Competition between grain growth and grain-size reduction in polar ice

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ABSTRACT. Static (or 'normal') grain growth, i.e. grain boundary migration driven solely by grain boundary energy, is considered to be an important process in polar ice. Many ice-core studies report a continual increase in average grain size with depth in the upper hundreds of metres of ice sheets, while at deeper levels grain size appears to reach a steady state as a consequence of a balance between grain growth and grain-size reduction by dynamic recrystallization. The growth factor k in the normal grain growth law is important for any process where grain growth plays a role, and it is normally assumed to be a temperature-dependent material property. Here we show, using numerical simulations with the program Elle, that the factor k also incorporates the effect of the microstructure on grain growth. For example, a change in grain-size distribution from normal to log-normal in a thin section is found to correspond to an increase in k by a factor of 3.5.

INTRODUCTION

Many classical studies of polar ice microstructure report an evolution of the mean grain size with depth according to what can be called the 'three-stage model' (Gow and Williamson, 1976; Herron and Langway, 1982; Thorsteinsson and others, 1997): in the upper few hundred metres, grain size increases steadily with depth; below a certain intermediate depth (400–700 m), the grain size stabilizes and remains roughly constant; finally, at great depths (approximately the last 300 m before reaching bedrock, where temperature exceeds –10°C (De La Chapelle and others, 1998; Duval, 2000) the grain size significantly increases again. Here we only deal with the upper two regions, where grain size first increases and then stabilizes.

The initial steady increase in grain size is usually explained by *static ('normal') grain growth* (Smith, 1964; Alley and others, 1986; Weaire and Rivier, 2009), defined as growth that is only driven by the reduction of free energy of the grain boundaries. The increase in grain size, expressed in mean radius, r, from a starting grain size, r_0, is usually described by (Anderson, 1986; Glazier and others, 1987; Weygand and others, 1998)

$$r^n - r_0^n = kt. \qquad (1)$$

The growth exponent n has a theoretical value of 2 in ideal static grain growth of grains with isotropic properties (Glazier and others, 1987). In natural systems, the exponent is usually found to be >2. Any other process or factor that influences grain growth tends to increase n, such as anisotropic boundary energies, pinning, etc. (Gow, 1969; Gow and others, 1997; Bons and others, 2001; Durand and others, 2006). The parameter k is normally treated as a temperature-dependent material property that is a function of only the boundary energy $\gamma(T)$ and the grain boundary mobility $M(T)$:

$$k = k_0 \gamma M, \qquad (2)$$

where T is the temperature and the factor k_0 is generally assumed to be constant. For ideal static grain growth the value of k_0 is ~0.5 in three dimensions and ~1.12 in two dimensions (Mullins, 1989; Weygand and others, 1998). Below we show that in practice k_0 is actually not a constant, but in fact depends on the microstructure (the ideal case being a particular instance). The factor k_0 itself is usually difficult to determine from experiments or measurements in nature (i.e. polar ice caps). This is because one normally only obtains k, which also includes the surface energy and grain boundary mobility. If k depends on microstructure through the parameter k_0, one cannot apply k obtained from one study to another situation where the microstructure may be different. In this paper we show that k_0 varies with microstructure and how ignoring this may lead to erroneous results if applied to polar ice caps.

If static grain growth were the only process operating in polar ice, the grain size should increase steadily with the age of the ice, and hence with depth. The observation in several ice cores that grain size stabilizes at a certain depth suggests that another process operates which balances the increase in grain size (Alley, 1992; De La Chapelle and others, 1998; Durand and others, 2006). If this other process leads to a reduction of grain size, a balance between grain-size increase and decrease will be reached at some point. The process usually invoked to explain the grain-size reduction process is polygonization or rotational/continuous recrystallization (Urai and others, 1986; Alley, 1992; Alley and others, 1995; Duval and Castelnau, 1995; Faria and others, 2002).

