Solid Earth Discussions

Solid Earth Discuss., referee comment RC1
https://doi.org/10.5194/se-2021-30-RC1, 2021

Comment on se-2021-30

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Referee comment on "A new finite element approach to model microscale strain localization within olivine aggregates" by Jean Furstoss et al., Solid Earth Discuss., https://doi.org/10.5194/se-2021-30-RC1, 2021

This paper presents a modelling approach for micro-scale strain localisation within olivine aggregates at high temperature. The framework is based on modified reduced crystal plasticity to account for non-dislocation glide mechanisms and the mechanical model is coupled with a missed velocity/pressure finite element formulation. The numerical tools are then applied to study localisation on various pre-existing shear zones for relevant laboratory conditions.

This contribution is quite technical but the work is rigorous and all components are well explained, with all steps thoroughly documented and all numerical parameter values justified from literature. The authors provide a comprehensive framework and should be commended for their good work. My main comment is about the impact of the results produced, with the final conclusions remaining unfortunately very much within the boundaries of common knowledge, that “fine-grained and crystallographic textured pre-existing bands favour strain localisation”. No-one denies the importance of texture and grain size on mechanical deformation and it would be nice to see more quantitative conclusions about the effects of those processes, including the cumulating feedbacks to tackle important questions like localisation initiation and whether such processes are causes or consequences of self-localising phenomena. The approach certainly shows great potential to get quantitative but it might require a bit more calibration work to draw the most useful conclusions.

Despite the extensive literature review presented to get values for all parameters, each experiment remains a specific case and values carry an uncertainty range (which can sometimes be wide). There is a large number of parameters used (22 listed in table 1, only taking into account temperature dependency globally) and some/most of those might require specific calibration for a given application, especially as the authors acknowledge (l.299-300) that some are more numerical than physical. As mentioned, l.427, the calibration problem is non-unique. This is possibly why the results don’t really match so well the laboratory results of fig. 2, which I found a bit disappointing after such a comprehensive and powerful model being presented. As the main quantitative calibration step before the subsequent predictive analysis, these results are particularly important,

yet they're currently not doing much justice to the nice framework introduced in my opinion. The authors should probably allow themselves the necessary freedom to set parameter values that work for the model. This includes not just playing with the identified degrees of freedom (eg. K1 and K2), but even with parameters whose values are supposedly fixed since reported in the literature. I agree that a unique CPFEM framework is numerically more efficient than existing numerical solutions for modelling dislocation climb (l.157) but it is important to tackle accuracy before efficiency and the (very complex) calibration stage has only been started. The breakdown and modelling of all processes involved cannot be decorrelated from the experiments to match and it would be nice to see a discussion about the shape of the experimental curves of fig. 2 to identify the (two) phases of all responses as well as the temperature effects (which don't affect the first phase as much as the second). Given the deep understanding of the authors on the processes modelled, it would also be nice to see more discussion about what type of experiments would actually be needed to calibrate more effectively the model parameters. Looking at fig.2, it looks like the calibration was done to minimise the L2 norm between the experimental and numerical results as a whole, which produces extremely large discrepancies at low strain as a side effect (with stress values about 400% too large at 1% strain on all three 1073K cases!). This type of mechanical response distorts enormously the results very early on and unfortunately casts a large shadow of doubt on all consecutive steps. Similarly, regarding the temperature effects, the values of K1 and K2 derived do produce some thermal weakening, but for the whole response, including the low strain part since the colder response (1073K) is mismatching this early response to begin with. Also, given the elegant physical model used, could the authors also comment on potentially better ways to include temperature effects for the various components?

Here are some other minor comments to help improve the manuscript:

- The introduction focuses on microstructure as a key factor to initiate localisation and mentions l.21 that "the microscale processes initiating this localisation are still debated". I fully agree but would go further as localisation can be initiated by much larger scale processes as well through multiphysics.
- L.30-33, it would be nice to open a bit the literature review to multiphysics studies (e.g. Santiago Pen Ì□a Clavijo's PhD thesis, http://hdl.handle.net/20.500.11937/78045) as chemistry becomes tightly coupled to mechanics at this scale.
- L.191: define P1 elements
- L.192: can you comment on remeshing step, benefits of keeping good quality elements vs handling of history in new nodes (interpolation drawbacks)?
- Eq.22: why not a volumetric integral? (Note that it's not completely natural for the reader to assume that the cylinder deforms the same way along its whole length in a paper studying localisation)
- Fig.4b: Are the two stars positioned on (1) the curve based on strain rate (i.e. taking the olivine deformation map as granted) or (2) also using computed differential stress values (which actually fall perfectly on the map)? (If (1), where are the stress values and where would the stars really be on the map?)
- L.361: I didn't quite understand why there's 20% higher strain (in the inner part compared to outer parts) for the model without shear zone. Shouldn't that be close to zero as a reference test? (I obviously misunderstood something, which is particularly detrimental as fig. 6 is arguably the most critical quantitative result of the study...) Please clarify.
- Optional: given the numerous acronyms used, maybe a table of acronyms / nomenclature table would help

- Optional: for all experiments described, a small sketch with boundary conditions would help
- Typos:
  - L.69: missing dot on gamma (slip rate)
  - L.82 spelling "Lasraoui"
  - (L.133: just curious, where does this notation for fourth order identity tensor come from?)
  - L.163-165, fix mangled sentence
  - L.281 disp_y=0 as well on other face?

In conclusion, the framework is very interesting and the authors presented it in an excellent manner. The complexity of the model, however, requires the calibration of numerous parameters and I'm afraid this tuning exercise was not performed at the same quality level. Consequently, many of the deductions remain rather generic and the authors point out correctly some possible reasons why the models cannot predict the development nor the persistence of a fine grain zone. The problem tackled is really complex and this new framework certainly adds enormous value. The geological conclusions, however, are not necessarily as impressive and the paper overall does not deliver the impact one could expect from the model. I would therefore recommend some major revisions to improve the calibration in hope that clearer and more impactful conclusions can be drawn.

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