Reply to the review of anonymous reviewer RC#1

Dear reviewer,

We would like to thank you very much for the thorough review and the critical comments. Your constructive suggestions and corrections strongly improves the quality of our manuscript. In the attached document, we present our changes and corrections to your individual comments.

Kind regards,

Lisa Winhausen and co-authors

SCIENTIFIC COMMENTS

General scientific points that require attention are as follows:

A) The authors often describe their work as addressing the microphysics or micromechanics of shear failure of the OPA material. However, there is no physics or mechanics in the paper at all – it is purely qualitative and conceptual. Rather, the authors address the MICRO-MECHANISMS involved in deformation and failure of the material studied and should really use this term to describe their work (it is a micro-mechanistic study).
→ This is a good comment and we agree on that. However, we feel that also the term 'micro-mechanistic' model implies physical and mathematical equations and laws. Therefore, we used the term 'Micro-deformation' model and replaced all text passages where 'microphysics' or 'micromechanics' is misused.

B) The experimental sample investigated was tested unconsolidated and undrained at 4 MPa confining pressure. There is no discussion as to how these test conditions (hence observed processes) might relate to conditions of interest in the subsurface, such as caprock or repository conditions. Perhaps the effective stress would be comparable (low) due to consolidation effects, but some discussion of this would be welcome – as would the likely pore pressure evolution in the experiment (perhaps based on volumetric strain data).
→ We agree with this statement and included a discussion on the testing conditions and to the application purpose.
"Many of these processes become effective at long time scales under natural conditions. In tunnelling however, low-permeable rocks such as OPA are subjected to undrained loading conditions during excavation. Thus, the triaxial compression tests have been performed as classical UU tests without prior saturation and consolidation. The pore water pressure development and effective stress inside the sample remain unknown. The test provide the undrained shear strength representative for the nearfield of a tunnel excavated at the consolidation conditions found at the MT-URL(Martin and Lanyon, 2003). Therefore, micro-deformation processes observed in the sample are considered similar to those found in the near-field of a freshly excavated tunnel in Mont Terri. This is further corroborated by the similarities between microstructural EDZ and BDZ (borehole damage zone) observations (Bossart et al., 2002, 2004; Yong et al., 2007; Nussbaum et al., 2011) and microstructures found in this study.".

C) The description of the experiment does not seem quite right in terms of boundary conditions applied to the sample. The authors seem to be saying that the test was carried out at constant confining pressure and at controlled circumferential strain rate, which is equivalent to controlled radial strain rate. Do the authors mean that axial loading system was servocontrolled to provide a constant radial expansion (or contraction rate)? This seems unlikely to me. Or do they mean that a constant axial strain rate (or stress rate) was imposed and the radial expansion/contraction was simply measured (not controlled)?
→ Our experimental description is correct (compare also Amann et al. 2012). The axial loading is applied in such a way that the sample exhibits a constant circumferential displacement rate. This approach is also described – even tough for unconfined tests – in "ISRM suggested method for the complete stress–strain curve for intact rock in uniaxial compression" (Fairhurstt & Hudson 1999) and

is especially practicable when the axial stress-strain is not monotonically increasing as commonly the case for soft, clay-rich rocks.

D) The terminology used to describe the various cracks, fractures and shear bands at different scales is somewhat confusing to the reader (at least this one!) and not very systematic. I would strongly recommend defining the terminology to be used for these features at an early stage in the manuscript. It would be useful if the authors could define cracks versus microcracks, as well as defining crack character – i.e. whether individual cracks are Mode I (opening) or Mode II (shear) cracks or mixed mode. The term "shear band" should also be defined and appropriately distinguished from a shear crack – at least in a morphological sense. Voids that open between grains due to local dilatation should also be defined as something like dilatational or dilated pores. Of course, the observed features may ALL have been influenced by unloading (removing axial stress and/or confining pressure), so that needs to be mentioned.

→ We agree with this comment and included a paragraph in which we explain the terminology used in our manuscript. We omitted the term 'cracks' and used the synonym 'fracture' instead.

"Prior to the qualitative description of macro- and microstructures encountered, we define the terminology for our observations and the subsequent discussion. First of all, we use – where possible and not explicitly implied in the section title – prefixes as 'macro' or 'micro' for structures which are visible with the naked eye or under the SEM, i.e. under magnification of at least x100. In general, we subdivide where possible the general term 'fracture' – the surface formed through an initially intact solid material – into 'tensile', 'shear' or 'hybrid fracture' according to their movement along the surface, i.e. normal, parallel or a mixture of both, respectively. Furthermore, we call broader zones of multiple fractures and deformed microstructure 'deformation band', in case for elongated zones with increased porosity 'dilation band', and where shearing is interpreted, we use the term 'shear band' (cf. Du Bernard 2002)."

