Reply to referee comments by Anonymous Referee #1 on TC-2016-167

(Strain localisation and dynamic recrystallisation in the ice-air aggregate: A numerical study. F. Steinbach et al.)

We thank Anonymous Referee #1 for a constructive review and regarding the proposed modelling approach and our conclusions as “sound and (…) reasonable”. In the following, we reply to the specific concerns addressed by the referee and state the corresponding changes in the revised manuscript. The referee comments are cited in italics and our reply is in blue font. If not indicated differently, any reference to page or line numbers are with respect to the discussion paper, not the revised version.

General Comments:

This paper presents micro-dynamical simulations of polycrystalline hcp ice containing air bubbles using a numerical approach based on the coupling of the numerical platform Elle, a front-tracking formulation that accounts for microstructure evolution due to different dynamic recrystallization processes (normal grain growth, strain-induced grain boundary migration, recovery, polygonization) and a viscoplastic model based on Fast Fourier Transform (VPFFT) to calculate the micromechanical fields (stress, strainrate, velocity, etc.) due to deformation of the constituent ice crystals by dislocation creep. In particular, the stored energy field calculated with VPFFT provides the driving force for the aforementioned recrystallization processes. Details of the integration between Elle and VPFFT and applications to different geomaterial systems have been reported in previous papers by the same team, including studies of the micro-dynamics of fully-dense ice polycrystals. This paper presents a new application of Elle/VPFFT, to study the ice-air system, aiming at a better understanding of the onset of dynamic recrystallization in, e.g. firn. One of the main conclusions with glaciological relevance of this study is that the presence of air bubbles induces a "composite material" behavior, which contributes to: a) higher strain localization in the ice crystals, and therefore faster onset of dynamic recrystallization compared with fully-dense ice, and b) weaker CPO–not caused by grain-boundary sliding–, as the volume fraction of air increases.

We thank the referee for this concise general comment and summary of the main topics and conclusions of our paper. We are pleased to read that our objectives and conclusions are apparently clearly explained in the manuscript.

Specific Comments:

While the proposed approach is sound and the main conclusions are reasonable, the specific treatment of the air inclusion phase, as far as its constitutive behavior and the treatment of the ice-air interfaces are concerned, needs to be better explained, including a better disclosure of the approximations involved. It is reported (section 2.6) that air bubbles are represented by an incompressible crystalline material with the same crystallography and slip systems as for ice, and that tau_s-air is set 5000 times smaller than tau_basal of ice. This seems to imply (more clarity is needed here) that the air is represented by hcp crystals deforming by basal, prismatic and pyramidal slip with equal critical resolved stresses.

The implications the referee is deducing from our description in section 2.6 are correct. For numerical reasons, air was described as crystalline material (section 2.6, page 8, lines 13-14) with slip systems similar than in ice Ih (basal, prismatic and pyramidal slip). For ice Ih, the pyramidal and prismatic critical resolved shear stresses were 20 times higher than for slip on the basal plane. The referee correctly assumes that the critical resolved shear stresses for all air slip systems were constant to approximate mechanical isotropy. As outlined in the manuscript, critical resolved shear stresses for the air phase were set 5000 times lower than for ice Ih basal slip. We agree that there is a need to better explain this approximation. Hence, we added a sentence on page 8, line 14. See our following reply for further explanations.

In turn, this implies the somehow unrealistic assumptions of: a) "anisotropic" bubbles (although the anisotropy remains small) and b) a unit cell unable to accommodate any volume change. The first approximation could have been avoided by adopting an isotropic viscoplastic behavior, or, even better, imposing zero stiffness (i.e. vanishing stress) to the unodes belonging to the air phase. With this said, I suspect (but I'd like to hear this from the authors!) that the predictions would not be dramatically affected.

We agree with the referee: Admittedly, this approach does not allow for a fully isotropic air material as deformation is only possible on defined slip systems. Our simplified approximation of the description of air inclusions is only correct if the results would not be dramatically affected by the unrealistic assumptions the referee was mentioning. Therefore, we updated our VPFFT code to impose zero stiffness to unodes in air inclusions (as suggested by the referee) to assume an air phase independent of any crystallography. For this comparison, the initial setups of F20 were used and deformed in one increment of pure shear to 1% vertical shortening to obtain instantaneous strain rates and stresses. We compared the results of the updated approach ("zero stiffness") with the VPFFT version used for the simulations presented in the manuscript (see attached figure R1.1). The results show:

(1) No significant difference in normalised von Mises strain rates, i.e. the location and intensity of strain localisation (cf. localisation factors "F")

(2) No significant difference in von Mises stresses for each unode obtained from the VPFFT output

(3) When using the VPFFT approach used for the simulations in the manuscript, mean pressure of both ice and air phase are zero. The variation in pressure in the air phase is very small and between one and two orders of magnitude smaller than in the ice phase.

