

## Review

# Pinch and swell structures: evidence for brittle-viscous behaviour in the middle crust

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by R. Gardner et al.

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## Introduction

Gardner et al. present an interesting numerical modeling study of the development of pinch-and-swell structures with a frictional-viscous rheology and attempt to relate their micro-scale models to natural microstructures of boudinaged mafic layers. Moreover, they extend their concept to the tectonic scale in order to study the brittle-ductile transition at mid-crustal levels. The authors apply a recently developed, sophisticated finite element modeling scheme, in which they implement *Mohr-Coulomb* brittle failure and subsequent viscous creep, i.e. *Newtonian* or non-*Newtonian* flow, of a mechanical stiff layer embedded in a weaker surrounding matrix during layer-parallel extension. A series of sensitivity studies of mechanical parameters is provided. Furthermore, Gardner and co-workers provide insights into naturally-boudinaged mafic layers from a mid-crustal high strain zone, in which they describe deformation styles and mechanisms by means of field observations and light microscopy. At first sight, the simulated pinch-and-swell structures resemble the natural examples to a certain high degree. The application of models those are capable of linking brittle with ductile features at various scales, as well as the comparison with natural examples of deformed rocks are of great relevance for the structural geology community, in general, and for the readers of *Solid Earth*, in particular.

However, I am concerned that the authors draw fundamental conclusions on the development of pinch-and-swell structures from the modeling results, which are based on the simplification of their prescribed rheological behavior. This problem particularly becomes evident when suggesting the application of the numerical model as a gauge for rheological parameters of natural samples, for instance. Without considering the classical literature about localization criteria for both brittle and ductile materials, they conclude that brittle failure is a necessary condition for the development of pinch-and-swell structures. With this respect, the onset of localization, i.e. the suggested pressure-sensitive necking process, remains hidden in the numerical scheme, although the authors stress that localization should arise out of an unperturbed, homogeneous system. Above this, I do not find the microstructural evidence of shear fracturing, representing the onset of boudinage, convincing at all. For these reasons, I suggest that major revisions have to be made in order to reconsider the manuscript after resubmission. In the following, I will focus on major and minor comments concerning content issues, referring to certain passages in the manuscript (*page, line No.*). My comments are meant to improve the manuscript and should therefore be considered during the revision process of the manuscript.

## Major comments

### 1) Microstructures

The interpretation of conjugate sets of brittle fractures of mode-2 (shear fractures), referred to as "through-going micro-shear bands" (1534, 3), based on the microstructural observations and the photographs of outcrop-scale structures presented in Figure 1, are not convincing and the following points should be addressed:

- (i) Where exactly are the conjugate sets of shear fractures, i.e. a set of two perpendicular planes oriented 45° to the boudinaged layer, visible on the larger (outcrop) scale (Fig. 1a,b,c) and on the micro-scale (Fig. 1e)?
- (ii) Where is proof that these shear fractures actually penetrate the entire mafic layer, on the microstructural or the outcrop scale? With this respect, drawing red lines on a field photograph is definitely not enough for such an important statement.
- (iii) I do not find the occurrence of single biotite grains indicative of brittle failure of the entire ca. 10 cm-thick mafic layers. Is the slight trace of an oblique (to the main foliation) oriented biotite clast indicative of a shear fracture that penetrates through the entire mafic layer? To me, the trace of the suggested shear band (dashed line in Fig. 1e?) is not clear. I cannot observe biotite precipitated along this zone.
- (iv) Is the amphibole clast, suggested to be intragranularly fractured (missing asterisks in Fig. 1e?), evidently fractured? Its thickness left and right of the supposed shear plane does not fit.
- (v) The suggested plane (dashed line; Fig. 1e?) runs vertical to the suggested extension direction, so is this a mode-1 structure? I suppose it is not, as I cannot observe any extensional features. Biotite should precipitate within such a structure in agreement with the direction of stress or shear. The orientation of this assumed failure plane is not in agreement with mode-2, nor am I able to follow the shear plane across the structure based on this micrograph. Moreover, I do not observe a conjugate set of these planes on the micro-scale.
- (vi) Mechanically weak phases are abundant all around the boudinaged layer (e.g. see biotite grain that defines the foliation in Fig. 1,d). Furthermore, according to Klepeis et al. (JSG 1999), the meta-sedimentary matrix of the St. Anne point host rock is composed of garnet, quartz, amphiboles and rutile. Does biotite also occur in the host rock (matrix)? Based on the micrograph taken at the outermost rim of a swell, close to the necking area, biotite seems to be also present in the host rock (Fig. 1e?), forming the foliation. Under the considered metamorphic conditions, at least quartz and biotite act as weak phases. For this reason, this kind of heterogeneous mineral distribution could also be treated as a homogeneous feature of the surrounding matrix and therefore be excluded for introducing instability. For clarification, please add a short description of the mineral composition and deformation mechanisms of the matrix. The latter will make the discussion of the results obtained from the sensitivity study of the power-law exponent more practical.

