Imperfections – deformation and microstructures in polycrystals

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6- Modeling

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a- Boundary conditions

Sachs vs. Taylor

Sachs model

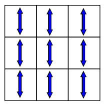
- All grains see the same stress
- Equilibrium conditions across grain boundaries
- Compatibility conditions between the grains violated, thus, finite strains will lead to gaps and overlaps between grains
- Each grain is treated as a single-crystal (Schmid factors, etc) without accounting for changes of stress within the polycrystal

Taylor model

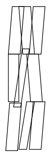
- All grains under the same state of deformation
- Compatibility conditions between the grains satisfied
- Equilibrium conditions across grain boundaries: stress can be different between both sides of the interface
- Each grain deforms to accommodate strain, and may build stress independently from each other

Sachs vs. Taylor (2)

Sachs
Homogeneous stress



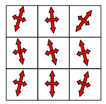
Same stress state in all grains



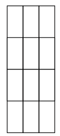
Each grain deform using a limited number of slip systems: those with the maximum Schmid factor.

Taylor
Homogeneous strain

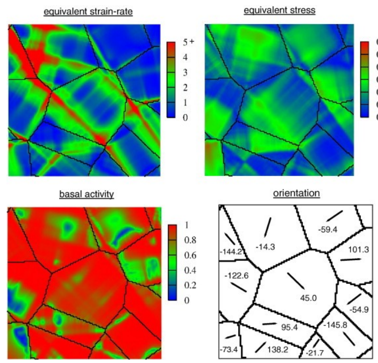
Stress is different from grain to grain



Many deformation mechanisms (5 or more) to ensure compatibility conditions between all grains.



True polycrystal



Model for ice polycrystal undergoing plastic deformation:

- Strain rate,
- Stress,
- Slip system activity,
- Orientation.

Intermediate state between Sachs and Taylor.

Heterogeneities inside each grain.

Lebensohn et al, *Acta Materiala*, 2009

Effect of strain rate

In a true polycrystal, deformation is accommodated by a large number of defects, dislocations, etc.

The transition between elastic and plastic behavior is not sharp, as in the Schmid model.

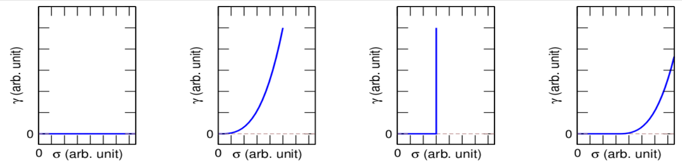
The behavior is well described with power-laws.

Each slip system then follows a law such as

$$\gamma = \gamma_0 \left(\frac{\sigma}{\tau}\right)^n$$

With
- γ : resolved shear strain rate on the slip system
- σ : resolved shear stress
- n : stress exponent
- τ : CRSS of the slip system
- γ_0 : normalization factor.

Constitutive models



Elastic	Visco-plastic	Elasto-plastic	Elasto-visco-plastic:
• No permanent deformation • No strain rate	• No elasticity • Power-law for strain rates	• Elasticity • True threshold at the CRSS • Strain rate is unconstrained	• Elasticity • Threshold for plastic flow at the CRSS • Power-law for strain rates
$\sigma = C\epsilon$	$\dot\epsilon = A\sigma^n$	$\sigma = C\epsilon$ $\begin{cases} \sigma < \sigma_c \Rightarrow \dot\epsilon = 0 \\ \sigma > \sigma_c \Rightarrow \dot\epsilon = \infty \end{cases}$	$\begin{cases} \dot\sigma = f(\dot\epsilon) \\ \dot\epsilon = g(\sigma) \end{cases}$

6- Modeling
b- Eshelby's inclusion problem

Eshelby's inclusion problem

Classical problems in continuum mechanisms
- Ellipsoidal elastic inclusions
- Inside infinite elastic body

The inclusion changes shape or orientation.

The surrounding material reacts to maintain equilibrium stress state.

Eshelby, in the 1950's found analytical solutions to many of these problems.

Works if the include is and remains ellipsoidal.

