ESF Activity: Micro-Dynamics of Ice (MICRODICE)
Title: **Influence of dynamic recrystallization on the microstructure evolution of polar ice: a numerical approach**
Reference Number: 4954
Host institution: Fachbereich Geowissenschaften, Eberhard Karls Universität, Tübingen (Germany)
Date of exchange visit: 01/06/2012 to 08/06/2012

1) Purpose of the visit

Conventional approaches used to simulate dynamic recrystallization in ice are based on simplistic descriptions of the medium and they are not able to fully describe the mechanical response of a heterogeneous material. Explicit full-field approaches are required for a better prediction of the microstructure evolution of ice at large strain. Over the last years, a new full-field numerical scheme that is able to simulate microstructure of ice is in development (FFT/ELLE). This numerical scheme is developed by collaborators of the ELLE project (www.microstructure.org/elle): the groups of Professor Paul Bons (Tuebingen), Mark Jessell (Toulouse) and Albert Griera (UAB, Barcelona). The purpose of the visit was give continuity to a previous Microdice's exchange visit by Jens Roessiger (Tuebingen) at UAB (June 2011), when the numerical scheme and first simulations were started.

The initial goals of the visit are summarized by,

1) Post-process of early numerical simulations. Development of new models simulating deformation and recrystallization of polycrystalline pure ice under simple shear boundary conditions. These conditions were not used in the first stage of numerical simulations, where only pure shear conditions were employed.
2) Update of several processes of the numerical code to be compatible with a new multi-thread library.
3) Definition of the data-transfer protocol between the FFT/ELLE scheme and the new approach to simulate grain boundary migration in a multi-phase medium. This is an important step for the future development of a numerical scheme able to simulate crystal deformation and recrystallization in heterogeneous polycrystalline aggregates (e.g. bubble ice).

Last two goals had the purpose to consolidate the collaboration between Tuebingen and Barcelona groups on the development of new tools for the numerical simulation of deformation and recrystallization of polycrystalline ice.

- Description of the work carried out during the visit

1. After revision and analysis of results from pure-shear simulations, we decide to focus on a new series of models using simple shear conditions. Three new numerical simulations were run using the computer facilities of the Tuebingen group. High resolution models were run up to large strain (γ=4.0). Initial microstructure was defined using more than 2500 grains and local crystal orientation by 256x256 elements (Fig. 1). Each simulation required between 2-3 days to be completed. The setup of the models was done trying to simulate different shear strain rates ($d\gamma/dt_{\text{model A}}=10\cdot d\gamma/dt_{\text{model B}}=25\cdot d\gamma/dt_{\text{model C}}$), and therefore, different degrees of dynamic recrystallization.

2. Previous and new data was post-processed, to enable subsequent microstructural and

mechanical analysis. This task required the improvement of several routines (e.g. stereographic projection, grain size calculator, etc). Bulk and local mechanical and microstructural properties were calculated and support materials (movies and graphs) were also created.

3. From a more technical point of view, part of the code was debugged and errors were fixed. The processes simulating grain boundaries migration and recovery were updated to run with multithread libraries. However, the upgrade of computational performance is still not satisfactory and improvements will be required in the future.
4. During the exchange visit, ideas on how to define the coupling between the FFT/ELLE scheme and the new approaches to simulate grain boundary migration in multiple phase medium were discussed. The complexity of the data transfer was found to be more complex than initially expected, and this work could not be completed during the visit.
5. Discussion and development of a manuscript draft describing the main results obtained so far.

Additionally during the visit, a short talk was done at the host institution. The talk was focused on the topics of the exchange visit ("Dynamic recrystallization of ice") and with the objective to increase the visibility of my visit, the Microdice program and the research developed by the Tuebingen group.

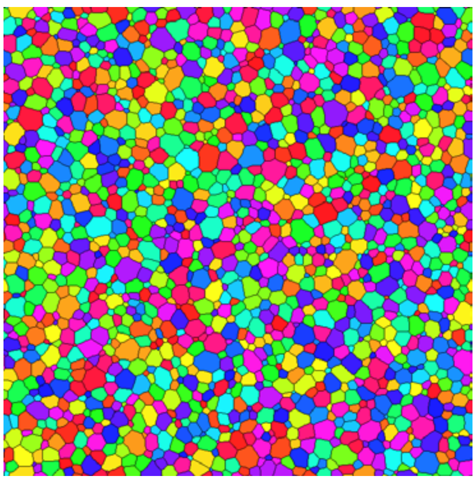

Fig. 1 Example of initial microstructure used in the numerical simulations. Colours indicate the c-axis orientation respect to the sample reference frame, while black lines indicate grain boundaries.