As the identification of shear fractures is of great importance for the numerical modeling scheme and the general concept, more insight and discussion have to be added.

Please consider providing more indicative microstructures.

## 2) Numerical modeling

In the numerical scheme (Moresi & Mühlhaus, PhilMag 2006), softening is induced by brittle yielding of the central layer. The sensitivity (rate) of softening is partly driven by the factor  $R_{CO}$ . In Table 2 the authors summarize the numerical experiments for different rheologies. However, the following points have to be critically reviewed:

- (i) In case of the numerical experiment with a viscous creep rheology exclusively, there is indeed no softening mechanism implemented. I miss the introduction and discussion of the classical concept of localization within rate- and temperature-insensitive materials and, more generally, the common assumption that pinch-and-swell structures form in a viscous manner, during continuous necking of a power-law layer, embedded in a weaker matrix (e.g. Schmalholz & Maeder, JSG 2012). These could be mentioned at page 1520, for instance. The authors finally imply that the initiation of pinch-and-swell structures in general is due to the brittle behavior of the material. If there is no softening in the dislocation or diffusion creep rheology accounted for by e.g. a negative power-law exponent or viscous shear heating, how can the layer localize? I fear that the authors draw a fundamental conclusion (e.g. 1532, 1-7) based on the limitations of the numerical concept.
- (ii) Unfortunately, the authors do neither discuss nor introduce how the onset of localization occurs and where? In case of a rate-insensitive material, the fundamental analysis of localization is missing. According to the finite element model of Moresi & Mühlhaus (PhilMag 2006), "healing" of former fracture planes was considered. Is this the case here?
- (iii) The authors lay emphasis on a model setup, in which localization results out of the constitutive description. However, they do not define the brittle localization criterion. Actually, the sketch of the model setup (Fig. 2b,d) indicates a surface roughness of the central layer. So, the initial condition is geometrically perturbed. For this reason, the introduction is misleading. Please specify how the model is perturbed, and how the onset of localization can be explained. (iv) Based on (iii), I am wondering why the resulting pinch-and-swell structure is rather asymmetric in terms of boudin spacing and the geometry of single swells and pinches. A higher level of softening explains unevenly spread sites of localization, whereas a lower level of softening results in a symmetric structure, respectively (1535, 7-9; 1537, 1-3). As the localization process remains hidden in the numerical scheme, please provide a better discussion of how the calculated asymmetries arise. If the layer surface is geometrically perturbed (iii), or healed fractures were assumed (ii), the site where localization occurs and the direction from where it propagates are predefined. Consequently, the initiation process itself is preconditioned and therefore cannot be studied.
- (iv) Concentrations of strain can be found at the layer-matrix interface (e.g. Fig. 6f). However, the authors do not discuss these matrix effects. Next, I miss a mesh sensitivity study and the scale of the finite element simulation. The suggested fracture is at the  $\mu\text{m}$ -scale. What is the finite element mesh size for small-scale

and tectonic-scale simulations? Please provide a mesh sensitivity study (e.g. in the supplement).

