Reply to the reviewers' comments TC-2015-143 Jansen et al. (Small-scale disturbances in the stratigraphy of the NEEM ice core: observations and numerical model simulations)

We would like to thank the reviewers for their very useful and constructive comments and are delighted to hear that both reviewers recommended publication of our manuscript after the suggested revisions. In the following we state all changes made to the manuscript and give a point-by-point reply to all concerns raised. The reviewer's comments are in black, our replies in blue. We also attached an updated manuscript with highlighted changes as a supplement to an additional post.

Reply to anonymous Referee #1:

The paper is interesting and important, and should be published. The data are fascinating, and the modeling provides insights.
However, I believe that additional issues should be addressed, and that the terminology should be considered more carefully. Terminology is not the most important issue, but I will start with the question of whether these features should be called "kink bands". This is a matter of convention and does not control the physics. However, I strongly advise against calling these "kink bands". The authors provide the quote "Kink-bands [...] can be expected to form in any statistically homogeneous rock which has a high degree of anisotropy and which is compressed in a direction parallel to the foliation" (Cobbold et al., 1971)." Most workers would immediately identify the layering in ice as the dominant foliation. Over time, there is stretching along that foliation and compression perpendicular to it, exactly reversed from the usual expectation of kink bands. The original usage of "kink band" in Orowan (1942) was for features formed in single-crystal compression parallel to the glide plane, but the features here originate almost perpendicular to the mean dominant glide planes of the crystals. Analog experiments have included workers generating kink bands in decks of cards by squeezing along the cards rather than perpendicular to them. (The Orowan, 1942, Nature paper (no. 3788, p. 643) is fascinating, and does include a hypothetical kink band with stress applied at 45 degrees to the glide planes as well as the observed bands with stress parallel to the glide planes.). The authors go on to state "When compressed parallel to foliation, the initial inclination of the kink bands is 45 degrees relative to the foliation. The ELLE model results show a similar feature: for the single maximum fabric vertical stripes develop in the first deformation stages, which only show a slight deviation of the c-axis from the vertical orientation." With the foliation horizontal, the ELLE model results start with near-vertical bands, not at 45 degrees as expected for kink bands. Furthermore, most definitions of kink bands note their tendency to occur in conjugate pairs, but the features in the ice cores do not form conjugate pairs, instead always having the same sense relative to the shear field. Using "kink band" for these features is highly likely to give most readers an initial idea about formation processes that is wrong. The definition of "kink band" as used in the full literature is sufficiently broad that one cannot absolutely insist that the usage here is wrong. But, the usage here is misleading, and should be avoided.

We agree that the paragraph explaining the kinking process was unclear in the first version of the manuscript and led to confusion, as indeed the initial orientation of the kink band is not at 45°, but at 90° to the foliation. It is in fact initially 45° to the maximum compressional stress. We rewrote parts of this paragraph to avoid misunderstanding. We omitted the Cobbold (1971) citation, as it gave the wrong impression that we are looking at a stress regime compressive perpendicular to the foliation. In our case, the foliation of the material is given by the basal planes of the initial single maximum fabric of the ice crystals, and the deformation is simple shear parallel to these planes.

The comments by the reviewer made it clear to us that we should have clarified better the two mechanisms of kink folding as described by Dewey (1965) in his extensive review of the formation of kink folds (p. 491):

" The first is produced by the development of kink-bands parallel to conjugate planes of maximum shearing stress (dihedral angle < 90”). [...] The second type of conjugate system arises as a direct result of bend gliding. Orowan (1942) and Barrett (1952) have demonstrated the importance of kinking in compressed metals where the plane of gliding is oriented parallel or sub-parallel to 01, i.e., initially parallel to the plane of vanishing shear stress. Barrett showed that kink-planes originate normal to the plane of gliding after elastic distortion ..."

In the idealised second mechanism, deformation is accommodated by "bend gliding", or "flexural slip" in geology. That is slip only parallel to the foliation as a single slip system. As there is zero strain rate perpendicular to the foliation (no thinning or thickening), the banding plane must be the bisector of the interlimb angle, and hence 90° to the foliation at the initiation of kink band formation. In case of foliation-parallel compression (most models and experiments), this second mechanism is inefficient to produce layer parallel shortening, as the kink bands would be perpendicular to sigma1. Conjugate kink bands develop with angles typically 45-70° to sigma1.