E) While it is clear that many of the observed cracks and shear bands are directly associated with the evolution of the macroscopic shear failure process, some features that the authors link to shear failure could potentially be present in the starting material or could have been caused by the application of confining pressure (i.e. to the hydrostatic component of consolidation). Crushed fossils, disrupted pyrite framboids, buckling of phyllosilicates etc all come to mind here. I do not doubt the authors' interpretation necessarily, but it would be desirable to add a few micrographs AT LEAST of an undeformed control sample to prove that the above features are not present in the starting material. Ideally one would like to see a few shots of a hydrostatically loaded microstructure too, if easily available.

→ We understand the reviewers point and argue here that the deformation markers such as micro fractures, crushed fossils etc. are absent in the starting material, i.e. undeformed host rock, as extensively described by Houben et al. 2013,2014. Considering the stress conditions of the over-consolidated host rock from MT-URL with similar stress conditions as used in our study (approximately 4 MPa) we argue that no deformation markers described here are due to isotatic loading as these are well below the past maximum in-situ effective stresses. Furthermore, Winhausen et al. 2021 performed hydraulic testing on shaly OPA at hydrostatic loading conditions of up to 24 MPa effective stress. They performed a microstructural analysis by comparing the unloaded and loaded sample, and found that hydrostatic loading and consolidation does not change the microstructure forming shear or 'damage' indicators as described above. For addressing this point, we added a paragraph to our manuscript and see no need in adding additional micrographs.

"The deformation markers (Fig. 4-7) are inferred to have formed due to shear failure since these are absent in the microstructure of tectonically undeformed OPA samples from MT-URL (Houben et al. 2013, 2014). Furthermore, Winhausen et al. (2021) analysed the microstructure of a shaly OPA sample, which has been used for hydraulic testing at maximum 24 MPa effective stress, and found no deformation features. Their comparison to a non-loaded twin-sample as well as to other microstructural studies on OPA indicate no structural damages due to isostatic loading at this effective stress (Winhausen et al. 2021).

F) Last but not least, some brief discussion is needed as to how fluid flow from consolidating regions of the sample to dilating regions of the sample may have facilitated shear localization (as opposed to dilatancy hardening), as this could be a key component in controlling the failure behavior and strength. Such aspects would be essential for any quantitative microphysical modelling in future, and notably for understanding strain rate effects.

→ We agree with the reviewer that the dilating regions play an important role, but see here the opposite effect: As the whole test was performed in less than 40 min, consolidation processes in this low-permeable rock do hardly play a role as the conditions within the sample can be considered undrained. However, we agree that the local dilatancy creates more pore space and, therefore, a reduction in pore water pressure and a local increase in effective strength in the sheared zones. We see here two competing mechanisms to act: The facilitated shearing (shear softening) due to the loss of cohesional bonds and the effective strength increase (shear hardening) within the shear zone. Based on the only sample analysed in this study, we argue that shear softening is the prevailing process but unequivocally strain rate effects play a great role (cf. Giger et al. 2018) when testing at consolidated boundary conditions. We will not extent the discussion in the manuscript but empathize this aspect in our ongoing studies under consolidated testing conditions. Nevertheless, we included a brief statement in this discussion to our text:

"The local increase of porosity in the deformation band leads to a local reduction in pore water pressure under undrained conditions and a related local increase in effective stress in the shear zones. The increase in effective stress involves a shear hardening effect, which represents the competing effect of shear softening due to the loss of cohesional bonds. Here, further research is required to investigate the dependency of permeability and porosity evolution with increasing amount of shear stress and the effect of undrained and drained conditions within the sample.

Detailed scientific comments/questions

1) Title: This seems unnecessarily long and not especially informative to me. Would something like "High resolution BIB-SEM study of micromechanisms leading to shear failure of Opalinus Clay in a triaxial test" not be more accurate and sufficient??

→ We change the title to be very similar to the suggested one

"Micromechanisms leading to shear failure of Opalinus Clay in a triaxial test: A high-resolution BIB-SEM study"

2) Abstract: Best clarify that failure occurred by shear failure and mention orientation of the shear fracture/band network (line 21).

