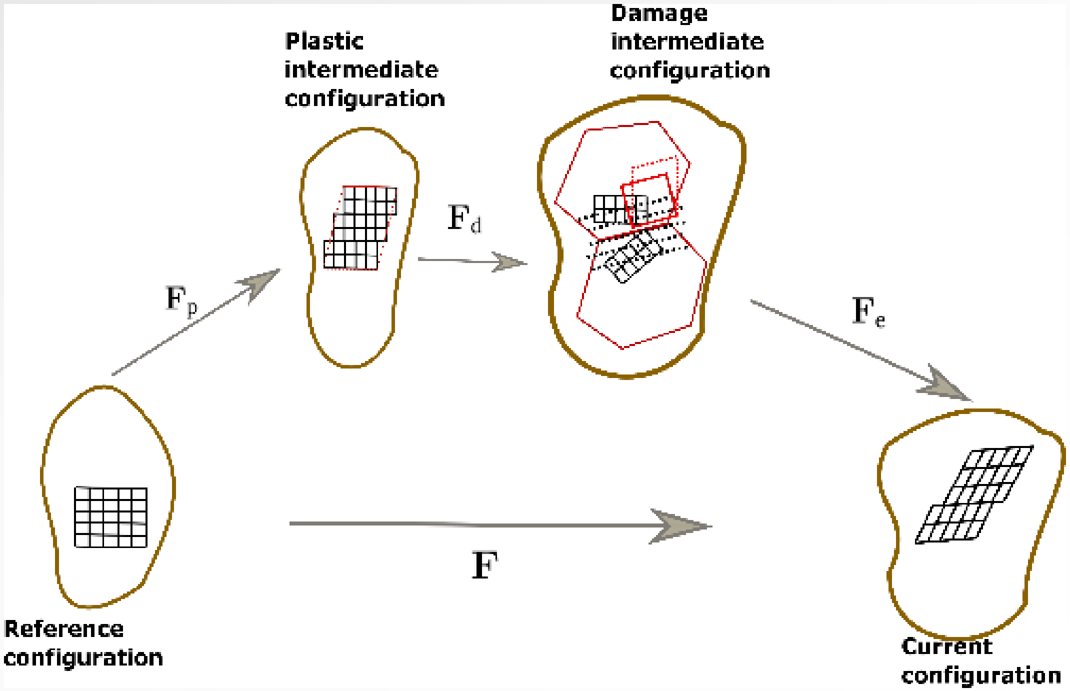


Interface band



$$\vec{\nabla}_0 \cdot l^2 \mathbf{D} \vec{\nabla}_0 \varphi_{nl} + \varphi_l - \varphi_{nl} = 0.$$

Eigen Strain Damage (Pandolfi, Ortiz et al.; Menzel, Ekh et al., 2002)



- Accomodation by eigen strain.
- In an anisotropic way (normal and tangential modes).
- (interface-) plane stretching effects.

Field problem

- Static Mechanical Equilibrium.

$$\vec{\nabla}_0 \cdot \mathbf{P}(\mathbf{F}) = 0.$$

- Nonlocal damage (regularisation/localisation limiter).

$$\vec{\nabla}_0 \cdot l^2 \mathbf{D} \vec{\nabla}_0 \varphi_{nl} + \varphi_l - \varphi_{nl} = 0.$$

Damage regularization solved using FFT

$$0 = \nabla \cdot l^2 \mathbf{D} \nabla \varphi_{nl} + (\varphi_l - \varphi_{nl})$$

$$l^2(\mathbf{X})\mathbf{D} = \bar{l^2}\mathbf{D} + \tilde{l^2}(\mathbf{X})\mathbf{D}$$

- Hetrogenous regularization lengthscale

$$0 = \nabla \cdot (\bar{l^2} + \tilde{l^2}(\mathbf{X}))\mathbf{D}\nabla \varphi_{nl} + (\varphi_l - \varphi_{nl})$$

$$\varphi_{nl}\left(1 - \nabla \cdot \bar{l^2}\mathbf{D}\nabla\right) = \nabla \cdot \tilde{l^2}(\mathbf{X})\mathbf{D}\nabla \varphi_{nl} + \varphi_l$$

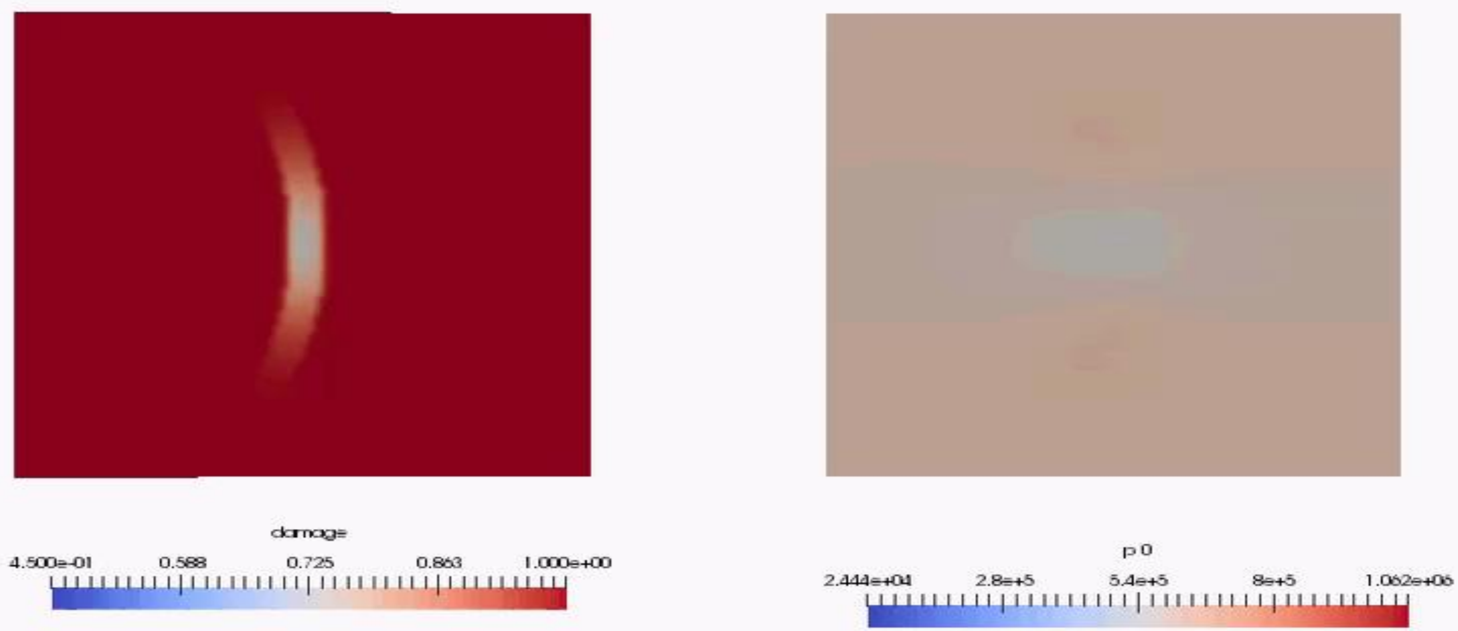
- Utilize Fourier transform

$$\mathcal{R}_{dam} = \varphi_{nl}^t - \mathcal{F}^{-1}\left(\frac{\mathcal{F}\left(\varphi_l + \nabla \cdot \tilde{l^2}(\mathbf{X})\mathbf{D}\nabla \varphi_{nl}\right)}{\mathcal{F}\left(1 - \nabla \cdot \bar{l^2}\mathbf{D}\nabla\right)}\right)$$

