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: Numerical simulation of deformation microstructures in polar ice

Application Reference N°: 6725

1) Purpose of the visit:

Ice dynamic knowledge requires the understanding of ice crystal microstructures. The bulk behaviour of large ice masses is the result of the behaviour of the ensemble of individual ice grains that strongly depends on crystal properties. The ice microstructure is constantly evolving through time, reducing the surface energy by grain growth or recrystallizing as a response of the strain energy increment due to deformation. Recrystallization changes the mechanical properties of the material (i.e. strength) depending on the amount of strain, temperature and time. Since ice is very close to its melting point, it is very sensitive to these changes.

Analyses of drill cores and experimental studies have been a key advance in ice behaviour research. However, much information remains unknown, especially regarding the recrystallization effect on the microstructure development. Since this effect determines the bulk behaviour of ice masses, its investigation is essential. Full-field numerical simulations, like the ones performed by the applicant, provide a better insight into the mechanics of ice, from the microstructure to the ice sheet scale. These simulations allow us to predict the microstructural evolution of ice polycrystals during deformation and dynamic recrystallization at large strain conditions.

The main aim of this visit was to incorporate three important processes into the full-field numerical simulation code (FFT) used by the applicant, to study ice deformation: (1) recrystallization (grain boundary migration), (2) nucleation and (3) recovery. These processes were coded into the ELLE software platform by Dr. Albert Griera (Lecturer at the Autonomous University of Barcelona), and coupled with the FFT software by him. The applicant needed his experience and instruction to be able to achieve this aim. The visit took place from June 30th to July 11th 2014.

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

1. Data resulting from experiments performed by the applicant have been postprocessed in order to carry out the microstructural and mechanical analysis. These models consist of viscoplastic deformation using a Full-Field approach (FFT) (Lebensohn, 2001) coupled with recrystallization processes (ELLE) (Jessell et al., 2001; Bons et al., 2008). We decided to focus on a series of pure shear experiments after a preliminary analysis of pure and simple shear simulations results. These models have an initial microstructure of 3260 grains defined by boundary nodes, and a resolution of 256x256 Fourier points (Fig.1A and 1B). The initial microstructure (Fig.1C) follows a loop that reproduces deformation by dislocation glide, grain boundary migration and recovery processes. An experimental run consists of iterative applications of small increments of 2% shortening of coaxial compression, followed by grain boundary migration and recovery.

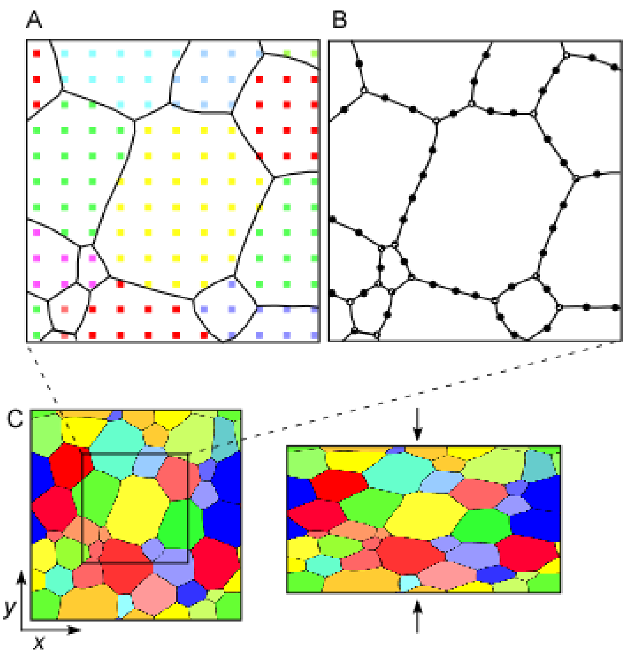

Fig1: Example of the initial configuration of a simulation. The ELLE model has two different layers: (A) the microstructure is discretized into a regular mesh of Fourier points for the FFT calculation, and (B) boundary nodes (triple or double nodes) that define polygons (grains). A pure shear deformation example is represented in (C), where colors indicate the c-axis orientation with respect to the sample reference frame, and black lines display grain boundaries.

