Review: "Study of a temperature gradient metamorphism of snow from 3-D images: time evolution of microstructures, physical properties and their associated anisotropy" by Calonne *et al.*

General comments

The authors investigate the evolution of snow under a temperature gradient by micro-computed-tomography (CT) and analyze a large number of microstructural parameters for that case. In addition, numerical simulations for two effective macroscopic properties (thermal conductivity and permeability) are compared to the predictions of two homogenization schemes which are computed from parameters derived from the 3D microstructure.

In short, I think this is a very interesting paper with new results which eventually warrant publication. In particular considering the self-consistent (SC) approach as an alternative to previous efforts based on two-point bounds is a very interesting route worth investigating. However, subtleties of the SC method should be elaborated in greater depth, and a comparison to previous results should be included. My main comments are:

Assumptions of the SC approach not valid. The SC approach is based on a certain symmetry assumption, namely that both phases have "the same shape" (p.1421, l.5). Likewise, the depolarization tensor $\boldsymbol{A}$, which characterizes the anisotropy of both phases is assumed to be equal for the ice and air contribution in Eq. (25). However, the analysis of the air and ice tortuosity tensors (Fig. 6), which are geometrical characterizations of the individual phases, clearly reveals that the ice-phase anisotropy $\mathcal{A}(\boldsymbol{\tau}_i)$ (cyan line) is different from the air-phase anisotropy $\mathcal{A}(\boldsymbol{\tau}_a)$ (purple line), in contradiction to the underlying assumption. This requires some clarification. In fact, where are the expected limits of applicability of the SC approach?

Missing explanations for the SC method. The SC scheme, if presented as an "analytical model", pretends to be a rigorous approach which can be applied without ambiguity. As far as I know this is not the case (cf. also first comment). In general, there is always some fundamental information missing in effective medium theories which cannot be provided by the method itself. Namely: what should be taken as the structural "ellipsoid-unit" which is represented by the depolarization tensor $\mathcal{A}$? As a consequence, the effective ellipsoid must be guessed in the first place. This is in contrast to the series expansion, which is a rigorous, formally closed-form solution, where Q is unambiguously related to the correlation function. Surprisingly, the guess "use the correlation lengths" actually works quite well, at least for the time series analyzed here. This is however already a finding which does not follow from the SC method. These things should be explained to the reader in sufficient detail. The claim that the SC approximation, equipped with the exponential correlation lengths as definition for the effective ellipsoid, yields an estimate of the effective quantities of snow "as is", without any adjustment of prefactors, is a strong statement. However the generality of the statement (p. 1432, l.10) cannot cope with the amount of data (7 samples, one density). The statement should acknowledge the limitations or a few more samples should be analyzed to demonstrate that the SC can actually replace the bound-based parametrization which was derived, after all, from 176 snow samples.

Comparison to previous results. It seems appropriate to include a comparison of your results to the parametrization we developed before. This is just plug'n'play since your approach is based on the same parameter Q. Likewise, in the introduction it seems appropriate to state, besides "need to refine the parametrization" (p.1410, l.26) and "more systematic investigations are required" (p.1410, l.4/5), that in fact (Löwe etal 2013) already implemented a "refinement" exactly in the vein of the present paper, i.e. using standard homogenization methods which predict the relevance of the anisotropy parameter Q that is computed from the correlation function. I completely agree though, that the bounds have an aesthetic drawback of requiring an empirical correction, which is motivation enough to aim at improvements.

Curvature analysis. The most unique contribution of the present paper is certainly the analysis of curvature distributions for TG metamorphism and the resulting time evolution of the asymmetry between sublimating and growing surfaces, which has never been addressed before. Unfortunately, simply plotting the bare distributions (Fig. 7/8) gives only limited insight. Explicitly providing the mean and the variance of all distributions as a function of time seems to be illustrative for various reasons:

1. First, this allows to make a statement about the rescaling properties of the distribution if plotted over the scaling variable $H/\overline{H}(t)$ where $\overline{H}(t)$ is the area-averaged mean curvature at time t. (Note, that rescaling the curvature-axis also requires to rescale the vertical axis if interpreted as a probability). It seems that this rescaling should be possible for the upward faces, but this rescaling will clearly fail for the growing surfaces, at least in the beginning. This is suggested by Fig.7 where the distributions at $t = 0$ and $t = 73$ have clearly different mean values but roughly the same peak heights, which is not compatible with a scaling form $p(H/\overline{H}(t))$ for the distribution.