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Rotational recrystallization is a deformation-driven process. Deformation by dislocation creep introduces dislocations in the crystal lattice, which can accumulate in planar zones or tilt walls that define regions within a grain with small differences in their lattice orientations. The lattice within these regions or subgrains within a grain thus rotate relative to each other. Progressive rotation of the subgrains with ongoing strain eventually leads to the formation of high-angle grain boundaries, and the subgrains they bound become real grains (Read, 1953; Duval and others, 1983). Rotational recrystallization can be regarded as a process that effectively splits grains into two or more grains (Mathiesen and others, 2004; Placidi and others, 2004). Each split increases the number of grains, N, in a volume by 1. The increase in N, and hence decrease in grain size, thus depends on the split rate f per grain:

$$\frac{dN}{dt} = fN. \quad (3)$$

The parameter f may depend on many factors, most importantly on strain rate and hence on deviatoric stress (e.g. through Glenn's flow law; Alley, 1992). However, in a first approximation it is usually assumed that the strain rate is approximately constant within the upper part of the core where our calculations apply (Lipenkov and others, 1989; Thorsteinsson and others, 1997; Montagnat and Duval, 2000). The split rate of a grain probably also depends on the size and deformation history of that grain. A split rate proportional to grain size was, for example, assumed by Mathiesen and others (2004) and Placidi and others (2004), while Morland (2009) studied the effect of ice flow history. However, the simplest (but not necessarily realistic) assumption is that f is a constant, not depending on grain size or any other factor. This simplification is permissible here, since this paper is mainly concerned with the influence of microstructure on growth rate, and we do not intend to model a particular ice core. For this case, a simple analytical solution exists for the stable grain size. Assuming that the grain growth exponent n is 2 in Equation (1), one derives (see Appendix)

$$\frac{dN_{(t)}}{dt} = -\frac{3ka^{2/3}}{2} N_{(t)}{}^{5/3} + fN_{(t)} \Leftrightarrow r_{(t)}{}^2 = \frac{3k}{2f}\left(1 - e^{\frac{-2f}{3}t}\right). \quad (4)$$

Here a is a geometrical factor relating the mean grain radius, r, to the number, N, of grains in a volume. For illustration, by applying this equation to the North Greenland Icecore Project (NorthGRIP) ice-core data (Fig. 1), one obtains a growth constant of $k \approx 5.0 \times 10^{-3}$ mm^2 a^{-1} and a split rate of $f \approx 1.5 \times 10^{-3}$ a^{-1} or once every 650 years. These numbers are within the range of those reported in the literature (Gow, 1969; Thorsteinsson and others, 1997; Svensson and others, 2003; Mathiesen and others, 2004). The question, however, is whether the values obtained are realistic and meaningful.

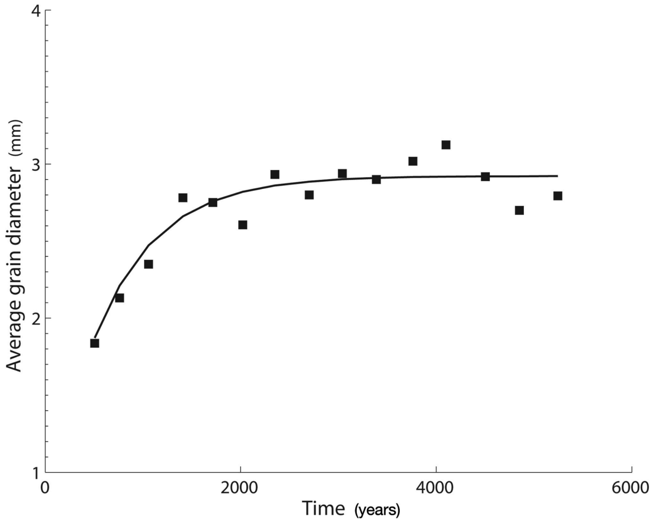

Fig. 1. Fit of analytical model (Equation (4)) to the average grain diameter as a function of age as observed in the NorthGRIP ice core (squares; data from fig. 3 in Mathiesen and others, 2004). Fit parameters are $k = 5.0 \times 10^{-3}$ mm^2 a^{-1} and a split rate of $f = 1.54 \times 10^{-3}$ a^{-1} or once every 650 years.

NUMERICAL SIMULATIONS

We used the numerical modelling platform Elle (Jessell and others, 2001; Jessell and Bons, 2002; Bons and others, 2008) to simulate the process of grain growth and grain splitting. The Elle software was developed to simulate the microstructural evolution in materials such as rocks. It has been applied to the simulation of a range of processes, such as static grain growth in anisotropic polycrystals or partially molten rocks (Bons and others, 2001; Becker and others, 2008), dynamic recrystallization (Piazolo and others, 2002, 2004) and strain localization (Jessell and others, 2005). The main distinguishing features are (1) that it uses a two-dimensional (2-D) image of the actual microstructure, and (2) that it uses operator-splitting to allow a range of different processes to operate on, and modify the microstructure. This means that simultaneously operating processes (such as grain growth and grain splitting) are modelled as isolated individual processes that sequentially modify the microstructures in very small increments.

