Review

A microstructure-based parameterization of the effective, anisotropic elasticity tensor of snow, firn, and bubbly ice

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1 Main Comments

In the paper under review, the authors characterize the contribution of geometric anisotropy on elastic moduli for snow, firn, and bubbly ice. Specifically, the authors propose a normalized upper Hashin-Shtrikman bound for elastic moduli that encompasses a range in porosity from 0 to 1. Under this scheme, the geometric anisotropy ratio and fabric tensor is related to the elastic moduli by using an Eshelby tensor. The behavior of the elastic moduli is simulated using finite element methods via volume averaging on 395 images taken with X-ray tomography. Although the methods presented herein are not novel (as indicated in the referenced models), the normalization scheme presented in the present work provides an excellent fit to the simulated outputs for elasticity of dilute dispersion of spherical cavities and is, relatively, computationally inexpensive. Moreover, all five components of a transversely isotropic elastic modulus for snow, firn, and bubbly ice used in the present work were predicted using 2 parameters rather than 5 (required for simulations referenced in the present paper) in calculating an orthortopic elasticity tensor. The authors note the influence of both geometric and crystallographic anisotropy in the range of densities from snow to ice. At lower porosities, the contribution of geometric anisotropy is greater than that of crystallographic with a volume fraction around 0.7 (and has appreciable contribution to the elasticity moduli even at densities past the bubble close off density for firn/ice). At higher porosities, the influence of these two effects switches, such that crystallographic anisotropy dominates the behavior of the elastic modulus at greater depths in the firn/ice. However, the point at which this transition occurs is not resolved in the present study and should be a discussion for future work. Although not entirely novel, the present study provides the cryospheric sciences a new method for characterizing the elastic moduli across the range of porosities for snow to ice and the relative contributions of geometric and crystallographic anisotropy across the full porosity range (0 to 1 for snow to ice, as defined in the present study). I would suggest publication, provided the authors resolve the following major and minor points.

1. The authors remark in Sec. 2.2.1 that empirical parameters in Eq.4. need to be estimated by fitting to experimental data. At least it should be explicitly stated that constraints on a_{ij} and b_{ij} have not been made, and there has yet to be a widely agreed upon model based on laboratory and/or field measurements of snow to ice porosities. This is a serious limitation in comparing model outputs in the present work for the elastic moduli to that of the FEM simulations (and other model comparisons, such as presented on in Fig. 3.). Moreover, it would be nice to get a brief description on the conditions under which the a_{33} and b_{33} components were obtained.
2. In Sec. 3.2, the two-point correlation function is defined and computed via fast Fourier transform of the 3D tomography images. It is noted that, if using the model presented in Eq.(9), (11), and (12), which showed the best agreement to FEM simulations of elastic moduli compared to other models presented on in the study, only two parameters are needed to determine all five components of the elasticity tensor, ζ and β. A possible limitation of using an anisotropy parameter as defined in Sec 3.2. and the accompanying appendix, is that it requires knowledge of the correlation lengths using 3D X-ray tomography images, which may not be widely available or accessible to those in the broader snow, firn, and ice communities.

3. The authors should consider including the temperature time series presented on in Figures 6 an 7 and discussed in the concluding remarks. To that end, it is not clear, at least from how the model in Sec. 2.6 and the accompanying Appendix are presented, how the elastic modulus (or, similarly, Eshelby tensor) depend on temperature. It is clear that there is an effect on anisotropy that is due to temperature effects, however, without a formulation for the dependence of the anisotropy ratio or Hashin-Shtrikman upper bound of the effective elastic modulus on temperature one would expect it difficult to implement the model presented on the in the current work.

4. It should be noted early on in the present study how you are defining porosity and the reference frame you are using.

5. In equation 8, it is assumed that the dependence on the eigenvalues for the ice volume fraction are of power-law type. Why? One can ad hoc assume the relation follows a power law, but a more detailed explanation should be provided.

6. In figure 3(b), all components of the elastic modulus from the FEM simulations are compared to the C_{33} components of the power law model presented in Eq. 4. It may be beneficial to clarify why the density power law agrees more with C_{44} components (rather than the C_{33} for which other comparisons are made) obtained from the FEM simulations.

7. It would be nice to see a plot of the upper HS bound with the polarization or fabric tensor (as Srivastava et al. (2016) notes, the choice in which one does not effect the representation of geometric anisotropy).