2. Second, you could actually quantitatively check your claim from (p.1431, l.7) about different metamorphism stages (destruction of connection between grains in the beginning) from your data: You could evaluate the Euler characteristic, as a measure for the connectivity, via the Gauss–Bonnet theorem

$$\chi = \frac{1}{2\pi} \int_{\Gamma} d^2x \, G(x) \tag{1}$$

(in your notation) which relates the integral Gaussian curvature to the connectivity/topology of the structure. According to your claim, you should see a two-stage evolution of χ, one related to *decreasing* connectivity (initial stage) and one related to a rather constant connectivity. Since χ can be written as a product of the surface area and the area-averaged Gaussian curvature this assessment can be done on-the-fly upon evaluation of the time evolution of the area-averaged mean and Gaussian curvature. A two-stage evolution w.r.t. the connectivity would be also interesting in comparison to the isothermal case (http://www.the-cryosphere-discuss.net/8/1795/2014/) where the very initial stage, if at all, is accompanied by an *increase* of the connectivity, at least for very low density snow.

3. Finally, you could also prove your claim from (p. 1427, l.12) that the structure becomes monodisperse by showing that the standard deviation of the curvature distribution (normalized by the mean) decreases with time. The mere fact, that the width of the distribution decreases and the mean moves to zero does not necessarily imply that the structure becomes "monodisperse".

Overall, the paper might also benefit from language improvements (some suggestions given below, cf. Technical comments) and from figure improvements (cf. last remarks in Specific comments).

Henning Löwe

Specific comments

p.1408, l.15: The "bed of ellipsoids" and the "self consistent scheme" are different things, the first is a microstructure model and the second a homogenization scheme. I wouldn't refer to them on the same footing as analytical models.

p.1412, l.20: Were the cores drilled in horizontal directions?

p.1412, l.14: What do you mean by "stuck"? What are the dimensions of the final cylindrical core? What are the temperature fluctuations for the sample in the cryo-cell?

p.1412, l.20-25: Where is the vapor condensation avoided? Inside the sample holder? A schematic of the cryo-stage might be helpful.

p.1413, l.1: The given references contain a lot of image processing, please indicate briefly what was used from what.

p.1413, l.22: I do understand what is meant here but a "surface area in x direction" might cause confusion for some readers, a surface area doesn't have a direction. One possibility is to define SSA_β^{-1} as a length scale λ_β, which is also a correlation length, as we have done it in (Löwe etal 2011). The other possibility is to spend more words on that, e.g. refer to specific surface area *estimates* SSA_β from different directions and explain the relation to the SSA in isotropic and anisotropic microstructures.

p.1414, l.22: Since the correlation function of snow is not an exponential, the notion of *the* correlation length is ambiguous. I would rather refer to it as one possible definition of *a* correlation length (see also previous comment).

p.1415, l.3: It might be helpful here to mention explicitly that the correlation length does not discern between ice and pore space.

p.1415, l.9/11: Use either K or G for the Gaussian curvature. In general H, K (instead of C, G) are more common.

p.1415, l.25: What is meant by "second order estimates"?

p.1416, l.3: "Variational approach" commonly refers to an underlying minimization principle, is this really meant here? What is minimized then?

p.1416, l.6: This is not a partial differential equation.

p.1418, l.10/11: The tortuosity is linked to the effective diffusion tensor of a *non*-reactive tracer, since for $k_a = 1, k_i = 0$ the internal boundary conditions leads to a zero flux Neumann condition for the diffusing species, i.e. the ice-air interface as a reflecting or non-reactive boundary. This is certainly not true for water vapor.

p.1418, l.14: Please give a citation for "it can be shown".

p.1420, l.1: Regarding the readjustment: The fit function $K^{fit}(\rho_s)$ obtained from previous data implicitly averages over all (unknown) values of Q, which were present in the previous data and which might be different from the present anisotropy values. So dividing by $K^{fit}(295)$ does not strictly remove only the influence of density. Any comment on that?

p.1420, l.18: As mentioned before, I wouldn't treat both models on the same footing of being "analytical models".

p.1420, l.21: (See general comments) This is not true, as far as I know. Using the correlation lengths for the effective ellipsoid is first and foremost an assumption, only for series expansions the relation to the microstructure is unambiguous and given via correlation functions.