- (v) The role of elastically stored energy was reported in various numerical studies. However, the authors refer to the work of Ranalli (1997) and assume that for "high strain" structures, the effects of transient deformation can be neglected. This is an outdated concept. This problem becomes evident as follows. In Figure 3b (data for black star), the material is intrinsically unstable, i.e. failure is obtained instantaneously. Data from within the swell (red star) indicate that the yield stress is reached just above a "stretch" of 1. Next, the sequence of boudinage formation (Fig. 4) indicates that between a stretch of 1.0 to 1.2, localization has already occurred. I do not see how these findings are in agreement with the definition of "high strain". Furthermore, pinch-and-swell structures are interpreted to indicate low-strain deformation. This becomes evident in studies of crystallographic preferred orientations of dynamically recrystallized grains within necking areas (e.g. Schmalholz & Maeder, JSG 2012) or around coarse-grained clasts (e.g. Bestmann et al., Tecto 2006). These grains reveal a weak preferred orientation and deformation mechanisms indicative of low strain conditions.

### 3) Linking microstructure and numerical model

In a study that relates observations made from naturally deformed rocks to numerical simulations, there are some insight into e.g. the deformation mechanisms, material properties and flow conditions, at least to some extent. This might be the greatest advantage of such an interdisciplinary study. Be that as it may, the study of real rocks and their microstructures defines a framework for the initial and boundary conditions of a numerical experiment. Thus:

- (i) The authors test the sensitivity of viscous creep, post failure, by varying the power-law exponent between 1 and 3. The stress exponent of the dislocation creep flow law was chosen for a certain typical range for grain size insensitive creep (see Tab. S1). As stressed further above, evidence pointing to dislocation creep processes being active during layer-parallel extension could underlie this post-fracture deformation mode. However, I am wondering why a stress exponent of  $n = 1$  was considered at all (p. 1521). Basically, the stress exponent should be in agreement with microstructural observations, i.e.  $n > 1$ . *Analysis III* (1528, 17-27) should be based on microstructural criteria, so: how realistic is scenario (1)? It has been shown before that only non-linear rheologies reveal a necking instability (Smith, GSABull 1977; Schmalholz et al., JSG 2008). Are there hints towards diffusion creep dominated deformation (grain boundary sliding) in the surrounding matrix or within the mafic layers?
- (ii) Studying the literature about numerical simulations of folding and boudinage, the *competence contrast*, i.e. the difference in effective viscosity between layer and matrix (Hobbs et al., JSG 2011 and references therein), was debated. This in mind, how realistic is a contrast in viscosity of about 125 (1531, 20-22)? Please provide a discussion.
- (iii) In case of ductile fractures (1534, 3), a certain amount of plastic deformation is accommodated before brittle failure, by e.g. mode-2 fracturing. Where is evidence of plastic deformation recorded in the central layer? And, where is evidence of massive plastic deformation in the simulated stress-strain curves (Figs. 3; 6)?

- (iv) Regarding the comparison with the work of Mancktelow (Geology 2006), brittle deformation is considered the necessary mode in order to localize ductile deformation (e.g. 1533, 22). A discussion of the dynamic class of localization for viscous materials is entirely missing. This discussion would shed light on the fact that brittle failure is not a necessary condition for proceeding ductile deformation, but one possibility. For this reason, the statement that the initiation of pinch-and-swell structures is of a brittle nature cannot be supported in general. Next, the provided microstructural criteria for shear failure of the layers are not convincing. Please consider restricting your conclusions to the limitations of your numerical scheme and the actual microstructural observations, i.e. boudinaged layers deform by different modes, given the geological boundary conditions.
- (v) Unfortunately, the application of the studied parameter range and boudinage geometries is not well explained (e.g. 1538, 24-27). A fluid-like behavior for the development of pinch-and-swell structures is suggested, once the layer is fractured. This implies that the structure is amplified by viscous creep ( $n > 1$ ) after initial fracturing. Based on this sequence and the role of power-law creep of the layer, how important is the factor  $R_{CO}$  then? To me it is not clear how the authors attempt to estimate rheological parameters from boudinage geometries, obtained in the field.

