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Full-field predictions of ice dynamic recrystallisation under simple shear conditions

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ABSTRACT

Understanding the flow of ice on the microstructural scale is essential for improving our knowledge of large-scale ice dynamics, and thus our ability to predict future changes of ice sheets. Polar ice behaves anisotropically during flow, which can lead to strain localisation. In order to study how dynamic recrystallisation affects to strain localisation in deep levels of polar ice sheets, we present a series of numerical simulations of ice polycrystals deformed under simple-shear conditions. The models explicitly simulate the evolution of microstructures using a full-field approach, based on the coupling of a viscoplastic deformation code (VPFFT) with dynamic recrystallisation codes. The simulations provide new insights into the distribution of stress, strain rate and lattice orientation fields with progressive strain, up to a shear strain of three. Our simulations show how the recrystallisation processes have a strong influence on the resulting microstructure (grain size and shape), while the development of lattice preferred orientations (LPO) appears to be less affected. Activation of non-basal slip systems is enhanced by recrystallisation and induces a strain hardening behaviour up to the onset of strain localisation and strain weakening behaviour. Simulations demonstrate that the strong intrinsic anisotropy of ice crystals is transferred to the polycrystalline scale and results in the development of strain localisation bands than can be masked by grain boundary migration. Therefore, the finite-strain history is non-directly reflected by the final microstructure. Masked strain localisation can be recognised in ice cores, such as the EDML, from the presence of stepped boundaries, microshear and grains with zig-zag geometries.

1. Introduction

There is an increasing scientific interest in polar ice sheets because of the role they play in controlling sea-level rise and paleoclimate records through deep drilling projects (e.g. NEEM, 2013). For a correct interpretation of these records, it is crucial to determine to what extent deformation processes, such as dynamic recrystallisation and heterogeneous flow, may affect or distort ice stratigraphy, especially in the oldest and, thus, deepest ice, which can undergo strong deformation (Cuffey and Paterson, 2010; Montagnat et al., 2014).

On Earth surface, the only stable ice phase is the hexagonal symmetry form *Ih*, which exhibits highly anisotropic viscoplastic deformation. The orientation of ice crystals is usually defined by the orientation of their c-axis, which is perpendicular to the basal plane. Deformation is mostly accommodated by dislocation glide on that plane, while the other slip systems (prismatic and pyramidal) are much harder to activate (e.g. Duval and Castelnau, 1995). A parameter accounting for the anisotropy of the crystal (A) can be defined as the ratio of critical resolved shear stress (CRSS) required to activate slip along non-basal versus basal systems. Experiments reviewed in Duval et al. (1983) indicate that the activation of non-basal systems requires stresses at least 60 times greater those on basal planes.

Polycrystalline ice with randomly orientated c-axes is considered to behave isotropically, as enough basal planes well oriented for slip are available. However, ice core analysis reveals that c-axes tend to rotate towards the vertical direction below a certain

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depth (S.H. Faria et al., 2014). Consequently, ice crystals tend to be oriented with their basal planes close to perpendicular to the maximum compression or shortening direction (e.g. Alley, 1988; Montagnat et al., 2014). Ice polycrystals in ice sheets and glaciers thus form a lattice preferred orientation (LPO) and develop a bulk intrinsic anisotropy with deformation (S.H. Faria et al., 2014). Near the ice-sheet base, simple shear deformation dominates and a strong LPO develops (S.H. Faria et al., 2014). It has been found that ice with a strong LPO deforms up to an order of magnitude faster than isotropic ice, and therefore, ice flow strongly depends on the LPO of the polycrystalline ice (Azuma, 1994; Castelnau et al., 1996).

Ice microstructure is affected by different recrystallisation processes, depending on the temperature and strain rate (H.G. Faria et al., 2014). Dynamic recrystallisation affects the evolution of the microstructure (grain-size and shape) and influences the development of LPOs (e.g. Montagnat et al., 2015). This process is very efficient in ice due to the natural deformation conditions of this mineral, i.e. temperatures close to its pressure melting point and deformation at low strain rates (Kipfstuhl et al., 2006). These are observable especially in comparison with fast artificial deformation in creep tests (Weikusat et al., 2009).

Near the flow divide of ice sheets, ice deforms under vertical compression and horizontal extension (Montagnat et al., 2014). On the contrary, simple shear boundary conditions dominate in zones away from the divide and close to the bedrock (e.g. Cuffey and Paterson, 2010). It is therefore crucial for understanding bulk polar ice behaviour to study the fabrics and microstructural evolution of polar ice in response to stress and time under different types of deformation (i.e. under different strain rates and ratio between vertical and shear strain rates or kinematic vorticity).