→ Both point were added to the abstract

"Observations on the cm- to µm-scale showed that the samples exhibited shear failure and that deformation localised by forming a network of µm-thick fractures which are oriented with angles of 50° with respect to horizontal."

3) Last statement about LIMITED similarity with natural fault zone microstructure and inferred role of pressure solution in nature is not very well supported in the main text. Perhaps add some additional evidence in the main text?

→ We added some additional similarities to the main text and the new following paragraph is discussion the existence of processes occurring in experimental vs. natural conditions.

"Some structures found in this study, such as the anastomosing fracture network, strained fossil shells and bending of phylosillicates resemble those found in highly strained OPA (Laurich et al., 2017; Orellana et al., 2018)"; see B)

4) Intro: I advise using the term "radioactive waste" rather than "nuclear waste". Nuclear suggests high level waste risk which is often not the case. Atomic nuclei are also hardly waste.

→ We replaced the term accordingly.

5) Page 2, line 48. Microstructure is perhaps the wrong term here. Mineral composition would be accurate. Line 52 – what measure of visible pore size shows a power law distribution??? Lines 61-62 – compressive loading of samples in what orientations with respect to bedding? And what is meant by plastic flow – please define as it has many meanings.
→ We replaced the text according to the suggestions and added the orientation of the samples tested in the cited reference

6) Page 3, Line 83: Is "slickensides" the correct term here for these very fine striations in the mirror slip surface? Are they optically visible or only in SEM and sub-optical? Line 88 - do you mean smectite interlayer water here? Please clarify.
→ We used the terminology as given by Jordan and Nüesch, 1991. Slickenslides is not referring to the striations but the shiny and mirror-like surfaces (on which striations might be visible). This is well explained in the text. Jordan and Nüesch 1991 observed these both optically and in the SEM. We added this missing information to the text. Concerning the water inter layers, the cited authors (Jordan & Nüesch 1991) mean the absorbed water between clay two layers but do not specify the clay mineralogy they are referring to. We changed the sentence slightly.
"These shiny and mirror-like surfaces (i.e. slickenslides), optically and microscopically visible, consist of denser packed clay material."; "[…] as 'sliding surfaces' on water interlayers of clay minerals and […]"

7) Page 4, Line 124: Mixed layer silicates?? Do you mean mixed layer smectites and mectite-illite??? Last line: what is the pore fluid? A brine with what composition?
→ We specified in the text which clay mineralogy is included; detailed subdivision of different clay minerals is not provided by the authors (klinkenberg et al. 2009) due to missing Rietveld analysis. The sample was not re-saturated by an artificial brine. Full saturation was demonstrated by porosity and water content measurements as explained in Amann et al. 2012, which is referenced in the text.
"[…] clay minerals (50-66%) composed of 2:1 layer with illite, muscovite, smectite, and illite-smectite mixed layer minerals are (20-30%), […] "

8) When first describing fracture/crack/bedding/loading orientation, please define what you mean by orientation or inclination in terms of an angle (say theta) defined in a small diagram. Present usage is confusing, perhaps due to language. It is important to be consistent in the use of this terminology throughout the paper. Confusing at present.
→ According to this and the third reviewers suggestions, we included a sketch (included in Fig. 3) for the definition of the inclination angle. Furthermore, the directions of bedding and loading were included in the figures, where still missing. We added a sentence to the text referring to the diagram added to fig.3
"In the following, all angles are defined as deviations from the horizontal, i.e. load direction of σ3 (see diagram in Fig. 3)."

9) Section 2.2. Please clarify boundary conditions imposed in the experiment – see point B above.
→ We comment on the selected boundary conditions in the discussion. Please, see point B)

10) Section 2.3, first line. Mechanically stabilized with epoxy ?
→ The sentence has been changed accordingly.

11) Section 3.1, last 3 lines. Specify branching fractures as the green ones if that is what is meant (all look branching to me). Fragments are only CRUDELY lens-shaped – best say this perhaps. Please clarify what is meant by "relay fractures".
→ We changed the text accordingly and inserted a small zoom-in illustration showing the relay structures observed on the macroscale to Fig. 3.

12) Section 3.2, first paragraph: How long were the samples stored before study ?? Please indicate in the material description. What reacted to produce gypsum? How do you know this occurred during sample storage?? Could storage have had any other effects that could corrupt the microstructure?

→ We added the missing information to the text (sample storage of five years) and explained why gypsum formation is likely to happen after core extraction (when exposed to air). Storage can lead to swelling or shrinking of OPA due to the changing stress and de-/saturation conditions. These effects are mentioned in our discussion.