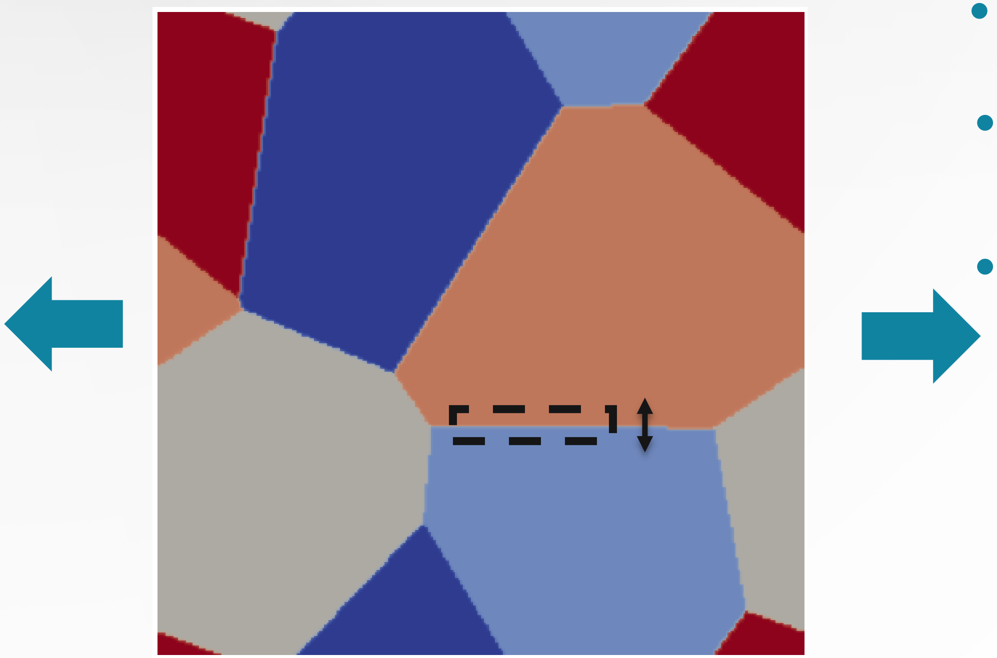
- Solved for its roots using Jacobian free Newton method.

