### The Impact of the Deformation History on the Microstructural Evolution of Polycrystalline Olivine and How It Affects the Interpretation of Mantle Seismic Anisotropy

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### Abstract

Relating seismic anisotropy with mantle flow requires a good understanding of the rock's microstructural evolution and the development of crystal preferred orientations (CPO), because plastic deformation of olivine is interpreted as the main cause for mantle seismic anisotropy. In this contribution, the influence of deformation history in the microstructure evolution and resulting seismic anisotropy is investigated by means of full-field numerical simulations at the microscale. We explicitly simulate the microstructural evolution of olivine polycrystalline aggregates during dynamic recrystallization up to high strain using the code VPFFT/ELLE (e.g. Griera et al., 2011; 2013; Llorens et al., 2016). Modeling results indicate that the evolution of a CPO is highly sensitive to the initial olivine fabric. When the initial fabric is formed by a random distribution of crystallographic orientations, there is a rapid alignment of the a-axes (or [100]) with the stretching direction of flow. However, when there is an initial CPO inherited from previous deformation, larger strains are required for the a-axes to become re-aligned with the stretching direction. Our numerical results agree with field and experimental observations (e.g. Boneh and Skemer, 2014; Skemer et al., 2012). The analysis of the seismic properties reveals that an increase of the strength of the initial inherited CPO produces a reduction of the azimuthal seismic anisotropy, compared to the case with an initial random fabric. It is concluded that the deformation history significantly influences the development of fabrics. Accordingly, seismic anisotropy interpretations must be carried out with caution in regions with complex deformation histories. References Boneh Y., Skemer P. 2014. EPSL, 406. Griera A, et al. 2011. Geology 39, 275-278. Griera A, et al. 2013. Tectonophysics 587, 4-29. Llorens, M.-G. et al. 2016 EPSL, 450, 233-242. Skemer P. et al. 2012. Geochemistry Geophysics Geosystems, 13:3.



## 1. Abstract

Relating seismic anisotropy with mantle flow requires a good understanding of the rock's microstructural evolution and the development of crystal preferred orientations (CPO), because plastic deformation of olivine is interpreted as the main cause for mantle seismic anisotropy. In this contribution, the influence of deformation history in the microstructure evolution and resulting seismic anisotropy is investigated by means of full-field numerical simulations at the microscale. We explicitly simulate the microstructural evolution of olivine polycrystalline aggregates during dynamic recrystallization up to high strain using the code VPFFT/ELLE (e.g. Griera et al., 2011; 2013; Llorens et al., 2016). Modeling results indicate that the evolution of a CPO is highly sensitive to the initial olivine fabric. When the initial fabric is formed by a random distribution of crystallographic orientations, there is a rapid alignment of the a-axes (or [100]) with the stretching direction of flow. However, when there is an initial CPO inherited from previous deformation, larger strains are required in order for the a-axes to become re-aligned with the stretching direction. Our numerical results are in agreement with field and experimental observations (e.g. Boneh and Skemer, 2014; Boneh et al., 2015; Skemer et al., 2012). The analysis of the seismic properties reveals that an increase of the strength of the initial inherited CPO produces a reduction of the azimuthal seismic anisotropy, compared to the case with an initial random fabric. It is concluded that the deformation history significantly influences the development of fabrics. Accordingly, seismic anisotropy interpretations must be carried out with caution in regions with complex deformation histories.

# 2. Numerical scheme: VPFFT/ELLE approach



The VPFFT/ELLE is a 2D code developed to simulate the microstructure evolution of rocks during plastic deformation and recrystallization. The code is integrated as an utility included in the numerical platform ELLE (see www.elle.ws), an open-source multi-purpose and multi-scale software for the simulation of the evolution of microstructures during deformation and metamorphism. The numerical approach is based on the coupling of a full-field viscoplastic formulation based on the Fast Fourier Transform and a front-tracking approach