One of the main observations of our study is that air inclusions cause and intensify strain localisation which provides driving forces for dynamic recrystallisation. The results of our comparison presented in figure R1.1 therefore indicate, that our treatment of the air phase as a very soft quasi-isotropic ice Ih crystal does not affect the predictions of the simulations. Using 5000 times softer slip for air "slip systems" than for ice basal slip and a stress exponent $n = 3$, we assume an even higher effective viscosity difference between the materials, which underlines why the results presented in figure R1.1 are essentially the same. As the results are almost identical, we did not re-run the simulations presented in the manuscript, but future simulations should use the new and updated VPFFT approach. Figure R1.1 will be provided as supplementary material.

In order to better discuss and present approximations made for the simulations (also the ones mentioned by referee #2), we added a paragraph to the new sub-chapter discussing model simplifications (4.5 Limitations of the modelling approach), where the simplified treatment of the air phase is discussed. We mention that for reasons outlined above our treatment of the air phase does not significantly affect the results.

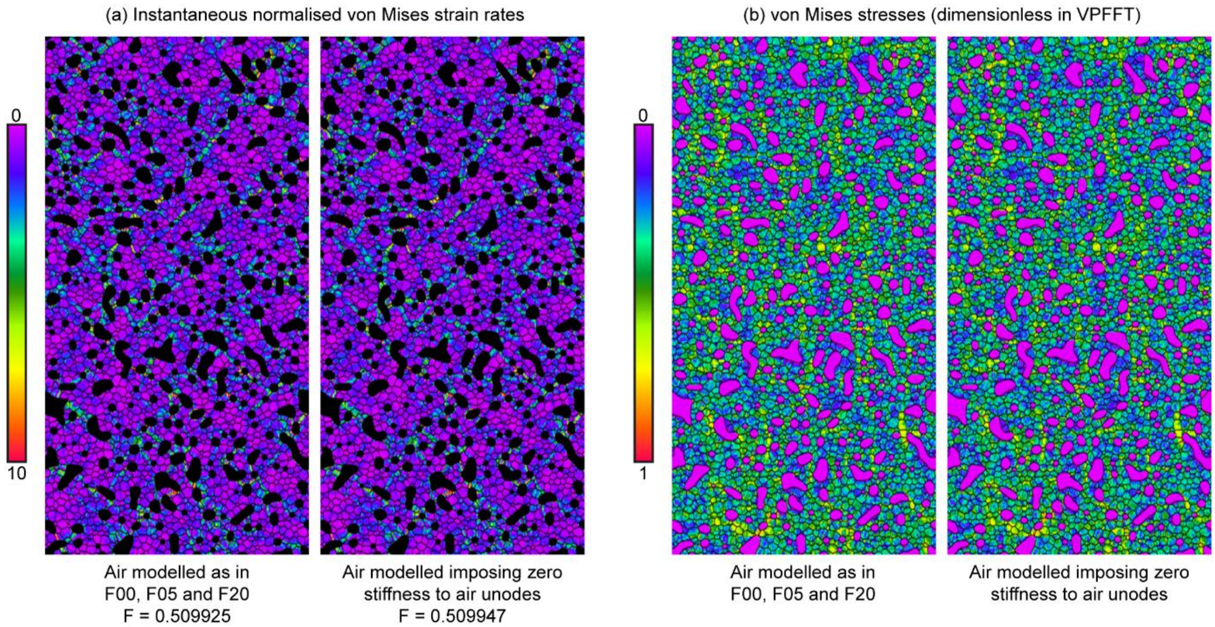

Figure R1.1: Comparison of the VPFFT model used for the simulations presented in the discussion paper with an modified algorithm that imposes zero stiffness to air unodes. These simulations comprised one step of VPFFT with an increment of 1% vertical shortening using the same initial setup as for simulation F20. We provide this figure as supplementary material and refer to it in the revised manuscript.

