

Small-scale disturbances in the stratigraphy of the NEEM ice core

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Small-scale disturbances in the stratigraphy of the NEEM ice core: observations and numerical model simulations

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July 2012. It is located on a topographic ridge, which dips towards the northwest so that the surface velocities on the ice divide have a non-negligible component of along ridge flow of about 6 m a^{-1} (NEEM community members, 2013). In July 2010 the bedrock was reached at 2537.36 m depth. The site has been chosen in order to recover an undisturbed Eem warm-period ice layer. However, it was found later that the ice below 2200 m was heavily disturbed and probably folded on a large scale (NEEM community members, 2013).

Visual stratigraphy of the NEEM ice core revealed folding also on a small scale, with fold amplitudes varying from less than 1 cm to a few decimetres (Samyn et al., 2011). These types of folds occur well above the large scale disturbances reported by the NEEM community members (2013). Similar structures have been found in the lower parts of other deep ice cores (Alley et al., 1997; Thorsteinsson, 1996; Svensson et al., 2005; Faria et al., 2010; Fitzpatrick et al., 2014). Stratigraphy bands are visualized by an indirect light source scattering on surfaces inside the ice, mainly particles and air bubbles/hydrates (Svensson et al., 2005). High impurity content is found in ice that originates from snow accumulated during glacial periods. Changing impurity contents between ice from glacial and interglacial periods have been linked to rheological differences (e.g. Paterson, 1991) and may lead to deformation heterogeneities, such as non-uniform thinning.

Due to their potential influence on the integrity of the climatic record, folds have been subject to modelling studies (e.g. Waddington et al., 2001). Thorsteinsson and Waddington (2002) explored the amplification of small disturbances in the layering of ice cores for isotropic and anisotropic conditions, investigating the potential for the existence of overturned folds near ice sheet centres. Azuma and Goto-Azuma (1996) concluded from model studies with an anisotropic flow law that an inclined single maximum fabric could lead to vertical strain even in simple shear and thus influence the stratigraphy. They also suggested that horizontal variations in the inclinations could then cause alternating thickening and thinning of layers, leading to folding or

recorded with a standardised exposure time and three focal planes within the ice core section with a vertical distance of 1 cm (Kipfstuhl, 2010). This allows to a certain degree a three-dimensional mapping of the visible layering in the ice core. The data are stored in high-resolution ($118 \text{ pixel cm}^{-1}$) bmp images. One drawback of this method is, of course, that it only shows disturbances in the ice if scattering surfaces are included. However, it is possible to even reveal structures at low dust content by means of image processing and filtering.

2.2 Automated Fabric Analyzer

The crystal fabric orientation of discrete samples was measured using a G50 Automatic Fabric Analyzer (Australian *Russell-Head* type, see e.g. Russell-Head and Wilson, 2001; Peternell et al., 2010, data set: Weikusat and Kipfstuhl, 2010). Samples cut from the physical properties part of the NEEM core were cut to $250 \mu\text{m}$ thin sections to measure c-axis crystal lattice orientations by polarized light microscopy, where the thin section is placed between systematically varying crossed polarizers (e.g. Wilson and Russell-Head, 2003). The data coverage is much better than in previous ice cores with continuous sampling of selected core sections (bags) to investigate meter-scale variations in fabric throughout the core. However, due to the time-consuming preparation of the samples it was not possible to produce a continuous record.

2.3 Microstructural modelling with ELLE and full field crystal plasticity

We use 2-D numerical modelling to investigate the development of strain localization in a polycrystalline aggregate during simple shear deformation. The simulation approach couples a full field method based on the fast Fourier transform (FFT) that simulates viscoplastic deformation, with two front-tracking codes that simulate dynamic recrystallisation processes (DRX), both included within the open-source numerical modelling platform ELLE (<http://www.elle.ws>; Bons et al., 2008). ELLE has been successfully used to simulate evolution of microstructures during deformation, such as

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recrystallization (Piazolo et al., 2008; Roessiger et al., 2011, 2014) or strain localisation (Jessell et al., 2005; Griera et al., 2011, 2013). The full-field crystal plasticity (FFT) code (Lebensohn, 2001; Lebensohn et al., 2008; Montagnat et al., 2014a) simulates deformation by pure viscoplastic dislocation glide. An experimental run consists of iterative applications of small increments ($\Delta\gamma = 0.04$) of simple shear deformation, each followed by a sub-loop of processes simulating dynamic recrystallisation (grain boundary migration and recovery). While grain boundary migration covers the motion of high-angle grain boundaries, recovery achieves decrease in intracrystalline heterogeneities by means of local rotation without motion of high-angle boundaries. The recrystallisation sub-loop may be called more than once to simulate the different balance between deformation and recrystallisation as a function of strain rate, since all simulations are performed with the same intrinsic mobility value (M_0) and boundary-diffusion activation energy (Q) (Roessiger et al., 2014; Llorens et al., 2015).

Exchange of data between ELLE and FFT is possible, as both use periodic boundary conditions and the physical space is discretised into a shared regular node mesh.