## Minor comments

1518, 2) Why does the second sentence begin with "However, ..."? This implies that some contrary thoughts, in contrast to the proceeding sentence, are following. Indeed, the flow properties of the lower and middle crust are in general described by viscous creep or more complex (elasto-visco-plastic) rheologies. I do not see how this common concept will change, even though the authors provide insight into a micro-scale structure. Introducing brittle failure, as in Moresi & Mühlhaus (PhilMag 2006), aims at the description of near the transition of brittle-ductile rheology. The typical rheological stratification of the crust, as illustrated in many textbooks (e.g. Passchier & Trouw, 2005, p. 114), is an extreme oversimplification and not a state-of-the-art concept of the rheology of the entire crustal section. For further studies, considering more appropriate rheologies, I have pointed out useful literature further above.

1518, 6) The term "flexible" should be avoided. Please refer to your numeric scheme as e.g. "Mohr-Coulomb failure and post-yielding viscous creep".

1518, 6-10) See the major comment further above.

1518, 12) What is the condition that limits further strain localization? What process or mechanism is responsible for the arrestment of material softening? Please specify.

1519, 1-18) I miss references of studies of the frictional-viscous transition (e.g. Brantut et al., JSG 2013; Bürgmann & Dresen, Annu. Rev. Earth Planet. Sci. 2008; Karrech et al., JGR 2011; Regenauer-Lieb & Yuen, PAG 2008). Taking those into account, the "flawed" assumptions could better be placed in a geological (and modeling) context.

1519, 12-14) Recent localization theories that encompass the effects of energy and

thermo-mechanical feedbacks and references pointing to them are entirely underrepresented in the manuscript. The concepts of viscous shear heating and the role of elastically stored energy (e.g. Regenauer-Lieb & Yuen, GRL 1998; Regenauer-Lieb & Yuen, PEPI 2000; 2004; Regenauer-Lieb et al., Nature 2006; Regenauer-Lieb et al., JGeoDyn 2012) are of great relevance for the introduction and the discussion of softening mechanisms.

1520, 13-23) The majority of numerical modeling studies is based on the idea of a growing instability (in terms of an unstable material or introduced geometric imperfection), covered by the linear stability analysis provided by e.g. Fletcher (1974). This concept has been applied in a whole range of numerical simulations. I suggest incorporating the linear stability analysis into the first paragraph *Theoretical Analysis*, and to outline its application in numerical models (e.g. Schmid et al., JSG 2004; Schmalholz et al., JSG 2008), which should both be cited as well.

1521, 23-26; 1537, 14-17) How does the term "heterogeneity" relate to the rheological stratification of the crust and the occurrence of pinch-and-swell structures in general? Please explain. The consideration at "all scales" rather sounds too far-reaching (see the discussion of softening in e.g. Montsi & Zuber, JGR 2002).

1522, 10) The term "edge" is not useful. Please refer to the necking area, in general, or e.g. the rim of a swell.

1522, 11-14) The fracture angles vary between 30-40. How does this correlate with the classical *Mohr-Coulomb* fracture model? I think more explanations of the model of Moresi & Mühlhaus (PhilMag 2006) are inevitable here.

1522, 22-23) Please provide evidence of an increasing grade of "fracturing" towards the necking area by means of e.g. image analysis. Can single, intragranularly fractured amphibole clasts really be related across the suggested "shear band" (dashed line)?

1522, 23-24) Please provide more micrographs.

