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"EosFit-Pinc: A simple GUI for host-inclusion elastic thermobarometry" by Angel et al. (2017)—Discussion

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Abstract

In this comment, we show mathematically that the equations of Angel et al. (2017) and Guiraud and Powell (2006) are equivalent. The tiny difference is due to different definitions of strain.

Keywords: Mineral inclusion, Raman barometry, quartz inclusion, equation of state, residual pressure, strain

Angel et al. (2017) proposes a new formula for calculating the residual pressure of inclusions in minerals. Software EoSFit-Pinc is also provided, which provides a convenient application of elastic geothermobarometry, e.g., for the quartz-in-garnet system. The work has great geological implications for various commonly observed inclusion-host systems, e.g., quartz-in-garnet. In the paper, it has been suggested that the previous corresponding formula to calculate residual inclusion pressure from Guiraud and Powell (2006) is incorrect. In this comment, we show mathematically that the difference between the equations of Angel et al. (2017) and Guiraud and Powell (2006) is more apparent than real. The two equations are algebraically and numerically different, but the difference is due to the types of applied volume strains rather than a mistake as proposed by Angel et al. (2017). It is demonstrated that the numerical difference between the two equations is extremely small (<0.2% for common mineral inclusions, e.g., quartz-in-garnet system). By adopting the logarithmic volume strain, rather than a linear volume strain, the equations of Angel et al. (2017) and Guiraud and Powell (2006) are shown to be algebraically and numerically identical. In the end, the three equations based on Angel et al. (2017), Guiraud and Powell (2006), and the proposed logarithmic strain formulation are numerically evaluated for quartz-in-garnet system to show the negligible difference.

In the previously published formulation from Guiraud and Powell (2006), the residual inclusion pressure is given by

$$\frac{3P_{\text{inc}}}{4G_{\text{h}}} = \frac{V_{\text{i}}\left(P_{\text{inc}}, T_{\text{room}}\right)}{V_{\text{i}}\left(P_{\text{trap}}, T_{\text{trap}}\right)} - \frac{V_{\text{h}}\left(P_{\text{room}}, T_{\text{room}}\right)}{V_{\text{h}}\left(P_{\text{trap}}, T_{\text{trap}}\right)} \quad (1)$$

where P_{trap} and T_{trap} are the entrapment pressure and temperature, P_{inc} is the residual inclusion pressure preserved in host mineral and can be retrieved from Raman spectroscopy measurement, P_{room} and T_{room} are the room pressure and temperature, G_{h} is the shear modulus of the host defined at room conditions, V_{i} is the inclusion volume, and V_{h} the host volume. Here, P_{room} can be taken as zero for simplicity.

In contrast, Angel et al. (2017) states that elastic relaxation must be undertaken at room temperature. This is done by using the pressure, so-called P_{foot}, found by tracing the entrapment isomeke down to room temperature, T_{room}. Therefore, the P_{foot} term is defined by

$$\frac{V_{\text{i}}\left(P_{\text{foot}}, T_{\text{room}}\right)}{V_{\text{i}}\left(P_{\text{trap}}, T_{\text{trap}}\right)} = \frac{V_{\text{h}}\left(P_{\text{foot}}, T_{\text{room}}\right)}{V_{\text{h}}\left(P_{\text{trap}}, T_{\text{trap}}\right)}. \quad (2)$$

Elastic relaxation at T_{room} is given in the following equation (see Angel et al. 2017, Eq. 6) by replacing the volume at the entrapment conditions (P_{trap},T_{trap}) in Equation 1 to the foot condition (P_{foot},T_{room}).

$$\frac{3P_{\text{inc}}}{4G_{\text{h}}} = \varepsilon_{\text{i}} - \varepsilon_{\text{h}} = \frac{V_{\text{i}}\left(P_{\text{inc}}, T_{\text{room}}\right)}{V_{\text{i}}\left(P_{\text{foot}}, T_{\text{room}}\right)} - \frac{V_{\text{h}}\left(P_{\text{room}}, T_{\text{room}}\right)}{V_{\text{h}}\left(P_{\text{foot}}, T_{\text{room}}\right)} \quad (3)$$

where ε_{i} is volume strain of the inclusion from P_{foot} to the residual pressure P_{inc}, and ε_{h} is the host volume strain from P_{foot} to P_{room}.