- Description of the main results obtained

From a *technical point of view*, the update and improvement of the code made the numerical simulations much more stable than before.

Main scientific results:

1) A series of two-dimensional numerical simulation of deformation and dynamic recrystallization of pure ice was done (Fig. 2). To our knowledge, these models are the first time than a full-field model is used to simulate microstructure evolution of pure ice during simple shear deformation up to large strain. Results will help us to improve our knowledge of the role of dynamic recrystallization on mechanic and microstructural evolution of polar ice.

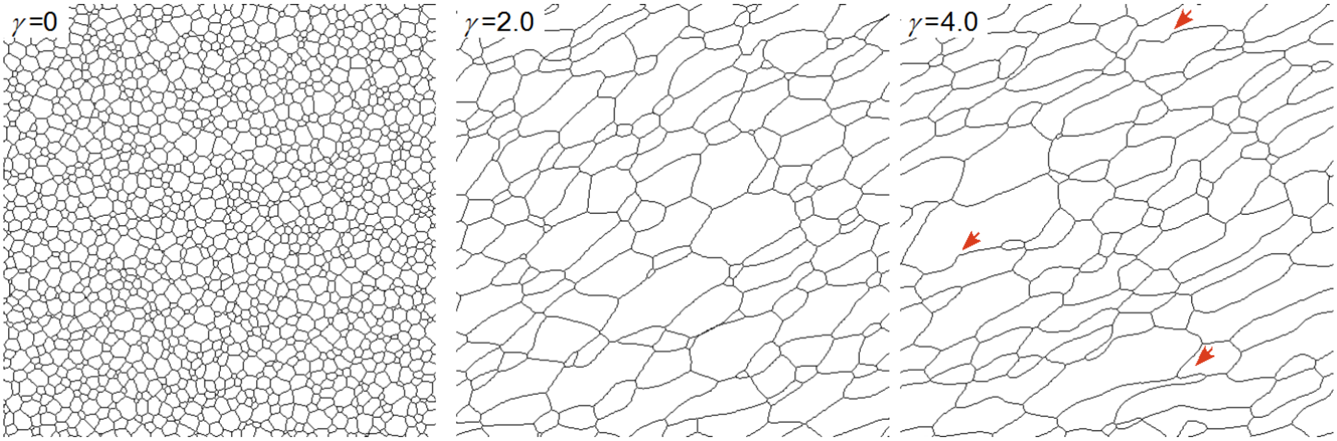

Fig. 2 Example of grain boundary evolution observed in "model B". Although a large strain was attained (indicated by gamma), strain localisation is not evident from the grain network and grain size coarsening is observed. However, local step geometry of grain boundaries and some elongated grains evidence this process (red arrows) are indicative of strain localisation. Shape preferred orientation of grains is also observed, with grain boundary oriented normal to the shortening direction.

2) Mechanical data shows that a stress peak is reached in all the simple shear simulations (Fig. 3). Initial strain hardening is followed by strain softening. This was not observed in pure shear simulations, where continuous strain hardening behaviour was observed during deformation. A dependence on the strain rate is also observed and larger decrease of stresses is observed with increasing strain rate.

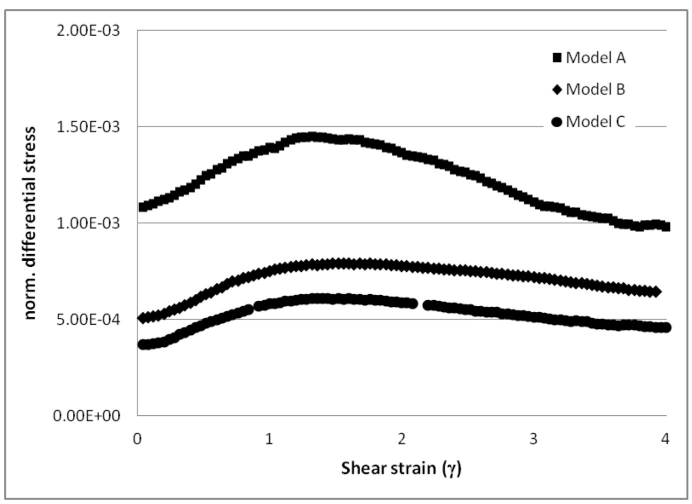

Fig. 3. Example of the mechanical stress-strain curves obtained from the three models ($d\gamma/dt_{\text{model A}}=10\cdot d\gamma/dt_{\text{model B}}=25\cdot d\gamma/dt_{\text{model C}}$). Stages of strain hardening and softening are observed.

