Fast Analytical Models for Texture Evolution in Anisotropic Polycrystals

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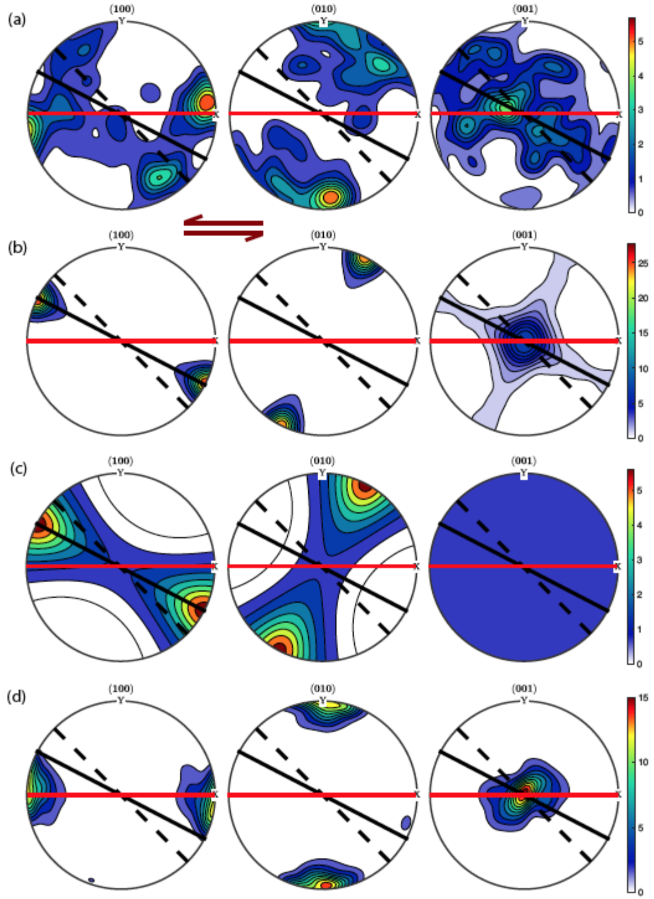


Aim

Context: To predict seismic anisotropy from geodynamical models, we need to be able to calculate how crystal preferred orientation (CPO) evolves during progressive deformation

Photo: Tim Walker

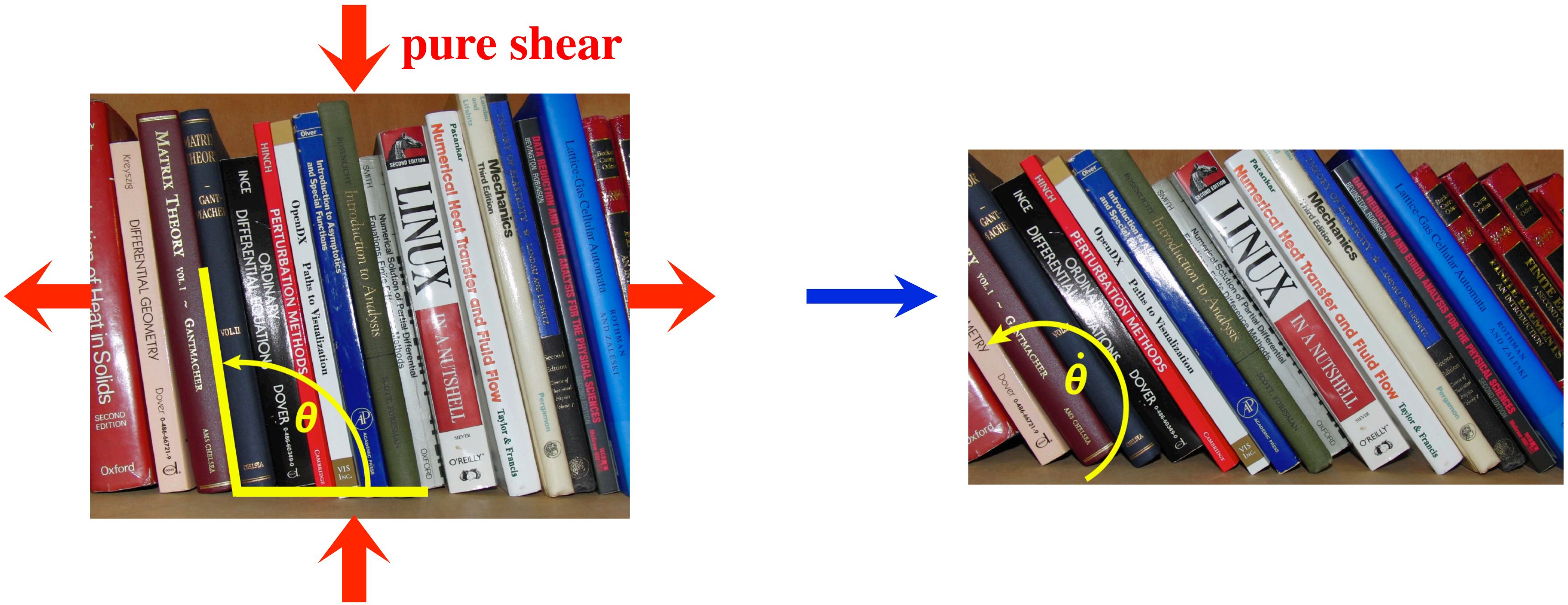
Difficulty: Self-consistent models (VPSC, SOSC) are too computationally expensive to include in 3-D convection codes