M2i

Test Simulation

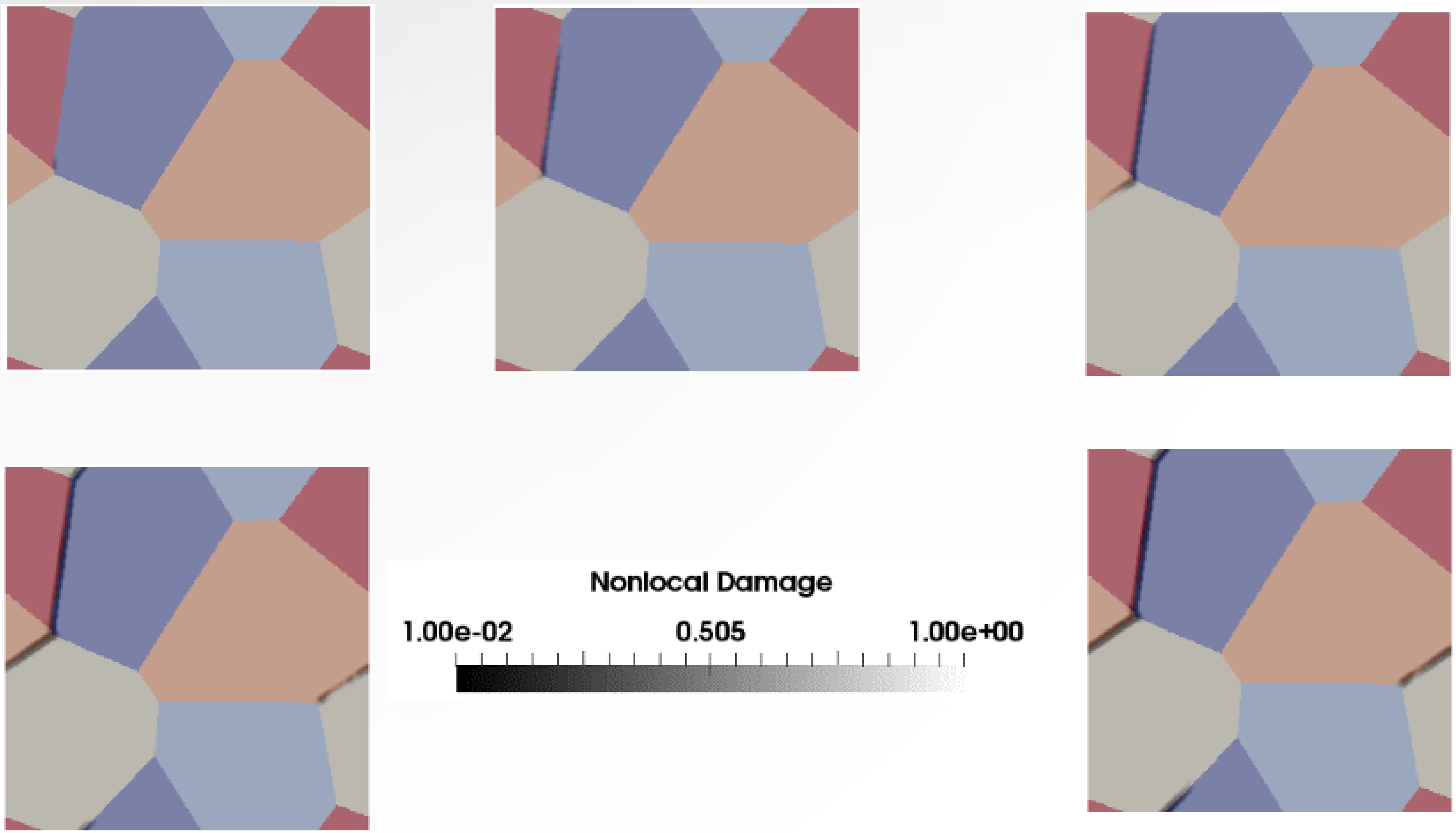


Polycrystal Simulation

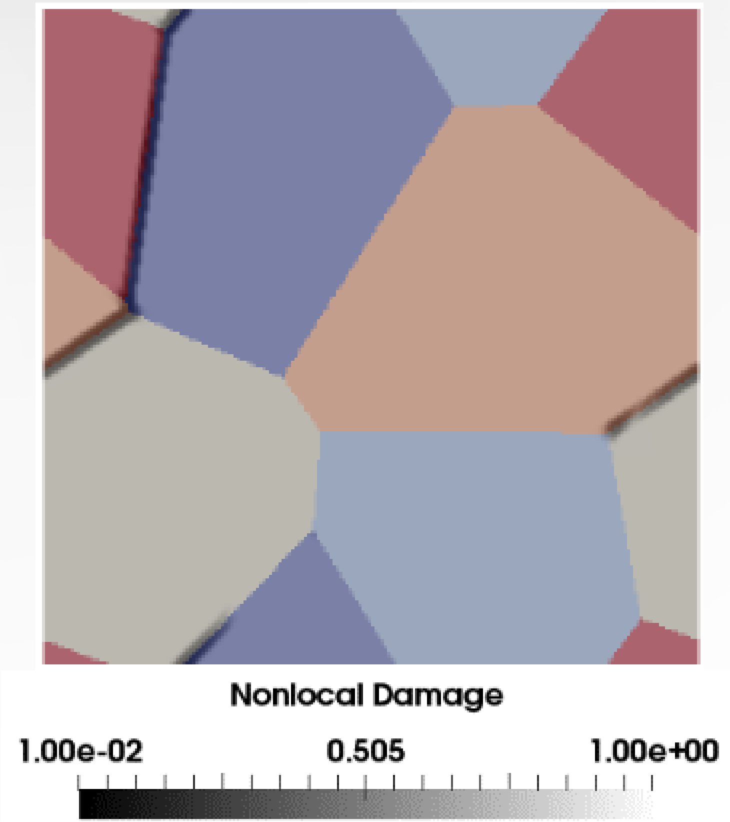


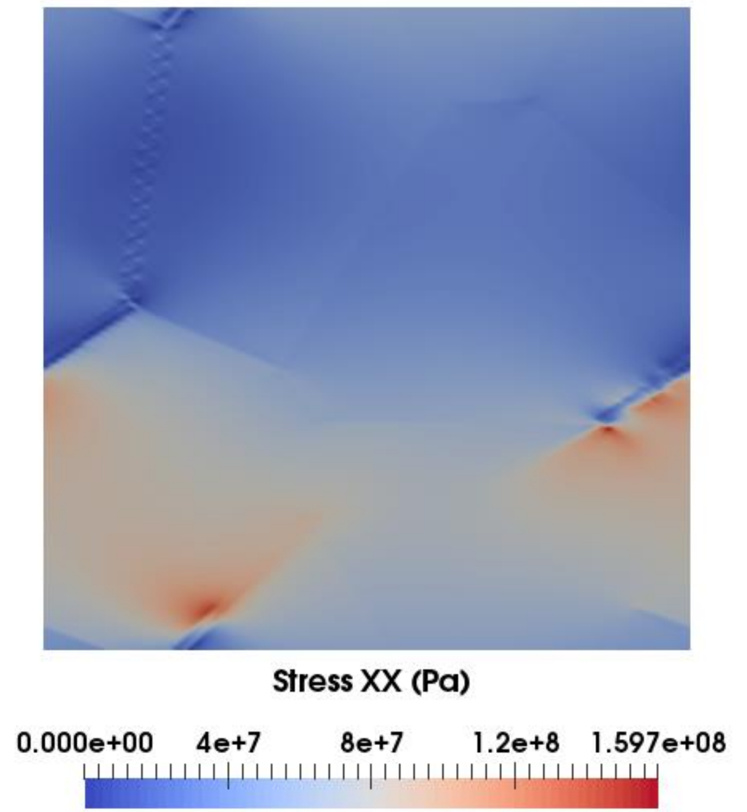
- Resolution: *256x256x2*
- Randomly orientation FCC
- Elasto-plastic-damage (crystal plasticity)
- Interface Band thickness: 4 voxels

Polycrystal Simulation: Damage evolution

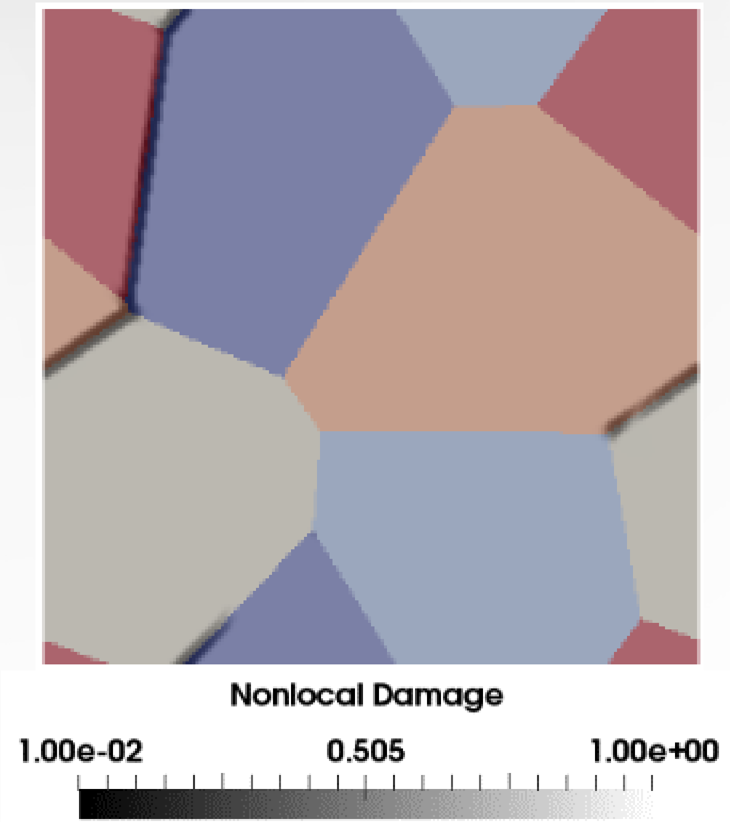


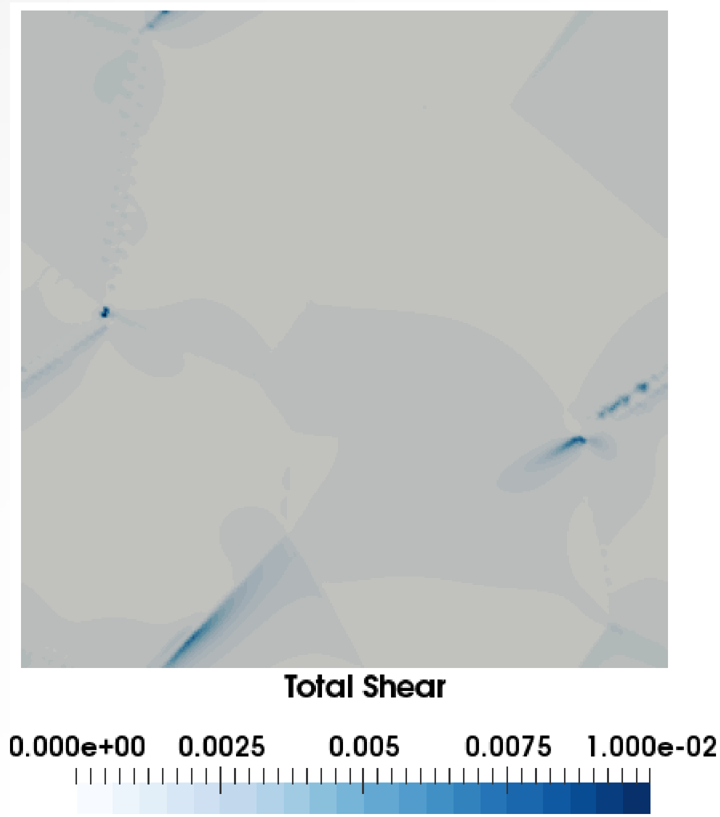
Polycrystal Simulation: Stess Unloading





Polycrystal Simulation: Damage vs Plasticity





Future work

- Coupling with damage models in the bulk
- Monolithic schemes for Multiphysics
- Implementation using petsc4py
- Time integrators (Fortran support)

Acknowledgment

Düsseldorf Advanced MAterial Simulation Kit, DAMASK

- Available as freeware according to GPL 3
- Integrates into MSC.Marc and Abaqus (std. and expl.)
- Standalone spectral solver

- Web: https://DAMASK.mpie.de
- Email: DAMASK@mpie.de

Thank you.
Questions?

