“Ice fabrics in two-dimensional flows: beyond pure and simple shear”
by Richards et al.

Review comments by M. Montagnat, January 2022.

Please find below the review of the new version of the paper. Since a lot of the comments I gave for the first review were not taken into account, I put at the end of the document the previous review I did, for the editor and the authors to do comparisons. The comments in concerned are underlined in yellow.

One of my concern on this paper is the feeling it gives me of a lack of clarity. Hypotheses are done with the model used here, and this is very fine for me, but many of them are not clearly stated. For instance:
- by assuming the rotation rate of the orientation distribution with equation 5, the authors are doing the assumption of a Taylor-type of mechanical interactions between grains. Indeed, the only terms that act on the rotation rate is the strain-rate (and the vorticity that rotate the full distribution). Another way of doing, that would still be a rather crude parameterisation, would be to follow Gillet-Chaulet et al. 2006 paper (eq 13) and put a stress component into the rotation rate. In this case, the mechanical hypothesis behind the orientation distribution rotation is in between a Taylor and a Sachs hypothesis.
The discussion about that in part 3.1, lines 230-245, is very deceiving... What is said lines 238-239 appears just wrong to me in a mechanical point of view. And the justification lines 240-245 is really astonishing! One can always parameterise any model to provide the result expected, it does not mean that the good "physics" is in the model!!! Please remove this sentence.
And please let’s assume the choice of the parameterisation as an "OK" hypothesis in order to simplify, especially since there exist no better way of doing so far.
From this choice depends the value of the parameters that have been tuned in Richard et al. 2021 on compression and simple shear cases, and this is fine! Providing it is clearly stated...
- Considering the migration recrystallization mechanisms (in particular lines 264-265), the authors know that what drives them is more complicated that only the “cumulated shear strain”... What drives nucleation and grain boundary migration occurring during dynamic recrystallisation is related to the STORED strain energy, that is related to geometrically necessary dislocations, the ones that help compensating the strain incompatibilities between grains, and their density is not simply related to the cumulated shear strain (some areas that are deforming “easily” cumulate a lot of shear strain and very few geometrically necessary dislocations, so very little stored energy...).
Once again, it makes sense, to my point of view, to use such a simplification in a model devoted to large scale flow modeling, but please mention it as an hypothesis and not as the truth!

- Considering figure 2, for vorticity → infinity, there should be no fabric formed since the material experiences rigid body rotation only? Where could the girdle come from? What constrains the rotation within this girdle, under rigid-body rotation? What is the relative weight of the two parameterised recrystallisation regimes in this weak girdle? And how is it impacted by slight changes in the parameters? Is it robust?

- Once again, this study lies on parameterisation performed in laboratory conditions, therefore very far from the “real world” it aims at representing. A sensibility study would therefore be necessary, to check, for instance, which of the rotation / migration recrystallization process is dominating and in which situation? Does that make sense with “real world” observations?
What happens when the parameters are shifted away from the linear fit? What is the impact on, for instance, the kinetic to steady-state?

This sensibility study is necessary to check the robustness of the modeling and therefore its ability to be predictive.
- Line 411-415: the 2D assumption is strong, and, as already mentioned in my previous review, was shown to give “correct” results only is some specific parts of the ice cores. This part is not an explanation of the limitations of the 2D assumption and the impact it could have on the results, it is more the expression of the authors’ opinion “is a good first step”... It may be, but please, explain us why and under which limitations.

<u>More specific comments:</u>

- Line 21: what does "validated" means? When can we consider a model to be fully validated? In particular, this model has not been validated in other deformation regime than simple shear and compression, while you are going to use it in very different conditions.

