Dear Pascal,

we thank you for the careful reading of the manuscript and the overall positive opinion on the work. Your valuable comments helped to significantly improve the manuscript. Below please find your comments pasted in black and with our replies in blue.

As a result of all reviewer comments, the major changes in the manuscript comprise: A revised introduction, an extension of the method section, a revision of Sec 4.4. We also realized that, due to to filename inconsistencies, some load states were previously ignored in the overall optimization. This is now corrected. Therefore the fit parameters slightly changed, but without any implication on the results.

Kavitha Sundu (on behalf of the authors)

Review of « A microstructure-based parameterization of the effective, anisotropic elasticity tensor of snow, firn, and bubbly ice » by Sundu et al. in The Cryosphere

Summary :

The effective stiffness tensor of snow, firn, and bubbly ice is controlled by the density, morphology, and elastic properties of the ice matrix. This control was previously studied and parameterized independently for different ranges of density: for snow (rho in [30, 500] kg/m3), firn (rho in [500, ~800] kg/m3), and bubbly ice (rho in [~800, 915] kg/m3). Here, the authors developed a new parameterization of this control that is valid on the full density range. They use the formal anisotropic Hashin-Shtrikman upper bound as a predictor of the stiffness tensor in empirical fit based on 395 finite-element simulations on tomographic images.

Main comments :

This article constitutes a valuable contribution to The Cryosphere with a sound methodology and interesting results. The paper is fairly well written to follow the work (typos to be corrected through proof review). Even if the new parameterization does not substantially outperform existing parameterizations in their porosity range of validity, it is valid on the full density range from snow to bubbly ice and does not exhibit artificial and arbitrary transition zones with density. In particular, the existing parameterizations for snow predict an effective stiffness larger than the one of ice if applied on high-density samples. Besides, the anisotropy is directly captured by the Eshelby tensor, which does not require additional fitting when using the 2-parameters fit (same beta and eta for all components) for the whole tensor. This new parameterization comes at the cost of a more complex implementation, particularly of the upper bound C_U using the Eshelby tensor derived from the correlation length of the structure. However, its computation expense remains far lower than a full finite-element simulation on the snow microstructure.

However, I have certain comments that would need to be addressed before publication :

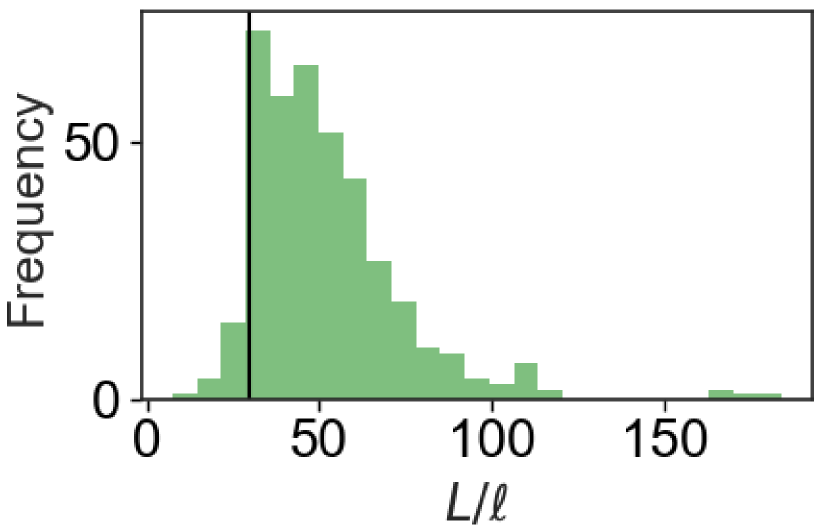
1. One goal of the presented work is to provide a new parameterization of the elastic tensor valid from snow to ice. To use it, one must compute the density, the correlation lengths of the given sample microstructure, the associated 4th-order Eshelby tensor, the corresponding Hashin-Shtrikman upper bound, and eventually, the empirical fit, and to juggle between Voigt and tensorial notations. The authors should provide the functions (e.g., Python or Matlab style) so the community can easily re-use this fit. Otherwise, I fear that simple density parameterization will remain the norm. The shown material must be enough to re-implement the fit, but it is prone to errors and headaches.

We fully agree and this was actually planned initially. Upon acceptance, we will provide (on envidat.ch) the python scripts together with the data and the necessary functions to compute the parametrized elasticity tensor as a function of density, anisotropy, shear and bulk modulus of ice for a straightforward adoption of the results in the community.