Simple shear parallel to the foliation is a special case where the preferred initial orientations for the kink bands of both mechanisms coincide: 90° to the foliation is also the orientation with the greatest effective shear stress. The two mechanisms effectively merge into one. One orientation of the conjugate set is parallel to the foliation and is therefore "invisible". The second orientation is at 90° to the foliation, which - if perfect - would neither stretch nor shorten. Small perturbations lead to kink folds in the foliation, with the foliation rotated in opposite directions in opposite limbs. However, only the rotation that is synthetic with the applied shear will amplify by the overall imposed simple shear, resulting in the kink bands that rotate synthetically with the shear, while simultaneously increasing the angle between the foliation (basal plane) in the kink band and its surroundings. Such kink bands that initially form at a high angle to the foliation have recently been reproduced experimentally by Misra and Burg (2012, Mechanics of kink-bands during torsion deformation of muscovite aggregate, Tectonophysics, reference added to the manuscript).

We thus regard our explanation for near-vertical kink band formation consistent with the Orowan (1942) reference suggested by the reviewer. In his fig. 5 Orowan illustrates the development of kink-bands for oblique foliation under compression and tension, which is an approximate analogue to simple shear parallel to the foliation. in this case the original orientation of the Kink band would be near-perpendicular to the foliation.

In summary, we still do think that it is legitimate to use the term “kink band” for the observational results as well as for the modelled features, and that this is consistent with the literature. We agree however that the Cobbold (1971) citation at the beginning of section 4.2 may have been somewhat misleading and rephrased the beginning of the paragraph to better explain the process of kinking in simple shear.

Moving to more interesting issues, the modeling uses simple shear only. This is fine as a starting point, but is certainly wrong. The authors are correct that basal shear increases downward and layer thinning decreases, but the folds very clearly form at a depth where layer thinning is significant. Stronger wording is needed that the experiments may generate hypotheses but cannot truly test them because stresses and strain rates are omitted that may be important.

At the moment it is not possible to combine pure and simple shear in the ELLE- FFT-simulations. We added a paragraph to the model description, giving more emphasis on the fact that the model setup is a simplified approximation of the real conditions. In the model results section 3.3 we again explain that in the deeper parts of ice sheet the deformation is dominated by simple shear, and our model is an approximation. However, we are confident that the shearing component in combination with the strong fabric is the essential factor for the nucleation and development of the kink bands. The influence of the vertical thinning under real ice sheet conditions may lead to an accelerated tilting of the kink bands due to layer thinning, which is explained in the text.
Rasmussen et al. (2013) show that the change in annual layer thickness decreases significantly below 1500 m, where the folds are observed, indicating the relative dominance of the shear component in deformation.

Perhaps more importantly, by enforcing simple shear, the model does not allow the folds to affect the flow at the 10-cm scale. The existence of a "stripe" of differently oriented grains in a small volume must affect the stresses or the strain rates nearby, and likely both, because of the flow response to the differences in c-axis fabric and possibly other important factors. In turn, if simple shear were to exist far from a stripe, the deformation near the stripe likely would have additional components, and as suggested by Alley et al. (1997), these components might contribute to growth of the folds and perhaps to larger-scale deformation. This limitation should be noted more explicitly; many processes that may be important to fold behavior are not allowed in the modeling.

We do mostly agree with the reviewer here, except the supposition that our model would not allow folds to affect flow on the 10-cm scale. The Full-Field Theory (FFT) model does calculate the full stress and strain rate field and, although the bulk shear strain rate is given, variations in the flow field do develop as a result of the formation of kink bands. Location, spacing and orientation of shear bands are not imposed in the model, but emerge from the small random perturbations in the initial lattice orientations of grains. These influence the strain rate and stress in their neighbourhood, leading to connected zones with rotated orientations of the basal plane: the kink bands or stripes. The Fig S3 is added to illustrate this process.
The objective of this study is to analyse the formation of these structures at the "hand specimen" scale and not at the large (km-) scale, where very likely additional parameters play a role, which are beyond of the scope of the microstructural model. To model larger-scale folds, the length scale and or resolution in the numerical model had to be changed. It can, for example, be envisaged that on larger scales ensembles of small perturbations form larger-scale folds.
We added a sentence to the summary explicitly mentioning our focus on the small scale.