Angel et al. (2017) claim that the method of Guiraud and Powell (2006) is wrong by not considering P_{foot} and the elastic relaxation is not performed at room temperature in Guiraud and Powell (2006). From this point, we will show that this claim is incorrect, and that the formulas in Guiraud and Powell (Eq. 1) and Angel et al. (Eq. 3) are, in fact, equivalent, if a small strain assumption is applied. First, observe that using the Cauchy or engineering strain, as done by both sets of authors, is not the only strain measure that can be used. Using Cauchy strain:

$$\varepsilon = \frac{V_{\text{final}} - V_{\text{initial}}}{V_{\text{initial}}} = \frac{V_{\text{final}}}{V_{\text{initial}}} - 1. \quad (4)$$

This is appropriate when the volume change ($V_{\text{final}} - V_{\text{initial}}$) is small, as it will be for inclusions of minerals. An alternative strain measure, logarithmic or true strain, is defined as

$$\varepsilon = \int_{V_{\text{initial}}}^{V_{\text{final}}} \frac{dV}{V} = \ln\left(\frac{V_{\text{final}}}{V_{\text{initial}}}\right). \quad (5)$$

This strain measure is generally used when the volume strain is large (for an example, the volume strain of highly pressurized gas), but when it is used in the current context, the difference between the equations of Guiraud and Powell (2006) and Angel et al. (2017) disappears. Note that these two strain measures (Eqs. 4 and 5) become identical for infinitely small strains:

$$\frac{V_{\text{final}}}{V_{\text{initial}}} - 1 \approx \ln\left(\frac{V_{\text{final}}}{V_{\text{initial}}}\right) \quad (6)$$

because $\ln(1+\alpha) \approx \alpha$ for small α. Note that this small strain assumption was also made in Angel et al. (2017) (Eq. 3) when approximating the volume strain from P_{foot} to P_{inc} (and other literature for elastic solution). Using the logarithmic strain for the equations of Guiraud and Powell (2006) and Angel et al. (2017), Equation 1 of Guiraud and Powell (2006) becomes:

$$\frac{3P_{\text{inc}}}{4G_{\text{h}}} = \ln\left[\frac{V_{\text{i}}\left(P_{\text{inc}}, T_{\text{room}}\right)}{V_{\text{i}}\left(P_{\text{trap}}, T_{\text{trap}}\right)}\right] - \ln\left[\frac{V_{\text{h}}\left(P_{\text{room}}, T_{\text{room}}\right)}{V_{\text{h}}\left(P_{\text{trap}}, T_{\text{trap}}\right)}\right]. \quad (7)$$

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Using the logarithmic volume strain in Equation 3 of Angel et al. (2017) gives:

$$\frac{3P_{\text{inc}}}{4G_{\text{h}}} = \varepsilon_{\text{i}} - \varepsilon_{\text{h}} = \ln\left[\frac{V_{\text{i}}\left(P_{\text{inc}},T_{\text{room}}\right)}{V_{\text{i}}\left(P_{\text{foot}},T_{\text{room}}\right)}\right] - \ln\left[\frac{V_{\text{h}}\left(P_{\text{room}},T_{\text{room}}\right)}{V_{\text{h}}\left(P_{\text{foot}},T_{\text{room}}\right)}\right] = \ln\left[\frac{V_{\text{i}}\left(P_{\text{inc}},T_{\text{room}}\right)}{V_{\text{i}}\left(P_{\text{foot}},T_{\text{room}}\right)}\cdot\frac{V_{\text{h}}\left(P_{\text{foot}},T_{\text{room}}\right)}{V_{\text{h}}\left(P_{\text{room}},T_{\text{room}}\right)}\right] \quad (8)$$

Equation 2 can be reorganized by moving P_{foot} on the same side of the equation:

$$\frac{V_{\text{h}}\left(P_{\text{foot}},T_{\text{room}}\right)}{V_{\text{i}}\left(P_{\text{foot}},T_{\text{room}}\right)} = \frac{V_{\text{h}}\left(P_{\text{trap}},T_{\text{trap}}\right)}{V_{\text{i}}\left(P_{\text{trap}},T_{\text{trap}}\right)} \quad (9)$$

and substituting this into Equation 8 gives:

$$\frac{3P_{\text{inc}}}{4G_{\text{h}}} = \ln\left[\frac{V_{\text{i}}\left(P_{\text{inc}},T_{\text{room}}\right)}{V_{\text{i}}\left(P_{\text{trap}},T_{\text{trap}}\right)}\cdot\frac{V_{h}\left(P_{\text{trap}},T_{\text{trap}}\right)}{V_{h}\left(P_{\text{room}},T_{\text{room}}\right)}\right] = \ln\left[\frac{V_{\text{i}}\left(P_{\text{inc}},T_{\text{room}}\right)}{V_{\text{i}}\left(P_{\text{trap}},T_{\text{trap}}\right)}\right] - \ln\left[\frac{V_{\text{h}}\left(P_{\text{room}},T_{\text{room}}\right)}{V_{\text{h}}\left(P_{\text{trap}},T_{\text{trap}}\right)}\right] \quad (10)$$