p.1421: The order of the section is odd, there is already quite some discussion of Eq (25) going on, before actually stating it.

p.1422, Eq (29): Since the z component is by far more important from a practical point of view, it would make sense to give the z-component explicitly in Eq (29) and rather state how the x, y components can be obtained by the replacement $Q \rightarrow (1 - Q)/2$.

p.1424, l.6: State what kind of a tensor product is meant here. Given, that you stress the "analytical" character of the the model you should later note in the discussion of the results that this is an ad-hoc modification.

p.1427: I am not sure if i got it right but are "occurrence ratios" meaningful quantities? Aren't these just bin frequencies which will depend on the chosen bin size of the curvature distributions? If not, you should show that. Is it possible to estimate the total fraction of faceted surface area. This would be an important result.

p.1427, l.16: Why do you discern between up/down only for the mean curvature? Please state (or show in a figure) that the Gaussian case is symmetric in view of up and down.

p.1428, l.14: Triple subscripts are cumbersome. Maybe denote the error by $E(\star)$, then this "only" leads to a double subscript.

p.1432, l.4: (and throughout) Referring to the simulations as "computed" is rather confusing since the "model" results are computed from the microstructure as well. I would discern between them by using something like "numerically exact" vs "modeled".

p.1442, Figures: In general: The fonts are very small, its hard to read numbers and labels. Some figures (like Fig 6) might also benefit from using different symbols for different quantities.

p.1444, Fig.4: If this will be the size of the figure in the final manuscript, the figure itself is clearly too small, it is impossible to see something. Maybe re-arrange images to fill one column? Or enlarge the present image to have a two-column figure?

p.1446, Fig.5: Same thing as before, everything is too small. The height of one subplot should be at least twice the present height.

p.1446, Fig.6: Wrong legend, should be $\mathcal{A}(\boldsymbol{\tau}_i), \mathcal{A}(\boldsymbol{k}), ...$ In the caption: coefficient $\rightarrow$ coefficients

p.1448, Fig.7: I think a semi-log scale might be advantageous in order to have visual access to the tails of the distribution.

Technical comments

p.1408, l.2: during a temperature $\rightarrow$ during temperature (cf. also the title)

p.1408, l.3: along the vertical $\rightarrow$ in vertical direction

p.1408, l.6: panel $\rightarrow$ set

p.1408, l.9: delete "a"

p.1409, l.2: What does "close environment" mean?

p.1410, l.5: specific anisotropic behaviors $\rightarrow$ anisotropic behavior

p.1410, l.14: undergone → encountered

p.1410, l.15: sampled → drilled

p.1410, l.18: delete “a”

p.1411, l.26: punctually → temporarily

p.1412, l.6: porosities → pores

p.1412, l.8: impregnation → casting

p.1412, l.10: delete 2nd “the”

p.1412, l.11: insure → ensure

p.1412, l.11: correct → good

p.1412, l.13: a drill mounted on a lathe operating → a drill which is mounted on a lathe and operated

p.1412, l.19: operates → is operated

p.1413, l.12: noted → denoted by

p.1414, l.2: delete “a”

p.1416, l.20: on → of

p.1418, l.12: is constituted of → constitutes of

p.1418, l.15: strongly → highly

p.1419, l.9: note → denote by

p.1421, l.22: The inversion symbol $(\bullet)^{-1}$ and sc-superscript read more like sc − 1. I suggest to use brackets: $\boldsymbol{k}^{\mathrm{sc}-1} \rightarrow [\boldsymbol{k}^{\mathrm{sc}}]^{-1}$

p.1422, l.17: reported → shown

p.1422, l.15: depicts → shows

p.1425, l.13: close from → close to

p.1425, l.26: “all directions combined” unclear, not a full sentence.

p.1426, l.11: see last comment.

p.1426, l.26: pointed out above with the Fig → pointed out above and shown in Fig

p.1427, l.6: proportion → ratio

p.1428, l.11: → In order to compare models and experiments quantitatively, we use the mean relative difference E, defined as

p.1430, l.5: can be considered as constituted by → can be considered as being comprised of

p.1430, l.22: proportion → volume fraction

p.1430, l.22: "way for heat conduction" unclear, not a sentence

p.1441, Fig1: forward → front