- Part 2.2.1: VERY IMPORTANT!!! This paragraph contains explanations that are contrary to what is known for ice and recrystallization mechanisms. It should be re-written and bibliography may be more correctly used. For instance: **Chauve et al. 2017 do not show that non-basal slip is active! They just show that under some specific conditions, geometrically necessary non-basal dislocations can be observed. It has already been mentioned in my previous review, and since I am co-author of Chauve et al. 2017, it is very important for me that the authors correct it!**
The mechanisms described lines 42 and 43 are not stricto-sensus deformation mechanisms. Only crystal plasticity in the list is a deformation mechanism. Recrystallization is a process of accommodation that facilitates the deformation, but does not produce a deformation per-se... For instance, during post-dynamic or static recrystallization there are a lot of microstructure modifications without any deformation produced. Please modify.
Line 42: Migration Recrystallization does not refer to grain boundary migration. Migration Recrystallization refers to a recrystallization associated with nucleation AND grain boundary migration, on a regime where grain boundary migration is fast. But nucleation does take place also. Above all, migration recrystallization refers to a mechanism that is driven by stored strain energy while grain boundary migration can occur driven by the reduction in grain boundary surface energy. It would be very important to clearly make the distinction and not mis-explain the migration recrystallization regime... Please see Humphreys and Haterly 2004 if necessary.
Line 45: the paper by Chauve et al. 2017 does not allow to say that non-basal dislocation activity is restricted to high temperature regime... This is just that the experiments presented in this paper are at high temperature. And once again, it just observes some non basal dislocations and no non-basal slip activity. So this sentence should be removed.
Lines 51-55: I am really puzzled to read this part, especially when dealing with ice! Recent results have shown (and some done by one of the co-authors, S. Piazolo), that strain heterogeneities in ice can not be resumed relatively to the main deviatoric stress (see Grennerat et al. 2012 for instance), and that strain distribution is very heterogeneous, with strain high in area of low stress, and the contrary... (see Piazolo et al. 2015, Montagnat et al. 2015, Chauve et al. 2017 Phil Trans). Similar observations exist also in other materials. So to say that "strain energy stored in a grain is directly related to the imposed strain" is somehow too vague and may be wrong... The reference given here, Gottstein and Shvindlerman 1999 is a book that I can not access to to verify. It could be stated as a working hypothesis, and justified, but not as the truth.

Previous review, August 2021:

This paper presents some simulations of ice fabrics in conditions relevant for the Antarctic ice sheet. The simulations are made by means of a numerical model inspired by the work of Placidi et al. (2010), that simulates the rotation of individual ice crystals included in a orientation mixture that is submitted to a given strain field, and includes a parametrisation of the effect of dynamic recrystallization on this rotation. This model has been applied recently in Richards et al. 2020 (EPSL) to reproduce laboratory observations.

This paper suffers from a lack of clear explanation of the strong assumptions that are included in the numerical simulations and the associated parametrisation.
Such assumptions, that I detail below, can have a significant impact on the results, and, since they are not clearly stated, they are not tested either, and this undermines the credibility of the study.

- It would be first necessary to recall the way the strain and stress interactions between grains are dealt with in the model.
 Unlike stated in Richards et al. 2020, the model, that derives from previous works of Faria et al. (2006-I,II,III), assumes an homogeneous strain rate, meaning that each crystal is submitted to the same strain rate. This hypothesis, apparently not clearly stated in any of those works, has been shown by Gagliardini (2008) in its response to Faria et al. (2006) to correspond to a Taylor-type of approximation, meaning uniform strain.
 Such an approximation can be clearly recognised as such, and then it is possible to evaluate its impact on the simulation of the mechanical response of the polycrystal, as done by Castelnau et al. (1996). In particular, Castelnau et al. 1996 showed that this approximation was not satisfactory for a highly anisotropic material such as ice since it requires the activation of non-basal slip systems at a non realistic level. By doing so, it strongly reduces the level of strain heterogeneities between crystals, the latter being the main driving force for dynamic recrystallisation. We can expect this approximation to impact the modelling of this mechanism.
Since Castelnau et al. work, it appeared clear that in situation where the full stress and strain field heterogeneities can not be taken into account, an homogeneous stress approximation is more adapted to simulating the mechanical response of ice (see maybe, for instance, the work of Pettit and co-authors).
In Richards et al. 2020, it is mentioned that the fact that the model considers a large number of grains for each orientation specie, reduces (or annihilates) the dependency on the grain orientation on the mechanical state and response (strain and stress). Gagliardini (2008) showed, based on Lebensohn et al. 2004 work, that this is not true and that only the dependency on the neighbourhood is reduced by considering many grains for each orientation.