The authors note that the ELLE simulations cause stripes to form, but do not explain what occurs at the grain-scale level in ELLE. Do the stripes initially arise from the random alignments that occur occasionally in a set-up such as that used? And if so, do interactions among these then strengthen the stripes over time by affecting orientations of grains in a nascent stripe or just beyond the end?
The prior work of Alley et al. (1997) addressed these issues, and found an important role for them and for the third-dimensional interactions that are ignored in the 2-d treatment here. Additional discussion should be added.

The initial orientation of the c-axes of the grains is disturbed with a noise of ±5 degrees. This noise is randomly distributed and does not show any initial vertical alignments. Figure S3 in the supplement to this manuscript shows a random distribution of c-axes. The stripes developing in the model appear to grow in length (i.e. the kink-band propagates along the model from a punctual nucleation). This propagation of the kink-band can be observed from the variation of c-axis orientation of grains along the bands: older segments of the kink-band have grains with their c-axis higher tilted/rotated than c-axis in grains inside younger segments.
We added this observation to the model results and discussion and also discuss findings from Alley et al. 1997 in more detail. We can only speculate on the 3-d nature of these bands, but assume that they are planar features, as stated in the manuscript

The authors state "The later onset of folding in the deeper ice cores shows that higher shear strain is required to produce visible folding due to the higher overburden pressure." Overburden pressure is almost certainly irrelevant, aside from a very small activation-volume effect on deformation; most ice-flow modeling omits overburden pressure entirely and focuses only on the local deviatoric stresses.

We agree that the term "overburden pressure" was an unfortunate choice. What is of relevance for the development of folds visible in the line scan data is the ratio between horizontal shear strain rate and vertical thinning. High vertical thinning rates would lead to a flattening of the structures, which then also prevents overturning. The paragraph has been rewritten, and "overburden pressure" has been replaced with "vertical strain-rates".

The authors state "The mechanism of kinking as a trigger for stratigraphic disturbances has already been suggested by Samyn et al. (2011)." True, but the role of these features as contributors to stratigraphic disturbances was a central theme in earlier work, including Alley et al. (1997), which grew out of the GRIP-GISP2 intercomparison effort and involved coauthor Kipfstuhl (Alley, R.B., A.J. Gow, S.J. Johnsen, J. Kipfstuhl, D.A. Meese and Th. Thorsteinsson. 1995. Comparison of deep ice cores. Nature 373(6513), 393-394). The consistency of shear sense noted in the previous paragraph in the new manuscript also was noted in that 1995 work for the GRIP and GISP2 cores.

We agree that the reference to Alley et al. (1995), should be added to the previous paragraph. The reference to Samyn et al. (2011) was specifically chosen for mentioning the term "kinking" as a trigger for disturbances. In the paper from Alley et al. (1997) kinking was explicitly excluded as a mechanism (see next paragraph). Their observation that the fabric stripes are connected to stratigraphy disturbances is already mentioned in the introduction of the manuscript.

Overall, this work presents important new data, of higher quality than in prior work. The use of ELLE also greatly improves on some parts of prior work, but with the difficulty that the stress state used almost certainly omits important effects. The larger picture of some aspects of their formation, their possible growth and how this might affect fold offset, and their larger role in the ice sheet are not addressed despite their importance.
So, significant revision is required, but the good work surely merits publication.

We added statements describing the limitations of the model to the discussion section. We also pointed out more clearly throughout the manuscript that the simple shear environment is an approximation to the in situ conditions, but also explain why we think this approximation is justified.

Reply to anonymous Referee #2:

Jansen et al. present linescan data from the NEEM ice core. The internal layers visible with this technique show signs of small scale folding and flow disturbances. They show that, where folds are present, the ice crystal orientations present a strong single maximum with inclined bands of grains where the c-axis orientation deviates from the single maximum. They use the ELLE model to discuss their data.
As noted by the first reviewer, the data are well presented and convincing. However the discussion to generalise their interpretation of the folds makes many assumptions on the stress/strain state in the ice cores (especially the role of vertical compression) which are not supported by the model results where only simple shear is applied. I think the discussion part should be revised. Below are my specific comments.