2. Information about grain shape and fabric evolution have been compared between experiments in order to understand the effect of dynamic recrystallization on ice deformation. We decided to use a new software to extract the simulation data. The texture analyses have been performed with the MTEX software (Mainprice et al., 2011), which works within the MATLAB platform. Data to build plots of Electron Backscatter Difraction (EBSD) images, Crystal Preferred Orientation (CPO), misorientation and grain size have been extracted from experiments, together with the calculation of the orientation tensor eigenvalues for all deformation steps. These tasks required the

improvement of several routines and scripts to be able to extract the necessary information. The complexity of the data processing was found to be more difficult than initially expected, and only part of the tasks could be finished by the end of the visit.

3. During the short visit the obtained results were discussed, focusing on the influence of dynamic recrystallization on the microstructure evolution. The improvement of images using the new texture analysis method revealed new results and new ideas arose. They will help us to improve our knowledge of the role of dynamic recrystallization on mechanic and microstructural evolution of polar ice.

4. A preliminary draft for a scientific publication with a selection of images for figures, data tables, main results obtained, relevant conclusions and principal discussion has been prepared.

2) Description of the main results obtained:

1. We have compared numerical simulations of pure shear deformation with different amounts of dynamic recrystallization of pure ice (Fig.2), focusing on fabric development and grain shape evolution during deformation.

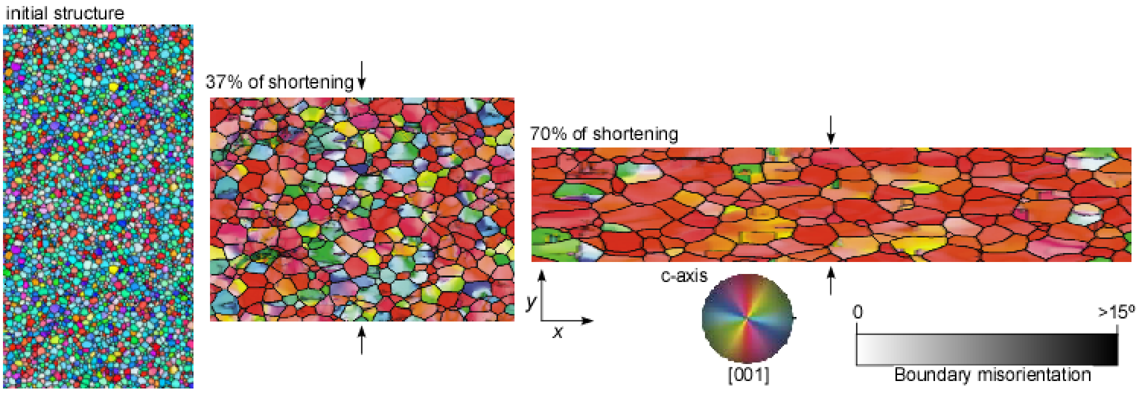

Fig2: Example of a pure shear experiment with 25 steps of grain boundary migration per deformation step. The images show the c-axis orientation at 0%, 37% and 70% of shortening. The simulation starts with a random distribution. At 37% of shortening the fabric starts to develop preferred orientation. At 70% of shortening crystals are preferred oriented parallel to the maximum shortening direction.

2. Analysis of the ice crystal preferred orientation symmetry were performed using the fabric types point (P), girdle (G) and random (R) for the ice [001] distribution. These values are calculated from the three eigenvalues as $P=\lambda_1-\lambda_3$, $G=2\lambda_2-2\lambda_3$, and $R=3\lambda_3$ (Vollmer, 1990). In all simulations the initial c-axis random orientation distribution of grains is destroyed firstly, followed by girdle fabric and tending to a single maximum pattern, parallel to the maximum shortening direction at high strain, being this evolution more marked at high number of dynamic recrystallization steps. (Fig.3).