The ELLE data structure consists of three layers: (1) a network of nodes (boundary nodes or *bnodes*) that are connected by straight boundary segments that define the high-angle grain boundaries that enclose individual ice grains, (2) a set of unconnected nodes (*unodes*) to map lattice orientations and dislocation densities, used for the FFT calculation, and (3) a passive marker grid utilised to track finite strain. Distances between nodes are kept between 5.5×10^{-3} and 2.5×10^{-3} times the unit distance (in a 1×1 bounding box), by removing *bnodes* when their neighbours are too close or adding *bnodes* when two nodes are too far apart. The space is discretised in a mesh of 256×256 Fourier points, resulting in a unit cell defined by 65 536 discrete nodes. Each *unode* represents a small area or crystallite with a certain lattice orientation, defined by Euler angles, and a dislocation density value. The ELLE data structure has fully wrapping boundaries. The $10 \text{ cm} \times 10 \text{ cm}$ initial microstructure has 1632 grains, each with a homogeneous lattice orientation, showing a c-axis preferred orientation almost perpendicular to the shear plane, in order to simulate an intrinsic anisotropic material.

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The misorientation between grains was set at $< 5^\circ$ (i.e. initial noise). Dislocation glide of ice-single crystal was defined by slip on the basal $\{0001\}$ $\{11-20\}$, prismatic $\{1-100\}$ $\{11-20\}$ and pyramidal systems $\{11-22\}$ $\{11-23\}$. In these simulations, the ratio A of critical resolved shear stress (CRSS) for non-basal vs. basal slip systems was set to $A = 20$.

The same stress exponent ($n = 3$) is set for all slip systems. The physical values used for recrystallisation are: intrinsic mobility M_0 ($1 \times 10^{-10} \text{ m}^2 \text{ kg}^{-1} \text{ s}$; Nasello et al., 2005), boundary-diffusion activation energy Q (40 kJ mol^{-1} ; Thorsteinsson, 2002), isotropic surface energy γ_e (0.065 J m^{-2} ; Ketcham and Hobbs, 1969) and temperature was set to $T = -30^\circ \text{C}$. To simulate recovery numerically, a modification of the approach proposed by Borthwick et al. (2013) was used. See Llorens et al. (2015) for a complete description of the methods.

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 time incremental for each recrystallisation step was set to $\Delta t = 6.3 \times 10^8 \text{ s}$, giving strain rates 3.17×10^{-11} and $3.17 \times 10^{-12} \text{ s}^{-1}$ for 1 and 10 DRX step models, respectively.

3 Results

3.1 Stratigraphy and fold classification

The stratigraphic data were visually inspected for all parts of the ice core containing cloudy bands, in order to categorise disturbances of the visible layers. It has to be noted that this method is only appropriate where sufficient layers are visible, since clear ice may have been deformed as well. Figure 1 shows an overview of the layering structures we find in the NEEM ice core. All images shown are confined to the core sections above the major disturbances in the Eemian ice beginning at a depth of approximately 2200 m. Around this depth the ice is heavily sheared and the layering becomes more and more diffuse. Below that it is no longer possible to see fold structures in the visual

width of the core sections limits our interpretation here, as the layers could have been flattened out by shear deformation. Figure 2c shows a stack of flattened folds, where the doubling of layers is not immediately obvious to the observer when focusing the left part of the image. There are also new generations of folds standing out through their well-defined and steeper axial planes and which are not yet overturned (Fig. 2c, on the left).

At even greater depth the layering becomes less distinct (Fig. 1f–h). In some parts of these sections the layers appear to be undisturbed but inclined, which may indicate that they are part of a larger deformation structure. The now very thin layers still show new generations of folds.

3.2 Crystal fabric orientation anomalies connected to folds

In comparison to previous deep ice cores, the amount of data gathered to analyse ice fabric is relatively high. To investigate small-scale variations entire bags of 55 cm from certain depths were processed. The general evolution of ice fabric with depth in the NEEM ice core was described in Montagnat et al. (2014b). The c-axis orientation distribution develops more or less linearly from an isotropic fabric to a single maximum at a depth of about 1400 m, which represents the transition from the Holocene to the last glacial (Rasmussen et al., 2013). Within the well-developed single maximum fabric we found inclined bands of grains with a deviating c-axis orientation. We assume that the bands are planar features, but as the thin sections are vertical cuts through the cylindrical core section the inclination of the bands is not necessarily equal to the inclination of the planes. Similar bands were described in the GRIP ice core (Thorsteinsson, 1996) and the GISP2 ice core (Alley et al., 1997). In case of the NEEM ice core, however, significantly more fabric data are available, which enables us to follow these structures through entire core sections.