This work:

Design faster algorithms based on:

- an analytical expression for crystallographic spin ☛ model ANPAR
- an economical analytical representation of CPO in terms of « structured basis functions » ☛ model SBFTEX

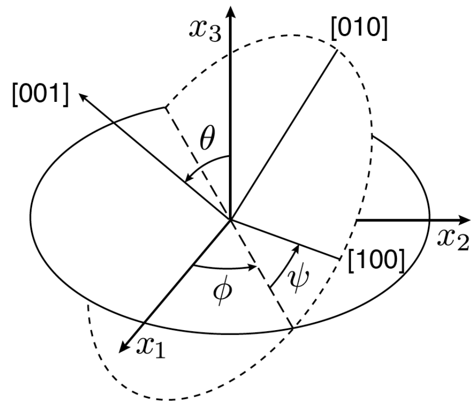
Mechanism of crystallographic rotation



Generalization to 3-D:

Orientation : three Eulerian angles $(\phi, \theta, \psi) \equiv \boldsymbol{g}$

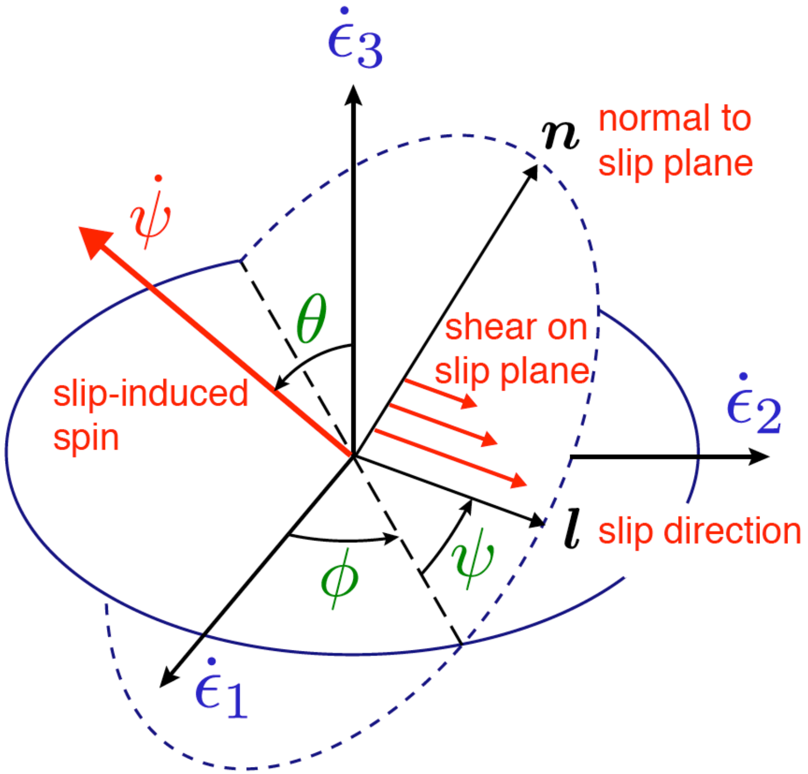
Spin : $(\dot{\phi}, \dot{\theta}, \dot{\psi}) \equiv \dot{\boldsymbol{g}}$



Analytical expression for crystallographic spin

Model: aggregate of crystals with one active slip system, deformed by triaxial straining

(principal strain rates $\dot{\epsilon}_1, \dot{\epsilon}_2, \dot{\epsilon}_3$)