1522, 27-28) Could the finer grain sizes observed in the necks be also due to some viscous processes?

1522, 27-28; 1530, 23-24; 1534, 3) Please stick to the common nomenclature. A shear band is commonly referred to as a ductile feature, i.e. a narrow intensely sheared region, in which plastic flow dominates (e.g. Fressengeas & Molinari, JMPS 1987), whereas as shear fracture is evidently brittle (sliding mode). If you want to use shear band for both ductile and brittle features, please add "brittle" / "ductile" in front of the term. In the current version of the manuscript, I find the nomenclature inconsistent.

1522, 27) Does this mean that the discontinuity, suggested at the outermost swell section, referred to as "edge", formed by shear bands? This would be a ductile feature and contradict the before made assumptions. See comment above.

1523, 18-21) Please provide microstructural evidence for dislocation creep processes being active (e.g. cross-polarized light micrograph / EBSD maps etc., showing sub-

grain formation / rotation recrystallization etc.). As dislocation creep is considered the main deformation mode after brittle fracturing, thus regarded as responsible for the symmetric necking areas, more emphasis should be laid on this microstructural feature.

1523, 23-25) This is an important statement and should be introduced or discussed in the proceeding introduction (please refer to my comment further above).

1524, 12-15) Does this mean that viscosity is recalculated after yielding? The softening process is not clear to me.

1530, 19-21) How do you explain that there is no change in layer width, although the numerical box is extended?

1531, 10-11; Fig. 4 first row) Why does the plot of the strain rate invariant reveal localization bands, whereas the plot of the 2D structure is continuous in terms of deformation? At which time steps were both plots obtained? You could either add the time steps (as e.g. a number) or plot both for the same time step, which is more convenient.

1531, 19; 1532, 9; 1537, 8; 1552; 1553) Terms like "good" or "better" should be avoided throughout the manuscript. They imply that parameters were fine-tuned in order to fit the natural geometry.

1532, 12) Please explain the term "complexity".

1532, 17-18) Is the "variability" in differential stress after yielding really related to the findings of Griggs and Handin (GeolSocAmMem 1960), or are these numerical oscillations? I suspect, the latter are responsible for the documented variabilities. In any case, there should be a discussion of mesh sensitivity be incorporated in the results section.

1534, 16-25) In the works of Schmalholz and co-workers (Schmalholz & Maeder, JSG 2012; Schmalholz et al., JSG 2008), a linear instability with an infinitesimal small amplitude is growing, which ultimately leads to localization. This kind of inherited localization phenomenon is covered by the hydrodynamic theory of Fletcher (AmJSci, 1974) and co-workers, which is not cited, unfortunately. Studying these works, it becomes obvious that the comparison with the aforementioned numerical models of viscous necking is not helpful with respect to the findings. This immediately raises the question, of how localization is obtained at the onset of boudinage (please refer to the major comment further above). Here, a more detailed comparison with work on brittle boudinage (e.g. Abe & Urai, JGR 2012) would be more useful.

1535, 3-5) This comment relates to the latter one, made above. The softening mechanism in Hobbs et al. (2009) is triggered at a critical stress-strain-strain rate condition, termed dissipative work, which was uncovered by a study of the critical strain needed to trigger a thermal runaway (e.g. Hobbs et al., JSG 2011). In contrast, Neurath & Smith (JSG 1982), repeated again in Montsi & Zuber (JGR 2002) or Schmalholz et al. (JSG, 2008), introduce a negative power-law exponent, inducing softening of a power-law material. As both concepts are encompassed by a viscous strain localization criterion, I do not understand how this relates to the initiation of boudinage by brittle failure? Is

the material intrinsically unstable, therefore always softening? The classical mechanics literature provides the criterion for brittle failure to occur, but it is not referred to (e.g. Rudnicki & Rice, JMPS 1975). Please modify your comparisons accordingly.

