FFT simulation of dynamic recrystallization in polar ice

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Abstract

Research on ice flow is a key to understand how climate changes affect polar ice. Numerical modelling provides a better insight into the mechanics of ice from the microstructure to the ice sheet scale. The mechanics of polar ice are very sensitive to temperature changes mainly due to active recrystallization processes, as the material is very close to its melting point. We present numerical simulations that predict the microstructural evolution of ice polycrystals during deformation and dynamic recrystallization at large strain, using a full-field approach.

A crystal plasticity code (Lebensohn, 2001) is used to calculate the response of a polycrystalline aggregate that deforms by dislocation glide, applying a Fast Fourier Transform (FFT). The coupling between FFT and the ELLE microstructural evolution platform allows us to include recrystallization in the aggregate, which is simulated by means of two main processes: (1) recovery and subgrain rotation, which locally reduces the crystal misorientation, and (2) grain boundary migration, which is driven by grain boundary curvature and intra-grain strain energies.

This contribution presents a comparison of numerical simulations under pure and simple shear conditions up to high strain at different strain rates. The results show a strong effect of recrystallization on the final microstructure, producing larger and more equidimensional grains, with smooth boundaries. Recrystallization masks the strain rate and finite strain heterogeneity resulting from the strong slip anisotropy of ice. However, this effect does not modify the single-maximum pattern of c-axes that are distributed at a low angle to the shortening direction in both pure and simple shear cases.
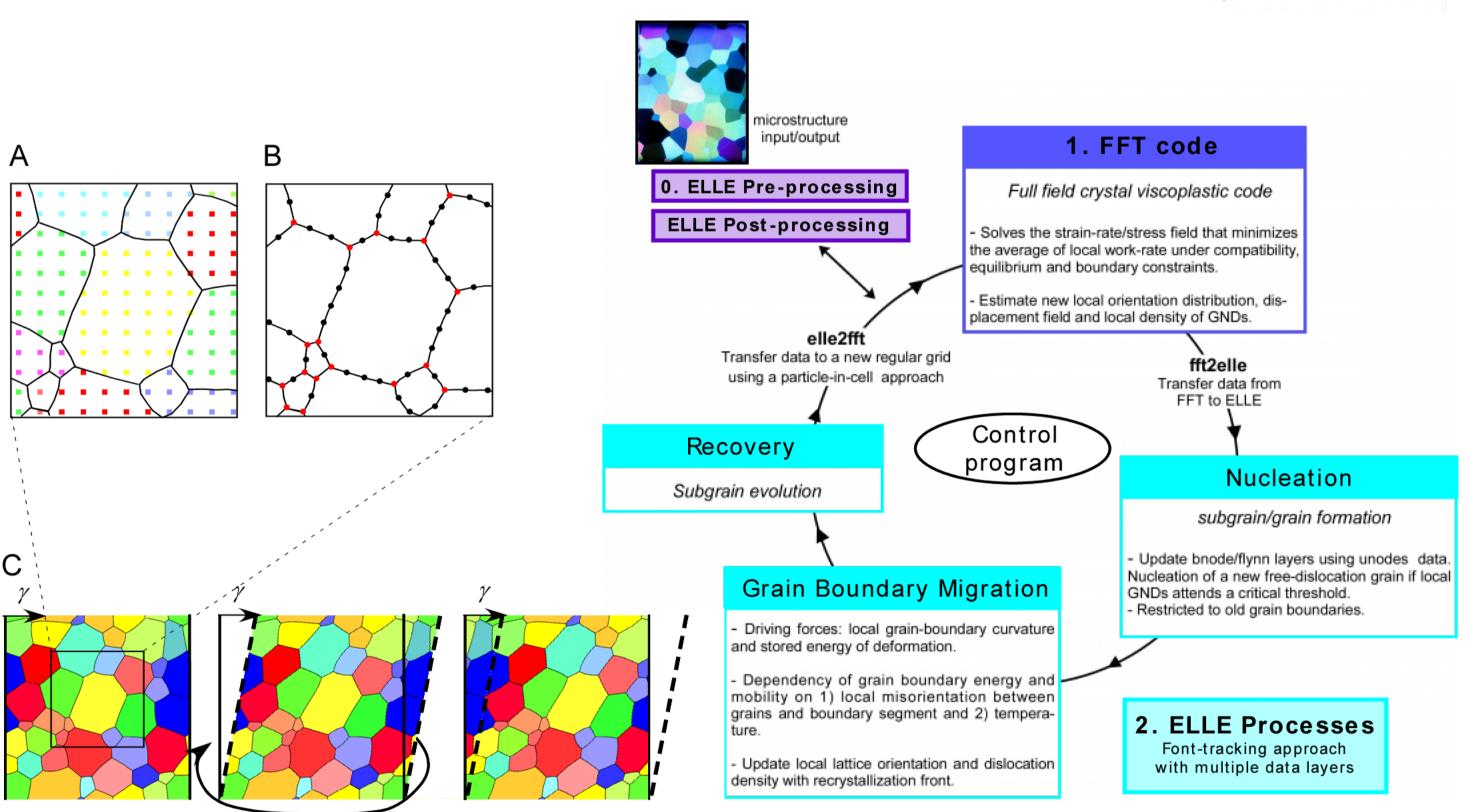
Methodology

