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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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Comments to Zhang et al., "Analytical solution for residual stress and strain preserved in anisotropic inclusion entrapped in isotropic host" submitted to Solid Earth.

The analysis developed in this manuscript to calculate the Raman shifts developed in ellipsoidal inclusions is correct under the assumption that the symmetry of the inclusion crystal is not broken by the strains imposed by the host crystal. Under these circumstances, it agrees with the extensive analyses published in both the materials science and geological literature.

With an isotropic host crystal (and we agree that normal metamorphic silicate garnets can be treated as being elastically isotropic for these purposes) the Eshelby solution for inclusion stress and strain shows that the symmetry of an ellipsoidal inclusion crystal will be broken when the crystallographic axes of the inclusion crystal do not coincide with the principal axes of its ellipsoidal shape. The manuscript is also correct in stating that the symmetry of faceted inclusion crystals will be also be broken; this is the consequence of stress and strain concentration at corners and edges of the inclusion, as well as of the orientation of the crystallographic axes of the inclusion with respect to the shape.

Such symmetry-breaking of the inclusion crystal must also affect the values of the components of the phonon-mode Grüneisen tensor which determine its Raman shifts arising from the strains applied to the inclusions. These Grüneisen tensors have only been determined for a limited number of crystals. Recent DFT calculations of these Grünesien tensors (Murri et al. 2018 for quartz; Stangarone et al. 2019 for zircon, Musiyachenko et al. 2020 for rutile) explicitly assume that the symmetry of the crystal is preserved. That means that the unit-cell strains are constrained as e1 = e2 to preserve the equivalence of the a- and b-axes of these uniaxial crystals. Therefore, these tensors cannot be applied to strain states where the e1 component is different from e2, or those with non-zero shear components, which will arise from the mechanical states presented in Figures 4 and 5 of this manuscript.

The magnitude of the effect of symmetry-breaking on the Grüneisen tensors of minerals has not been calculated in recent DFT simulations. But there is direct experimental evidence that it can be significant compared to the shifts without symmetry breaking (e.g. Briggs and Ramdas, 1977, on quartz). If symmetry-breaking was not an issue, then the Raman peaks of cubic host minerals such as diamond and garnets would not exhibit any change in the deviatoric strain fields around inclusions (e.g. Angel et al 2019). But the Raman shifts in diamond (e.g. Nasdala et al., 2005) and garnets (Campomenosi et al., 2020) around inclusions have been measured and are signifi-

cant. They are correlated with the symmetry-breaking visible in thin sections as optical birefringence haloes. Therefore, the calculations in the current manuscript of Raman shifts of inclusions whose symmetry is broken is not correct. The magnitude of the error is unknown.

In summary, for the cases in which the symmetry of the inclusion crystal is not broken, this manuscript provides results that are in agreement with previous studies with a variety of methods. For inclusions whose symmetry is broken, this manuscript does not allow for the additional Raman shifts that will arise from the symmetry breaking. This means that Figures such as 4 and 5 should not be used to interpret the Raman shifts in quartz inclusions trapped in garnets and the authors should clearly identify in the manuscript all of their examples and calculations in which the inclusion symmetry is broken.

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