1536, 25-26) I find this passage a more appropriate way to deal with the localization problem observed at the St. Anna point rocks. Please consider revising your fundamental conclusions elsewhere.

1537, 14-17) As criticized before, I do not agree that brittle fracturing has to be a necessary precondition for ductile flow, because there exists a criterion for strain localization in ductile rocks indeed (e.g. Hobbs et al., JSG 2011). Next, please add studies of viscous necking phenomena (using low-temperature plasticity;  $n = 10$ ) under greenschist facies metamorphic conditions (e.g. Schmalholz & Maeder, JSG 2012) here.

## Tables

1546, Tab. 1) As the viscosity ratio ( $R_{CO}$ ) was increased up to 125 and tested for its sensitivity in the manuscript, please modify the second row for the values of  $R_{CO}$  accordingly.

1547, Tab. 2) The last row with numerical experiments No. (iv) shows that there is no development of pinch-and-swell structures. This is due to the fact that there is no softening mechanism implicitly accounted for in the viscous creep description in the modeling scheme. Please refer to my major comment further above.

## Figures

1548, Fig. 1) The labels of minerals (Fig. 1a) are not visible in the sketch. Please add a label (Fig. 1e?) to the last micrograph. Asterisks are not included in the graph (?). (c) How do you explain the strong asymmetry of the studied necks? The boudin spacings and aspect ratios are highly heterogeneous, which suggests that the transient response was somehow altered. This might be due to the imposed geometric imperfections at the layer-matrix interfaces (see also my major comment further above)? (d) What does "Modes" refer to (e)? Is this  $\mu\text{m}$ -wide "shear band" really seen at outcrop scale? On the outcrop photo, no trace of this feature can be found. Within the so-called "shear band", fractured clasts of amphibole should, at least, lie within the suggested shear plane (dashed line) and should easily be matched (size, orientation). An additional micrograph, showing a necking area under cross-polarized light, could help to provide further insight into the dislocation creep processes.

1549, Fig. 2) (b,d) The layer-matrix surface is not a straight line, thus geometrically perturbed. The perturbation technique that explains location and direction of localized deformation should be mentioned in the text. (c) The stress-strain curve reveals a complex transient deformation stage (linear elasticity and strain hardening). In agreement with the numerical modeling scheme, there should be only linear elasticity illustrated (linear increase of stress with loading).



1550, Fig. 3) (c) Why is the plot of the stress invariant rather blurry than localized?

1551, Fig. 4, first row) Why does the plot of the strain rate invariant reveal localization bands, whereas the plot of the 2D structure is still homogeneous?

1553, Fig. 6) Please indicate from where (which model setup and location within the boudinaged layer) the stretch-differential stress data (g) are coming from. (f) Why do the rheological data for  $R_{CO} = 1$  suggest continuous softening, although there is no softening mechanism implemented in the viscous part (and thus not detectable in graph -f-)? Is the layer thinned to a certain high degree (with elevated strain rates) and therefore apparently softening? In graph (f), I observe localization at the layer-matrix interface. If the material is homogeneous and the geometry unperturbed, how do you explain such localization patterns? (g) The rheological data for  $1 < R_{CO} < 10$  reveal continuous softening, whereas the data  $R_{CO} = 20$  are rather bumpy. Only the data for  $R_{CO} = 100$ , i.e. the highest contrast in cohesion before and after yielding, are in steady state. This finding limits the potential application as a deformation (rate) gauge for natural viscous rocks, because constraints on matrix flow can only be obtained from steady-state creep within the necking areas. I suggest including this to the discussion and limiting the application to the boudinage geometries, due to brittle fracturing. For these reasons, I am wondering about how much pinch-and-swell structures are actually being addressed with this respect? For  $R_{CO} > 100$ , I suspect that the data are more stable. Be that as it may, does it make sense (from a microstructural or material properties perspective) to apply contrasts in cohesion of larger than 2 orders of magnitude?