



Research Networking Programmes

Short Visit Grant or Exchange Visit Grant

(please tick the relevant box)

Scientific Report

The scientific report (WORD or PDF file – maximum of eight A4 pages) should be submitted online within one month of the event . It will be published on the ESF website.

Proposal Title: Dynamic recrystallization during simple shear deformation: a numerical approach

Application Reference N°: 7150

1) Purpose of the visit:

The bulk behaviour of large ice masses is the result of the behaviour of the ensemble of individual ice grains. This is strongly influenced by the viscoplastic anisotropy of these grains and their lattice orientation. In ice sheets, the orientation and tightness of c-axis maxima become dependent on the flow regime. In general, the ice flow pattern is expected to be simple shear near the base and pure shear at the surface and along divides in the ice sheet. Ice develops a lattice preferred orientation during flow. The ice microstructure evolves through time as a consequence of recrystallization processes.

Laboratory experiments and deep drill cores through glaciers and ice sheets are the most important sources of information on ice microstructures. However, a major limitation of experiments is that deformation rates are inevitably higher than those typically occurring in nature by several orders of magnitude, especially in the case of slowly flowing polar ice sheets. Numerical simulations, like the ones performed by the applicant, provide a solution to this problem, since they are not limited by scale, stress or strain rate. A full-field viscoplastic deformation model has been coupled with the ELLE software platform to simulate coetaneous deformation, recrystallization (grain boundary migration) and recovery. These models allow us to predict the microstructural evolution of ice polycrystals during pure and simple deformation and dynamic recrystallization at large strains.

Previous simulations in pure shear conditions have been successfully performed and the obtained data have been post-processed and prepared for publication by the applicant. However, it is necessary to perform simulations in simple shear conditions, in order to compare and understand the differences between microstructures forming in these two flow regimes. This visit aimed to perform numerical simulations of ice deformation and recrystallization in simple shear conditions, using the aforementioned numerical simulation codes. The coupling between FFT and ELLE was coded by Dr.

Albert Grier (lecturer at the Universitat Autònoma Barcelona). Through this visit, the applicant has collaborated with him to be able to achieve this aim. The visit took place from February 15th until March 1st 2015.

1) Description of the work carried out during the visit:

Prior to the visit, the applicant performed experiments of viscoplastic deformation using a Full-Field approach (FFT) (Lebensohn, 2001) coupled with recrystallization processes (coded within the ELLE software platform) (Jessell et al., 2001; Bons et al., 2008) under simple shear boundary conditions. During the visit, the data resulting from these experiments were post-processed in order to carry out the microstructural and mechanical analyses. These models have an initial microstructure of 3260 grains defined by boundary nodes, and a resolution of 256x256 Fourier points (Fig. 1A and 1B). 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 1C. The initial microstructure (Fig.1C) follows a loop that reproduces small increments of dextral simple shear deformation ($\gamma = 0.04$) by dislocation glide, to an initially square model. The square boundary is maintained constant at the end of each deformation increment. After this deformation Grain Boundary Migration and Recovery processes reduce the stored strain energy produced by deformation.