Minimize difference of crystal and aggregate deformation rates

$$\boxed{\begin{aligned}\dot{\psi} = A \Big\{ &\frac{3}{4}\dot{\epsilon}_3 \sin 2\psi \sin^2\theta \\ &+ \frac{1}{8}(\dot{\epsilon}_2 - \dot{\epsilon}_1)[4 \sin 2\phi \cos\theta \cos 2\psi \\ &+ \cos 2\phi (\cos 2\theta + 3) \sin 2\psi] \Big\}\end{aligned}}$$

Amplitude A:

= 5 if global strain rate compatibility is enforced

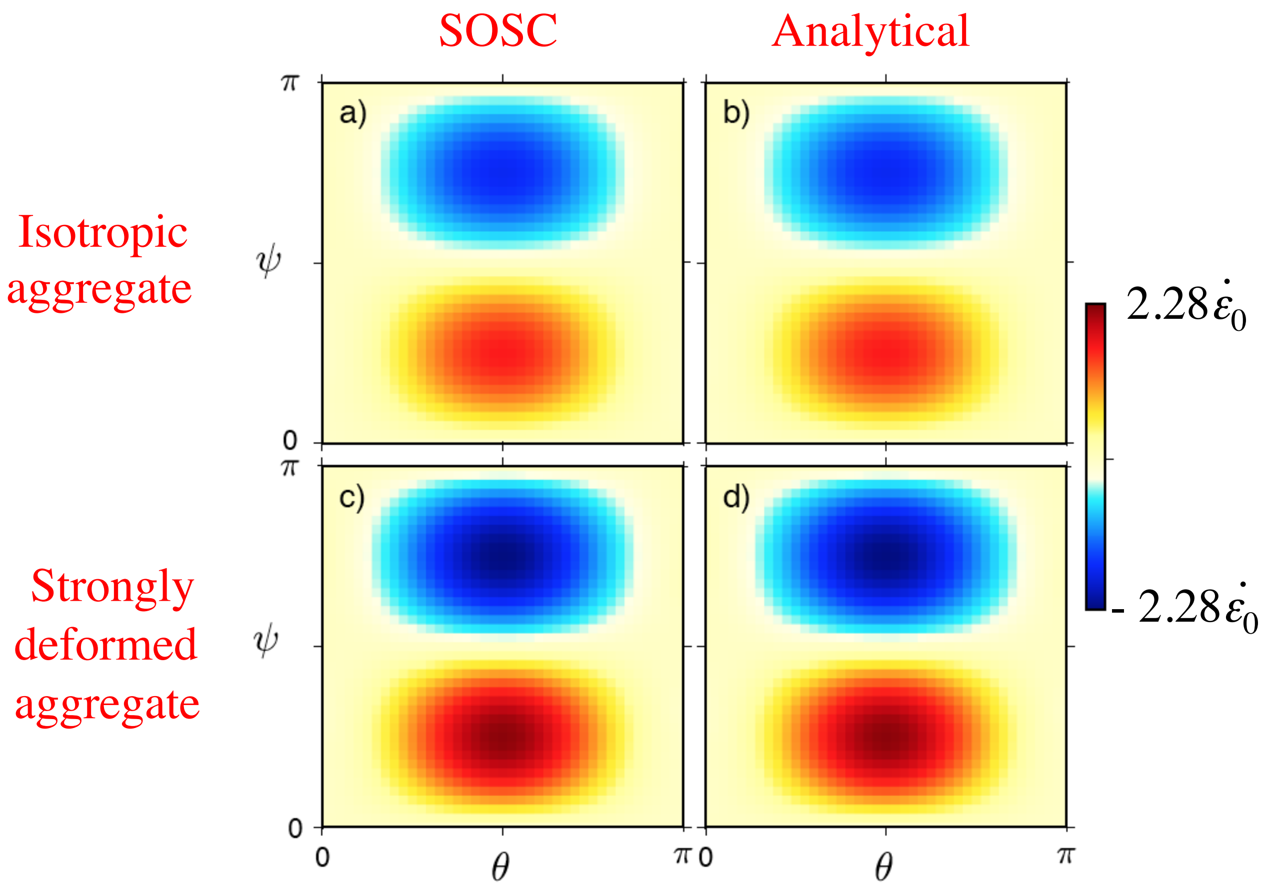
= 1 if not enforced