2. The computation of the effective isotropic transverse elastic tensor from finite-element simulations is not described in enough detail.
    1. First, what sample size (mm) and boundary conditions are used? Indeed, the convergence of the apparent sample properties into effective material properties with the simulation volume depends on the applied boundary conditions and sample density. In particular, the low-density samples of Alp-DIV likely deviate from the proposed parameterization because of the too-small sample size (Fig. 2). With this information, the robustness of the simulations can be evaluated.

The FEM simulations were performed by employing periodic boundary conditions as originally implemented in the used FE code, which we mentioned now in extended description of the FE method.

The sample size vary for each sample and were taken as is from the original data sets. This information is now included in the paper. To assess the impact on the RVE we show the convergence criterion from Wautier et al 2015 in the figure below:

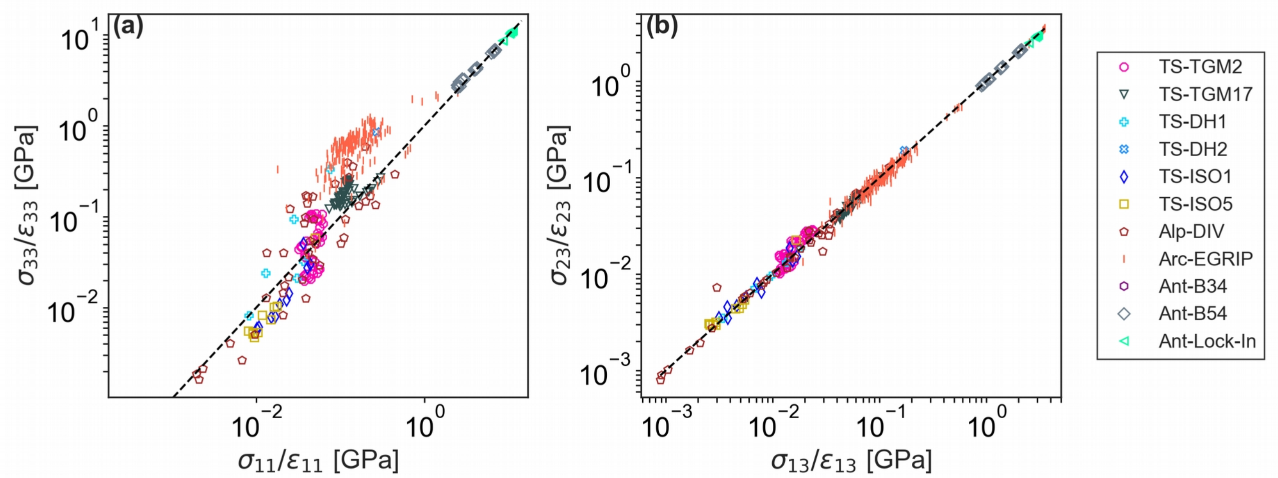


According to their estimates on correlation functions, convergence to an RVE can be assumed when the ratio of linear sample size L and the correlation length l exceeds 30. From distribution of our data shown above (figure not included in the paper) we infer that 92% of all the samples fulfill the requirement of RVE (>30 L/l), while 8 % are below the limit. However, only one sample from Alp-DIV in the low volume fraction range falls into this group, and there is no systematic sub-set of particular samples in these 8%. This information on RVE is now explicitly included in the methods.

2. The isotropic transverse tensor is estimated from 5 load states (Sec. 3.4) by finding the five independent components of C that minimize the L2-norm of sigma-C:epsilon. The five load states are not described. It is unclear whether a bad choice of these load states may favor better approximations of certain components when approximating the full tensor to the isotropic transverse one. What is the difference between getting the full tensor (21 components) based on 6 unit load cases and taking the theoretically non-zero components under the assumptions of transverse isotropy (e.g., Wautier et al., 2015)? In addition, the assumption of transverse isotropy makes sense for snow (deformation by gravity generally aligned with temperature gradient), but is it relevant for bubbly ice on ice sheets that may also flow in a certain horizontal direction?

We now included the definition of the five load states that were used for the optimization. In principle we are just using the Cartesian basis vectors in 6 dimensional stress space (e_1… e_6). We were combining, though, e_4 and e_5 to a single load state (e_4+e_5) leading to the same equations. We acknowledge and explicitly mention now that the choice of load states naturally implies a different weight for different elasticity components in the least squares optimization (As an example: C33 is only involved in the e_3 load state). The description of the optimization is also extended.