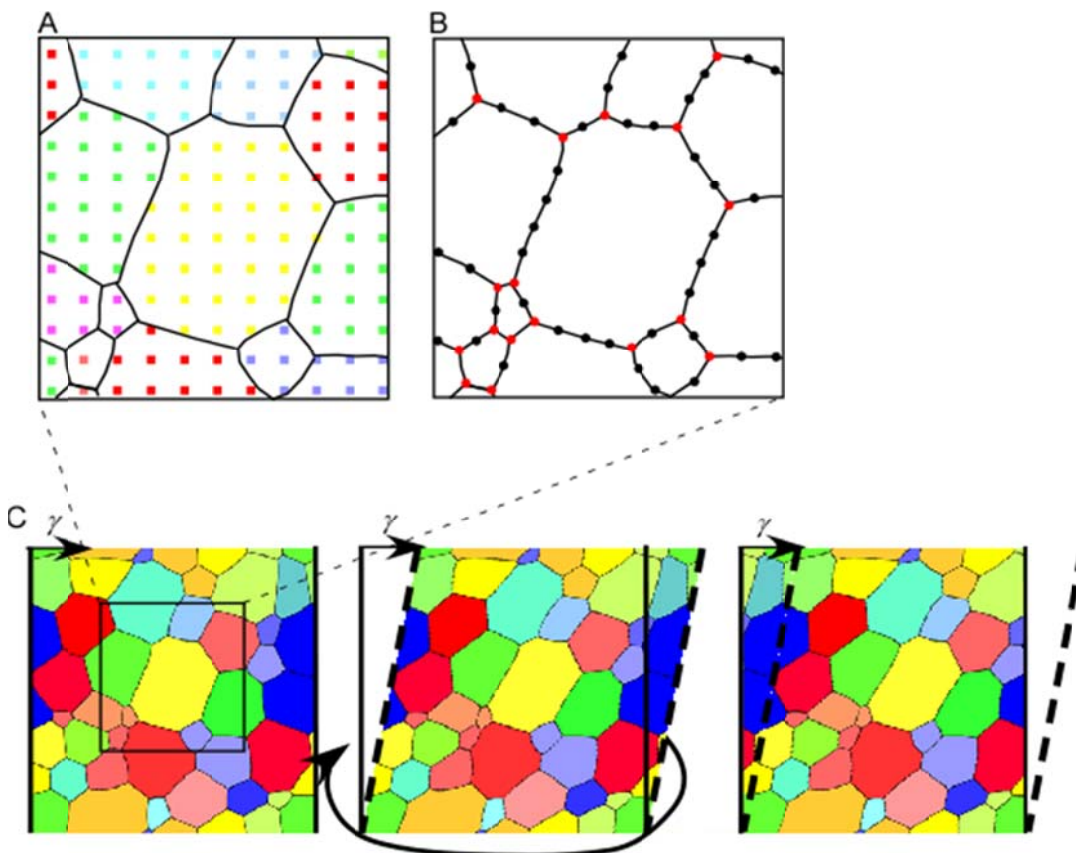


Fig1: Example of the initial configuration of a simulation. The ELLE model has two different layers: (A) the microstructure is discretized into a regular mesh of Fourier points for the FFT calculation, and (B) boundary nodes (triple or double nodes) that define polygons (grains). A simple shear deformation

example is represented in (C), where colors indicate the c-axis orientation with respect to the sample reference frame, and black lines represent grain boundaries.

The data resulting from the simulations were extracted using the MATLAB software MTEX (Mainprice et al., 2011). Data to build plots of Electron Backscatter Diffraction (EBSD) images, crystal preferred orientation (CPO) and inverse polar figures (IPDF), misorientation and average grain size were extracted from the numerical experiments. Scripts and routines were developed in order to be able to extract the necessary information.

The results of the four experiments, with different ratios between dynamic recrystallization and deformation performed (0, 1, 10 and 25 DRX steps per deformation step) were discussed, in order to observe the influence of dynamic recrystallization on the microstructure evolution.

The main results obtained and relevant conclusions are being prepared in the form of a manuscript for publication in a high-impact scientific journal.

2) Description of the main results obtained

In order to compare the influence of different parameters on the structure evolution, we analysed the results from experiments at different strain rates (deformation/grain boundary migration ratio). The critical resolved shear stress for basal vs non-basal slip systems ($A=20$) and stress exponent ($n=3$) are fixed parameters in these experiments. We focused on fabric development and grain shape evolution during deformation.