- The way the dynamic recrystallization is simulated is also based on important assumptions, not always in agreement with laboratory or field observations. It would be necessary to explicitly mention these approximations, and justify their use.
First, in the main part of ice sheets, where temperature and strain rates are low, the main recrystallization mechanisms is continuous (or rotation) recrystallization, characterized by a low driving force for grain boundary migration (see for instance De la Chapelle et al. 1998). In such a regime, the fabric is supposed to evolve only slightly owing to recrystallization, and to remain mainly dominated by deformation (see also Montagnat et al. 2012, for the Talos Dome core).
It would therefore be important to evaluate, in some appropriate locations, the relative influence of the simulated rotation recrystallization versus migration recrystallization in the obtained fabrics. If migration recrystallization, the way it is simulated here, has too much weight on the resulting fabric in location where rotation recrystallization is expected to dominate, the model can be questioned.
In areas where migration recrystallization dominates (high temperature / high strain rate), the grain boundary migration kinematic dominates the softening process, so that the fabric and microstructure end up resulting from the stress state, and loose track of the deformation history (see what happens at the bottom of the GRIP, NEEM, Dome C ice cores for instance, or also in high shear conditions,

Hudleston 1977 for instance, or even Hudleston 2015, see also Alley 1992). Can we expect, in such conditions, an evolution of fabric with strain?

- Second, concerning the physical mechanisms. Migration recrystallisation is supposed, in the presented model, to be governed by a “deformability” related to the total deformation accumulated in the grain. Dynamic recrystallization mechanisms (nucleation and GBM) are related to the local accumulated dislocations in the form of geometrically necessary dislocations (responsible for local misorientations) and statistically stored dislocations. The densities of SSDs and GNDs are not, by default, correlated with the total amount of strain experienced by the grains. It has been recently shown by Harte et al. 2020 for Ni-based alloy by coupled EBSD observations and Digital Image Correlation strain measurements (stored energy is different from cumulated strain).
In various experiments performed on ice, or full-field modeling, it was shown that there is no relationship between the amount of deformation (measured by Digital Image Correlation for instance) and the Schmid factor of a grain. There is therefore no “hard grains”, or “soft grains”, since the local behavior is much more controled by the grain interactions and the resulting stress redistribution. The uniform strain assumption neglects this aspect too.

My point of view concerning these approximations made relatively to dynamic recrystallization is that they can be useful and justified in the simplified numerical modeling approach used in this work. Nevertheless, it has to be clearly mentioned that they ARE approximations, and their effects should be tested.

- The way the boundary conditions are selected is very unclear to me. Considering that fabric is being formed during deformation in depth of the ice sheet, how can a surface velocity map be representative of the in-depth flow conditions? Can the authors be clearer about that?
The 2D approximation is also strong. It was shown by the Elmer-Ice community to be OK in the case of specific types of flow, like divides (where there is little divergence or convergence). Can it holds for more complex situations such as fast ice streams? What effect could it produce on the fabric evolution? This should be justified and tested.

- What “highly-rotational” conditions represent “in reality”? Does that correspond to area where a block of ice rotates freely on itself? Can that happen in the depth of ice sheets? If yes, where?

- About the capacity of the model to predict steady-state fabrics. Steady-state fabrics depend strongly on the mechanical state the ice is experiencing, and the flow history. I therefore don’t understand how could the model be realistically predictive considering the strong assumptions made (1) on the mechanical state (Taylor-type of approximation) and (2) on the recrystallization mechanisms.
In order to test the predictability of the model, it would be necessary to test how robust it is to variations in the parameters, and to the 2D approximation, and to the use of surface velocity vorticity. Such a robustness test was already missing in Richards et al. 2020.