The microstructure is defined by a contiguous set of polygons that are themselves defined by boundary nodes that link straight boundary segments (Fig. 2). The polygons typically represent individual grains. Changes in the microstructure are achieved by (1) changing the properties of polygons or boundary nodes, (2) changing the position of boundary nodes, which implies a change in shape of the polygons, and (3) creating, removing or reordering boundary nodes and segments. A change in shape can be the result of deformation, for which the finite-element code, Basil, is available in Elle (Houseman and others, 2008). A change in shape can also be the result of the movement of boundaries (grain boundary migration), for example in the case of grain growth.

The movement of grain boundaries is modelled by sequentially selecting each boundary node, and applying a small incremental displacement that depends on the driving force for migration and the intrinsic boundary mobility. In this study we test the validity of Equation (4) by combining a static grain growth routine that moves grain boundaries, and a split routine that divides grains into two daughter grains.

The normal grain growth routine simulates ideal isotropic growth (without grain boundary energy anisotropy). For each time-step, the routine goes through the list of all boundary nodes and calculates the local radius of curvature, r_c, using the node and its immediate grain boundary neighbours. The velocity, v, of the node in the direction of the centre of the curvature is calculated using

$$v = \frac{M\gamma}{r_c} \text{ and } \Delta x = v \cdot \Delta t. \quad (5)$$

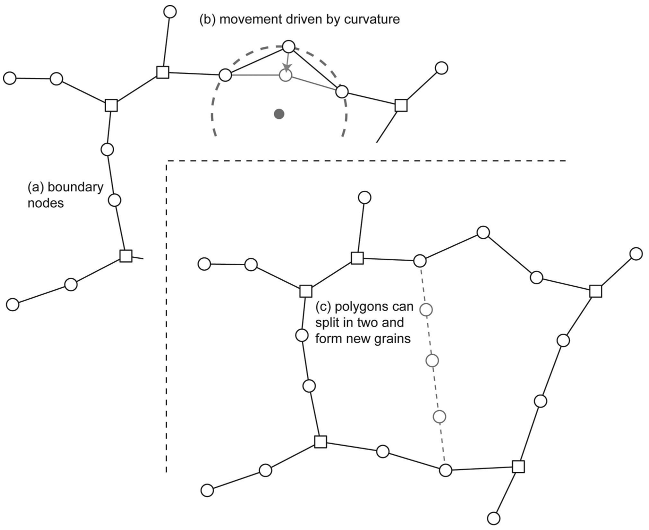

Fig. 2. Basic structure of the Elle model. The model consists of polygons which represent grains, and these polygons are in turn defined by boundary nodes (a) that are connected by straight boundary segments. Only boundary nodes with two or three neighbours are allowed in the model. The boundary nodes can move (b) and their movement is determined by the curvature of the boundary of the polygon at that point. Grains are split by the introduction of a new straight boundary that links two existing nodes (c).

The node is then moved over a distance Δx for a small time increment Δt. This routine results in ideal growth with a linear increase in mean grain area A, implying a growth exponent of $n=2$, and $k_0=1.22$ (Figs 3 and 4a). This would be the growth exponent as expected from theory (Humphreys and Hatherly, 1996). However, growth exponents measured in natural ice may deviate from that value due to other processes not taken into account here.

The effect of rotational recrystallization was implemented by randomly splitting each grain with a probability of f every time-step for each grain. This probability determines the rate of grain-size reduction by splitting. For this, each grain is selected in turn, and a random number generator determines whether the grain will be split. If so, one of its nodes is randomly selected and a new boundary is constructed across the grain, in a random orientation. Each time, the program checks whether the intended split will cause topological problems, such as intersection of the new boundary with another boundary or that a tiny grain has insufficient available nodes to split between. As a result, some splits are cancelled and a set value of f of $1.54 \times 10^{-3}\ \mathrm{a}^{-1}$ results in an effective split rate of $1.52 \times 10^{-3}\ \mathrm{a}^{-1}$, meaning that on average 1.3% of attempted splits are cancelled when a steady state has been established.