One of the first examples of such a band, shown in Fig. 3a, appears at a depth of 1800 m. The c-axis orientation of grains within the bands is tilted anti-clockwise relative to the single maximum, which is indicated by the blue-greenish colours in the

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3.3 Model results

To understand the development of the observed fabric anomalies and the related disturbances in the layering, we simulated the fabric evolution under simple shear with an initially well developed single maximum orientation distribution. A random noise of $< 5^\circ$ was added to grain orientations. The setup of the simulation does not fully represent the probably kinematic boundary conditions in the region of the ice core where we observe the structures, which would be a combination of vertical compression and simple shear (Montagnat et al., 2014b). We, however, model these structures in simple shear for simplicity. This approach is reasonable, since there is a non-coaxial flow component in the region (NEEM Community Members, 2013). Moreover, the choice of simple-shear boundary conditions is also justified by the fact that the bands start to appear in the lower third of the ice sheet where shear stress becomes the dominant driver for deformation (Montagnat et al., 2014b).

In the model simulation vertical bands similar to the ones observed in the ice core begin to stand out after a shear strain of $\gamma = 0.6$, but start to appear already after small strains (Fig. S3). The c-axes of the grains in the bands are slightly tilted clockwise, in a synthetic sense with the imposed dextral shear. These bands intensify during the next steps and begin to tilt due to the continuing shear deformation (Fig. S2). Continuing shear causes further tilting of the c-axes orientations within the bands. The rotation of the c-axes is twice the inclination of the band, which is typical for flexural-slip kink folds (Fig. S4; Dewey, 1965; Tanner, 1989). Figure 8a–c show the c-axis orientations for the sample after shear strains of $\gamma = 1$, $\gamma = 2$ and $\gamma = 3$. The bands seem to develop in different generations, which can be distinguished by their inclination as the new bands are steeper. There are areas between the bands where orientations of c-axes rotate anti-clockwise (magenta coloured), but on a larger scale and with less well-defined boundaries. In later stages of the simulation the oldest bands begin to disintegrate with the grains recrystallizing back to a vertical c-axis fabric.

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Figure 8d–f shows the development of a passive marker grid during the simulations. The blue lines were perfectly horizontal at the beginning of the simulation and can be regarded as an analogue to the stratigraphic layering observed in the ice core. It is apparent that the bands with abnormal grain orientation are connected with folding in the layering. At first these disturbances appear as small steps, but they develop into overturned folds with a short and steep limb with progressive deformation. They correspond to the well-developed bands in the fabric, and to a long, less inclined limb, representing the area in between the bands. The disturbances in the layering are permanent, and therefore the bands are visible in the passive grid even when they no longer exist in the orientation plot. 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 may explain the existence of horizontally layered sections in the deeper parts of the NEEM ice core seen in the linescan images discussed above.

Figure 8g, h and i shows the equivalent von Mises strain-rate for the deformation steps $\gamma = 1$, $\gamma = 2$ and $\gamma = 3$. The strain-rate appears to be localized around the margins of the bands where bending strain is the highest, which is most apparent for newer bands with steep inclinations.

4 Discussion

4.1 General discussion of folds

The shape of the observed folds in the NEEM ice core is typical for similar folds, as the layers are thickened in the hinge region and thinned in the fold limbs. Similar folds are passive features, where all layers of the package are deformed in a similar way (Fig. 9a). They form by passive shearing of the layering and can evolve to become overturned z-folds or even sheath folds (Quinquis et al., 1978; Bons and Urai, 1996; Alsop and Carreras, 2007). Competence or viscosity contrast between the different

very similar in ice thickness to GRIP, the onset of folding for the latter is 300 m deeper, which may be due to its dome position. In the region of the NEEM ice core there is an even higher along-ridge flow. A comparison of shear strain rates profiles with depth at the NEEM, GRIP and North GRIP locations can be found in Montagnat et al. (2014b).

5 The EDML ice core stands out in the comparison shown in Fig. 10, as the folding begins significantly higher than the establishment of a single maximum fabric. However, Faria et al. (2010) report that a strong girdle fabric has formed in the region of the onset of folding, thus the fabric does show some anisotropy there as well.

10 The scale of the disturbances found in the layering of the NEEM ice core is very similar to the ones observed at EDML (Faria et al., 2010) and North GRIP (Svensson et al., 2005), for both of which a linescan dataset of comparable quality as for the NEEM ice core is available.

4.2 Kink bands as a source for folding

15 “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).

Ice is a mechanically highly anisotropic mineral, as is polycrystalline ice with a strong single-maximum c-axes distribution. Kinking has been observed in single ice crystals as well as in polycrystalline aggregates under compression (Wilson et al., 1986). When
20 compressed parallel to foliation, the initial inclination of the kink bands is 45° 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. In a perfectly anisotropic material with slip only possible along a single plane (the basal plane in case of ice), kink
25 folds develop where the axial plane forms the bisector of the angle between the two limbs (Fig. 9c) (Frank and Stroh, 1952; Dewey, 1965; Cobbold et al., 1971). Initial kink bands, with interlimb angles still close to 180°, thus form by geometric necessity at

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approximately 90° to the layering, and thus along the c-axes maximum in the lower part of ice sheets. However, kink bands are still hardly visible at this stage.