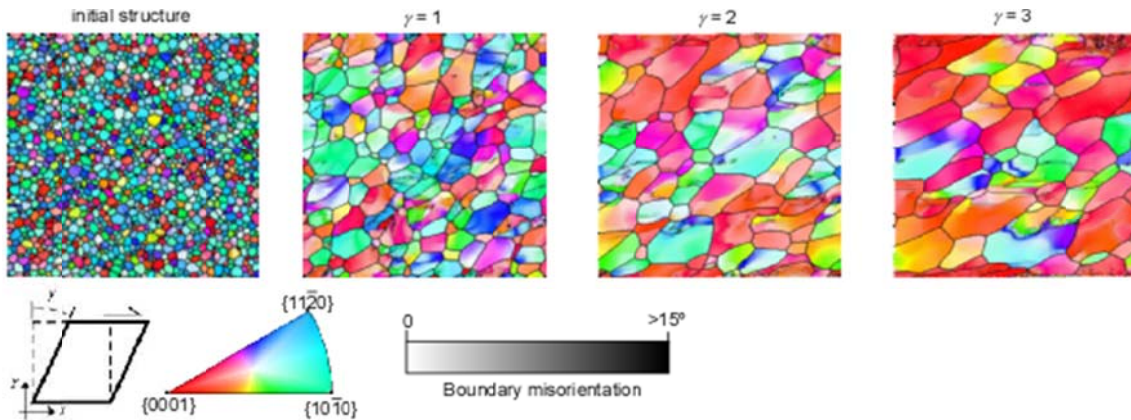


Fig2: Example of a simple shear experiment with 25 steps of grain boundary migration per deformation step. The images show the EBSD map at $\gamma=1$, $\gamma=2$ and $\gamma=3$ of shear strain. The simulation starts with an initial microstructure with a random c-axis orientation distribution. At a shear strain of $\gamma=2$ the fabric starts to develop preferred orientation. At a shear strain of $\gamma=3$ crystals are preferentially oriented almost perpendicular to the shear plane.

Dynamic recrystallization produces larger and more equidimensional grains, with smooth boundaries. Shape preferred orientation of grains is also observed, with grain boundaries oriented perpendicular to the maximum shortening direction. In simulations with lower number of dynamic recrystallization steps grains are elongated on strain localization bands parallel to the shear plane. (Fig.3).

