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Interactive comment on "Analytical solution for residual stress and strain preserved in anisotropic inclusion entrapped in isotropic host" *by* Xin Zhong et al.

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We thank the reviewer for the comments that greatly improve the quality of the work. Our replies to the comments are in blue and the original comments are in black.

The manuscript of Zhong et al. presents analytical and numerical solutions for the deformation and stress of ellipsoidal inclusions in an infinite host. These solutions are applied to so-called Raman elastic thermobarometry, which is a method to estimate the peak P-T conditions of exhumed rocks. This thermobarometry is an alternative method with respect to P-T estimates based on thermodynamic Gibbs energy minimizations and is, hence, important to validate and cross-check P-T estimates obtained

from different methods. The authors present solutions for an anisotropic inclusion in anisotropic host and further present approximate solutions for so-called faceted inclusions (inclusions with corners). The analytical solutions are tested with numerical simulations based on the finite element method. The Raman elastic thermobarometry is an important and more and more applied method to estimate P-T conditions of exhumed rocks and is, hence, of interest for a wide readership. The authors also provide several of their numerical algorithms, which allows readers to reproduce the presented results and to apply these algorithms for their own research. The open access to these algorithms is a great benefit of this contribution.

However, the authors should discuss in more detail the limits of applicability of their solutions and potential magnitudes of errors when applied to natural host-inclusion studies, which are likely more complex. Ideally, the authors should provide something like a "check-list" for the application of their solution to natural host-inclusion systems.

We have added a new section "5. Limitation of applicability" to discuss this issue as suggested by the reviewer. This includes the discussion and limitation of some of the assumptions that we have taken so far, e.g. infinite and isotropic host, linear-elasticity and inclusion shape. This is practically a check list to remind readers of the potential issues of elastic thermobarometry, and we believe there will be certainly more refinement to work on in the future.

I have also read the comment to this manuscript by Angel et al., which discusses in detail some limits of the presented models, for example arising due to different orientations of the axes of crystallographic orientations and the principal axis of the ellipsoidal shape. I find this comment very useful and urge the authors to clearly explain and discuss these limitations.

We have provided a detailed reply to Angel et al. and added new text into the manuscript to address this issue. We agree that this is worth mentioning but, in our view, the symmetry breaking issue has no adverse effect on our work: 1) Its estimated effect on the final Raman shift seems minor after comparing the experimental and DFT calculations (see table above in the reply to Angel et al.). 2) Obtaining the Raman shift using residual strain or stress is intrinsically a post-processing procedure that does not affect our analytical solution at all (so our main focus is not impacted). 3) Lastly, there are simply no available parameterizations of the physical properties such as elastic stiffness, thermal expansivity and particularly the Gruneisen tensor under non-symmetric deviatoric stress.

Making algorithms available is great for the research community, but always generates the risk that users may apply such algorithms wrongly to natural systems for which the algorithms are actually not correctly applicable. Therefore, the authors should address the limitations and applicability of their solutions in detail during a revision of their manuscript. Apart from this major comment, I have a few minor comments, which the authors might also consider during a revision.

Minor comments:

Line 86-88: These are strong assumptions for the stage of entrapment. Maybe these assumptions could be discussed and justified in the Discussion section.

We agree with the reviewer that we use an assumption that upon entrapment, the inclusion and host were subject to the same stress field. However, it can be argued that this assumption is a reasonable one considering that when the inclusion was engulfed by the host during its growth, they must be possess the same stress state under mechanical equilibrium as elastic stress equilibration is a fast process compared to mineral growth. This is made clear in the main text after this sentence.

Line 97: For readers not expert in anisotropy in minerals, it would be useful to explain the angles, maybe even with a little sketch showing the anisotropy axes and the corresponding angles.

We have added a sentence explaining the meaning of the angles.

Line 107: Please explain what the PVT relationship is. Best would be to just add the formula to avoid any ambiguity.