Kink bands passively rotate, if there is a layer-parallel shear component, which does not necessarily have to be the dominant deformation component. As the kink band rotates by an angle α to the long limb, the short limb has to rotate by 2α , as is observed in the NEEM core and numerical simulations (Fig. 8d–f). With progressive rotation of the kink bands they become more distinct. Rotation of the short limb occurs by sliding parallel to the basal plane with a sense opposite to the overall shearing direction (Fig. 9c). Kink bands finally “lock up” when the interlimb angle reduces to 90°, i.e. when the kink bands are approximately 45° to the layering. In the numerical simulations we see that kink bands begin to disintegrate at this stage, with recrystallization and recovery consuming the grains with deviating orientations and flow homogenizing again (see Fig. 8). However, marker lines, such as the layers in the NEEM core, will still record the kink bands, which now continue shearing and develop into passive folds.

In summary, the model results indicate that the evolution of kink bands is a consequence of a fabric with a strong anisotropy with superimposed small random disturbances. In this way grains orientated unfavourably for basal glide are rotated by rigid body rotation and internally reversed shear into a more favourable position in relation to the bulk shear strain. Thus, kinking appears to be an essential process in ice deformation under shear.

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 development of kink bands is a process providing such variations in the fabric.

A difficulty in comparing the results of the simulation with the observational data is that with fabric measurements we can only capture a 2-D section of a 3-D feature. Assuming that the kink bands are planar features, the angle at which the cylinder of the ice core is cut relative to the inclination of the plane determines its appearance in the 2-D section. Thus, the inclination of the observed bands in the plane is not sufficient

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to describe the full orientation of the kink-band plane, but instead gives a minimum inclination of the plane. This also has to be taken into account when interpreting the fold structures on the linescan images.

Within one 55 cm section of the ice core (bag) the cutting plane through the core is consistent and so are the samples used to prepare the thin sections for the fabric measurements. Figure 7 shows that within one bag the inclinations of the kink bands are consistent as well, strengthening the assumption that they are connected to the local stress environment and to the sense of shear, projected onto the plane of the thin section or linescan image. In both examples different generations of kink bands can be detected, differing in inclination of the bands as the older bands have subject to more shear strain since their formation, and the corresponding shift in c-axes orientation, as it is seen in the model results as well.

The mechanism of kinking as a trigger for stratigraphic disturbances has already been suggested by Samyn et al. (2011). Together with the microstructural model results the observations can be interpreted with an improved understanding of the kinking process. Alley et al. (1997), who described similar bands in the GISP2 ice core, state that the observed bands are most likely not kink bands, as they would require a compressional regime in the horizontal direction. However, the model results clearly show that kink bands can form in simple shear conditions. At the moment it is not clear why the bands sometimes appear dark in the linescan images, but from deeper parts of the core where the crystals are larger in size the linescan images give indication the backscattering can be subject to the crystal orientation.

5 Summary and conclusions

The onset of small-scale folding can be observed at the start of the lower third of the NEEM ice core, which is similar to the fold evolution observed in EDML. Below a depth of about 2160 m it is no longer possible to track stratigraphic layers. The shape of the observed structures indicates that they are not buckle folds, which means that they are

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in Belgium (FNRS-CFB and FWO), Canada (NRCan/GSC), China (CAS), Denmark (FIST), France (IPEV, CNRS/INSU, CEA and ANR), Germany (AWI), Iceland (RannIs), Japan (NIPR), Korea (KOPRI), the Netherlands (NWO/ALW), Sweden (VR), Switzerland (SNF), UK (NERC) and the USA (US NSF, Office of Polar Programs).

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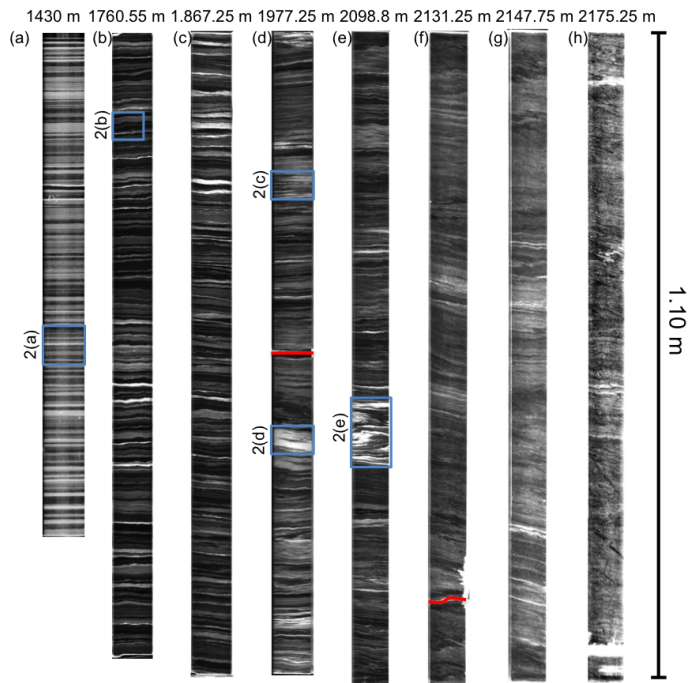


Figure 1. Visual stratigraphy overview. Linescan images of different depths. A Gauss filter was applied to images shown in panel (a), (d), (e), (f), (g), and (h) to enhance the visibility of the layers. Red lines indicate fractures. Blue squares and associated figure codes indicate location of enlargements shown in Fig. 2. The 1.10 m line at the right indicates the scaling of the images and is also the typical length of a recovered core section.