To further support the assumption on TI symmetry underlying the work, the following figure (a) compares the ratios sigma11/epsilon11 with sigma33/epsilon33, obtained from the (e_1) and (e_3) load states respectively (without prior assumptions on symmetry). When comparing potential symmetry breaking between x and y (e.g. by plotting sigma13/epsilon13 and sigma23/epsilon23 (see Figure (b)) no significant difference can be observed.



This further indicates that TI symmetry is a reasonable assumption for the present data. We agree though that for bubbly ice, in principle more complex symmetry cases are hypothetically possible as you mentioned. This was however not observed here.

3. The different models were fitted on the simulation data using a log-transformation of the elastic tensor component with a least squares regression. The density distribution of the samples is not uniform in the full density range. In particular, around 80% (?) of the samples exhibit a density between 250 and 500 kg/m3 (Tab. 1, Fig. 2). Besides, some data are highly correlated because they belong to the same time-series. The collected is already huge and the largest so far to my knowledge; however, could you discuss this point? Can we rely on this parameterization for any collected snow data, or is the fit impacted by the sampling? Moreover, the improvements of the new parameterization do not show up in the regression coefficient (Tab. 2) or the scatter around the predictor (phi or C^U in Fig. 2). Sampling.

   The percentage of samples with density between 250 and 500 kg/m3 is 68%. In this intermediate density range, the most significant influence of structural anisotropy is expected, in contrast to the low and high-density range, at which the structural anisotropy is be less dominant. It is known, that the evolution of structural anisotropy is mainly driven by temperature gradient metamorphism (Leinss et al 2020) and that some lab samples included in our data here have served as an independent validation for the rather strong temperature gradient metamorphism observed in the Arctic tundra (Leinss et al 2020). Therefore, we expect that this parameterization is sufficiently generic to capture typical, anisotropic structures in snow.
   The rather moderate change in the regression coefficient indeed reflects that anisotropy has a only a sub-dominant influence on elasticity, while density is still the main parameter. However, capturing these sub-dominant influences may be very important though for advanced microstructure characterization by alternative means. This is better explained now in the introduction.

4. The authors state that « the limit of $\varphi \rightarrow 1$ the microstructure must tend to an isotropic state » (l.160-161). I disagree with the statement or I have not understood it. Bubbles in ice may be very flat and tend to, for instance, horizontal micro-cracks (porosity tends to zero, but anisotropy can remain constantly high). This point motivated the choice of the HS bound as a predictor but there is no prior reason for that. It appears that the collected samples (Fig. 6) of high density (phi > 0.7) are also characterized, but the sampling may be too limited to draw definite conclusions on the structure anisotropy at high density. Moreover, Fig. 6 is based on this specific feature of the HS bounds. It shows that the anisotropy of the bubbles does not affect the anisotropy of the elastic tensor. I am not convinced this is sound. Please clarify.

   This was not well formulated: We meant the effective *elastic* behavior of the microstructure must tend to an isotropic state for $\varphi \rightarrow 1$, i.e. the elastic anisotropy

must obviously vanish for zero-porosity, polycrystalline ice. It is true that the geometrical anisotropy may remain non-zero for φ → 1. This is somewhat visible in our bubbly ice samples where a slight geometrical anisotropy remains, even for the highest densities. But in this density range our data may not be exhaustive enough to see if the slight vertical anisotropy is generalizable to other sites. Due to the processes in polar firn, the remaining geometrical anisotropy for φ → 1 must be weak and much lower as for intermediate densities. The effective elastic behavior involves both, density and geometrical anisotropy, and the combined effect must converge to an elastically isotropic elastic state for vanishing volume fraction of the inclusions. From our understanding this limiting behavior is strict, and automatically accounted for through the HS bound. We reformulated the sentence to make this clearer.

5. The elastic tensor depends on density as a power law with an exponent in [3, 5]. An error of 5% on density may cause an error of 15% to 25% on the elasticity components. Measuring density, even with tomography, is subjected to errors in this order of magnitude (e.g., Proksch et al., 2015; Hagenmuller et al., 2016). The « relative » error due to anisotropy should be discussed with respect to the errors on density and not shown as the main source of uncertainty.

This is a very good suggestion, we included the comparison in the discussion. To this end we considered the extreme anisotropy and density cases in our data and computed the propagated uncertainty on the elastic constants ΔC from our parametrization, for both, namely i) having a density error of 5% or ii) neglecting anisotropy. The results are:

Case 1: Highest anisotropy in our data
$\alpha = 1.87$, $\varphi = 0.39$
$\Delta C\_\alpha = 88.7\%$
$\Delta C\_\varphi = 18.18\%$

Case 2: Lowest anisotropy in our data
$\alpha = 0.45$, $\varphi = 0.66$
$\Delta C\_\alpha = 58.45\%$
$\Delta C\_\varphi = 28.55\%$

These values confirm that neglecting anisotropy may lead to considerably larger errors than a typical error in the density measurement.