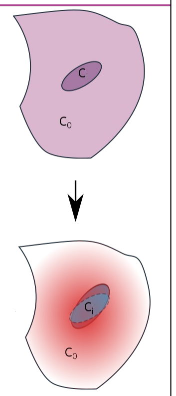
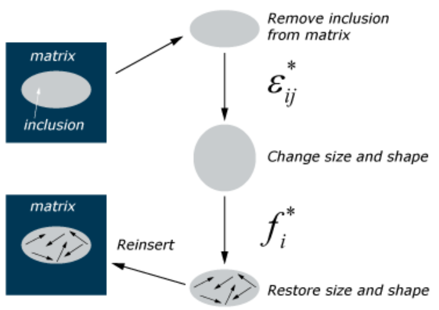


Illustration adapted from Wikipedia

Eshelby's problem: main idea



Example

For an isotropic and spherical inclusion

$$\mathcal{S}_{ijkl} = \frac{5\nu - 1}{15(1-\nu)}\delta_{ij}\delta_{kl} + \frac{4-5\nu}{15(1-\nu)}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

Pour an ellipsoidal inclusion with some symmetries (*a* = *b*)

$$\begin{aligned}
\mathcal{S}_{1111} &= \mathcal{S}_{2222} = \frac{\pi(13-8\nu)}{32(1-\nu)}\frac{c}{a} \\
\mathcal{S}_{3333} &= 1 - \frac{\pi(1-2\nu)}{4(1-\nu)}\frac{c}{a} \\
\mathcal{S}_{1122} &= \mathcal{S}_{2211} = \frac{\pi(8\nu-1)}{32(1-\nu)}\frac{c}{a} \\
\mathcal{S}_{1133} &= \mathcal{S}_{2233} = \frac{\pi(2\nu-1)}{8(1-\nu)}\frac{c}{a} \\
\mathcal{S}_{3311} &= \mathcal{S}_{3322} = \frac{v}{1-v}\left(1 - \frac{\pi(4\nu+1)}{8\nu}\frac{c}{a}\right) \\
\mathcal{S}_{1212} &= \frac{\pi(7-8\nu)}{32(1-\nu)}\frac{c}{a} \\
\mathcal{S}_{3131} &= \mathcal{S}_{2323} = \frac{1}{2}\left(1 + \frac{\pi(\nu-2)}{4(1-\nu)}\frac{c}{a}\right)
\end{aligned}$$

And so on. Can be used to evaluate the strain state in the inclusion.

Formulas from a class of Weinberger & Cai
Elasticity of Microscopic Structures
University of Stanford

6- Modeling
c- Self-consistent approaches

Principles

Issues with polycrystal plasticity modeling

- Heterogeneous state: a true polycrystal does not follow neither the Sachs nor the Taylor bound.
- Anisotropic behavior: each grain is anisotropic, with its own elasticity, deformation mechanisms, etc.
- Effect of microstructure: how to account for grain shapes, sizes, etc?

Simplified solution:

- Self-consistent model.
- Each grain = ellipsoidal inclusion inside homogeneous matrix.
- Eshelby-type solution.
- In each grain: elastic, elasto-plastic, visco-plastic, elasto-visco-plastic.
- Matrix: polycristal, average of all grain properties.

One implementation

Los Alamos Visco-Plastic Self Consistent code (VPSC) :

- Developed by Ricardo Lebensohn and Carlos Tomé since the mid 90's.
- Free, fairly easy to use, with manuals.
- Works for all crystal systems.
- Other codes are available (Metz, Ensam Paris...).

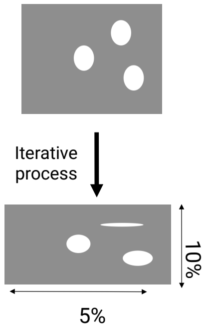
Underlying theory:

- Visco-plastic model: no elasticity, power-law relationship between stress and strain rate.
- Infinite choice of deformation mechanisms.
- Infinite choice of deformation geometry.

Extensions:

- EPSC: elasto-plastic
- EVPSC : elasto-visco-plastic
- ....

Algorithm



Parameters

- Structure, lattice systems, elasticity
- Plasticity mechanisms: geometry, CRSS, etc
- Starting texture (ex. 1000 random grains)
- Deformation path

Plasticity model

- Visco-plastic, elasto-plastic, elasto-visco-plastic.