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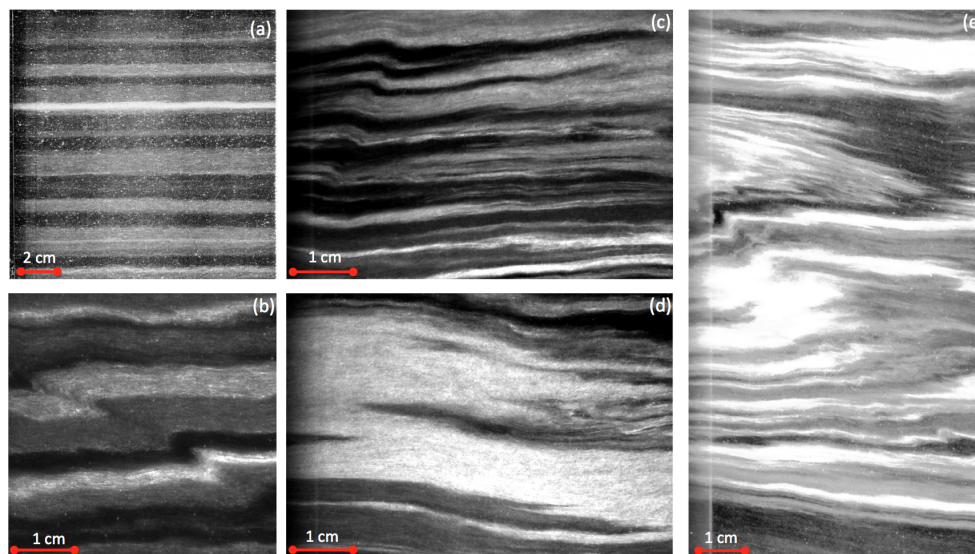


Figure 2. Close-ups from the overview Fig. 1. **(a)** Undisturbed layering. **(b)** Angular z-fold consistent throughout layering. **(c)** Different generation of folds. **(d)** Strongly disturbed layer significantly thickened. **(e)** Strongly disturbed layering with different generations of folds.

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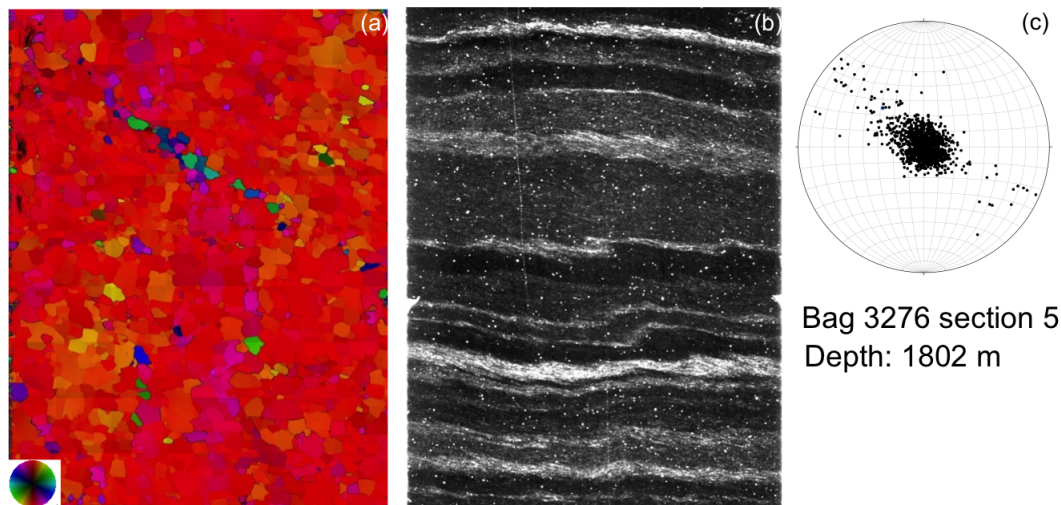


Figure 3. Comparison of fabric data and visual stratigraphy in detail, Bag 3276, approximate depth 1803 m. **(a)** Fabric data in a vertical section, **(b)** linescan image in a vertical section, **(c)** stereoplots of c-axes orientations (horizontal plane).