8. Please provide a more explicit relation for effective elastic moduli (presented as Eq. (2) in the original text) to Young's modulus, bulk modulus, and Poisson's ratio. To that end, it would be useful to to see these relations plotted as a function of mass fraction for all discussed models.

9. On line 148, it would be useful to see a figure of the geometric result of $\alpha > 1$, $\alpha < 1$, and $\alpha = 1$, to illustrate the result of prolate inclusions, oblate inclusions, and isotropic bubble distributions. Better yet if a movie of this transition could be provided across a range of porosities.

2 Minor comments

I3: "... geometrical) that give rise to macroscopically anisotropic elastic behavior." to "... geometrical), which can give rise to elastic behavior due to macroscopic anisotropy."
I16: "...the elastic modulus is the probably..." to "the elastic modulus can be used to represent the mechanical properties of snow, firn, or bubbly ice, and so knowledge of the effective elasticity tensor plays a crucial role in..."
I22: "In particular,...anisotropy..." to "In Schlegel et al. (2019), the role of elastic anisotropy was emphasized. Specifically, the retrieval of elasticity..."
I24-26: "...anisotropic, on one hand...orientation" to "an anisotropic with respect to ice matrix geometry (e.g. ...) and crystallographic orientation [there needs to be a citation here]."
I29: "Recent work wave propagation..." to "Recent work by Hellmann et al. (2021) on measuring wave propagation in glacier ice suggests that at low porosity [give value] the effective elastic... is influenced by geometric effects (such as porosity)." Reduce the intensives (e.g. "already"). They weaken your argument.
I37: "Using the Finite-Element (FE) methods..." to "Using Finite-Element (FE) methods via volume averaging, a solution for static linear elasticity yields the material effective elastic properties."
I48-49: "the HS bounds incorporate the non-linear interplay between structural anisotropy and density." HS bounds incorporate the non-linear relation between density and bulk and shear stress, but you need to be more careful defining how anisotropy is represented in the limit of these bounds in the introductory remarks (or refer to the description in Sec.2.4).
I51-56: This entire paragraph is one sentence. Although this is fine, consider breaking it up to make your points more clear to readers.
I62: "by comparing it with the above mentioned shortcomings of previous work" to "... with previous work in which these parameters are not captured," or something similar. Refrain from adding subjective words.

I69: "... is defined by Hook's law" to "is defined by Hook's law, using Hill's lemma,..." Add the reference frame.
Eq.1. Consider adding the region over which the continuum is occupied. Also, consider adding a remark on the use of the notation in eq.1. in connecting volume averaged strain energy of a heterogeneous material at micro length-scales to that of a macroscopically heterogeneous material under uniform strain.
I86: Specify how you are defining ice volume fraction (see Major comments for a related remark).
I86: "...parameterization often..." to "parameterizations use a power law..."
Eq.6. Consider showing the limit explicitly.
I128-129: It can be left to the reader to refer back to the cited text. However, to avoid ambiguity, consider providing a brief description on how these parameters were obtained.
I132: "Hashin-Shtrikman..." to "when using Hashin-Shtrikman (HS) bounds, the effective elastic properties of porous materials can be derived based on volume fraction and microstructural anisotropy (incorporated through n-point correlation functions)."
I130: Consider re-phrasing the subsection header to specify the case of geometric(?) anisotropy, since the distinction is clearly made on I140-141.
Eq.10. Consider expanding on eq. 10 with 8. Also, make reference to accompanying definitions given in the appendix.
I155: "...the formulations including anisotropy, three different anisotropy ratios..." to "including geometric anisotropy, three different anisotropy ratios (alpha = 0.1, 1, and 1.6) were evaluated..."
I161: "...tend to an isotropic state" to "the geometric fabric must tend to an isotropic state"
I161: "the U bound" to "the upper bound (C^U).
In Fig.1. Gpa should be GPa
Eq.11. Define the normalized HS bound before introducing the transformation.
Eq.13. This assumes no mass exchange between the two phases, correct? If so, please note this. I.e. that you assume no sublimation (a process that occurs in glaciological contexts and is a deviation in model applicability to natural environments).
I213: Consider including the definition of $Q(\alpha)$ used here, for completeness.
I216-217: What temperature is this valid for? It would be useful to run FE simulations over a range of shear and bulk moduli that correspond to a range of temperatures. (See major comments)
I221-222: Consider adding a table summarizing the model equations, names, unknown parameters, and porosity range over which they are valid, and their main assumptions.
In Fig 3. Refer back to table 1. It is unclear in Figures 2 or 3 what the legend means. These codes should also be explained in the body of the text in Sec. 4.1.
In Fig 3.b. it is clear this is the only value for the elastic modulus for which the empirical parameters (a_{33} and b_{33}) are known. However, either consider omitting this plot (3.b), since it adds confusion as to which models provide the best agreement to simulations of C, or obtain empirical parameters for a_{ij} and b_{ij} from other experimental datasets. Also, please explain a possible reason that C_{33} from the density power law agrees more with C_{44} from the simulations.
I247: Refer to eq.(5) here.
I248-249: "...and with the literature P-wave velocity of ice...". Please include the conditions under which this was measured. Although readers could refer to Diez's work, without context of it's conditions of validity, it is opaque.
In Fig 4. "Gpa" to "GPa"
I258: "...for reasons discussed in Fig. 1" to "..., as mentioned in the caption of figure 1,"
I259: "...gives the right prediction" to "...parameterization provides an elastic modulus that agrees well with simulated values, taken from images of EastGRIP samples that were close to the surface. At these depths, anisotropy values are low ($\alpha < 1$), and are consistent with..."
I261:"... for deeper snow" to "at greater depths, the geometric anisotropy increases."
I262:"...demonstrate a good performance..." I am not sure what you mean by this, or at the least it is slightly vague. Please explain what you mean by good performance here.
I265: "... reasons discussed in Fig. 1" Omit and consider stating clearly the reason for greater error values for the ZC model with greater densities. Also, reasons cannot be discussed in figures (it is up to you to discuss what the figures mean). Please re-phrase.
In Figure 5: "...Bottom: Error plot which is given by the difference between the simulated elastic modulus..."