= intermediate if several slip systems are active

Analytical expression for the spin: Validation against SOSC

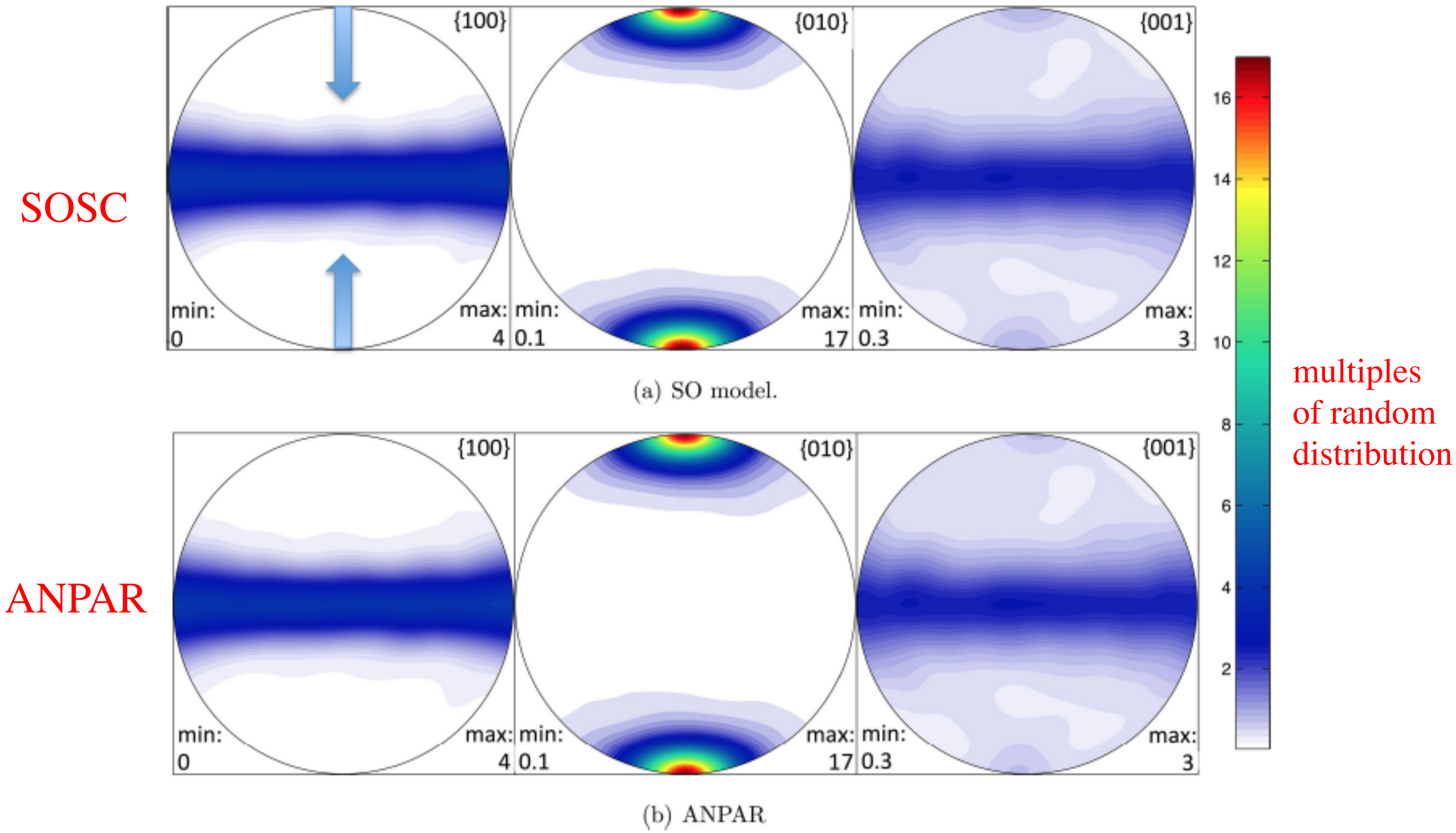
Test case: uniaxial compression (shortening rate $\dot{\varepsilon}_0$)

Quantity shown: spin $\dot{\psi}$ for slip system (010)[100] of olivine

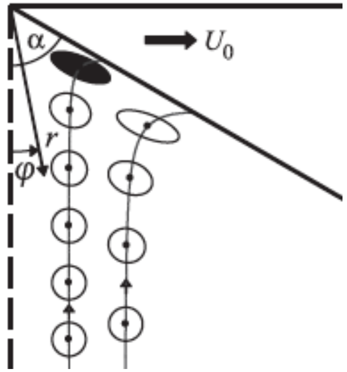


The analytical model reproduces *exactly* the orientation-dependence of crystal spin predicted by the SOSC model