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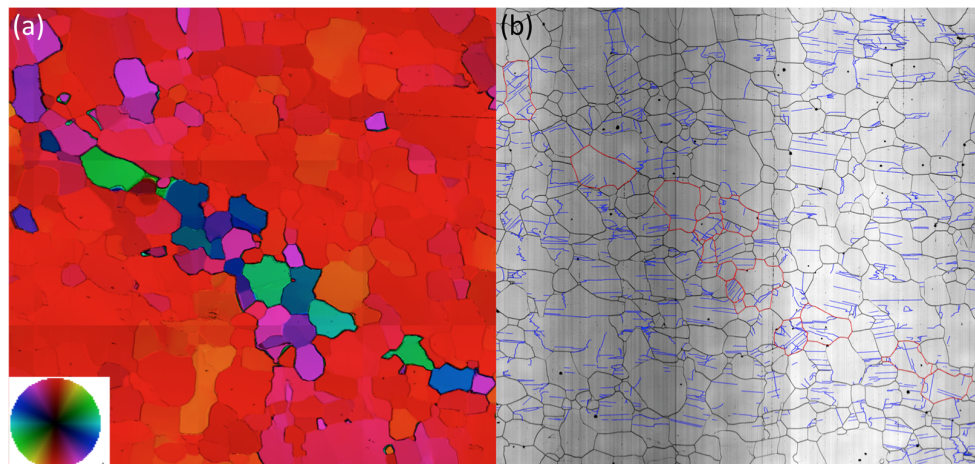


Figure 4. (a) Close-up of kink band grains at approximately 1803 m depth (bag 3276). Inset shows the colour code for c-axes orientation (b) subgrain structures (blue) visible on LASM (Large Area Scanning Microscope) data. Black lines indicate grain boundaries; the red outlines highlight the kink band grains.

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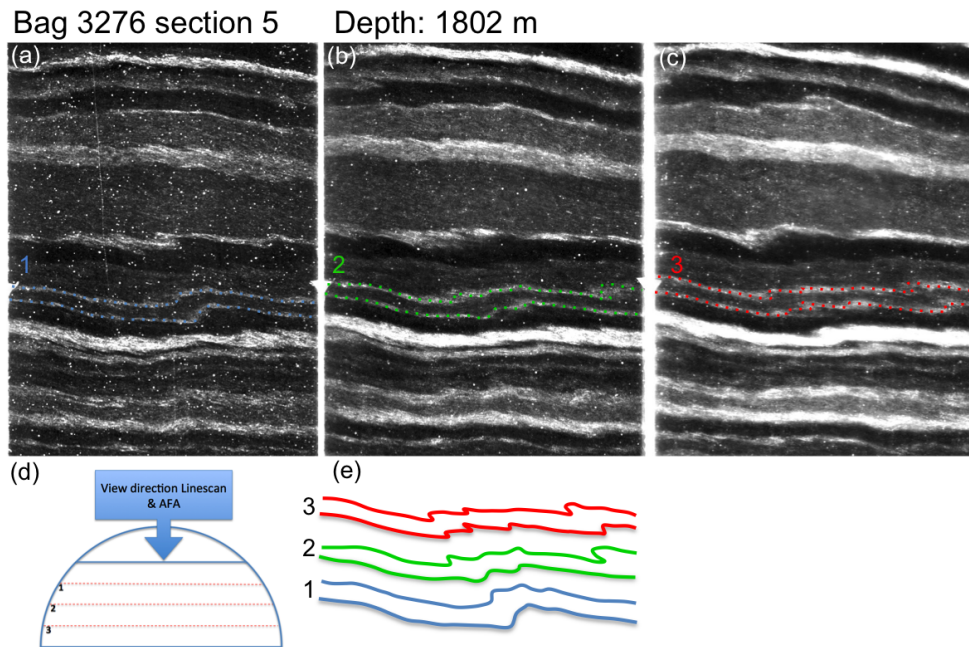


Figure 5. Linescan images from the same sample as shown in Fig. 3 from three focal depths with one highlighted layer **(a)** close to the surface, **(b)** in the centre of the core section, **(c)** close to the lower surface. **(d)** Sketch of the core sections, the upper part represents the physical properties sample, from which the thin sections are prepared. **(e)** Change of shape of the highlighted layer for the different foci.

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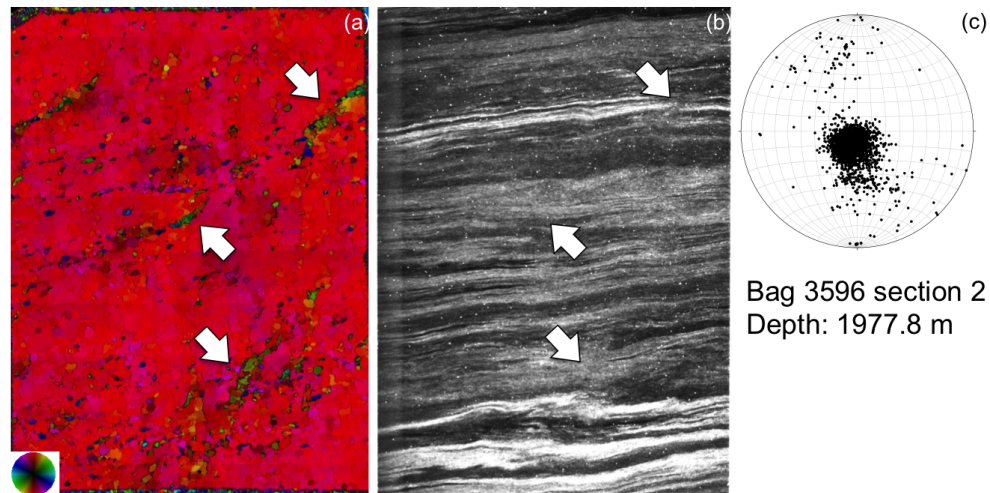