Page 5819, lines 15-19 :".... (e.g. Paterson, 1991) and may lead to deformation heterogeneities such as non-uniform thinning". Paterson (1991) discuss the feedback between initial viscosity contrast and fabric development, which makes initially softer ice even softer in simple shear. This process has been modelled by Durand et al., Clim. Past., 2007. This has been discussed for large scale flow, and the results show that it is not because ice is softer that it will thin faster, as this will requires, because of mass conservation, some kind of extrusion flow.

We agree that the non-uniform thinning is a controversial issue and probably only important for very special geometries like, for example, small ice caps or cirque glaciers, where extrusion flow might be possible (Waddington, 2010, Life death and afterlife of the extrusion flow theory, Journal of glaciology, 56(200), 973-996). Instead of the non-uniform thinning, we now give shear localization as an example for the effect of rheological differences.

Page 5819, lines 24-25: "Azuma and Goto-Azuma (1996) concluded from model studies with an anisotropic flow law". Azuma and Goto-Azuma (1996) did not used a flow model, they proposed an anisotropic flow law where stress and strain-rate are not co-linear (i.e. the viscosity is a tensor). With this flow law they show that simple shear stresses can produce vertical strain-rates because of the no-co-linearity. They propose a simple sketch where, because of this effect, a layer submitted to simple shear but with different fabrics could exhibit thinning and thickening leading to boudinage. However there is not flow-model (i.e. solving for momentum and mass conservation) in their application.

We agree, and have added "Azuma and Goto-Azuma (1996) concluded from a proposed anisotropic flow law".

Page 5823, lines 12-16: "Starting with the same initial microstructure, models with two different ratios between dynamic recrystallisation (grain boundary migration and recovery) and viscoplastic deformation were performed: 1 and 10 DRX steps per deformation (FFT) step ...". The difference between the two ratios is not discussed in the results section and we don't know for which set-up the results are given.

All model results shown in the manuscript are calculated using the 10 DRX steps. This means that more dynamic recrystallization is performed per deformation step than in the 1 DRX case. In the run with 1 DRX step the bands appear at the same locations as well, but are less intense. An explanation for this is that grains located in kink bands rotated to harder positions are favoured for survival by DRX, increasing the intensity of these bands during the simulation. We omitted the reference to these runs in the manuscript, to keep it concise. We think it would be beyond the scope of this study to examine the sensitivity to DRX in detail.

Section 3.1: It would be interesting to give an idea of the thickness of the annual layers for the different depths. Are the visible layers annual layers?

The thickness of the annual layers is changing from about 2 cm at 1400m depth to less than 1 cm at 2100 m (Rasmussen et al. 2013), below that dating is difficult due to the large scale disturbances (Neem community, 2013). Thus, at least in the undisturbed layers in fig. 1 a the alternating cloudy and clear bands are in the order of the annual layering. We added this to the text in section 3.1.

Section 3.1: When the authors discuss features in the Figures (especially Figure 2), they should put some symbols on the Figure to avoid any ambiguity on which feature is discussed (e.g. line 24 "central greyish layer").

We have included a symbol indicating the "central greyish layer" and other features in fig.2.

Page 5825, Line 2: "...been flattened out by shear deformation.". If it is simple shear it should not produce any thinning of thickening?

In this case we did not describe a layer thinning, but a distortion of an overturned fold, in which limbs can become near-horizontal again due to ongoing shear. We rephrased the sentence to clarify this. Thickening or thinning in simple shear depends on the localization of deformation and layer orientation with respect to the shear plane. If simple shear deformation is heterogeneous, there is localization of deformation and therefore thickening or thinning can occur.

Figure 4. Red lines should be thicker to make them more visible.

We have changed red lines to be thicker in fig.4.

Page 5827, lines 9-10 : "This approach is reasonable, since there is a non-coaxial flow component in the region (NEEM Community Members, 2013)." I don't understand the term co-axial here?

Co-axial refers to pure shear deformation (zero internal vorticity) where there is no rotation of the incremental strain axes from an initial to final strain state. Non-coaxial flow refers to cases, including simple shear deformation, where the principal strain axes rotate relative to material lines and therefore do not represent the same material lines with progressive strain (internal vorticity). To avoid confusion we rephrased the sentence.