As expected, a stable grain size is established as a result of the combination of growth and splitting (Figs 4b and 5). For $M\gamma = 3.2 \times 10^{-3}\ \mathrm{mm^2\,a^{-1}}$ ($k = 3.90 \times 10^{-3}\ \mathrm{mm^2\,a^{-1}}$) and $f = 1.52 \times 10^{-3}\ \mathrm{a}^{-1}$), the average stable grain diameter is $3\ \mathrm{mm}^2$. To compare this result with the analytical model, we must rewrite Equation (4) for the 2-D case:

$$A = \frac{k}{f}\left(1 - \mathrm{e}^{-ft}\right) \Rightarrow A_{t\to\infty} = \frac{k}{f}. \qquad (6)$$

The average stable grain area predicted by the analytical model (Equation (6)) is similar to the value obtained with the

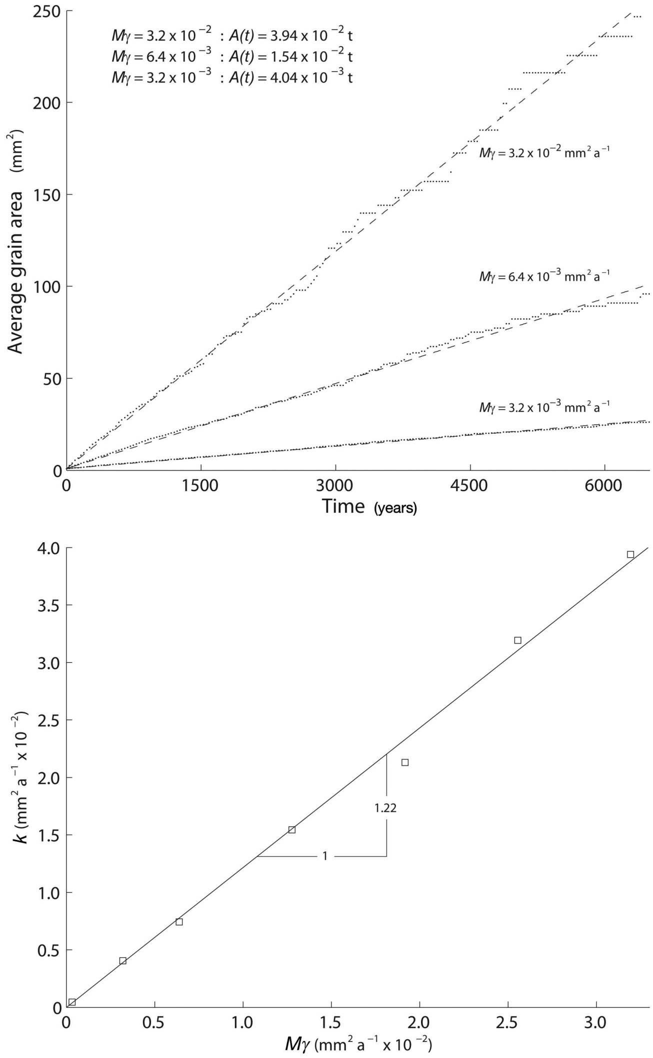

Fig. 3. (a) Growth curves for models of pure static grain growth. For $M\gamma = 3.2 \times 10^{-3}$, 6.4×10^{-3} and $3.2 \times 10^{-2}\ \mathrm{mm^2\,a^{-1}}$, the average grain area increases linearly with time. (b) Plot of k values measured from simulations as a function of the set value of $M\gamma$. The slope of 1.22 is the value of k_0.

Elle simulation, although the stable state is only reached after ~4000 years in the simulation. To achieve stabilization of the grain size after ~2000 years, as in the case of the NorthGRIP data, one has to roughly double both k and f. The discrepancy between the analytical model (Equation (4)) and the numerical simulation can be explained by considering the microstructure (Fig. 4). Static grain growth produces a regular foam texture. The frequency distribution of grain diameter has a maximum at about the average grain area (Fig. 6), and the normalized grain-size distribution is time-invariant (for steady-state growth). When a stable grain size is reached due to a balance between grain boundary migration and splitting, the grain size distribution changes significantly, with an increase of the frequency of very small grains, but also an increase in grains much larger than the average.