3) Microstructure evolution strongly varies between different models. For high strain rate conditions, development of S-C geometries are easy identifiable and evidence strain localisation However for models with high recrystallization rates (models B and C; Fig. X), strain localisation is not evident from grain network, even though large strains are achieved. Grain coarsening dominates and partly erases strain localisation markers. Only geometry of grain boundaries forming steps and local elongated grains show this process (red arrows in Fig. 2). Shape preferred orientation of grains is also observed, with grain boundary oriented normal to the shortening direction. Normalized strain rate maps also point in evidence this process. Crystal-lattice preferred orientation is also modified during deformation and can help to explain the mechanical differences observed during deformation. High anisotropy of ice and preferred orientation of basal planes parallel to the shear plane allow strain localisation and

softening.

Our results indicate that dynamic rerystallization is able to significantly modify the mechanical and microstructural evolution (grain size, strain field, CPO, etc) of ice during deformation.

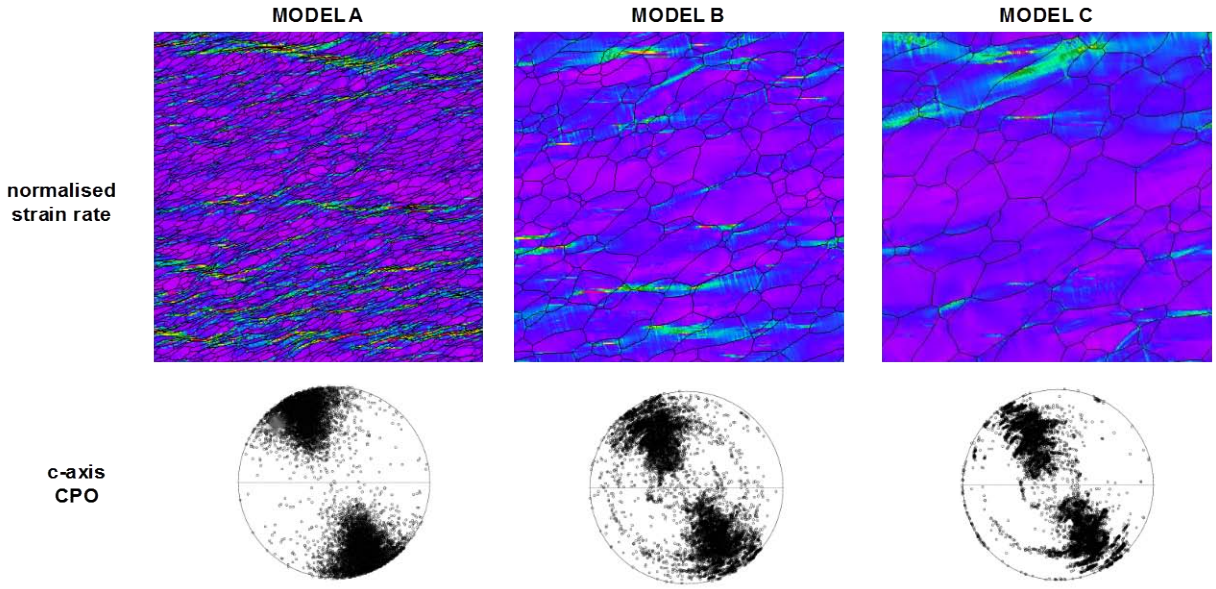

Fig. 4 Comparison of the normalised strain rate field and the crystal preferred orientation observed in the three models. For all models shear strain was 2.0. High strain rate on left and lowest on right.

- Future collaboration with host institution (if applicable)

One objective of this exchange visit was to consolidate the collaborations between the Tuebingen and Barcelona groups. It's expected to explore new ways to consolidate the collaboration between both groups (i.e. via national and/or european research funds).

- Projected publications/articles resulting or to result from your grant

Based on the work done during the exchange visit and the previous exchange visit by Jens Roessiger at UAB, a joint publication is in preparation for a peer-reviewed journal. The required models have been run and data post-processing is close to completion. The objective is to submit during the next two months (July-early September) to the "Earth and Planetary Science Letter" one's of the first quartile publications of the Geoscience discipline.

The provisional title and authors of the manuscript:
Roessiger, J., Griera, A., Bons, P.D. Impact of recrystallization during deformation of ice polycrystal: a numerical approach.

- Other comments (if any)

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