We use the software packages ELLE (Jessell et al., 2001; Bons et al., 2008; http://www.microstructure.info/elle) and FFT crystal plasticity code (Lebensohn, 2001). FFT is used to calculate the response of a polycrystalline aggregate that deforms by dislocation glide, applying a Fast Fourier Transform.
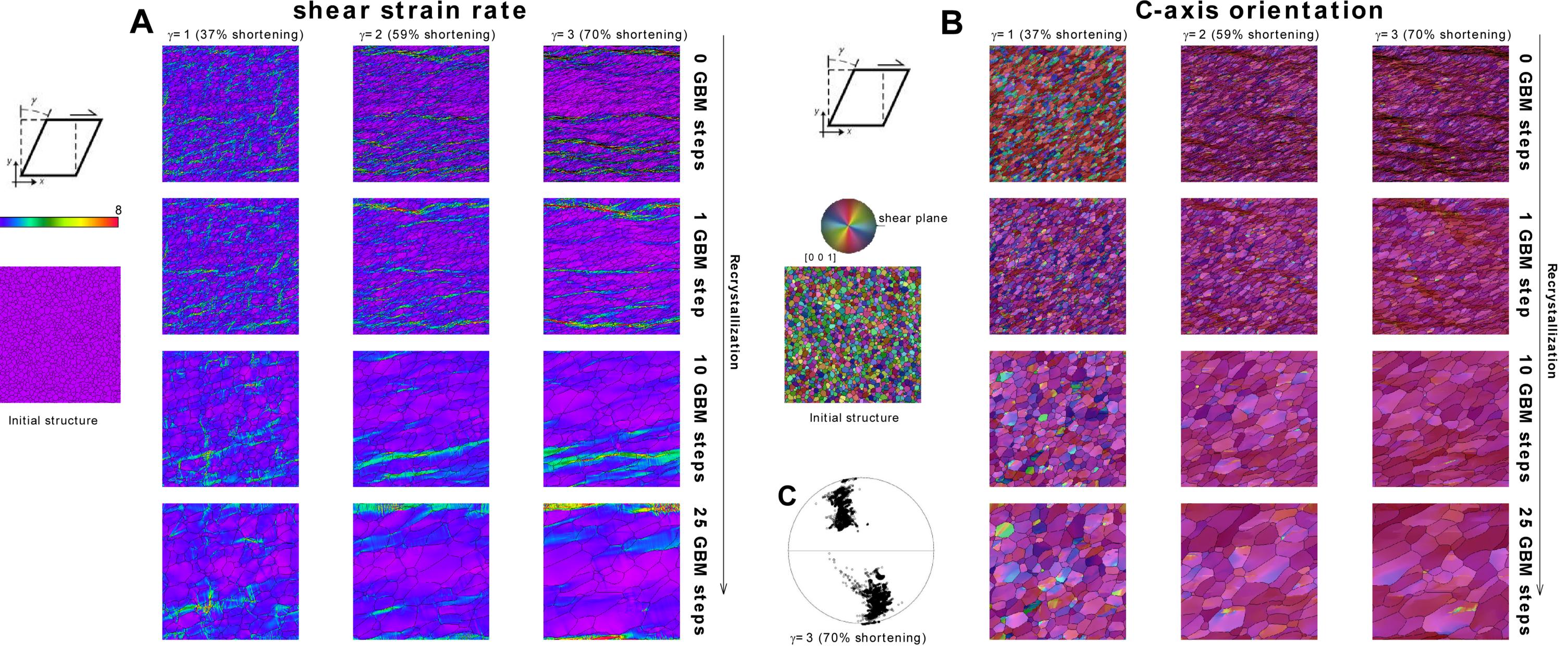
The numerical models consist of two layers: A: unconnected node grid (Fourier points) used for FFT calculations at each time and step, and B: a polygon segment network used to define elements. Boundary conditions are periodic in the horizontal and vertical direction. Properties are assigned to Fourier points.