The second approximation is more delicate. The air phase/unit cell incompressibility implies the inability of the present approach to consider volume changes that are inherent to ice flowing under its own weight. Moreover, the incorporation of a constitutive description admitting compressibility would have also allowed improving the convoluted treatment of the behavior of the ice-air interfaces described in section 2.4.1, accounting explicitly for the effect of the bubbles' internal pressure, both in terms of mechanical behavior and as a controlling factor of the recrystallization process. Furthermore, the shortcomings associated with the simplified treatment of the air bubbles as an incompressible phase may be responsible for the somehow puzzling results, in the cases of the F05 and F20 microstructures, showing the overall porosity almost unaltered after ~50% vertical shortening. This makes the comparison with the EDML ice core at 80m depth presented in Fig. 8 questionable. This needs to be acknowledged and further model improvements to mitigate these limitations be discussed, before this paper is accepted for publication in The Cryosphere.

We thank the referee for pointing out an important assumption made in our simulation approach. Also referee #2 commented on the assumption that air is modelled as an incompressible material. In consequence, no porosity changes are possible during our simulations. The referees' concerns are clearly justified and correct. In the following we aim to better explain why we chose to use this assumption and discuss possibilities to mitigate this limitation. This reply can also be found at end of the reply to referee #2.

By imposing pure shear, we assume a deformation mode that conserves the total area of the simulation box, which does theoretically not allow for any volume change and implies conservation of mass for both phases. However, firn is characterized by most vertical shortening achieved by compaction of the pore space causing a significant air volume loss. In general, we would like to remark, that the evolution of our numerical microstructures cannot be regarded as an evolution with depth (as would be the case in natural firn and ice). In fact, the microstructure in each simulation step can be regarded as the microstructure that results from the deformation of a material with an unknown previous porosity to the actual situation. We refrain from any study of depth evolution of porosity, inclusion shape or distribution and remark, that the scope of the manuscript is a study of deformation and recrystallisation processes within the ice at the presence of a very weak phase.

Theoretically, the compaction of a pore is a function of the surface energy driving inward bubble surface movement and the inner bubble pressure counter-acting this movement. The latter depends on parameters such as the overburden pressure, bubble shape and connectivity. In a state of equilibrium, a bubble's size is does not change implying static conditions. Since the simulations do not incorporate gravitational forces, overburden pressure is unknown and the theoretical "area energy" is used to counter act surface energy (cf. section 2.4.1, equations (3) and (4) and Roessiger et al., 2014). The pre-factor *c* can be regarded as an approximation of a compressibility factor that controls how quickly this equilibrium is reached (Roessiger et al., 2014). The lower the factor *c*, the less "area energy" is counter acting the surface energy that tends to decrease the overall cross sectional area of the bubbles. In turn, this means more cross sectional area change is allowed causing a stronger violation of the conservation of mass requirement.

To fulfil the conservation of mass requirement in our simulations, any movement of the ice-air interface that is not mass conserving should actually be inhibited. This would however lead to complete "freezing" of the interfaces, an even more unrealistic assumption. Therefore, we allow movements of the ice-air interfaces that preserve the overall porosity, but still allow for sufficient shape changes of the bubbles. Preparatory tests yielded $c = 0.1$ as a compromise to achieve this. With this, we use a 10 times higher factor *c* than Roessiger et al. (2014), who modelled static conditions without deformation.

The current VPFFT code does, unfortunately, not include a compressible phase or voids. This is not an intrinsic limitation of the model, and a version without this limitation is under development. The current model is, therefore, not capable of simulating compaction, and we limited ourselves to area-conservative pure shear. Admittedly, this raises questions on the comparison of the simulations with the EDML firn image (Fig. 8). In the revised manuscript, we discuss the limitations associated with assuming incompressibility and explicitly highlight, that the comparison with the firn image has to be taken qualitatively and as a comparison of inferred processes and their expression in the microstructure.

Specific actions taken in the revised manuscript:

1. As a reaction to both referees' concerns, we created the new sub-chapter "4.5 Limitations of the modelling approach" to discuss approximations made in our simulations. A condensed version of the explanations above is part of this chapter.
2. The role of the pre-factor *c* and our choice of $c = 0.1$ is now better explained in section 2.4.1 and in the new section 4.5.
3. The comparison with the EDML firn image (Fig. 8) has moved to another new sub-chapter in discussion (section 4.2). We present the natural firn image as a first qualitative comparison with an Elle/VPFFT simulation on ice microdynamics. The intention of this comparison is trying to identify processes observed in the simulations also in natural firn (i.e. strain localisation in the vicinity of bubbles associated with enhanced dynamic recrystallisation). The limitations caused by the modelling approach are discussed and we state that we refrain from any quantitative comparison.