Note that P_{foot} does not appear in this equation. In fact, any intermediate point along the entrapment isomeke, instead of (P_{foot},T_{room}), gives the same result as in Equation 10. The results in Equations 7 and 10 using the logarithmic strain measure are identical. The slight numerical difference in results gained with the equations in Guiraud and Powell (2006) and Angel et al. (2017) relate to the quality of the approximation:

$$\ln\left(\frac{V_{\text{final}}}{V_{\text{initial}}}\right) \approx \frac{V_{\text{final}}}{V_{\text{initial}}} - 1. \quad (11)$$

For mineral inclusions (e.g., of quartz in garnet) with a volume strain of ca. 2%, the relative difference between the equations is less than 0.0002, resulting in only a few MPa difference (for a 100 GPa bulk modulus), which is certainly negligible for the purpose of Raman thermobarometry.

Numerical calculations of residual pressure isopleths as functions of entrapment *P-T* based on the three formulations—(1) Angel et al. (2017), (2) Guiraud and Powell (2006), and (3) logarithmic strain formulation—have been performed for quartz-in-almandine system. The results are shown in Figure 1. It is shown that discrepancy indeed exists because of the different strain measures that have been used in the three formulas. The differences among the three curves naturally increase toward higher entrapment *P* because the small strain measure (Eq. 11) becomes less accurate. However, the discrepancy is still on the level of ~0.01 GPa up to 3 GPa entrapment conditions, which is significantly smaller than the uncertainty arising from the Raman spectroscopy (Fig. 1b).

We conclude by asserting that the previous equation of Guiraud and Powell (2006) is not incorrect and is also consistent with Angel et al. (2017). Workers using Raman thermobarometry need to be aware that the difference between the two equations of Angel et al. (2017) and Guiraud and Powell (2006) is not due to a mathematical error. We emphasize that the arguments above do not imply that the derivations provided in Angel et al. (2017) are mathematically incorrect. It is up to the user to decide which formula (Angel et al. 2017, Guiraud and Powell 2006, or the logarithmic strain in Eq. 10) to choose when performing elastic thermobarometry.

In geology, due to the small strains in minerals, geometrical nonlinear strain measures (e.g., logarithmic strain) do not necessarily need to be used for elastic problems. In fact, as shown, it does not matter which measure of volume strain is used in Equation 11. Cauchy and logarithmic strain have both been used extensively in the literature, and there are other definitions of strain as well. Unlike geometrical nonlinearity, material nonlinearity (e.g., elastic stiffness as a function of *P-T*) should be accounted for. Here, we show that geometrical nonlinearity does not have a major impact on the equations to use in Raman thermobarometry (Fig. 1). There are more critical issues to resolve for the future development of such thermobarometry [e.g., the effect of anisotropy (Murri et al. 2018), viscous relaxation (Zhong et al. 2018), and so on rather than the small difference due to use of different definitions of volume strain].

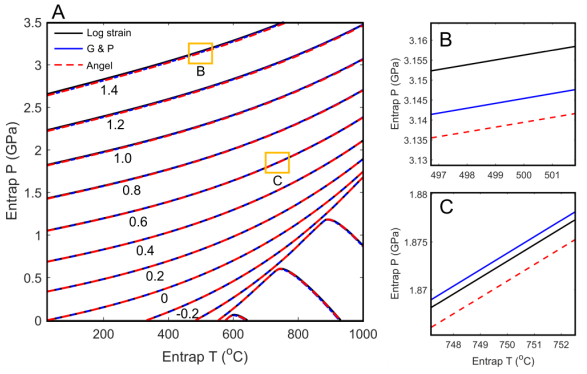

Figure 1. (**a**) Comparison between isopleths for residual inclusion pressure (in GPa) based on equations using logarithmic strain (Eq. 7), Guiraud and Powell (2006) (G&P, Eq. 1), and Angel et al. (2017) (Eq. 3) for quartz-in-almandine system. The differences among the three formulas increase toward higher pressure due to the fact that different volume strains depart from infinitesimal value, i.e., the difference between the three formulas increases toward higher volume strain. (**b** and **c**) Enlarged image shows the numerical difference among the three equations. The EoS of quartz is based on Angel et al. (2017b) and almandine garnet is from Milani et al. (2015).

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