to "Bottom: Error in FEM and PAR parameterized elastic modulus calculated from the difference between simulated elastic modulus..."
I274: "...with zero relative error by" to "with zero relative error for isotropic..."
I278: "...we show the geometrical Thomsen parameter ϵ_{geom} (see Eq.3) in Fig. 7." Referencing this figure does not assess the geometrical vs crystallographic anisotropy in your calculations, or at least it is not clear what you mean by this. Consider "... we plot the geometrical Thomsen parameter, obtained from Eq. 3, against the porosity, the output of which is given in Figure 7."
I295-296: No parentheses are needed around the authors names.
I299: "In contrast... are explicit formulas." to "In contrast, the limiting behavior of the Hashin-Shtrikman bounds can provide an explicit formula for effective moduli."
In Fig. 7. Make sure the symbols you are using are consistent. For example, varepsilon is used to label the vertical axis, but epsilon is used in the text.
I303: "...collapsing onto" to "...collapse onto"
I304: "...as a function of normalized HS upper..." to "... as a function of the normalized HS upper bound..."
I305: "...parameterization Srivastava et al..." to "parameterization used in..."
I317: "...yields a eigenvalue zero..." to "yields zero eigenvalue..."
I323: "...where MIL resulted circle with no signatures of anisotropy." It is not clear what you mean by this. Please explain the outputs from the cited text more clearly. For example, "...observed by Klatt et al. (2017), in which a Boolean model of MIL with arbitrary rank fabric tensors, produced figures of circles when evaluated on Reuleaux triangles. Moreover, the MIL analysis used in that model was insufficient in detecting interfacial anisotropy."
I327: "...overall our parameterization shows" to "overall, the parameterization used in the present work (C_{ij}^{PW}, given by Eq. (11)-(12)), had excellent agreement ($R^2 = 0.99$) when fit to all components..."
I335: "... evident for temperature gradient time series (TGM2 and MMTO17) from Fig. 6 (a)...". Which one is MMTO17? This timeseries is not listed in the referenced figure (or, at least, it is not clear which time series you mean). Also, without a description of the temperature timeseries in the body of this work, the dependence of the elastic modulus used in the PW model (and even α) on temperature is not entirely clear, other than vertically oriented structures being favored at high temperature gradients.
I371-375: "in principle... However, typos..." These sentences are not needed. Unless you plan to also compute crystallographic fabric at low porosity (such as in future work), with remedied typos from the referenced text, it detracts from the overall discussion.