The advantage of ELLE is that very high strains can be achieved through continuous remeshing and wrapping boundaries, showed in figure C.

A simple shear experimental run consist of iterative applications of small increments of dextral simple shear deformation (γ = 0.04) to an initially square model. The square boundary is maintained constant at the end of each deformation increment. A pure shear experimental run consist of iterative applications of small increments of 2% of shortening of coaxial compression. After this deformation Grain Boundary Migration and Recovery processes reduce the stored strain energy produced by deformation.

In order to compare the influence of different parameters on the structure evolution, we varied the boundary conditions (pure or simple shear) at different strain rates (deformation/grain boundary migration ratio). Critical resolved shear stress for basal vs non-basal slip systems (A= 20) and stress exponent (n= 3) are fixed parameters.

Simple shear simulations

shear strain rate

A

γ= 1 (37% shortening) γ= 2 (59% shortening) γ= 3 (70% shortening)

0 GBM steps / 1 GBM step / 10 GBM steps / 25 GBM steps

Recrystallization

Initial structure

C-axis orientation

B

γ= 1 (37% shortening) γ= 2 (59% shortening) γ= 3 (70% shortening)

0 GBM steps / 1 GBM step / 10 GBM steps / 25 GBM steps

Recrystallization

shear plane

[0 0 1]

Initial structure

C

γ= 3 (70% shortening)

Shear strain rate field, normalized respect to the bulk strain, (A) and c-axis orientation (B) plots for dextral simple shear experiments at different steps of deformation (γ).
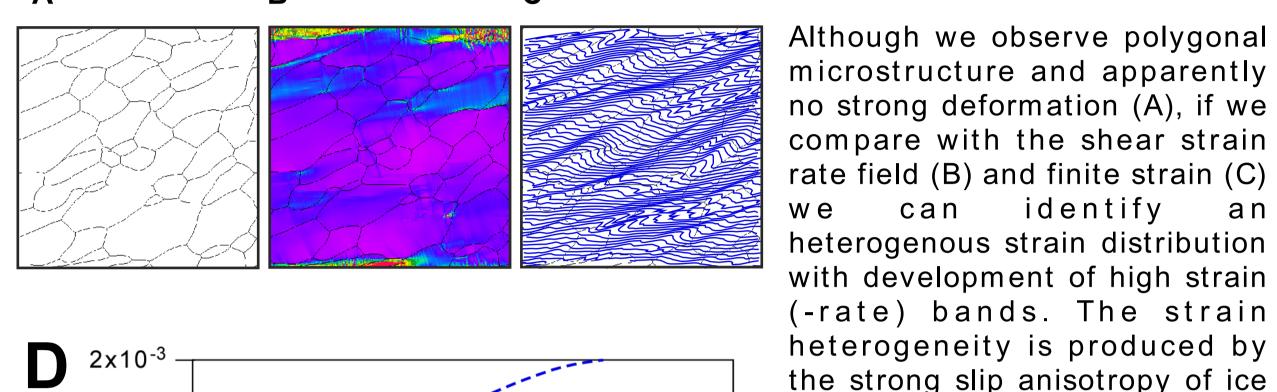
The initial 1x1 structure follows a loop that reproduces dislocation glide, grain boundary migration and recovery processes.