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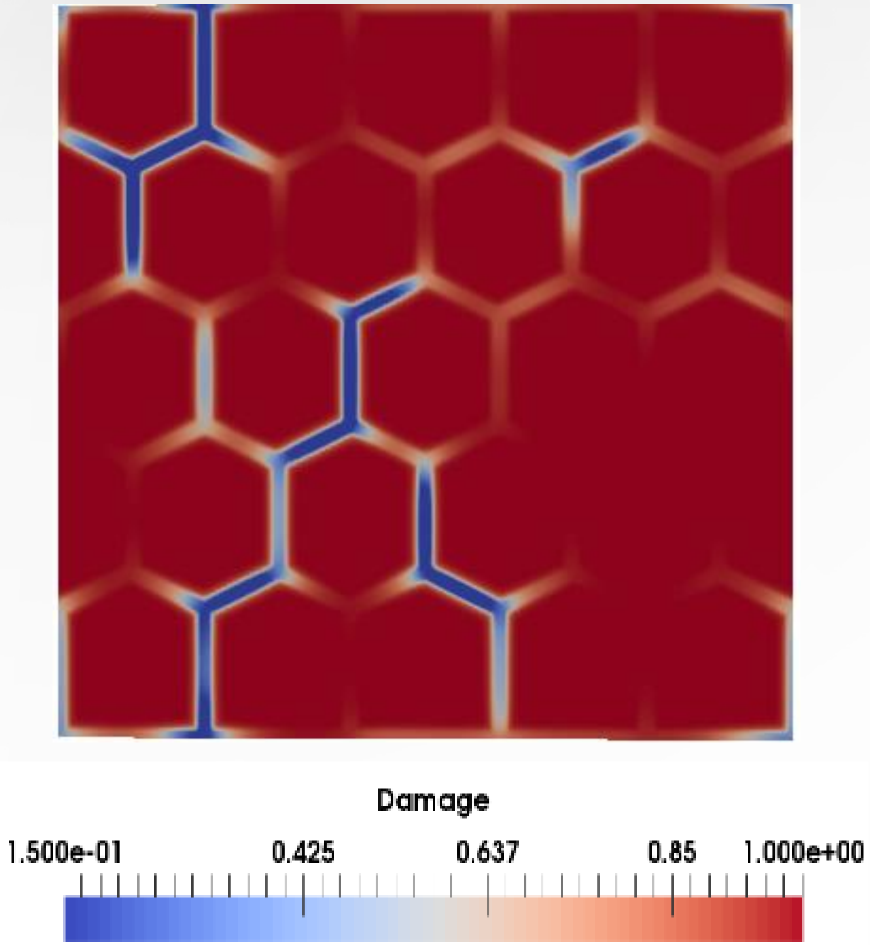
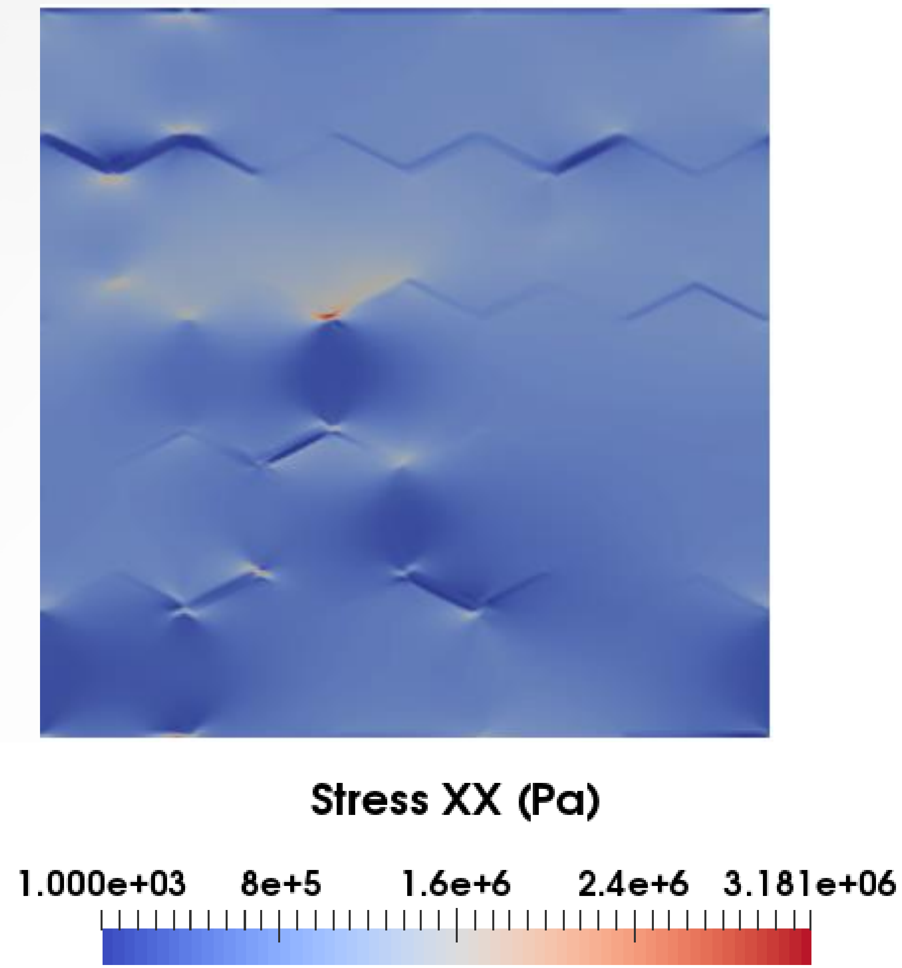
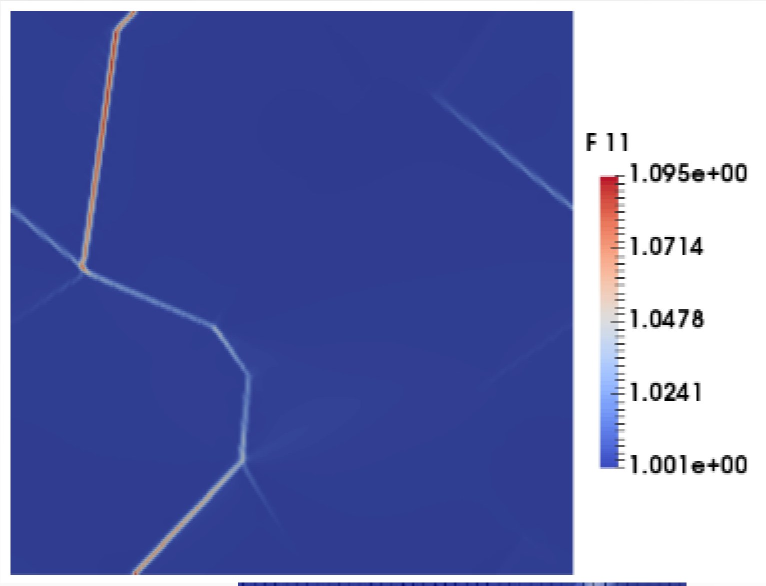
Simulation (hexagonal polycrystal loaded horizontally)

