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Influence of bubbles on grain growth in ice

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ABSTRACT

Numerical static grain growth simulations of ice with air bubbles as a second phase show a significant drop in grain-growth rate compared to bubble-free ice. The magnitude of this drop in growth rate is dependent on the bubble boundary mobility, the volume fraction of air, the average bubble size and the bubble size distribution. The rate of grain growth decreases at first, as the microstructure evolves towards a steady state. Only then does grain growth follow the expected linear increase of mean grain area with time. In experiments, this decrease in growth rate could erroneously be interpreted as growth with a deviating growth exponent.

1. Introduction

Natural ice is rarely a single-phase material. It generally contains chemical impurities and dust, as well as air inclusions. In glaciers and ice sheets, air is trapped in the form of bubbles during the compaction from snow to firn to ice (Arnaud et al., 2000). In lake- or sea-ice, air bubbles may also occur due to gas accumulations along the water–ice interface (Schulson and Duval, 2009). With ongoing burial, air bubbles are compressed and may eventually convert to clathrates, in a transition zone that for polar ice sheets lies approximately in the range 600–1200 m depth (Barnes et al., 2002; Faria et al., 2009; Hondoh, 2009; Lipenkov et al., 1992). Air bubbles, clathrates, dust and other chemical impurities all influence recrystallisation of ice (Durand et al., 2006; Faria et al., 2010). While one expects that small particles such as microscopic inclusions and clathrates may mostly modify the grain boundary velocity, air bubbles form a significant volume fraction in the upper few hundred meters of ice sheets and glaciers, and could therefore influence recrystallisation even more (Arena et al., 1997; Azuma et al., 2012).

Grain size increases significantly in the upper few hundred metres of polar ice sheets (De La Chapelle et al., 1998). The increase in grain size is assumed to be driven by a reduction of grain boundary surface energy, a process usually termed static or normal grain growth (Alley et al., 1986a; Smith, 1964). This process is thought to dominate over flow-induced dynamic recrystallisation or polygonisation (Urai et al., 1986), which increasingly affects the ice microstructure with depth (Alley, 1992; Duval and Castelnau, 1995; Faria et al., 2002). The depth at which dynamic recrystallisation becomes significant is still under debate (Kipfstuhl et al., 2009). The stabilisation of grain size at depth has been observed in several deep ice cores. It is thought to result from a balance between grain growth and grain size reduction by dynamic recrystallisation (Gow et al., 1997; Gow and Williamson, 1976; Mathiesen et al., 2004; Montagnat and Duval, 2000; Thorsteinsson et al., 1997). Such a dynamic equilibrium between grain size increase and decrease is also invoked to explain grain sizes in other minerals, for example olivine, in deforming rocks (Herwegh and Handy, 1996; De Bresser et al., 2001).

Knowledge of the rate of grain size increase by grain growth is of clear relevance to be able to interpret grain sizes, grain size evolution and microstructures (Urai et al., 1986; Stöckhert and Duyster, 1999; Herwegh and Berger, 2003; Herwegh et al., 2011; etc.). The increase of grain size (diameter D_t) with time (t) from an initial size (D_0) is usually expressed in the form (Anderson, 1986; Glazier et al., 1987; Evans et al., 2001):

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$$D_t^n - D_0^n = kt \text{ with } D_t^n \approx kt(\text{if } D_0 << D_t) \quad (1)$$

The growth parameter (k) is determined by the grain boundary energy (γ) and the grain boundary mobility (M) with $k = k_0 M\gamma$. M [m^{2}s/kg] and γ [kg/s^2] are material properties. The temperature dependence of k is determined by the activation energy Q (since $k \propto \exp^{-Q/RT}$, with R the universal gas constant and T the absolute temperature). In the literature, Q is assumed to be about 40–50 kJ/mol, which is based on observations on polar ice sheets (Gow, 1969, 1971; Paterson, 1994). Recent experiments by Azuma et al. (2012) indicate that Q for pure ice is much higher at about 110–120 kJ/mol.

The dimensionless parameter k_0 is usually assumed constant with a theoretical value of $k_0 = 4.48$ or 2 in a two- or three-dimensional aggregate, respectively (Mullins, 1989). However, in reality k_0 is not a constant, but depends on the microstructure (Arena et al., 1997; Roessiger et al., 2011). Only if the microstructure is a foam texture will k_0 equal the theoretical value. The growth exponent (n) depends on the grain growth mechanism (Evans et al., 2001). In a pure grain aggregate, grain growth is controlled by the curvature of grain boundaries. If all boundaries have the same mobility, the growth exponent should be two. This can be derived from a simple dimension analysis, considering that the unit of k is m^2/s. Inserting this in Eq. (1) gives $n = 2$.