Page 5828, lines 10-13: "The development of the kink bands is represented in the model run, but the flattening of the structures probably takes place faster under real conditions due to the additional vertical flattening caused by the overlying ice column." This is not clear. Do the authors assume that there is differential thinning? Or that the bands rotate faster because of compression. Is it not possible to test this with the model and apply both simple shear and compression?

A mentioned before in reply to reviewer 1, it is unfortunately not yet possible to combine pure and simple shear in an Elle simulation. Thus we make the assumption of simple shear boundary conditions, and justify the approximation by the fact that the observed kink bands occur in a depth dominated by simple shear deformation. We assume that in natural conditions the bands may rotate faster because of the vertical strain rate, which is small but not zero. The thinning of layers does not favor the nucleation of bands, but contributes to their inclination change over time. We rephrased the sentence to better explain the relation.

Page 5829, line 14: "the evolution of an anisotropic fabric (red line) for several ice cores". Not clear how the position of the red line has been chosen. In many cores the development of the fabrics is continuous, so that is it very difficult to give a threshold to define a "single maximum fabric" (caption Fig.10).

In case of the NEEM and the EDML ice cores there is a relative abrupt change in the fabric. For the other cores a depth is used where the eigenvalue reaches a plateau or the displayed data in the literature display a single maximum. The values are based on the literature cited in the caption of figure 10 and in the text. We added a sentence to the text explaining this, and also two more references.

Page 5829, line 17: "Greenland reveal that the onset of visible folding is dependent on the relation between vertical strain rates and shear strain rates (Fig. 10)." Not clear as no indication has been given on this ratio for the different cores. Maybe the depth at witch vertical strain-rates and shear strain-rates becomes equivalent could be evaluated following Montagnat et al., 2014b?

Yes, this is a good point. In the case of the three ice cores (NEEM GRIP and NGRIP) displayed in Montagnat et al. (2014b) the folds begin at the depth where the dominating strain rate changes from vertical to shear, thus at the cross-over of the curves. We added this to the discussion in the text, and discuss the other ice cores in terms of their surface velocity and location (dome, divide, flank). See also the reply to the next comment and related comments of reviewer 1.

Page 5829, lines 21-23: "The later onset of folding in the deeper ice cores shows that higher shear strain is required to produce visible folding due to the higher overburden pressure." I don't see the role of the overburden pressure here. I understand that the authors suggest that the amount of shear should be higher if the vertical strain-rates are higher?
However the overburden pressure do not produce strain-rates, only the deviatoric stresses do. A good proxy for the surface vertical strain-rate is the ratio between ice accumulation and thickness, while the shear stress increase with depth and surface slope (at first order). So that ice thickness only is not sufficient to evaluate the ratio between vertical strain and shear strain.

Reviewer 1 also highlighted this problem and we agree, the paragraph on the comparison of the onset of folding in different ice cores has been rewritten.

Section 4.2 kink-bands...: I have difficulties to follow the discussion here as the citation by Cobbold et al. 1971 speaks of compression to explain the formation of the kink bands while only simple shear is applied here with the model. I think the first paragraph should be reformulated and maybe illustrated by a cartoon to explain the formation of the bands and their orientation.

We agree, this citation was confusing and we did rewrite the paragraph. We did not insert another sketch but think that figure 9 should be sufficient, at least after rewriting the paragraph. See also the reply to reviewer 1.

Page 5831, lines 21-25: “Azuma and Goto-Azuma (1996) suggested that horizontal variation in the single maximum direction could explain heterogeneous layer thinning or thickening of initially horizontal layers, eventually leading to folding.” The authors already show that they are able to produce some small scale folds with their model in simple shear. Because the flow law proposed by Azuma and Goto-Azuma (1996) applies to fabrics and thus polycristals, I think the mechanism was more suggested for larger scale folds (at least the layers should be larger than a polycristal). So I think this do not apply here.

Azuma and Goto-Azuma mentioned that the horizontal variations in the single maximum could lead to folding, but without mentioning a mechanism providing these initial variations. The kinking we describe in this manuscript could be one possible mechanism providing these. We did rewrite the paragraph to better explain this. The Elle simulations are simulating deformation of a polycrystal, with a very narrow variation in original orientations of the single crystallites.

Page 5833, line 15, “but the results are in line with findings from ice flow models on the larger scale (Azuma and Goto-Azuma, 1996)”. See previous comments.
See above.