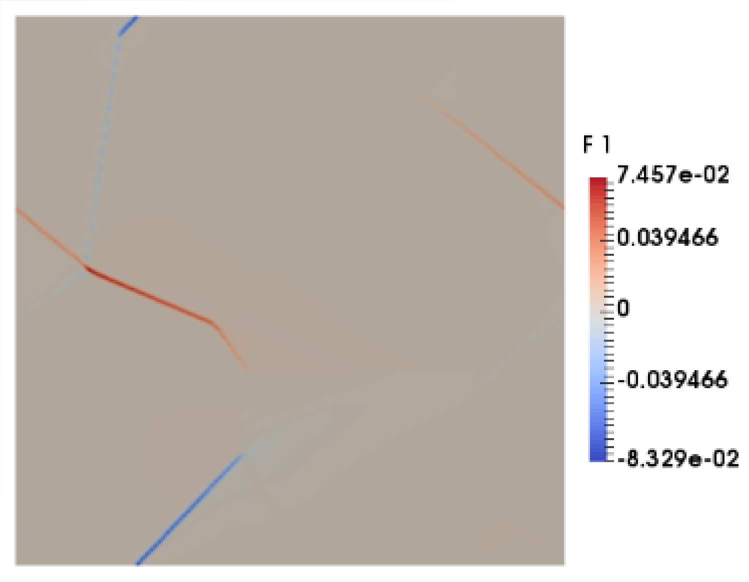


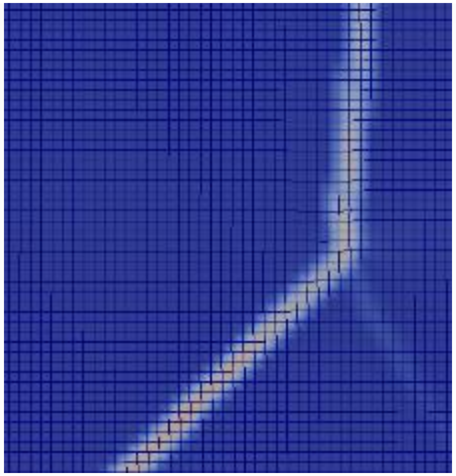


Simulation

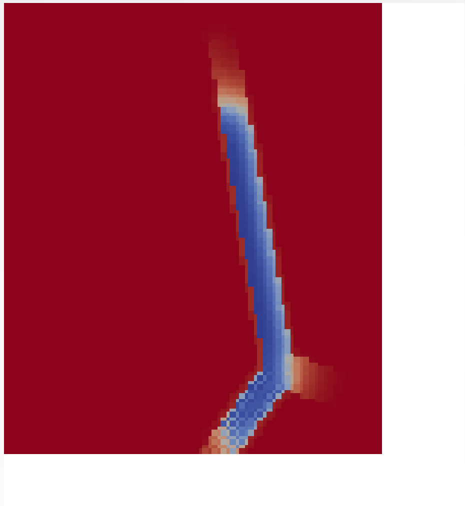
Strain localisation



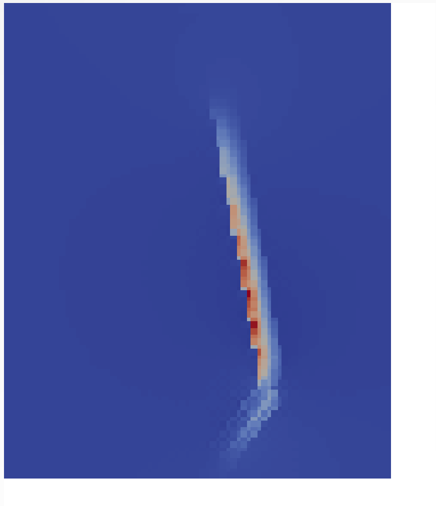




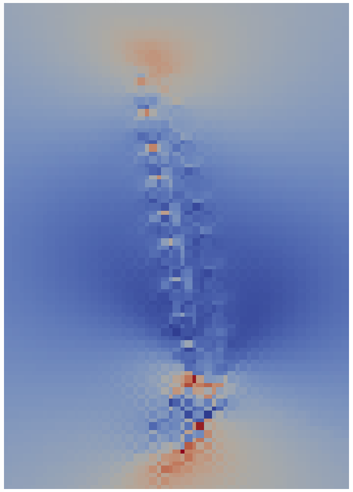
Brittle Simulation



Damage



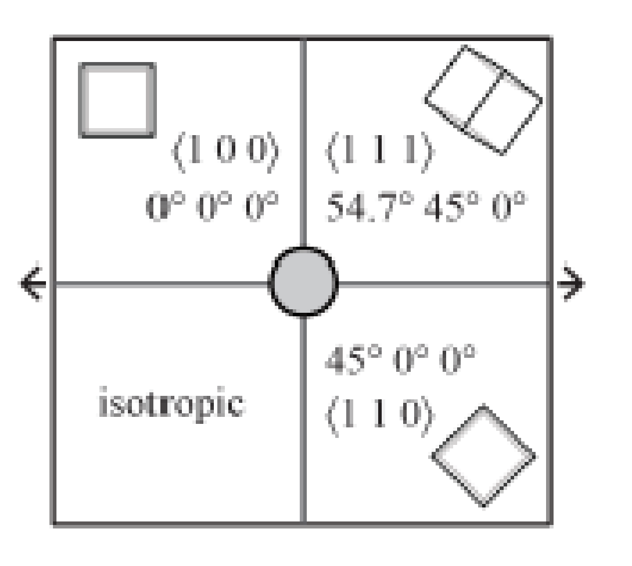
Strain (F11)

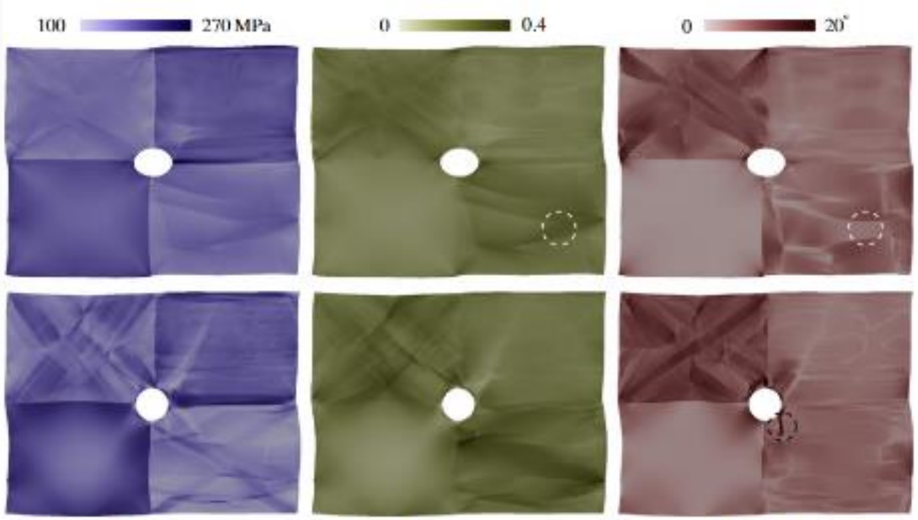


Stress (P11)

Mesoscale mechanics

- Crystal plasticity.
- FFT based Spectral method





(a) Equivalent stress σ_{vM} (b) Equivalent strain ε_{vM} (c) Rotation angle between initial and current grain orientation

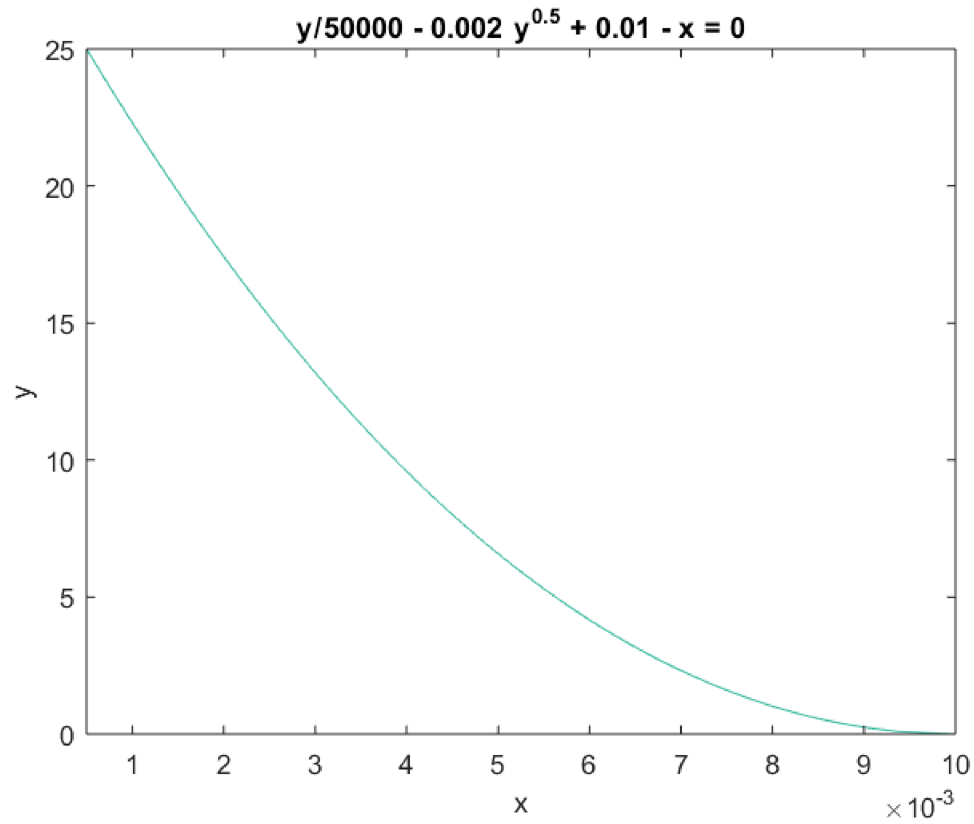
Shanthraj et al. [2015]