ANPAR vs. SOSC: Uniaxial compression (45% shortening) of an olivine polycrystal



ANPAR vs. SOSC: Corner Flow Model

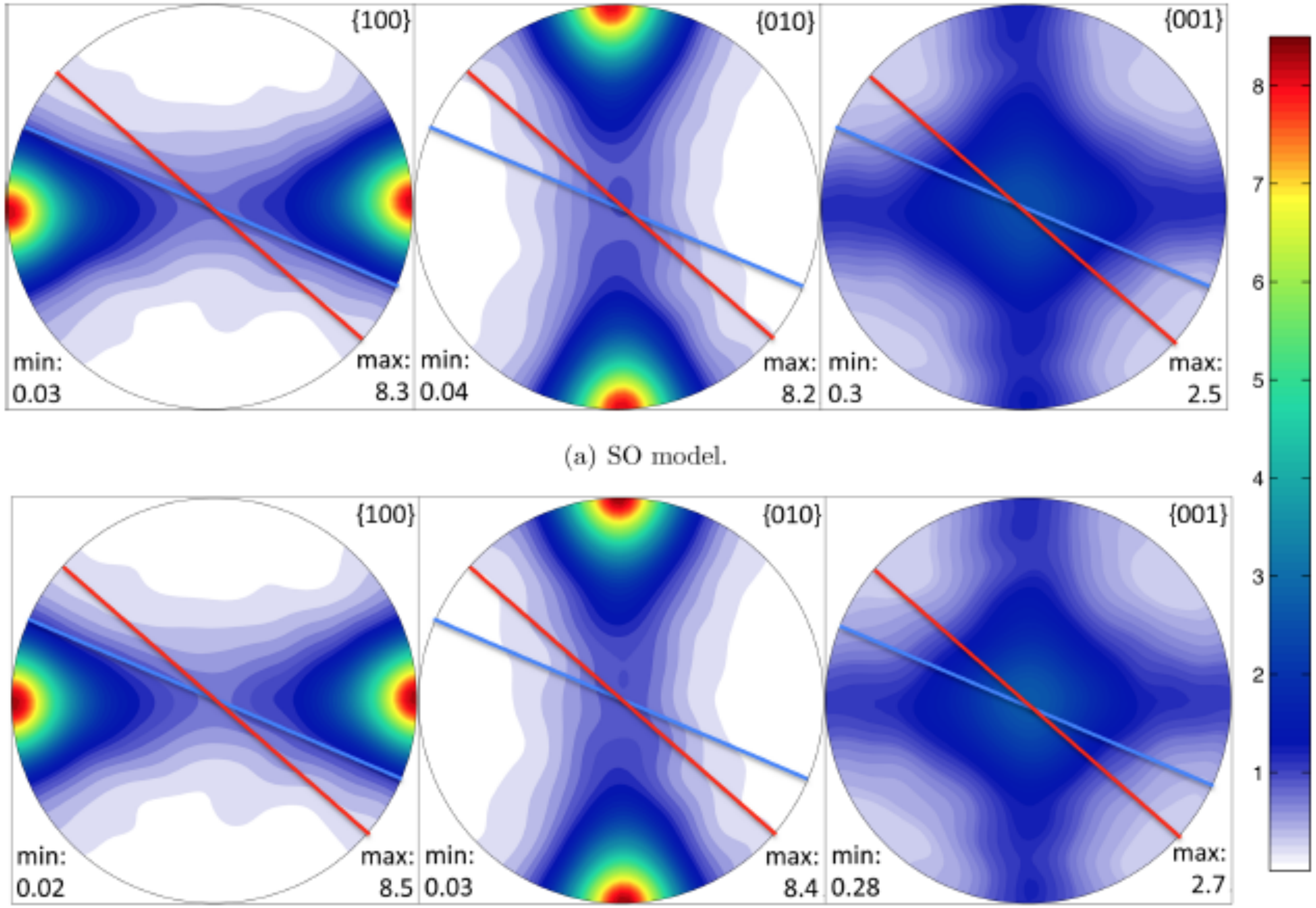


long finite strain axis

shear plane

SOSC

ANPAR



multiples of random distribution

Analytical description of CPO

Idea : represent CPO using « structured basis functions » that:

