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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.

Anonymous Referee #2

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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 an isotropic 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 impor-

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tant 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. 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. 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.

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.

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

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?

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?

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?

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.

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

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?

Line 389: comma instead of point.

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

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.

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