Experimental-Numerical

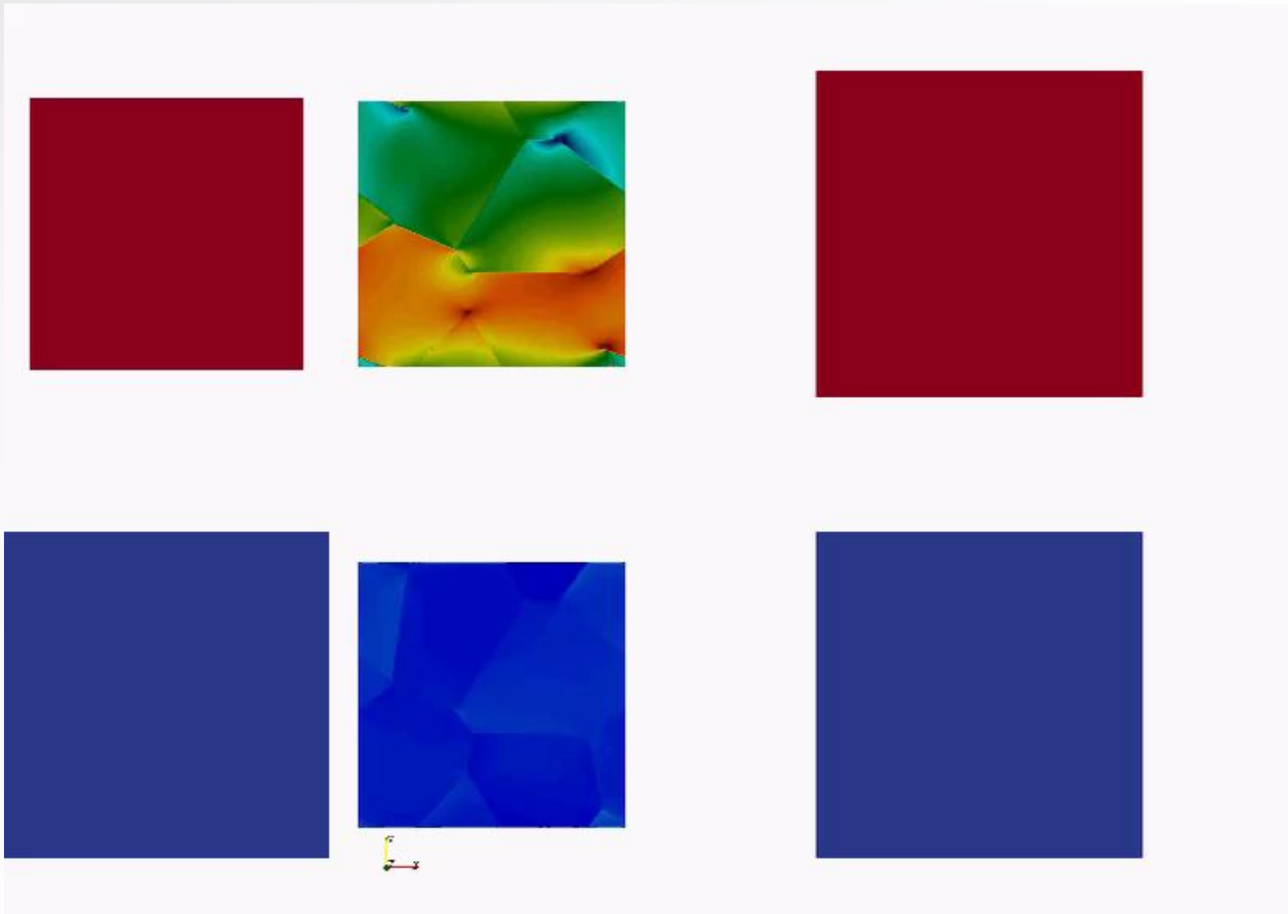
Example: Basal slip in Magnesium

Wang et al. [2014]

Rate independent



Rate independent



Local Damage

- 1 for undamaged material
- 0 for fully damaged
- Monotonously decreases (irreversibility)

▸ Local damage:

$$\dot{\varphi}_l = \begin{cases} \frac{-1}{O_{c_{fin}} - O_{c_{init}}}\dot{\kappa}, & \text{if } O_{c_{init}} < \kappa < O_{c_{fin}}. \\ 0, & \text{otherwise.} \end{cases}$$

▸ History variable:

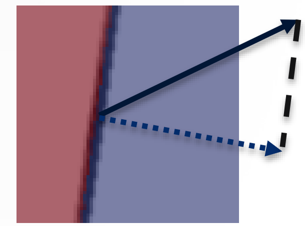
$$\dot{\kappa}(t) = \left\langle \dot{O}_n \right\rangle + \left| \dot{O}_t \right|$$