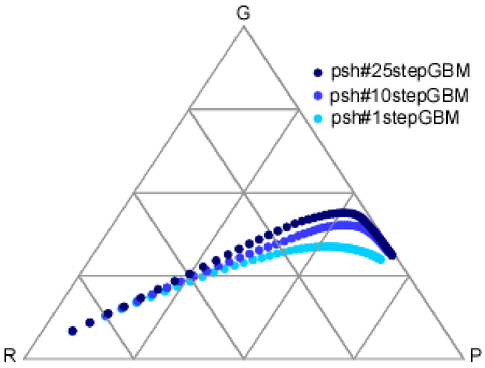

Fig3: Ice CPO symmetry expressed as the proportion of point (P), girdle (G) and random (R) components for [001] crystallographic axis. Different blue colours represent simulations with different amount of dynamic recrystallization: 1, 10 and 25 grain boundary migration steps per deformation step.

3. Dynamic recrystallization produces larger and more equidimensional grains, with smooth boundaries. Shape preferred orientation of grains is also observed, with grain boundaries oriented normal to the shortening direction. In simulations with lower number of dynamic recrystallization steps grains are elongated on strain localization bands. (Fig.4).

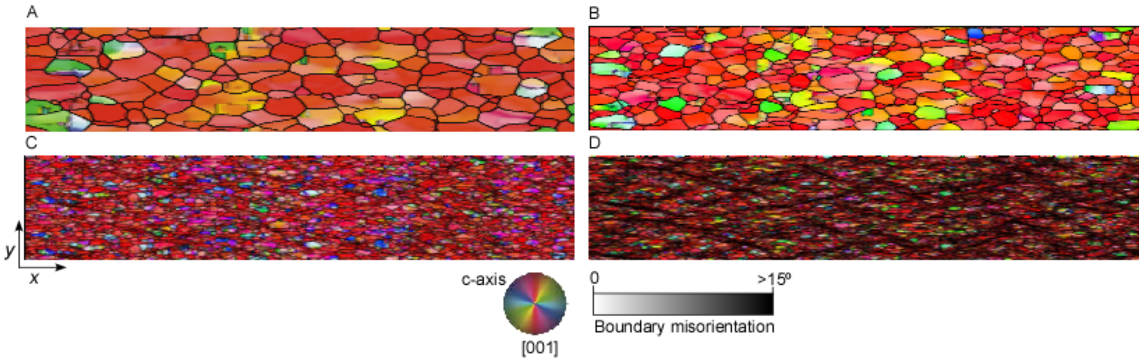

Fig4: Comparison of the grain shape and c-axis orientation map at the end of the simulations (70% of shortening) observed in the four models with different ratios between dynamic recrystallization and deformation: (A) 25, (B) 10, (C) 1 and (D) 0 grain boundary migration steps per deformation step.

4. Results show that dynamic recrystallization strongly influences the mechanical and microstructural evolution (crystal preferred orientation, grain size and shape, etc…) of ice during deformation.

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

The objective of this short visit was to consolidate the relationship and collaborations between Barcelona and Tuebingen research groups. It is expected to continue with the feedback and research collaboration. Moreover, several joint manuscripts are being prepared, to be published in high-impact journals.

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

Results and conclusions from these experiments are planned to be submitted with the contribution (provisional title) "*Llorens, M.- G., Griera, A., Weikusat, I. and Bons, P. Dynamic recrystallization of ice aggregates during viscoplastic deformation: a numerical approach*" to a special issue on ice microstructures and micro-deformation mechanisms in Philosophical Transactions of the Royal Society of London. This special issue arises from the MicroDice session at EGU 2014.

6) Other comments (if any):

References:

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