Computation time ~ minutes

At each deformation step

- In each grain:
  - Solve the Eshelby inclusion problem
  - Activate plasticity mechanisms, as needed
  - Rotate the grain, balance stresses, change shape
- In the polycrystal
  - Compute the average stress
  - Compute texture

Qualities and limitations

Ignored parameters:

- Microstructural details: grain sizes, shapes, arrangement.
- Heterogeneities inside a grain
- Grain boundary behavior

Qualities

- Does not require unknown information (details on microstructure)
- Fast calculations
- Good results for texture
- Very useful for
  - the interpretation of experimental data
  - integration in large scale calculations

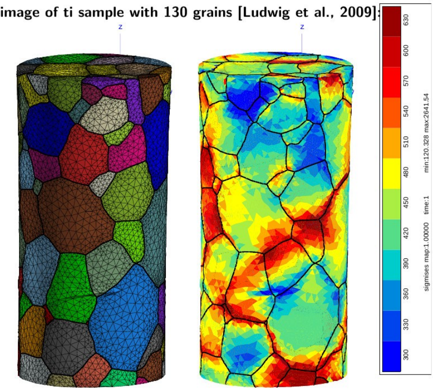
6- Modeling
c- Full field calculations

FEM : illustration (1)

Computation under tension

Proudhon, Cailletaud, Forest
Mines Paris-Tech
TD Elts Finis

mesh from DCT image of ti sample with 130 grains [Ludwig et al., 2009]:



FEM : illustration (2)

Numerical Diffraction Model

Proudhon, Cailletaud, Forest
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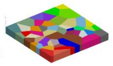
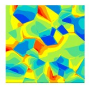
A 3 steps model (more in [Vaxelaire et al., 2010])

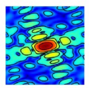
1. Generate 3D polycrystalline model
   - 2D Voronoi cell generation in (x, y) plane
   - extrusion along z to simulate columnar grains
   - $\langle 111 \rangle$ texture with random in plane orientation



2. Compute displacement field $\mathbf{u}(x, y, z)$
   - Z-SeT/ZéBuLoN software suite
   - Cubic Elasticity
   - Parallel computation for large meshes



3. Carry out Fourier Transform of $\exp(\imath \mathbf{G}.\mathbf{u}(\mathbf{r}))$
   - transfer $\mathbf{u}$ field on a regular grid
   - complex FFT using fftw library [Frigo and Johnson, 2005]
   - now available as a `post_processing` routine within Z-SeT



FEM : illustration (3)

Model parameters

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physical parameters

- 50 grains
- film dimensions: $500 \times 500 \times 50\ \mu m^3$
- cubic elasticity with $C_{11} = 192\,340$ MPa, $C_{12} = 163\,140$ MPa and $C_{44} = 41\,950$ MPa
- gold crystal atomic spacing $a = 0.408$ nm

mesh parameters

	m_5	m_3	m_2	m_1	m_0
number of elements	1172	5940	27430	224410	1820200
elements in grain 06	32	93	460	3860	31290
elements in grain 39	12	45	160	1340	10880
parallel computation	no	no	no	yes	yes

FEM : illustration (4)

Shape of the illuminated grain

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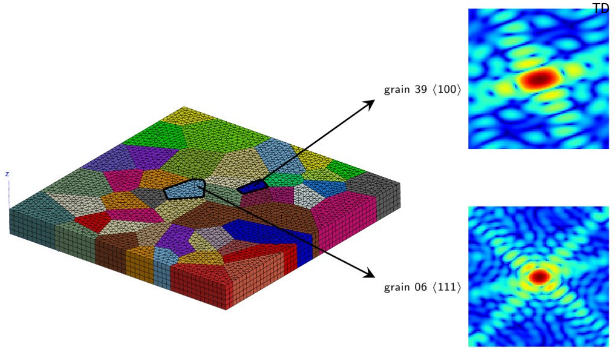


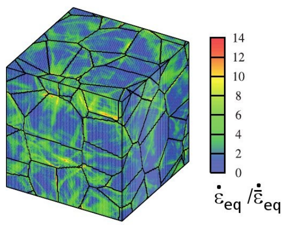
FEM + Plasticity

Full field methods

- Finite elements
- Elasticity
- Plasticity mechanisms (slip systems, twins, etc)

Applications

- Comparison to high resolution experimental data
- Understand mechanisms at the intra-granular scale (stress and stress heterogeneities)
- Validation and calibration of mean field models



Example: strain rates distributions in olivine polycrystals

Castelnau et al, 2009