New insights into ice rheology can be gained from interpretations of deformed natural ice from ice cores (S.H. Faria et al., 2014) or from experiments of natural or artificial ice deformed in the laboratory (Azuma, 1994; Treverrow et al., 2012; Montagnat et al., 2015). However, ice experiments in the laboratory are performed at high strain rates compared with that in natural conditions (Budd and Jacka, 1989) and high finite strains cannot be achieved. Numerical simulations can complement the study of ice rheology, as they can be performed at different strain rates and up to high strain. The aim of this contribution is to systematically study the effects of dynamic recrystallisation on the mechanical behaviour, resulting microstructures and strain localisation of polar ice under simple shear deformation, by means of numerical simulations. We focus on the evolution of fabrics and microstructures in response to finite strain and time, and the associated development of intrinsic polycrystalline anisotropy. We specifically capture the strain localisation indicators in the developed microstructures, and discuss how the resulting finite strain localisation that can potentially affect the spreading of climate signals at the small scale (Faria et al., 2010).

2. Numerical procedure

We use a two-dimensional numerical model (software platform ELLE, Bons et al., 2008; http://www.elle.ws) that simulates viscoplastic deformation coupled with dynamic recrystallisation (*DRX*), in order to investigate the microstructural evolution of an aggregate of pure ice grains. The numerical approach is based on the coupling of a full-field viscoplastic code using the Fast Fourier Transform algorithm (VPFFT; Lebensohn, 2001; Lebensohn et al., 2008) and several ELLE modules (Bons et al., 2008) that simulate recrystallisation processes such as recovery and grain boundary migration (Llorens et al., 2016). The VPFFT formulation provides a solution of the micromechanical problem by finding a strain rate and stress field that minimises the average local work-rate under the compatibility and equilibrium constraints (see Lebensohn, 2001). The algorithm assumes deformation by dislocation glide along pre-defined slip systems. Here we use the crystallography (unit cell dimensions and symmetry) of ice Ih and consider slip of dislocations along the basal, prismatic and pyramidal planes. The deformation-induced lattice rotation and the estimation of geometrically necessary dislocation densities calculated from the stress and velocity fields provided by the VPFFT algorithm are used to simulate intra-crystalline recovery and grain boundary migration. The ELLE platform has previously been used to simulate several deformation microstructure processes, including grain growth (Roessiger et al., 2011), dynamic recrystallisation (Piazolo et al., 2002), strain localisation (Griera et al., 2011; 2013) or folding (Llorens et al., 2013a; 2013b). In this study, grain boundary migration and recovery processes are used in order to simulate the microstructural evolution by recrystallisation. Grain boundary migration (*GBM*) is simulated using a front-tracking approach based on the algorithm by Becker et al. (2008). Grain boundary migration is driven by reduction of grain-boundary energy and stored strain energy, reproducing the motion or displacement of high-angle grain boundaries (HAGB). Regions swept by grain boundaries are assumed to restore lattice distortions (i.e. dislocation densities are zero). Recovery reduces the intra-granular stored energy in a deformed crystal by the annihilation of dislocations and their rearrangement into low-angle subgrains (Borthwick et al., 2013). A limitation of the model is that nucleation of new HAGB from lobate boundaries or due to highly deformed grains is still not implemented.

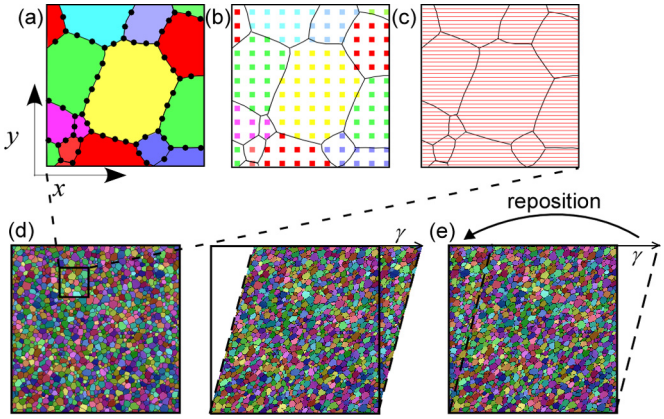

Fig. 1. Data structure. ELLE microstructures consist of three different layers: (a) boundary nodes (triple or double nodes) that define polygons (grains), (b) a regular mesh of unconnected nodes used for the VPFFT calculation, and (c) a passive marker grid used to track the finite deformation, where only initially horizontal grid lines are shown. The initially unit length model (d) is repositioned after the deformation step, bringing the model back into the unit cell (e).

The data structure of the models consists of two basic layers (Fig. 1): (a) a contiguous set of polygons (termed *flynns*) that are themselves defined by boundary nodes (*bnodes*) and are connected by straight boundary segments, and (b) a set of unconnected nodes (*unodes*) that provide a high-resolution grid for storing physical properties within grains. Additionally, an extra layer of unconnected nodes is used as a passive marker grid to track the finite deformation (Fig. 1c). A resolution of 256 × 256 Fourier points (*unodes*) was used to map lattice orientations, resulting in a unit cell defined by 65,536 discrete *unodes*. Each *unode* represents a small area with a certain lattice orientation, defined by three Euler angles following the Bunge convention, and local parameters, such as stress or dislocation density. The VPFFT code uses these *unodes* for the viscoplastic deformation calculations. The change of the position of *bnodes* is calculated according to the deformation velocity field and grain boundary migration. The data structure of both the