"[…] by chemical reactions during sample storage before or after the experiment. When exposed to air, pyrite will oxidise creating sulphate, and the presence of Ca-ions from calcite (and dolomite) will lead to the formation of gypsum. Timing of this process could not be determined and, therefore, these regions were excluded from microscale analysis."

13)Page 6, Line 183: Microcracks were often oblique to bedding…. Which set is meant here?
→ We changed the text accordingly.
"Micro-fractures, which belong to fracture set 1), were often […]"

14) At several points in the description of the microstructure (Results – Figs 4 and 5), reference is made to increased porosity and grain-matrix separation at specific sites around clasts and clast-like/sigmoidal micro-lithons. These sites seem to correspond to interfaces under local extension – i.e. at roughly 45 degrees to the overall (macroscopic)shear failure plane orientation. This should be described as such, if indeed a widespread feature, making reference to previous work that has observed and constructed models for this type of feature (e.g. Den Hartog & Spiers 2014; Haines et al., 2013). These featureshave key mechanical significance in defining the onset of mechanical weakening due to a decrease in dilation angle (see papers by Den Hartog et al).
→ We understand what the reviewer is referring to but do not entirely agree with his/her observations. In fact, in Fig. 4 can be seen that grain boundary-matrix slitting appears in all directions (calcite fossil in centre for instance parallel to "shear plane" as of larger, rounded quartz grain in lower third shows a rim with orientations from parallel to 90° to shear band direction. Similar observations can be made in Fig. 5a), where quartz grains in the upper right corner are completely surrounded by porous rims. We can see the 45° degree trend in one calcite grain (upper right, label "cal"), but again the siderite grain (lower right, label "sid") shows a grain-matrix separation which is parallel to the macro shear zone. We also want to state here that we present microstructures of an incipient "shear zone", the MS of the sample does not show fully developed shear bands or gouge.

15) Page 8, line 235: "Plastic reorientation of clay aggregates". What exactly is meant here? Why is this plastic not frictional intergranular sliding? "Ductile" deformation is inferred from reorientation to form an SPO, I guess? The term "plastic" is used elsewhere in the ms to refer to intracrystalline plasticity of the phyllosilicate grains> perhaps make more consistent? Line 236 – "grain boundary sliding". This term is generally used for a high T process involving grain boundary dislocations. Better use "intergranular sliding" here as it is likely a frictional or fluid-lubricated sliding process. Lines 239-242 – I am surprised that no reference is made here to the top quality work on deformation of claystones such as COX by the Paris Est (Ecole des Pont) Team (recent papers by Philippe Braun, Pierre Delage and co-workers). Relevant work should be added.
→ In line 235, we deleted "plastic" which was not appropriate in this sentence. Throughout the manuscript, we distinguish between brittle (breakage/fracture with prominent surfaces) and ductile deformation (bending and reorientation). We changed all parts according to make the text consistent. We replaced "grain boundary sliding" by "intergranular sliding". Indeed, we know the work of Braun, Delage et al. However, they performed hydro-mechanical experiments on (mostly) isostatically-loaded samples to derive the material's poroelastic properties and dependencies on temperature. Up to our knowledge, they performed no triaxial deformation experiments in which they analysed the (micro)structural deformation and we see therefore no valuable contribution to our manuscript.

16) Page 9, Line 260: It is assumed that unloading elasticity is equal throughout the sample. Perhaps make this "roughly equal" as the elastic stiffness of the porous zones will certainly be much lower than the undeformed matrix. Line 268-269 – reference is made here to the amounts of elastic versus inelastic deformation in the sample. This could be evaluated from the elastic part of the unloading curve, perhaps. Not done? Could this be added to add a littlle more quantitative information?
→ We changed the sentence according to your suggestion. Unfortunately, we have no data from the unloading part of the experiment, hence, we cannot evaluate this quantitatively.