Specific comments:

- Abstract: “a definitive classification of all fabric patterns”. This sentence lacks humility... in particular owing to the lack of clarity of the text regarding the assumptions made (see my comments above), and their effects on the obtained simulation results. On top of that, the 2D simulations highly limits the ability to provide this full classification, and also the fact that strain states were deduced from surface observations, very likely not relevant for flow in the depth of the ice sheet.
“Highly-rotational fabrics... produce a weak fabric”. Can we expect a fabric to produce a fabric? Not clear to me.

- Part 2.1: The presentation of the processes made in this part is simplistic regarding the many other observations and analyses that exist in the literature (see my comments above). It is OK if it is clearly presented as assumptions made to simplify the processes and better introduce them into the modeling approach. It is a very classical approach to simplify the physics in order to be able to take it into account in a modeling approach. But it needs therefore to be clearly stated, justified, and tested when the results are presented.
What is the “real situation” responsible for some “rigid-body rotation”?

- Part 2.2: Various studies were done in the past that include torsion and compression, or shear and compression, and therefore that consider a more complex scheme that pure or simple shear. None of them are mentioned in part 2. I can suggest Budd et al. (2013), Duval 1981 for instance, but others are mentioned in Hudleston 2015.
At domes, in fact close to domes since deep ice cores are never exactly at the dome location, if girdle is observed it is that not only compression occurs, but also lateral extension. This can signify that the core was cored slightly on the flank, or that dome has moved with time (see for instance NEEM, Vostok, EDML, NorthGRIP). For nearly every deep ice core drilled close to a dome, a shear component was observed close to the bedrock, that participated to strengthen the single-max fabric (see for instance Talos Dome).
Can we consider ice deep in the ice sheet to be fully unconfined?
Please cite Gusmeroli et al. 2012 for sonic measurements of fabrics.

Part 2.2.2: How do you extrapolate surface velocity measurements to get access to in-depth flow history? What are the limitations? Where can it be used, and where it can’t, and why?

Part 3: See my comment above, please provide here the main assumptions that are made in this model, from a mechanical point of view (how are the mechanical strain and stress field distributed in the microstructure, what is the flow law considered, how are the interactions taken into account, what are the boundary conditions, etc...), and from a physical point of view (what are the assumptions made to formulate the recrystallisation mechanisms, and why).
Some assumptions made, like the parametrisation with the deformability for instance, or the one for the temperature effect, are very strong and very likely control the results. It would be clearer to emphasise them and test their relative impact.
As it is presented, it appears to me as if the model was a parametrisation of the rotation of crystals, under homogeneous imposed strain, and not a mechanical modeling (such as Elmer-Ice or VPSC) able to provide interactions between the stress and strain field and the fabric evolution (see Martin et al. 2009 for instance).

Part 4: the limitations associated with the 2D formulation are not mentioned. Can it be applied in every stress and strain configurations considered? See my comment above.

Part 4.3 and discussion: to my point of view, in order to test the robustness of the results presented, the authors should provide results within which the parametrisation is modified, and the effect of the assumptions made tested. In particular, the steady-state obtained is highly dependent on the way the recrystallisation is modeled, on the parameters that control the effect of temperature. By changing them slightly, are the steady-state still reached in the same conditions?

Part 5.2: I don’t think that the model can be, as it is, predictive in terms of relation between finite strains and steady-state fabric owing to the fact that it neglects the complexity of the deformation history along flow lines, that it considers a homogeneous state of strain. Taylor-type of approximation, by neglecting the strong anisotropy of ice, very likely underestimate the fabric

development rate (see Castelnau et al. 1996). It therefore seems to me hardly transferable to ice core interpretation.
Instead of citing Faria et al. 2014, please refer to some of the original work that deserve the credit, since Faria et al. 2014 is a review.

- Part 5.4:
Before Minchew et al 2018, you could refer to Russell-Head and Budd, 1979, Alley 1988, Van der Veen and Whillans 1990, etc...
By the way, the work of Minchew et al. 2018 seems to contradict the hypothesis of an evolutive effect of migration recrystallization, and go in favor of the fact that the fabric, in conditions where this recrystallization regime is dominant, is dominated by the state of stress (also mentioned by Alley 1992). Indeed, it shows that in shear zones, the fabric is very rapidly steady.

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