In impure grain aggregates, grain growth is a much more complicated process, due to the interaction between the grains and the impurities (Herwegh et al., 2011 and references therein). Impurities, such as dust particles, chemical impurities, or second phases such as air bubbles, may hinder or completely stop grain boundary movement (Zener pinning; Olgaard and Evans, 1986, 1988; Brodhag and Herwegh, 2010). If impurities inhibit grain boundary movement, growth comes to a complete halt when all boundaries are pinned (Weygand et al., 1999; Herwegh et al., 2011). In this case equation (1) does not apply, but grain size will asymptotically approach a fully pinned state. The maximum grain size ($D_{\max}$) is usually related to the fraction of second phase (f) and the size of the second phase particles or regions (d_s) by the Zener equation, where z is a scaling parameter:

$$D_{\max} = z\frac{d_s}{f^m} \quad (2)$$

See Olgaard and Evans (1986), Manohar et al. (1998) and Evans et al. (2001) for the background of the Zener equation and variations proposed in the literature.

If particles can be dragged along by the boundaries (Zener drag), the boundaries keep moving, but at a reduced rate as they accumulate more and more particles. If the second phase occupies a significant fraction of the material, as is the case for air bubbles in ice, the overall growth rate is assumed to be controlled by the increase in d_s of the minor phase (Hiraga et al., 2010a). In a two-phase material, such as ice with air bubbles, grains and bubbles represent phase regions. Isolated phase regions (air bubbles) can grow by two basic mechanisms:

- Diffusional material transfer between phase regions. The driving force for this is the higher surface energy of small compared to large phase regions, which have a larger radius of curvature (Ostwald ripening). If transport is by volume diffusion, theory predicts a growth exponent $n = 3$, while $n = 4$ is expected for grain-boundary diffusion (Evans et al., 2001). However, much higher growth exponents have been reported in the literature (Hiraga et al., 2010a; Ohuchi and Nakamura, 2007; Olgaard and Evans, 1988; Tullis and Yund, 1982; Yamazaki et al., 1996).
- Migration and merging of phase regions. Grain boundaries may drag phase regions, which may lead to them merging to form larger volumes (Brodhag and Herwegh, 2010). No diffusional exchange between phase regions is required for this mechanism.

Depending on the mechanism of migration of the second phase, surface-energy driven grain growth does not necessarily follow the normal grain growth law (Eq. (1)). For example, in case of migration of bubbles in ice, the migration rate is a function of bubble radius, diffusivity of water molecules in air, etc. (Hsueh et al., 1982; Alley et al., 1986a). In this case, the growth rate (dD/dt) is no longer proportional to $1/D$ (Eq. (12) in Azuma et al., 2012) and if Eq. (1) were to be applied, high apparent growth exponents are the result.

Few studies on grain growth in ice specifically address the influence of air bubbles (Arena et al., 1997; Azuma et al., 2012). It is usually assumed that grain boundary migration in nature is in the fast migration regime, also called regime 2 (Alley et al., 1986b). In this regime, migrating boundaries can sweep across bubbles and these do not remain on the boundaries but slow them down. The inferred regime 2 migration is based on the observation that air bubbles occur inside ice grains (Alley et al., 1986b). However, in the upper part of polar ice sheets, around the firn–ice transition, most bubbles are actually residing on grain boundaries (Arnaud et al., 1998; Kipfstuhl et al., 2009), which suggests that boundaries can usually not sweep across bubbles and leave them behind.

In this paper we investigate grain growth in ice with air bubbles with numerical simulations. Our model only includes grain boundary migration driven by the reduction in grain boundary curvature and thus excludes air transfer between air bubbles (Ostwald ripening). Rather than attempting to provide a grain-growth law for ice, as a function of parameters such as bubble content, temperature, etc., we discuss the behaviour of a two-phase grain aggregate, with particular attention to the influence of the two-phase (ice–air) boundary mobility relative to the single-phase (ice–ice) boundary mobility.

2. Method

For our simulations we used the open-source modelling software package Elle (Bons et al., 2008; Jessell et al., 2001; Piazolo et al., 2010). It has been used for the simulation of recrystallisation processes in ice, rock-forming minerals, and partially molten rocks (Becker et al., 2008; Bons et al., 2001; Jessell et al., 2003; Piazolo et al., 2004; Roessiger et al., 2011). The 2-dimensional microstructure is defined by a contiguous set of polygons (termed *flynns*) that are themselves defined by boundary nodes (termed *bnodes*). Bnodes are linked to two or three neighbours by straight segments (Fig. 1). Spatial resolution is defined by the *switch distance* (D_{sw}), here set at 0.005 of the unit-sized square model. Spacing between bnodes is held between 1 and 2.2 × D_{sw} by either inserting or removing bnodes when they are too far apart or too close, respectively. With a starting grain aggregate of about 420 grains, this means that grains have on average about 26 bnodes. A neighbour switch is induced when two converging grain boundary triple junctions are less than D_{sw} apart. Attributes can be assigned to both boundaries and flynns. Flynns represent individual ice grains or air bubbles. Boundaries can be (1) ice–ice grain boundaries, (2) ice–air interfaces, or (3) air–air boundaries, which are sometimes necessary for numerical reasons, but have no physical meaning. Periodic boundary conditions are applied in both horizontal and vertical directions, meaning that a grain boundary that reaches the left or bottom edge continues its motion on the right or top edge, respectively. The model can thus be considered a unit cell in an infinite grain aggregate.