17) Section 4.3 - Micro-mechanical model. This is a misnomer, I feel, as the model presented is a conceptual model containing no real micromechanics – a term that implies a quantitative approach. This header is perhaps best modified to "4.3 Micro-mechanistic model" - which is probably what is meant by the authors. Perhaps it would be wise to add to this section the caveat that the conceptual model developed is based on a low P experiment with no pre-consolidation, and to clarify the imposed boundary conditions (constant P, controlled axial or radial? strain rate etc etc). It has to be recognized that different microstructures may develop under different conditions, or it should be argued why this would not be the case.
→ We agree and inserted the missing information to this paragraph. We also changed the section title and replaced the phrasing in the text accordingly; see also point A)
"For the unconsolidated, undrained deformation of OPA under differential compressive load at a total confinement of 4 MPa, we propose the following deformation mechanisms based on our microstructural observations […] "

18) Fig 9 vs. Fig 1. This depicts the micromechanistic model proposed. However, the stress strain-curves used to illustrate the various stages of evolution looks rather different from the original experimental data depicted in Fig.1. Is the stress axis perhaps the total axial stress as opposed to the differential stress plotted in Fig. 1?? Please clarify as the stress levels mentioned seem not to match up as is. It would be useful to clarify the orientation of Sigma-1 in the microstructural sketches also. In Fig. 1, how was the stress level labelled "crack initiation" established? This should be mentioned somewhere?
→ Yes, the plot in Fig9 shows the total axial stress instead of the differential stress, we added "total" to the axis title; apart from that, the plot shows the same data as in Fig.1. We inserted the orientation of sigma1 to the sketch. "crack initiation" or "fracture initiation" as used in this manuscript has been adapted from Amann et al. 2011. They determined this threshold as the deviation from the linear-elastic behaviour of the volumetric strain curve. We added the explanation to the text.
"Amann et al. 2012 showed that fracture initiation, the point where the volumetric strain curve deviated from linearity ("crack initiation" in Amann et al. 2012), occurs long before stress peak at approximately 2 MPa differential stress independent from confining stress."

19) Section 5 - Implications and conclusions. As indicated above and in my general scientific comments, this section would benefit from some brief consideration of the extent to which the observed processes and proposed mechanistic model can be expected to apply under shallow upper crustal (geo-storage system) conditions. The authors do state that more work is needed on consolidated samples and on naturally sheared/faulted samples to test the broader applicability of the model. However, in future experiments, would not higher P-T conditions and deformation/loading rate not be important too, bearing in mind issues like smectite hydration state changes and internal fluid pressure equilibration, for example?
→ We agree with this point and included a paragraph to section5
"Our high-resolution study gives insights into the macro- and microscale structures with some similarities to excavation or naturally induced structures. However, OPA - deformed up to peak stress - also shows structural differences to naturally deformed OPA, which shows drastically reduced porosity. Strain amount and rate in natural fault systems, as well as elevated temperatures or clay-mineral hydration processes may influence the deformation mechanisms and structures. On the other hand, natural veins as an indication for paleo-fluid flow in the early faulting stage (Clauer et al., 2017) support localised dilation as similarly found in this study. Future experiments covering a broader range of

boundary conditions on consolidated samples are required to analyse the deformation processes under shallow upper crustal conditions, and to formulate an effective stress dependent deformation model.

20) Still Section 5: In Line 353 of page 12, how does the present study support implementing damage into constitutive modelling in the references mentioned? Do the authors mean "support" here or "provide input to constrain" such models, perhaps?
→ We changed the sentence according to your suggestion.
"The results of this study support more recent efforts […] to provide input to constrain damage in constitutive models […] "

21) Figures 2-7: It would be useful if the orientation of the principal compression direction is indicated in all key micrographs, either directly in the micrographs or appropriately via the captions. Angles defining fracture and shear band orientations should be marked on key micrographs also, so that the intended meaning of terms like inclination (to what? Horizontal? Vertical? Bedding?) is clear. What is OM in Fig. 5a?
→ We inserted a sketch indicating the orientation of bedding and macro-shear band orientation in each key micrograph with according colour labels as presented in Fig.3, and added a description of such in the figure captions. We replaced OM by "organic matter".

TECHNICAL ISSUES (language, typographics etc)
Overall the paper is well written and in good English. Nonetheless a few small improvements can be made as follows:
i) Fault gouge spelling: Gouge NOT Gauge → corrected throughout the text
ii) "Associated with" is the correct usage, not "associated to" → corrected accordingly
iii) "Indicated "should not be used to mean "correspond to". Use the latter. → exchanged where necessary
iv) A typo: Saddle-reef pores. Better define the term also as it is from structural geology and is not familiar in rock mechanics. → corrected and definition inserted
v) "Acting on"… not "acting to..". → corrected
vi) "growed" >>>> grew → corrected
vii) Page 11 – reformulate first sentence. English awkward/unclear. → sentence reformulated
Finally, I would recommend a thorough spelling/grammar check at the end of the road. I wish the authors good luck in revising the paper and hope that my comments are helpful and not too burdensome. Please note that I have elected not to do a second review, not out of disinterest but from "review overload".