Figure 6. Comparison of fabric data and visual stratigraphy in detail, Bag 3596, approximate depth 1977.8 m. **(a)** Fabric data in a vertical section, **(b)** linescan image, in a vertical section **(c)** stereoplot of c-axes orientations (horizontal plane).

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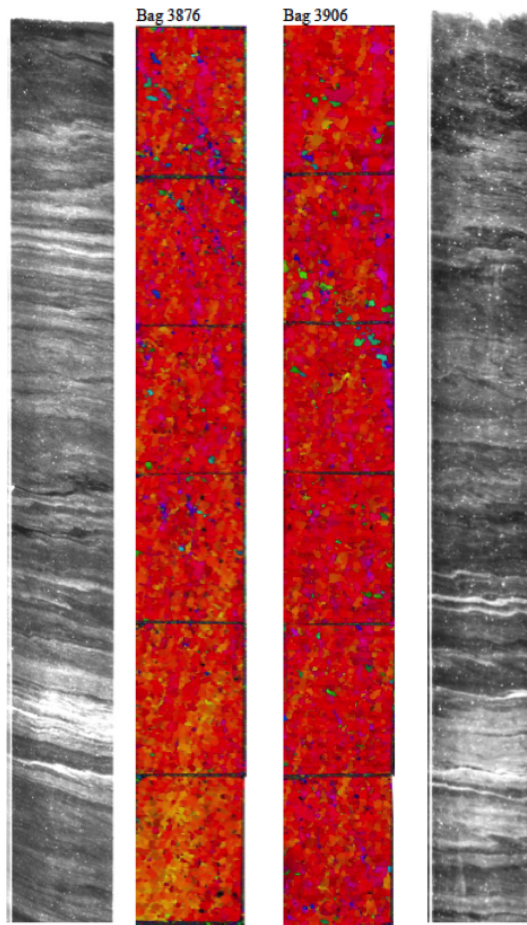


Figure 7. Comparison of entire 55 cm core sections (full bags) of linescan (a, d) and fabric data (b, c).

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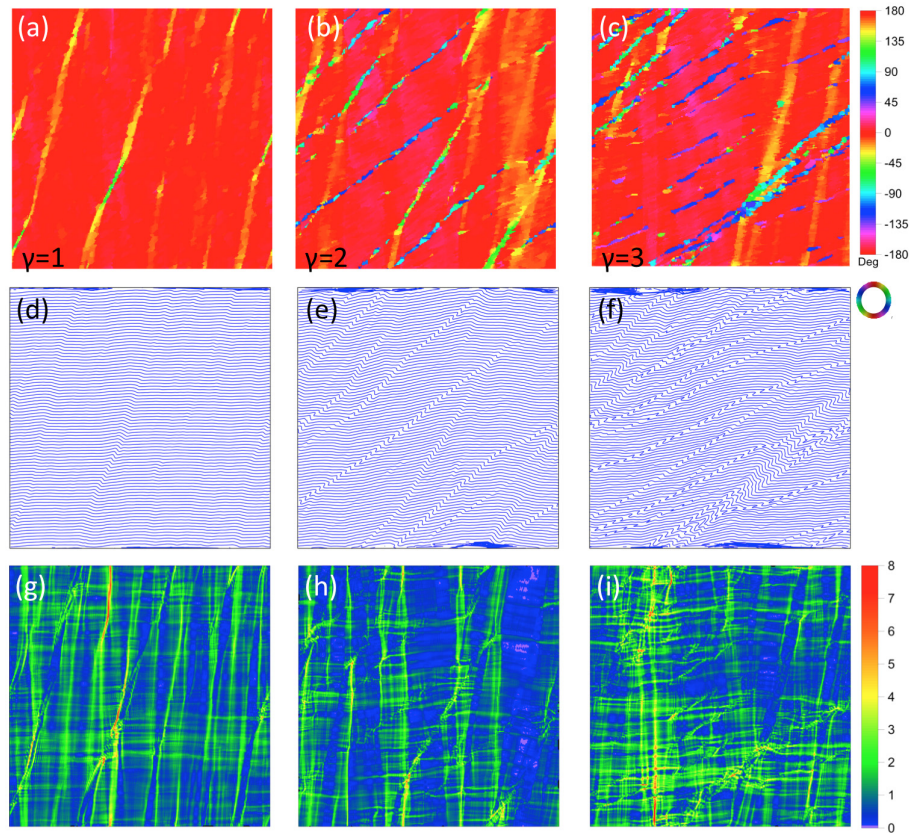


Figure 8. ELLE model results for the simple shear experiment. Panels (a), (b) and (c) show c-axes orientations for shear strains of $\gamma = 1$, $\gamma = 2$ and $\gamma = 3$. Panels (d), (e) and (f) show the distortion of the passive grid marker. Panels (g), (h) and (i) show the equivalent von Mises strain-rate field.