Minor comments :

l11 : « the crystallographic anisotropy » -> « to the maximal theoretical crystallographic anisotropy .» Indeed, your estimation of crystallographic anisotropy is very rough.

Changed accordingly.

l22 : « the last example … » -> « Schlegel et al. have stressed ».

Changed accordingly.

l24-26 : « ice matrix geometry … crystallographic orientation ». There are references for geometrical anisotropy but no for crystalline anisotropy.

Agreed. References included.

l26-28: « fabric is low/high ». What does it mean? Anisotropy is high /low?

Changed to "strong" (this is how it is commonly referred to) and "anisotropy" added in brackets.

l29: « recent work wave propagations » -> ? « Hellmann et al. (2021) measured wave propagation on glacier ice and suggested … »

Reformulated

Figure 1: The range of density on which the existing parameterizations are supposed to work (according to their respective authors) is never shown in Figure 1 or explained in the text (e.g. Section 2.2). Add this info.

This information has been added in the Sec 2.2.

l34: « elasticity ». Delete word.

Deleted

l34: « for retrieving sub-surface density and anisotropy ». In general, it is unclear to me if the parameterization is bijective, i.e., is there one unique anisotropy tensor and density for a given elasticity tensor?

We guess no. But in geophysics (like the work cited here) retrievals are rarely based on exact inversions, but rather on suitably constrained optimizations of (strictly) ill-defined problems by exploiting the properties of the forward model. A potential elastic inversion is somewhat similar to the electromagnetic inversion put forward in (Leinss et al 2016) where also a very small impact of the structural anisotropy on the effective permittivity tensor (with known anisotropic forward model) could be exploited to retrieve the geometrical anisotropy of snow. This is elaborated a bit further in the extended version of the introduction.

l57: « Section 2 gives a theoretical overview of the elasticity tensor » -> « Section 2 gives the background of the elasticity theory ».

Changed accordingly.

l.66: « Where the » -> « whose »

Reformulated.

Eqn. 1: Give the assumption underlying this equation (Hill's lemma).

Hill's lemma stated now.

l72-73: Explain what is « transversely isotropic » and that z is vertical (?).

The coordinate system is now properly defined at the beginning of the section.

Eqn. 2: Report also sigma and epsilon (as in Eqn. 1), so that the Voigt notation is explicit (there may be some variations with some 1/2, 2 coeff.).

Voigt notation is explicitly defined now.

l77: « common relations ». It would be convenient to have these relations in the appendix. Indeed, the paper change from one notation to another (C_ij, Lamé, bulk modulus, etc.) and it is sometimes difficult to follow.

Relations are stated in the appendix now.

l80-83: Only one Thomsen parameter is used after. Only present this one and explain in a few words what it represents.

We followed the suggestion.

l94 : « 33 component » -> « the component C_33 »

Reformulated.

l122: « elasiticity » -> « elasticity ». Check the orthograph in the whole paper with dedicated software to avoid typos.

Changed and spell check carried out.

l132: « HS bounds predict the effective elastic properties ». No, they are bounds (with one equal to zero).

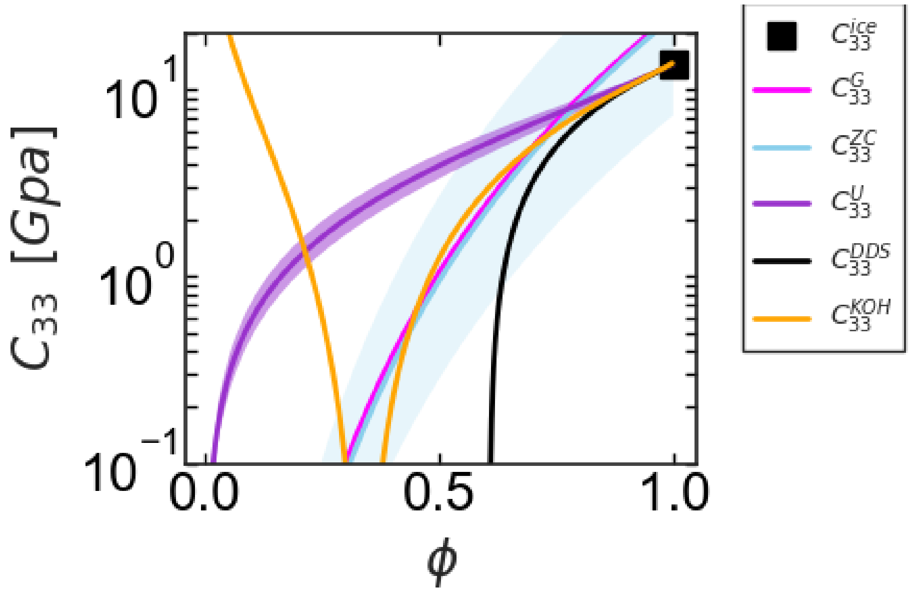
From our perspective, bounds still *predict* the effective elastic properties. The HS bounds are even realized for specific microstructures. This implies, that the prediction can be even exact. So in some cases a *prediction* via bounds is very good, in other cases less good. We therefore keep our formulation.