The change in microstructure changes the growth behaviour. The relatively abundant small grains have a high boundary curvature and quickly disappear. Yet many new small grains constantly appear because in the model every grain has the same chance of being split, independent of its size. The effect of the widening of the grain-size spectrum is an increase in the growth rate that balances the split rate in

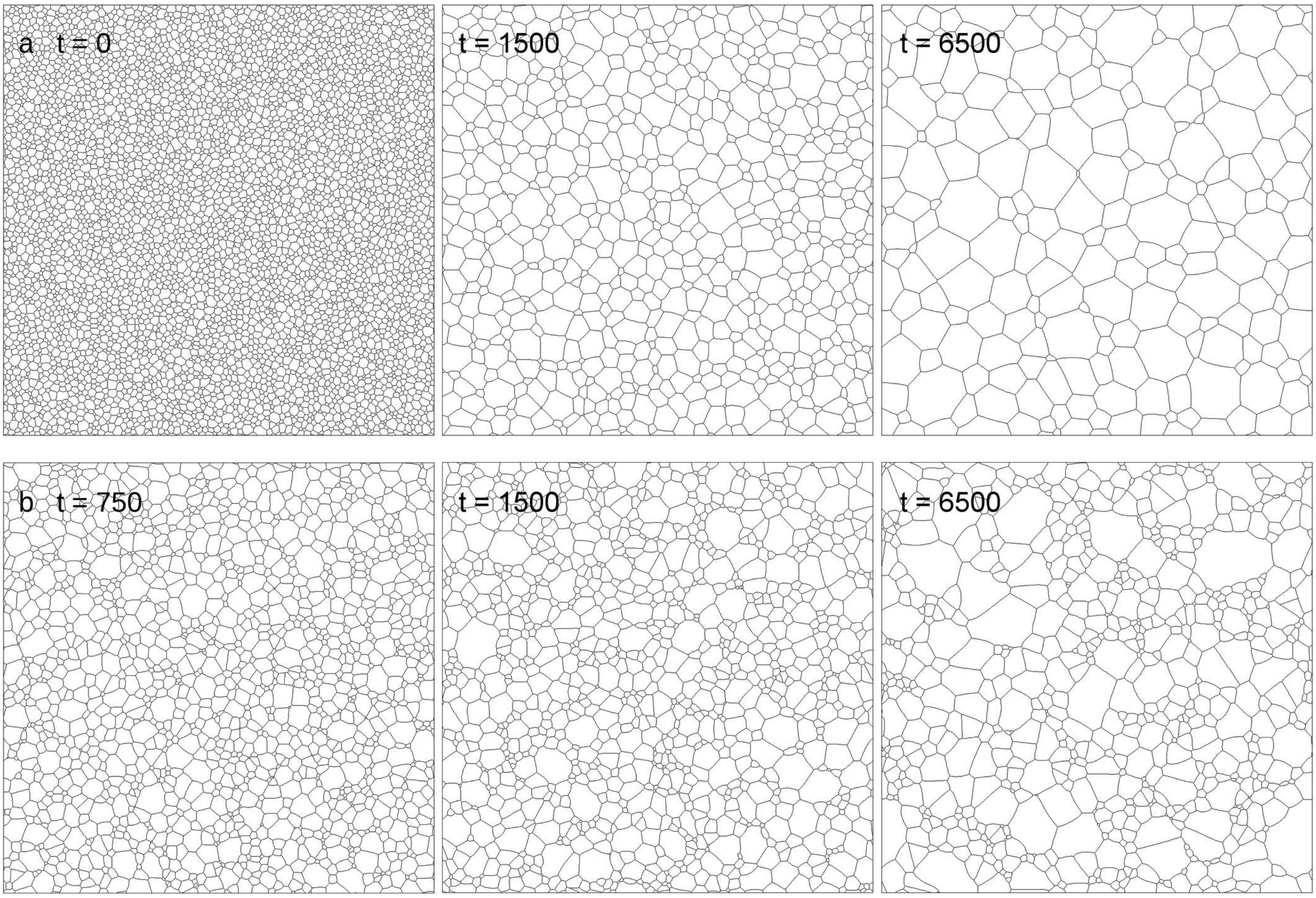

Fig. 4. Results of numerical simulations with Elle. (a) Static grain growth only, for 6500 years and $M\gamma = 3.2 \times 10^{-3}\ \mathrm{mm}^2\ \mathrm{a}^{-1}$. (b) Simulation with same starting aggregate and settings as for (a), but with splitting at a constant $f = 1.54 \times 10^{-3}\ \mathrm{a}^{-1}$ added, which leads to the establishment of a stable grain size after ~4000 years, and a different microstructure compared to static grain growth. Size of box is 72 mm × 72 mm.