- satisfy automatically the symmetry of the imposed deformation
- can represent arbitrarily sharp textures
- are analytical solutions of the evolution equation for the ODF:

$$\frac{\partial f}{\partial t} + \nabla \cdot (\dot{\boldsymbol{g}} f) = 0$$

☛ Number of SBFs required

= Number of active slip systems

Structured basis functions

General form (for time-independent spin amplitude *A*)**:**

$$f = f(\phi, \theta, \psi, \quad A, \quad c_1/c_2, c_2/c_3)$$

Eulerian angles **spin amplitude** **finite strains**

Exact expression:

$$f = f_0[\cosh A\Gamma - \sin 2(\psi - \chi)\sinh A\Gamma]^{-1}$$

$$\Gamma = \left[r_{12}^2 F^2 + (r_{12}G + r_{23}H)^2\right]^{1/2}$$

$$\{\cos 2\chi, \sin 2\chi\} = \Gamma^{-1}\{r_{12}F, r_{12}G + r_{23}H\} \qquad r_{ij} = \ln(c_i/c_j)$$

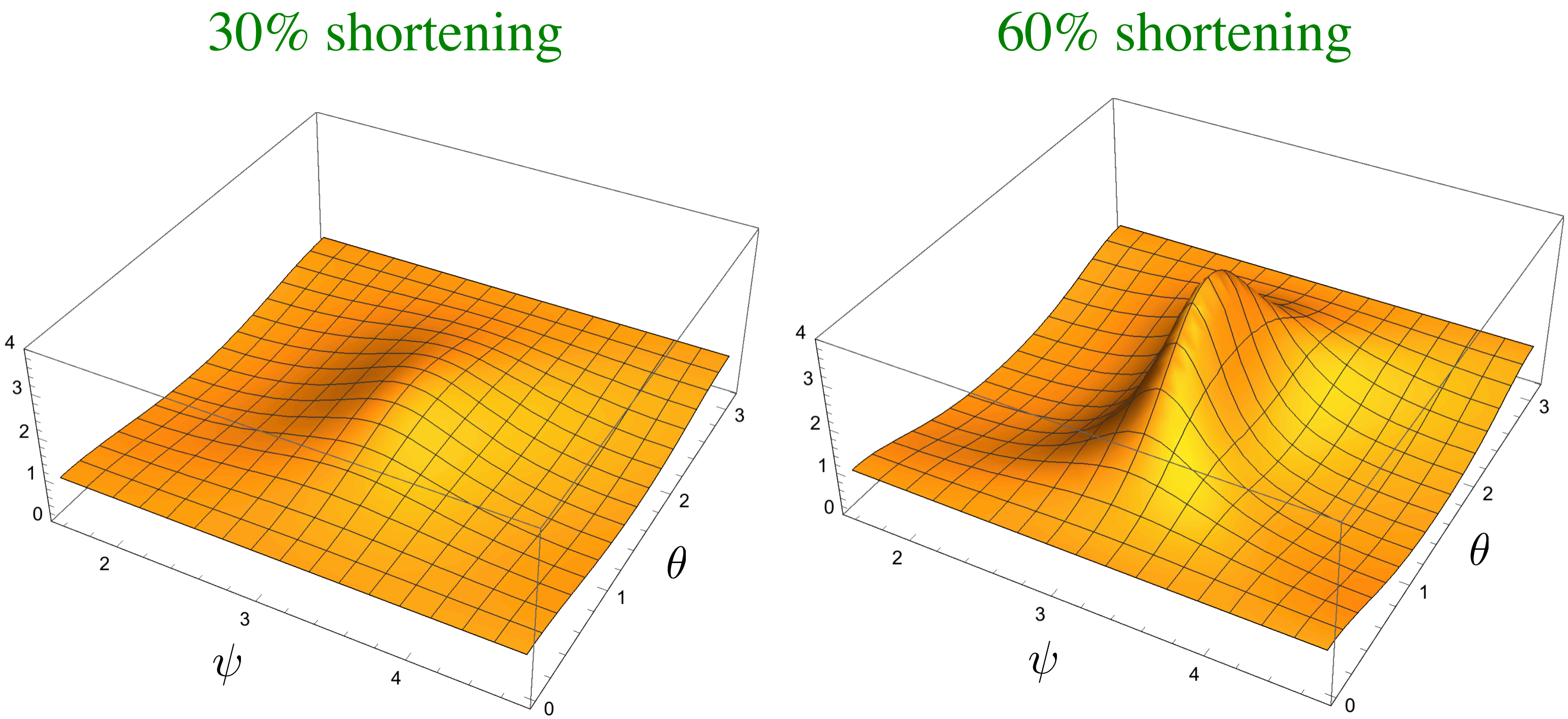
$$F = -\sin 2\phi\cos\theta \qquad H = -\sin^2\theta$$

$$G = \sin^2\phi\cos^2\theta - \cos^2\phi$$

Interpretation:

SBF = virtual CPO produced by the action of a single slip system

Structured basis function vs. strain (uniaxial compression)



☛ SBF automatically gets sharper as strain increases

SBF expansion of the orientation distribution function

$$\mathcal{F}(\mathbf{g}) = 1 + \sum_{s=1}^{3} C_s(p_{12}, p_{23}, r_{12}, r_{23}) \left[f(\mathbf{M}_s \mathbf{g}, r_{12}, r_{23}) - 1 \right]$$

ODF

isotropic part

precalculated expansion coefficients

anisotropic part of SBF for slip system *s*

$$p_{ij} = \ln \frac{\tau_i}{\tau_j}$$ (relative strengths of slip systems)

$$r_{ij} = \ln \frac{c_i}{c_j}$$ (axial ratios of finite strain ellipsoid)

$$\mathbf{M}_s =$$ rotation matrix for slip system *s*

☛ Given the finite strain and the slip system strengths, the full ODF can be calculated

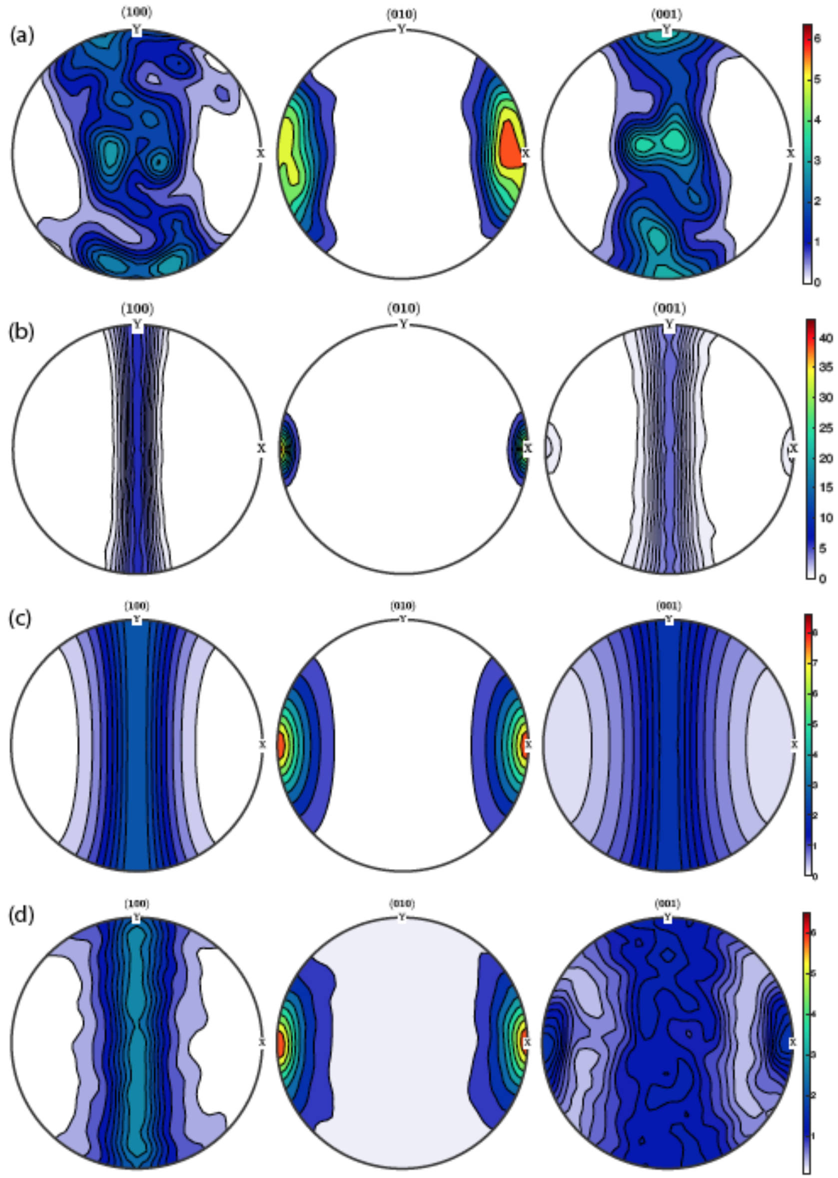
SBFTEX prediction: Uniaxial compression (58% shortening)

Laboratory experiment
(Nicolas et al. 1973)