Briefly, the VPFFT-formulation provides an exact solution of the micromechanical problem by finding a strain-rate and stress field associated with a kinematically admissible velocity field, which minimizes the average local work-rate under the compatibility and equilibrium constraints. Based on the evolution of the local misorientation and strain-rate gradient fields, the geometrically necessary dislocation densities are calculated, which in turn are used to predict the driven energy of the recrystallisation processes. Current version of the VPFFT/ELLE can simulate the visco-plastic deformation and recrystallisation of an aggregate defined by multiple crystalline phases and materials (e.g. melt, air). Recrystallisation processes included are grain boundary migration (driven by surface, strain stored or mass defect/excess), intracrystalline recovery and nucleation of new grains. The code has been extensively used to simulate the microstructure evolution of polycrystalline ice during deformation and recrystallisation (Llorens et al., 2016, 2017), partial-melt aggregates (Llorens, et al., 2018), deformation and recrystallisation in two-phase aggregates (Steinbach, et., 2016), grain dissection during abnormal grain growth (Steinbach, et., 2017), porphyroclast/-blast rotation in anisotropic materials (Griera et al., 2011; Griera et al., 2013), or as strain gauge indicator in deformed halite aggregates (Gomez-Rivas et al., 2017), among others. The code is freely distributed within the Elle package, although if you want to use please contact us (info@elle.ws).

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### 3. Model Setup

The influence of an inherited microstructure was investigated using a superposition of two (a) stages of dextral simple shear deformation. During the first stage ( $\gamma$ 1), shear direction was applied parallel to the sample  $x_1$  direction. Afterwards, during the second stage ( $\gamma$ 2), simple shear direction was applied to the  $x_2$  direction (i.e parallel to the Y direction ). A reference model, defined by random initial orientation of grains, was deformed under constant simple shear conditions. Initial models with inherited microstructures were defined using intermediate stages of the reference model ( $\gamma$ 1=1,2,4,6 and 8). As models are 2D, the initial CPOs were defined doing a 90° rotation around the Z axis. Microstructure, CPO and seismic analysis were performed using the MTEX code. Seismic properties were estimated using the Voigt-**Reuss-Hill approach** 

# 4. Results: a) Microstructure and CPO evolution

γ<sub>1</sub>=0, γ<sub>2</sub>=0

γ<sub>1</sub>=8, γ<sub>2</sub>=0.04



scan for simulation movies

### First Stage Deformation ( $\gamma$ 1)



### (.Y.Z deformation axis



 $\gamma_1$ =8  $\gamma_2$ =1







a) Evolution of the angle *a* between fast propagation direction and the shear direction (X). FSE indicates the evolution predicted by the Finite Strain Axis. Grey area indicates the average dispersion observed from real azimuthal measurements. b) Evolution of the azimuthal Swave anisotropy (AVs %). AVs is reduced between 40% to 60% of the expected values.



Polycrystalline aggregate was defined assuming olivine mineralogy. Sample length was L=10<sup>-2</sup> m. A non-linear viscoplastic rheology (n = 3) was used. Deformation was assumed to be accommodated by glide along four main slip systems: (010)[100], (001)[100], (010)[001] and (100)[001]. Critical resolved shear stress (CRSS) was defined  $\tau_{CRSS}$ =1 for slip-systems with Burger's [100]-axis, while, while  $\tau_{CRSS}$ =2 and  $\tau_{CRSS}$ =3 for (010)[001] and (100)[001], respectively. A dummy slip-system defined by <111>{1-10} with  $\tau_{CRSS}$ =50 was used to preserve strain-compatibility. For DRX module, grain boundary mobility was M $\gamma$ =4·10<sup>-20</sup> m·s, with surface energy  $\gamma$ =1 J/m<sup>2</sup> (from Karato, 2008). Threshold for high angle boundaries to nucleate was defined to 7.5<sup>o</sup>.



### 5. Conclusions

In this study, full field micro-dynamic models were used to investigate the influence of an inherited fabric on the microstructure evolution and seismic properties during superposition of simple shear deformation. The results show that large strains are required previously to realign the fast direction axis (or [100]-axis) with the current flow direction (X). At level of azimuthal anisotropy (AVs%), the anomalies are permanent and there is not recovery of the values observed for constant kinematic deformations

# 6. References

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