Equation (4). This can be seen if one stops the splitting when a stable grain size has settled but grain growth is allowed to continue (Fig. 7). The initial growth rate is over three times higher than the stable growth rate that is reached after the mean grain area has about quadrupled. This implies that the factor k_0 is not a constant, but a function of the microstructure. For the stable foam texture that results from static grain growth only, k_0 is 1.22. When the microstructure is the result of a competition and random splitting, the effective value of k_0 increases to 4.2 (an increase by a factor of 3.5).

DISCUSSION

The modelling in this paper is in no way intended to argue that the microstructure and grain size of the upper hundreds of metres of polar ice is determined by a balance of static grain growth and a constant grain-splitting rate. For this reason, we do not attempt to fit the results of the numerical simulations to obtain a growth constant or an average split rate of once every so many years. The dynamics of rotational recrystallization are much more complex (Faria and Kipfstuhl, 2004; Weikusat and others, 2011) than can be grasped by a simple constant split rate that is equally applied to all grains.

The intention of this paper is to show one of the pitfalls of numerical simulations that do not include the effect of

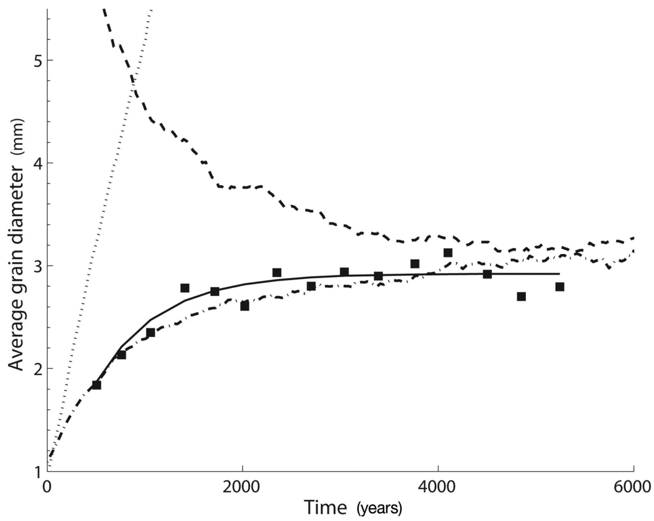

Fig. 5. Evolution of the average grain diameter with time. Static grain growth ($M\gamma = 3.2 \times 10^{-3}\ \mathrm{mm}^2\ \mathrm{a}^{-1}$) results in a linear increase of grain diameter (dotted line) (Fig. 4a). Adding a constant split rate (f=1.54 × $10^{-3}\ \mathrm{a}^{-1}$) for all grains (Fig. 4b) results in the establishment of a stable average grain diameter (dash-dot line). Applying the same settings to an initially large grain microstructure (dashed line) results in the same steady state as for the initially small grain microstructure. For comparison the data from the NorthGRIP core (Fig. 1) have been plotted as well (squares) along with their fit (solid line).

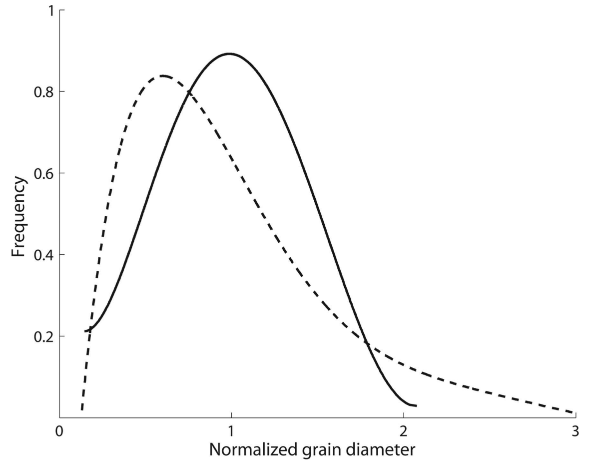

Fig. 6. Normalized frequency distributions of grain diameter. Solid line is the average of 16 simulations of only static grain growth (Fig. 4a). Dashed line is for eight simulations after a steady state has been reached by the competition of static grain growth and splitting (Fig. 4b).

microstructure. The simple analytical model of growth versus splitting produces a curve that can be fitted to data from ice cores. At first sight, it appears that the use of a simple splitting constant, *f*, would be the most problematic simplification. However, our simulations show another simplification that is rarely considered, namely lack of coupling between the growth 'constant', k_0, and *f*. The parameter k_0 is determined by the microstructure. As the microstructure is a variable, k_0 is not a constant, but a variable as well. This observation is of importance because many models that incorporate grain growth, assume k_0 to be constant (Cotterill and Mould, 1976; Randle and others, 1986; Montagnat and Duval, 2000). The numerical simulations show that changing the grain-size distribution from normal to approximately log-normal increases k_0 by a factor of ~3.5. Clearly, other factors may influence k_0, such as grain boundary morphology and grain shape.