l160: « influence of anisotropy increases monotonically ». Clarify if its relative anisotropy.

Formulation changed.

Fig. 1: show in log scale to be consistent with the rest of the paper. Show the expected range of validity of the models.

We tested this as shown in the Fig below. However, we believe that at this point of schematic introduction, the log scale is more confusing to the readers. Hence, we prefer the non-log scale.



« Illustration » -> « Evolution »

Changed.

Table 1 : « Isothtermal » -> « Isothermal »

Corrected.

Section 3.4. Give reference to the choice of the ice properties.

Reference included.

Fig. 2: Are the first row and last column really necessary? You could gain space to make the subfigures larger.

We think they are illustrative (also in view of another reviewer's comment): The three columns progressively shows how the data collapse is attained by 1/ including the correct symmetry/anisotropy 2/ rescaling by the underlying ice parameters (in particular through the first row). This now better described. But we also increased the space for the subfigures by relocating the legend.

Fig. 3: comparing C_FEM to C_G_33 (power law) is somehow unfair (scatter due to the fact that, e.g. C12 != C11). Indeed refits of the power law on each component show very little scatter (Tab. 2).

There was a typo in the x-label of the Figure 3d subplot. We now corrected from C_G_33 to C_G_ij. Indeed, also for (e) or (f) we have C12!=C11. But here the data collapse is attained even without fitting components individually. This illustrates that the underlying symmetry supplied by the fabric/Eshelby tensor is the relevant ingredient (see comment above)

Fig. 6b: I am not sure this figure makes any sense. Anisotropy at high density affects elasticity anisotropy, but it appears that porous ice is not anisotropic (due to ice physics). See main comments. Can you make the same figure but with the FEM as the ground truth?

This is also related to your comment further above: At high density, the elastic anisotropy due to geometry must vanish (as shown by the figure) and the difference between the anisotropic and the isotropic formulation tends to zero. The geometrical anisotropy in porous ice (at least for the samples analysed here) remains very weak, but still visible. This is exactly how you expected it to be in your comment above. The figure cannot be done using FEM data since the data does not fill the plane continuously.

Sect. 4.6: This is not clear to me why epsilon_cryst should decay with increasing porosity. For sure, it cannot go above the value for a single mono-crystal. Moreover, you do not need this decay to draw your conclusion (geometric anisotropy is dominant for most of the densities). Simplify.

Assume a volume-filling monocrystal with zero porosity, which is represented by epsilon_cryst as the the maximally, possible anisotropy. Now add a mechanically isotropic inclusion phase (air). As a result, the elastic anisotropy must decay. We still believe that this schematic is illustrative since it re-emphasizes the necessity of revisiting the dominant anisotropy for very high density. This is maybe less of a concern for snow, but this is very important for fabric analysis of ice. We changed the text to make this clearer.

l287 : significantly

Changed accordingly.

l340-342: You discuss here possible improvements. Does it really make sense with the given current performance and the uncertainty on the measurements? Delete paragraph?

We agree, paragraph deleted.

l388: « The new parameterization constitutes a significant simplification ». I would not say it is simple but rather, « it is a crucial tool »

Reformulated.

Reference :

- Hagenmuller, P., Matzl, M., Chambon, G., Schneebeli, M., 2016. Sensitivity of snow density and specific surface area measured by microtomography to different image processing algorithms. The Cryosphere 10, 1039–1054. https://doi.org/10.5194/tc-10-1039-2016
- Proksch, M., Löwe, H., Schneebeli, M., 2015. Density, specific surface area and correlation length of snow measured by high-resolution penetrometry. Journal of Geophysical Research: Earth Surface 120, 346–362. https://doi.org/10.1002/2014JF003266

References added.

Pascal Hagenmuller