Grain Boundary Migration moves boundary nodes that define polygons (i.e grains) following the direction of reduction of Gibbs free energy (Becker et al., 2008; Roessiger et al., 2014). Recovery reduces the misorientation of c-axis, assuming that processes like annihilation of dislocations and polygonization take place.

Four different ratios between dynamic recrystallization and deformation are performed (0, 1, 10 and 25 Grain Boundary Migration steps per deformation step) in order to observe the influence of the amount of recrystallization in the structure evolution.

The results show that an increment of recrystallization produces larger grains, with smooth boundaries. However, the increment of recrystallization does not modify the single-maximum pattern of c-axes (figure C), that are distributed at low angle to the shortening direction (initially 45° respect to the shear plane).

Pure shear simulations

A

37% shortening   59% shortening   70% shortening

0 GBM steps / 1 GBM step / 10 GBM steps / 25 GBM steps

Recrystallization

Initial structure   High

B

37% shortening   59% shortening   70% shortening

0 GBM steps / 1 GBM step / 10 GBM steps / 25 GBM steps

Recrystallization

Initial structure

[0 0 1]

C

70% shortening

Shear strain rate field, normalized respect to the bulk strain, (A) and c-axis orientation (B) plots for pure shear experiments at different steps of deformation.

In pure shear experiments, the initial structure has the same configuration as in simple shear. However, the size of the initial structure is 2x1, instead of 1x1, allowing us to reach the same deformation as in simple shear experiments. The initial structure follows a loop that reproduces dislocation glide, grain boundary migration and recovery processes, as in simple shear experiments.

Four different ratios between dynamic recrystallization and deformation are performed (0, 1, 10 and 25 Grain Boundary Migration steps per deformation step) in order to observe the influence of the amount of recrystallization in the structure evolution.

The results show a similar effect of the recrystallization as in simple shear simulations: larger grains and smooth shape boundaries. However, this effect does not significantly modify the single-maximum pattern of c-axes (figure C), that are distributed at low angle to the shortening direction (parallel to the compression).

Strain rate and finite strain heterogeneity

A   **B**   **C**

Although we observe polygonal microstructure and apparently no strong deformation (A), if we compare with the shear strain rate field (B) and finite strain (C) we can identify an heterogenous strain distribution with development of high strain (-rate) bands. The strain heterogeneity is produced by the strong slip anisotropy of ice and it is masked by dynamic recrystallization.

Pure shear simulations are characterized by an initial strain hardening stage followed by steady state at large strain (dashed lines, (D). Simple shear simulations are characterized by an initial strain hardening stage reaching a peak of differential stress and finally strain softening behavior (continuous lines).

D

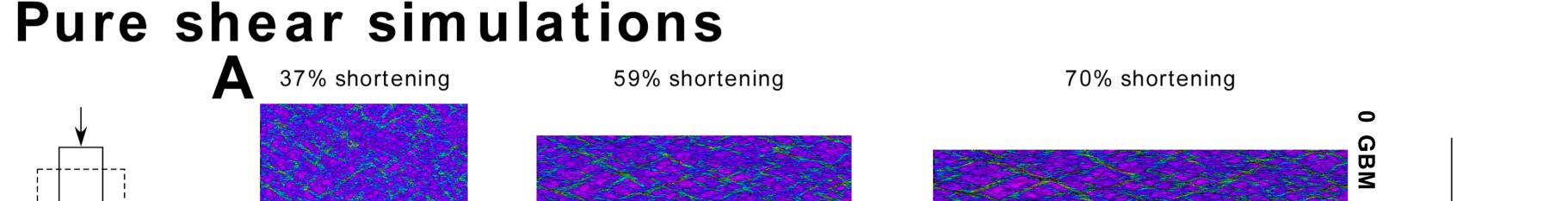y-axis: normalized differential stress
2×10^{-3}, $1,5 \times 10^{-3}$, 1×10^{-3}, 5×10^{-4}, 0
x-axis: Shear strain γ 0, 1, 2, 3

— 1 gbm step / deformation step
— 10 gbm steps / deformation step
— 25 gbm steps / deformation step
- - - pure shear — simple shear

Conclusions

- The simulation results show a **strong effect of the recrystallization** on the final microstructure.