The simulation of static grain growth shows that the resulting grain-size distribution is relatively narrow. A normal distribution of measured grain diameters is predicted for static grain growth (Humphreys and Hatherly, 1996). However, grain diameter distributions in ice are usually log-normal, even at relatively shallow depths (Arnaud and others, 1998), for example at 115 m depth in the NorthGRIP core (Thorsteinsson and others, 1997; Svensson and others, 2003). This indicates that the microstructure of ice is already strongly affected by processes other than only static grain growth, well above the transition to a stable grain size. This observation supports the suggestion by various authors (Kipfstuhl and others, 2006, 2009; Durand and others, 2008; Weikusat and others, 2009a,b) that dynamic recrystallization and other processes (Arnaud and others, 2000; Faria and others, 2010) already commence at relatively shallow depth.

The observation that k_0 is dependent on the microstructure may have consequences for the interpretation of grain growth experiments to determine the growth exponent *n*. If the experiment is started with a non-equilibrium microstructure, k_0 may initially be much higher. As the microstructure stabilizes to that characteristic of static grain growth, k_0 decreases (Fig. 7). If the initial phase of microstructural equilibration is included in an analysis where *k* is assumed to be constant, one would erroneously obtain an exponent *n* that is larger than the real value. For example, the applicable value for k_0 in a polar ice cap would be different from one obtained in a static grain growth experiment, because the microstructure, and hence grain growth in nature, is influenced by additional factors, such as dynamic recrystallization, presence of impurities and bubbles (Cuffey and others, 2000).

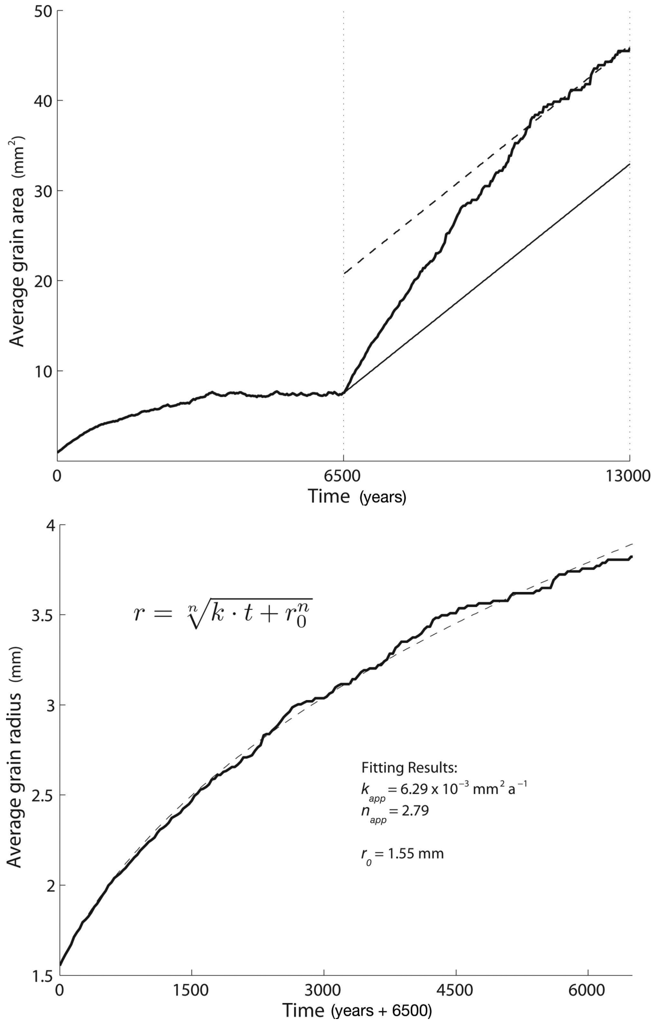

Fig. 7. (a) Grain growth experiment ($M\gamma = 3.2 \times 10^{-3}\ mm^2\ a^{-1}$) where splitting ($f = 1.54 \times 10^{-3}\ a^{-1}$) is turned off after 6500 years. The dashed line shows the growth rate of $k_0 = 1.22$, which is achieved ~4000 years after splitting is stopped, at which stage a foam texture has been established. Just after stopping the splitting, the growth rate is much higher, corresponding to $k_0 = 4.2$. (b) Detailed plot of the experiment in Figure 7a after 6500 years (splitting has been stopped). Equation (1) has been fitted to the experimental curve, giving apparent *k* and *n* values that are incorrect: n_{app} is 2.79 instead of 2 and k_{app} ± is 6.29×10^{-3} instead of $3.90 \times 10^{-3}\ mm^2\ a^{-1}$.