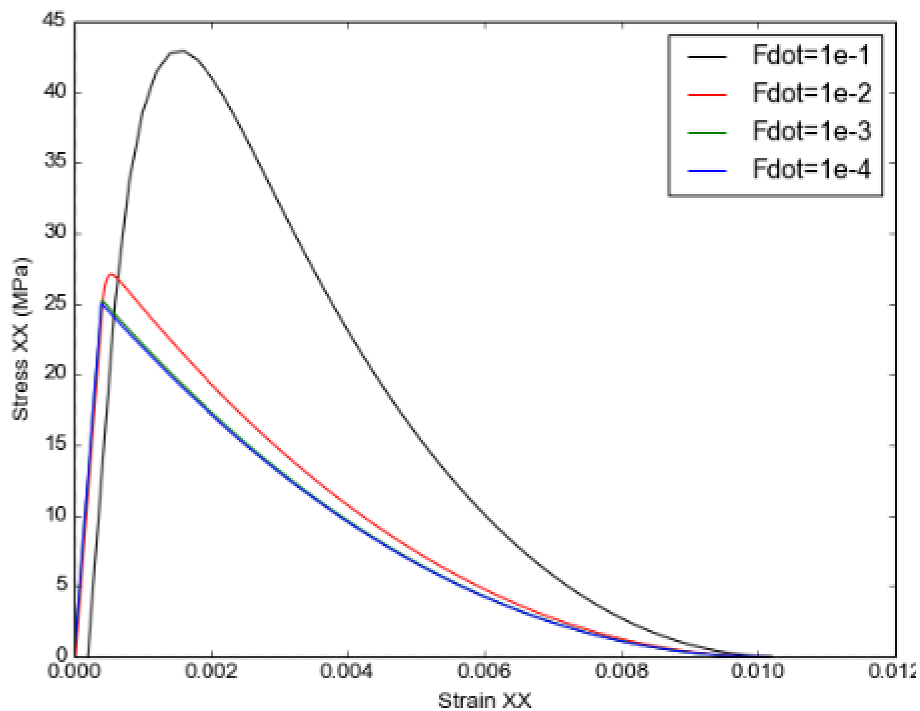
$$\kappa(0) = 0$$

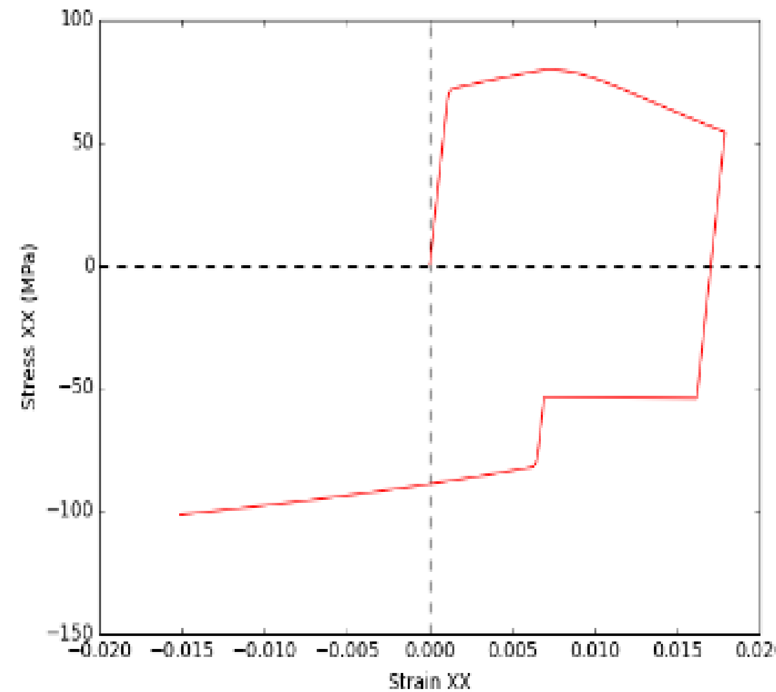
Normal opening strains

- Normal opening strain rate

$$\dot{O}_n = \dot{O}_{0_n} \left\langle \frac{|\tau_n|}{\varphi_{nl}^2 \tau_{c_n^o}} - 1 \right\rangle^n \mathrm{sgn}\left(\tau_n\right) \mathcal{H}(0_n)$$



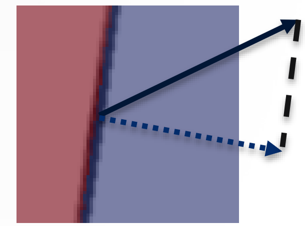


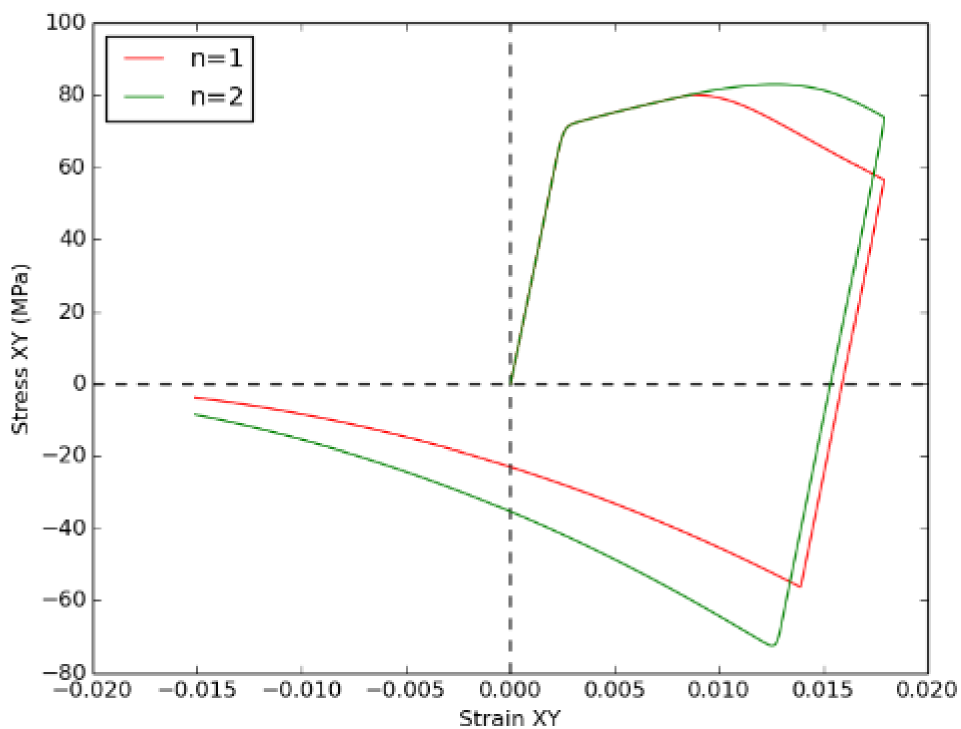


Tangential opening strains

- Tangential opening strain rate

$$\dot{O}_t = \dot{O}_{0_t} \left\langle \frac{|\tau_t|}{\varphi_{nl}^2 \tau_{c_t^0}} - 1 \right\rangle^n \operatorname{sgn}(\tau_t)$$





Stress Integration (the Local problem)

$$\mathbf{F}_{\mathrm{e}} = \mathbf{F}\mathbf{F}_{\mathrm{p}}^{-1}\mathbf{F}_{\mathrm{d}}^{-1}$$

$$\dot{\mathbf{F}}_{\mathrm{p}} = \mathbf{L}_{\mathrm{p}}\,\mathbf{F}_{\mathrm{p}}$$

$$\dot{\mathbf{F}}_{\mathrm{d}} = \mathbf{L}_{\mathrm{d}}\,\mathbf{F}_{\mathrm{d}}$$

$$\mathbf{F}_{\mathrm{p}} = \left(\mathbf{I} - \Delta t\mathbf{L}_{\mathrm{p}}\left(\mathbf{M}_{\mathrm{p}}\right)\right)^{-1}\mathbf{F}_{\mathrm{p0}}$$

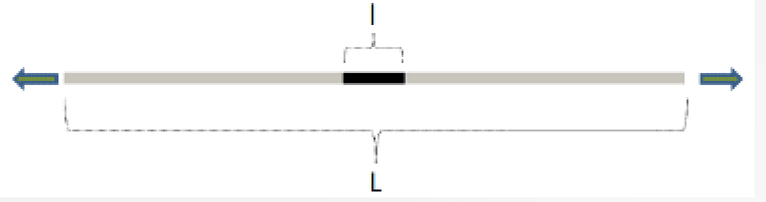
$$\mathbf{F}_{\mathrm{d}} = \left(\mathbf{I} - \Delta t\mathbf{L}_{\mathrm{d}}\left(\mathbf{M}_{\mathrm{d}}\right)\right)^{-1}\mathbf{F}_{\mathrm{d0}}$$

$$\mathbf{R}_{p} = \widetilde{\mathbf{L}_{\mathrm{p}}} - \mathbf{L}_{\mathrm{p}}\left(\mathbf{M}_{\mathrm{p}}\left(\widetilde{\mathbf{L}_{\mathrm{p}}}, \widetilde{\mathbf{L}_{\mathrm{d}}}\right)\right)$$