- Dynamic recrystallization **masks the strain rate and finite strain heterogeneity** resulting from the strong slip anisotropy of ice, being this masking higher at high number of dynamic recrystallization steps.

- The strong **effect of recrystallization on the microstructure does not significantly modify the single-maximum pattern of c-axes**, that are distributed at low angle to the shortening direction in both pure and simple shear cases.

- In pure and simple shear simulations, **dynamic recrystallization produces larger and more equidimensional grains**, with smooth boundaries.

References

- Becker, J K., Bons, P. D. & Jessell, M. W., 2008, A new front-tracking method to model anisotropic grain and phase boundary motion in rocks. Computers & Geosciences 34, 201-212.
- Bons, P.D., Koehn, D., and Jessell, M. W., eds., 2008, Microdynamics Simulation: Berlin, Springer, 406 p.
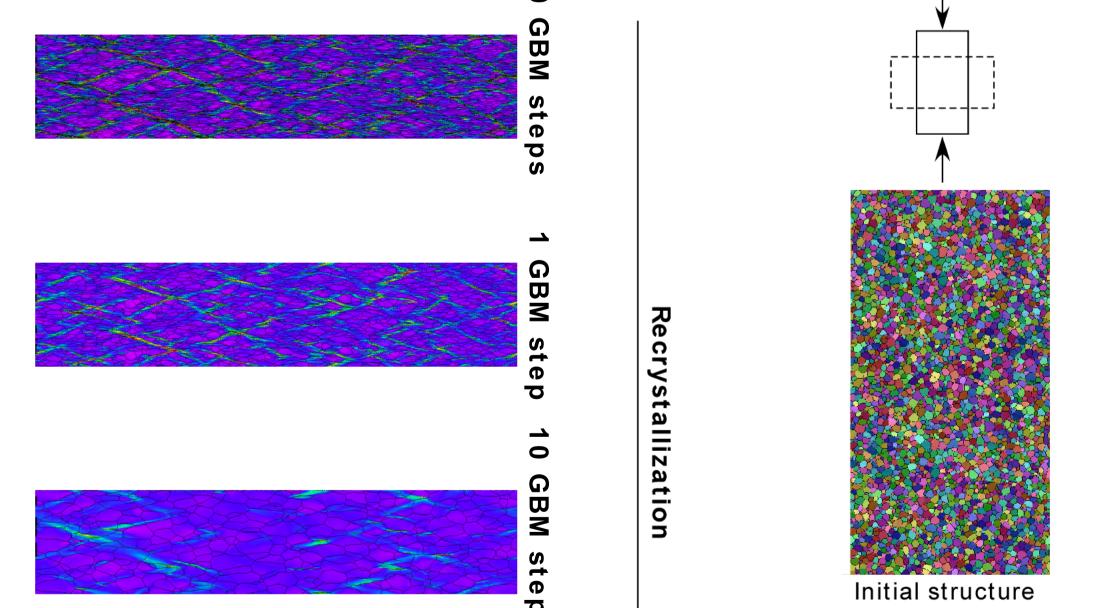- Jessell, M. W., Bons, P.D., Evans, L., Barr, T., and Stüwe K., 2001: Elle: a micro-process approach to the simulation of microstructures: Computers and Geosciences 27, 17-30.
- Lebensohn., R. A., 2001. N-site modelling of a 3D viscoplastic polycrystal using Fast Fourier Transform. Acta Materialia 49, ,2723-2737
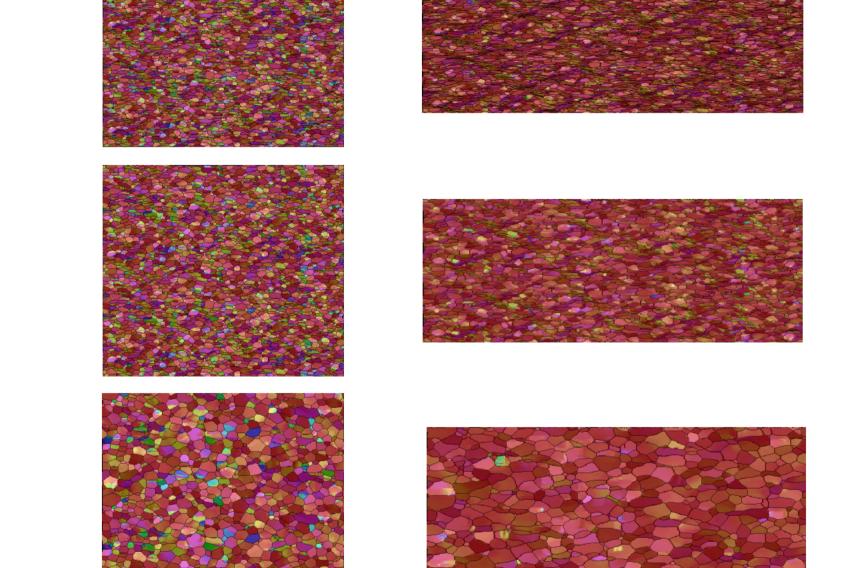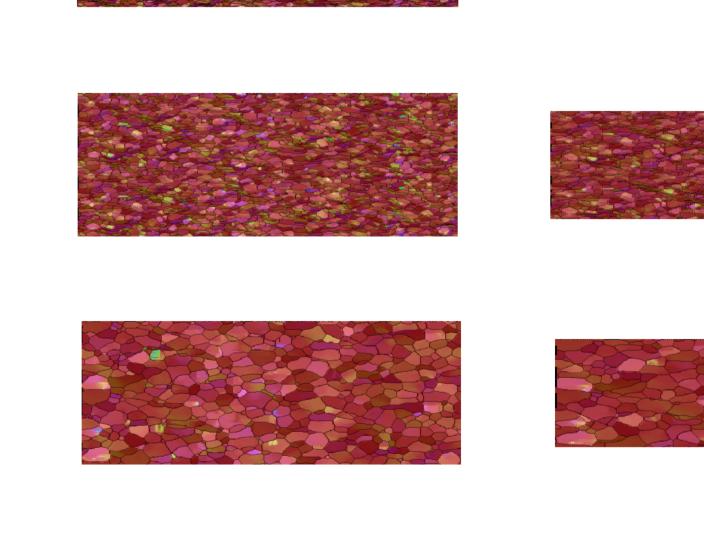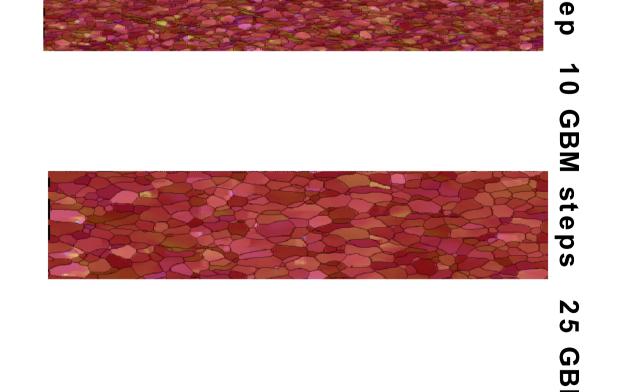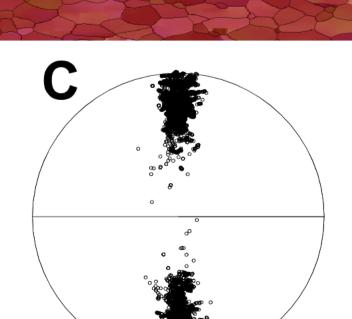- Roessiger, J., Bons, P. D. & Faria, S. H., 2012 Influence of bubbles on grain growth in ice. Journal of Structural Geology in press.