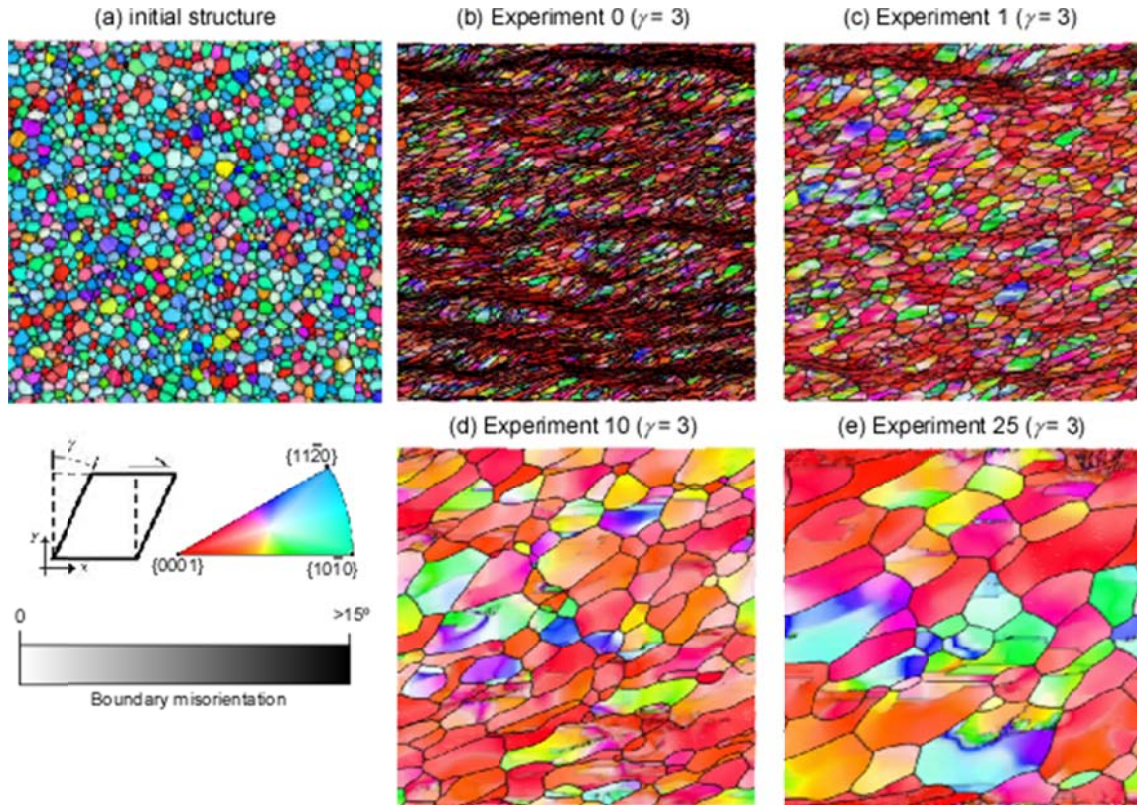


Fig3: Comparison of the grain shape and c-axis orientation map at the end of the simulations (shear strain of $\gamma=3$) observed in the four models, starting with the same initial microstructure (a), and different ratios between dynamic recrystallization and deformation: (b) 0, (c) 1, (d) 10 and (e) 25 sub loops of dynamic recrystallization per deformation step.

Deformation without grain growth produces elongated grains and the average grain area remains constant during deformation, while DRX produces larger and more equidimensional grains. Fig. 4 shows the relationship between grain size and grain elongation depending on the amount of DRX. When DRX is activated deformation is masked, because elongation is reduced, being the aspect ratio in experiments with DRX less than 2.

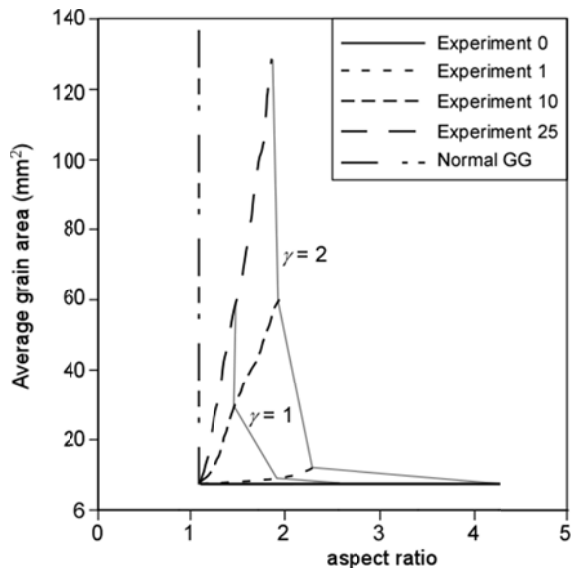


Fig4: Average grain area vs elongation ratio evolution during deformation for experiments 0, 1, 10 and 25, together with an only normal grain growth curve (Normal GG experiment).

The results show that dynamic recrystallization strongly influences the microstructure and lattice preferred orientation evolution of ice during deformation.

4) Future collaboration with host institution (if applicable):

5) Projected publications/articles resulting or to result from your grant:

The results and conclusions from these experiments are planned to be submitted as a contribution to a peer-reviewed journal related to the topic.

6) Other comments (if any):

References:

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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.

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Mainprice, D., Hielscher, R., Schaeben, H., 2011. Calculating anisotropic physical properties from texture data using the MTEX open-source package. In: Prior, D. J., Rutter, E. H., Tatham, D. J. (Eds.), *Deformation Mechanisms, Rheology and Tectonics: Microstructures, Mechanics and Anisotropy*. Vol. 360 of Special Publication. The Geological Society of London, pp. 175.