CONCLUSIONS

We simulated the process of pure static grain growth and grain growth in competition with another process, namely splitting grains at a constant rate. The numerical simulations show that the growth parameter k_0, normally taken to be a constant, is in fact a function of the microstructure. When the microstructure is only affected by static grain growth, k_0 is 1.22. The change in microstructure resulting from additional splitting increases k_0 by a factor of ~3.5.

The numerical simulations show that the log-normal grain-size distributions observed in polar ice at shallow depth (≥100 m) are not in accordance with the expected distributions for static grain growth. At least one other process must operate to widen and skew the distribution towards a log-normal distribution. This supports the idea that dynamic recrystallization already operates and influences the microstructure at shallow depth.

The growth exponent and grain boundary properties (surface energy and mobility) are usually determined from experimental growth curves. If the microstructure changes during these experiments, k_0 should not be assumed constant. Making this assumption leads to an overestimate of the growth exponent n.

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APPENDIX: DERIVATION OF EQUATIONS (4) AND (6)

The number, N, of grains per unit volume equals

$$N = \frac{1}{ar^3}, \tag{A1}$$

where a is a shape factor that depends on the shape of grains. If only static grain growth operates, Equation (A1) can be combined with Equation (1), which gives, assuming $n=2$:

$$N = \frac{1}{a\left(kt + r_0^2\right)^{3/2}} \Longleftrightarrow \frac{\mathrm{d}N}{\mathrm{d}t} = \frac{-3ka^{2/3}}{2} N^{5/3}. \tag{A2}$$

Adding the effect of splitting Equation (3) has an additional term, and the number of grains per time is

$$\frac{\mathrm{d}N}{\mathrm{d}t} = -\alpha N^{5/3} + fN, \text{ and hence } -\int \frac{\mathrm{d}N}{\alpha N^{5/3} - fN} = \int \mathrm{d}t, \tag{A3}$$

where $\alpha = 3ka^{2/3}/2$.

This equation can be solved with the standard indefinite integral:

$$\int \frac{\mathrm{d}x}{x(x^p - b^p)} = \frac{1}{pb^p} \ln\left(\frac{x^p - b^p}{x^p}\right). \tag{A4}$$

By using $p = 2/3$, $f = N$ and $b = (f/\alpha)^{3/2}$ the relation between t and N results in

$$t = \frac{-3}{2f} \ln\left(\frac{N^{2/3} - \frac{f}{\alpha}}{N^{2/3}}\right) \Longleftrightarrow N^{-2/3} = \frac{\alpha}{f}\left(1 - \mathrm{e}^{\frac{-2f}{3}t}\right), \tag{A5}$$

and by using Equation (A1) grain-size evolution finally gives

$$r^2 = \frac{3k}{2f}\left(1 - \mathrm{e}^{\frac{-2f}{3}t}\right). \tag{A6}$$

Note that variable α is replaced by full expression (A3), and the shape factor, a, used in Equation (A1) is cancelled out of the equation.

The derivation of Equation (6) for two dimensions is similar to the above. In two dimensions, Equation (1) still holds and if $n=2$ we can write for the mean grain area, A:

$$A - A_0 = kt. \tag{A7}$$

The number, N, of grains per unit area equals $1/A$, which gives

$$N = \frac{1}{kt + A_0}. \tag{A8}$$

Taking the time derivative and adding the increase in number of grains as a result of constant splitting, Equation (3) results in:

$$\frac{\mathrm{d}N}{\mathrm{d}t} = \frac{-k}{(kt + A_0)^2} + fN = -kN^2 + fN. \tag{A9}$$

The last equation can be solved with the indefinite integral of Equation (A4) to obtain:

$$\frac{1}{N} = A = \frac{k}{f}\left(1 - \mathrm{e}^{-ft}\right). \tag{A10}$$

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