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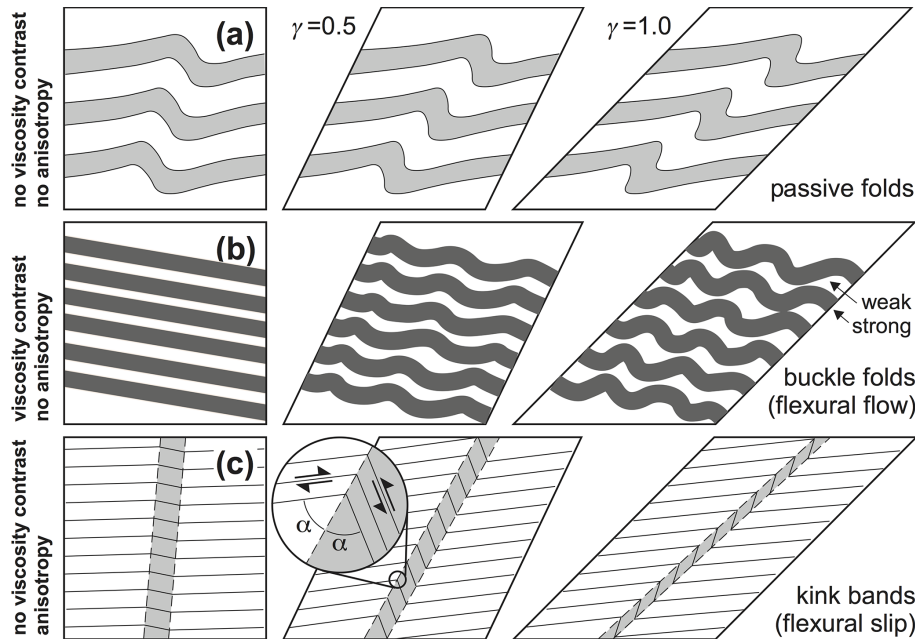


Figure 9. Basic folding mechanisms discussed in the text. **(a)** Passive folds form by shearing of disturbances in layering, without an active mechanical influence of that layering. Fold geometry is that of similar folds. **(b)** Buckle folds form by shortening of alternating strong and weak layers, in which the strong layers buckle and weak material flows into fold hinges. Fold geometry is that of parallel folds. **(c)** Kink bands form in case of strong intrinsic anisotropy, but do not require viscosity contrasts between layers.

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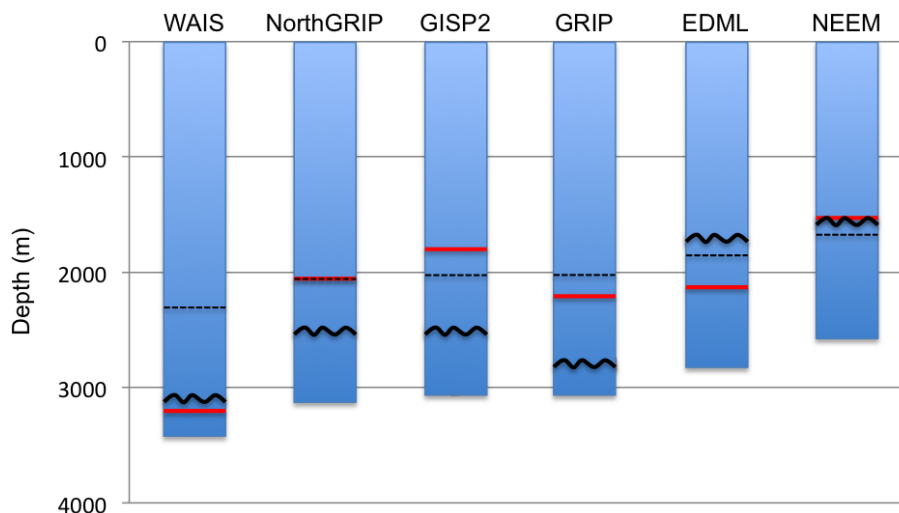


Figure 10. Comparison of the onset of visible folding in ice cores with published visual stratigraphy. The red line indicates single maximum fabric, the black line indicates onset of folding, the dashed black line indicated the lower third of the ice core. Data from Thorsteinsson (1996) (GRIP), Alley et al. (1997) (GISP2), Svensson et al. (2005) (North GRIP), Faria et al. (2010) (EDML), Fitzpatrick et al. (2014) (WAIS).

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