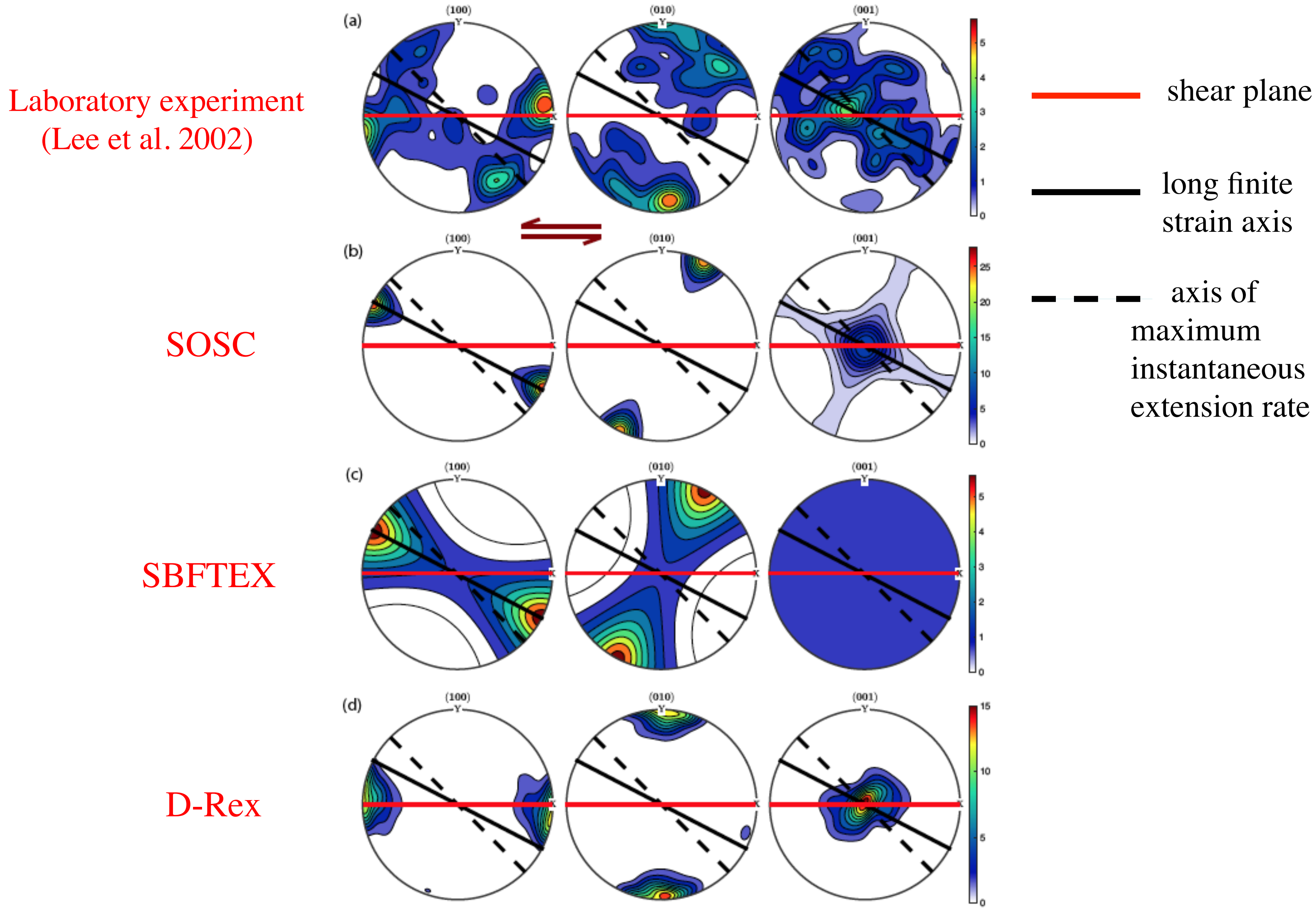
SOSC

SBFTEX

D-Rex



SBFTEX prediction: Simple shear ($\gamma = 140\%$)



Summary and Perspectives

Advantages of the structured basis function approach:

- ☛ Representation of CPO is
  - ◆ smooth (uses continuous functions)
  - ◆ economical (typically 3 coefficients)
- ☛ Expression for crystallographic spin agrees exactly with the SOSC model
- ☛ Calculations are ~ 10^7 times faster than SOSC
- ☛ Can be applied to both upper- and lower-mantle phases

Future work:

- ☛ extension to two-phase aggregates
- ☛ parameterization of recrystallization
- ☛ user-friendly open-source implementation