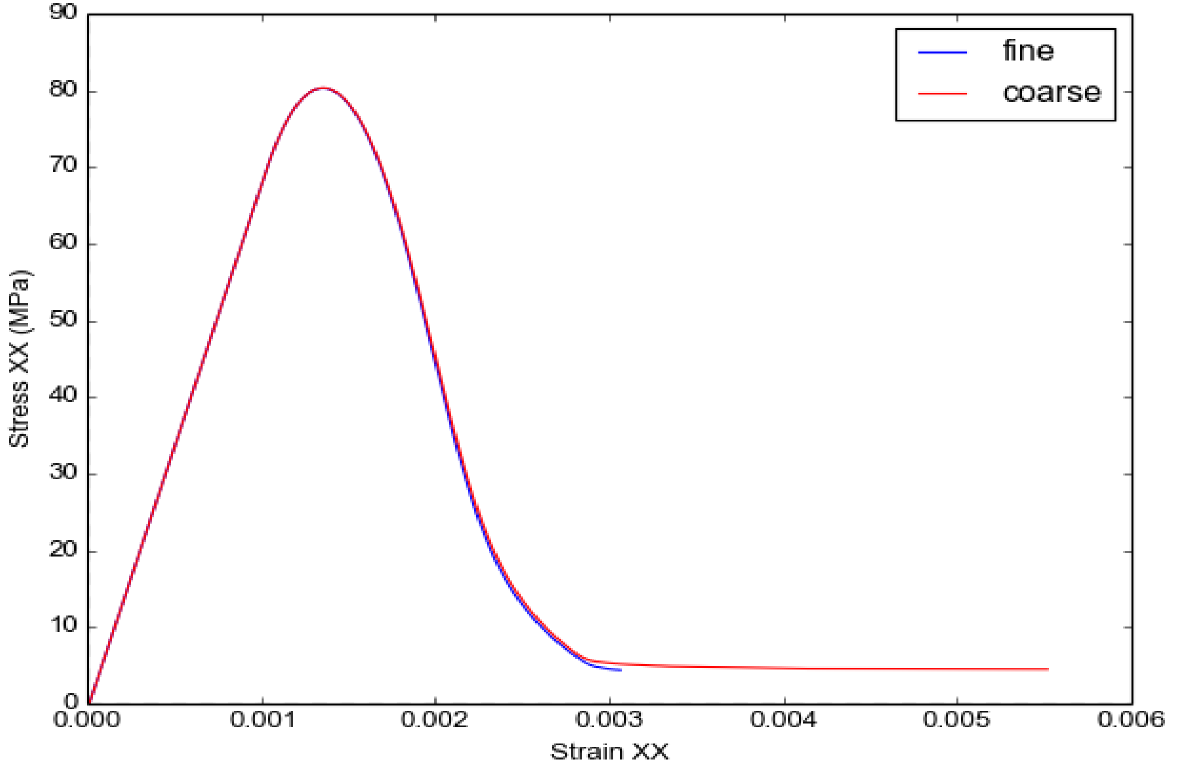
$$\mathbf{R}_{d} = \widetilde{\mathbf{L}_{\mathrm{d}}} - \mathbf{L}_{\mathrm{d}}\left(\mathbf{M}_{\mathrm{d}}\left(\widetilde{\mathbf{L}_{\mathrm{p}}}, \widetilde{\mathbf{L}_{\mathrm{d}}}\right)\right)$$

$$\boldsymbol{\xi}\left(t_{n}\right) = \boldsymbol{\xi}\left(t_{n-1}\right) + \Delta t\,\dot{\boldsymbol{\xi}}\left(\mathbf{M}_{\mathrm{p}}, \mathbf{M}_{\mathrm{d}}, \mathbf{F}_{\mathrm{p}}, \mathbf{F}_{\mathrm{d}}, \mathbf{L}_{\mathrm{p}}, \mathbf{L}_{\mathrm{d}}\right)$$

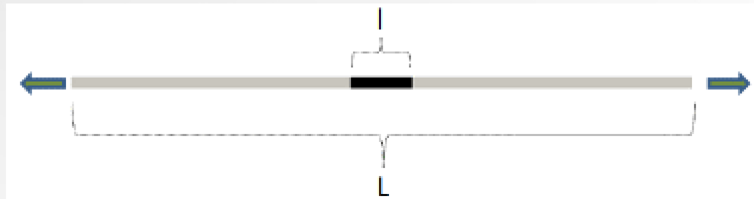
Mesh Objectivity

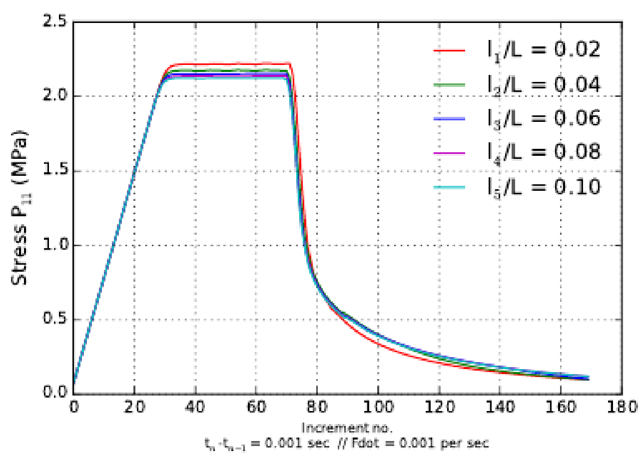


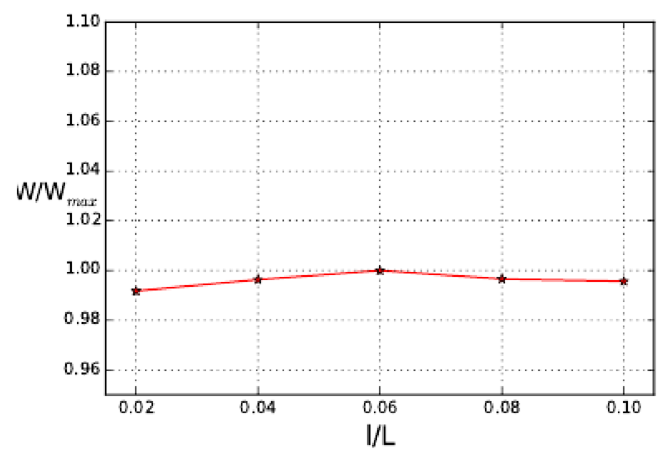
- Coarse mesh (10 fourier points in the band)
- Fine = 2x coarse



Work of separation with band thickness



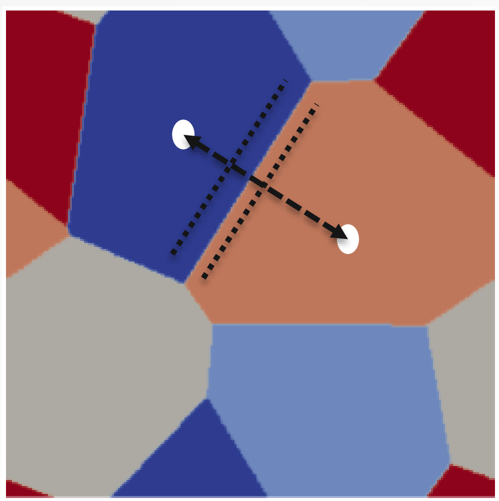




- recovery of work of separation for different width of interface band.
- scale the damage parameters (critical opening strain) with the width of interface band.

Voxelized field of the normals

- Generator points of standard voronoi tesselation.



- First order cartesian moments.
  [*Libermann et al., 2015*]

2	3	3	3
2	2	3	3
2	2	4	4
2	2	4	4

1	0	0	0
1	1	0	0
1	1	0	0
1	1	0	0

0	0	0	0
0	0	0	0
0	0	1	1
0	0	1	1