We have added a line describing the PVT relationship. It is difficult to add a simple formula to describe the relationship because: 1) there are many distinct PVT relationships, each applied to different minerals; 2) the relationships are highly non-linear and often implicit, so it is not possible to use one simple formula to describe the PVT relationship. Therefore, we have not added any specific PVT formula to avoid potential confusion.

Line 171: Could you add a sentence explaining the origin of the Grüneisen tensor for the non-specialists. For example, is this tensor derived from theoretical calculations or determined from experiments?

Done. We have added new text here to describe this tensor. Both ab-initio and experimental data on the Gruneisen tensor exist and they seem to match quite well, even if they are done at distinct stress condition. See the table in the reply to Angel et al.

Line 214: A main result is quantifying the impact of the aspect ratio. However, the impact of the aspect ratio is not very transparent from the presented equations. Is there a possibility to provide an equation, which shows the impact of the aspect ratio on the Eshelby tensor clearer, or in a more transparent way?

There is unfortunately no explicit form describing the impact of aspect ratio on the Eshelby tensor (not to mention the final expression for the residual stress), e.g. see the work of Mura 1987, who has attempted and the current formula is at its most simplified form as given in the Appendix. Therefore, we did not change this part.

Line 235-231: Could you provide a simple and/or intuitive explanation why the aspect ratio is least sensitive for quartz but most sensitive for rutile. What is the controlling mechanical difference between quartz and rutile responsible for the different sensitivity?

It's not very intuitive why the rutile is more sensitive to aspect ratio as it requires deriving an explicit form of stress variation from spherical case due to shape change, which cannot be easily done. One possibility is that rutile is highly anisotropic, which makes the residual stress more sensitive to the change of aspect ratio. We have added this into the text. However, we also noted that care must be taken for this explanation because we have not tested all minerals and in case of other minerals, readers are encouraged to perform their own calculation.

Line 242: Could you provide a typical value of a wavenumber variation, which "defines" the transition from significant to insignificant variation? Maybe as percentage with respect to the corresponding Raman peak.

We have added a sentence here to clarify this point. The main point is that as long as the variation stays below the detection limit of standard Raman machine after Gaussian fitting of the Raman band position (e.g. 0.2 cm-1), we consider the effect insignificant. This is made clear in the main text now.

Line 272: Please add a sentence explaining what the second-order moment is and why the second-order moment is needed and not the first-order moment.

We have removed the second-order moment to simplify the text for readers. It is practically a method that minimize the mismatch between the irregular inclusion shape with the effective ellipsoid.

Line 305: So I guess "interestingly" implies that you did not expect such better approximation. Could you provide now an explanation why you got this better approximation, or do you still not know why this approximation is better?

This is an observation that volumetric stress average provides a better approximation than the central point. This is interesting that this measure is better considering the fact that when performing Raman measurement on inclusions, we are in fact averaging over the effective volume under the laser. Therefore, it is interesting and, in fact, useful

that the average volume is a better proxy than just a central point. For an explanation, we can so far provide a speculation that it is due to the consideration of the stress variations at the inclusion-host wall (on the inclusion side) that drive the volumetric average closer to the equivalent stress based on the effective ellipsoid. However, it is difficult to prove it because the inclusion shape is arbitrary and faceted so there is no easy analytical description of the stress field.

Line 389: comma instead of point.

Corrected.

Conclusions: The conclusion section could be shortened by stating only the main conclusions and the main new results.

We have slightly shortened the last section. However, this section is more inclined to geological implications to provide a summary for the geologists who might not be interested in the mathematical derivations, but only the geological relevance. Therefore, we still prefer to keep most of the text so that it is easier to follow and readers may hopefully benefit more for their own petrological works.

Numerical codes: The Matlab script "Fit Ellipsoid" uses, for example, the command "syms" which requires the Symbolic Math Toolbox; so this script cannot be run with a basic Matlab license. It would be great if the authors could modify the codes, if possible, so that they can be used also with a basic Matlab student license.

We thank the reviewer for reminding us this issue. We have revised the code so that now it does not need the symbolic toolbox and everyone with basic MATLAB can use it. We now use the function handle, which is available with standard MATLAB version.

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