Appendix to

EosFit-Pinc: A SIMPLE GUI FOR HOST-INCLUSION ELASTIC THERMOBAROMETRY

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In this Appendix we show the error in the approach of Guiraud and Powell (2006) to calculating inclusion entrapment conditions from measured inclusion pressures P_{inc} when the host is at final conditions P_{end} and T_{end}.

Angel et al. (2017) found the volume strain of the inclusion for the isothermal changes in pressure from P_{foot} on the entrapment isomeke to the final P_{end} on the host, and to P_{inc} in the inclusion *at the final temperature* T_{end}:

$$\varepsilon_{inc} = \varepsilon_{host} + \frac{3(P_{inc} - P_{end})}{4G_H} \tag{A1}$$

The volume strains are given by the volumes of inclusion and host at the start and the end of this descent from the isomeke:

$$\begin{aligned} \varepsilon_{inc} &= \frac{V^i_{Pinc}}{V^i_{Pfoot}} - 1 \\ \varepsilon_{host} &= \frac{V^h_{Pend}}{V^h_{Pfoot}} - 1 \end{aligned} \tag{A2}$$

If we substitute these into equation (A1) we get:

$$\begin{aligned} &\frac{V^i_{Pinc}}{V^i_{Pfoot}} = \frac{V^h_{Pend}}{V^h_{Pfoot}} + \frac{3(P_{inc} - P_{end})}{4G_H} \\ &\text{which, for later clarity, we can re-arrange to:} \\ &\frac{3}{4G_H}(P_{inc} - P_{end}) = \left[\frac{V^i_{Pinc}}{V^i_{Pfoot}} - \frac{V^h_{Pend}}{V^h_{Pfoot}}\right] \end{aligned} \tag{A3}$$

Along the entrapment isomeke from entrapment conditions to the P_{foot} at T_{end}, the fractional volume changes of the two phases must be the same, by the definition of the isomeke (Rosenfeld and Chase 1961). Therefore:

$$\frac{V^i_{Pfoot}}{V^i_{Ptrap}} = \frac{V^h_{Pfoot}}{V^h_{Ptrap}} \tag{A4}$$

Now multiply the first term inside of the square bracket in (A3) by the ratio for the inclusion, the second one by the (numerically equal) term for the host, and multiply the outside by the inverse:

$$\frac{3}{4G_H}\left(P_{inc}-P_{end}\right)=\frac{V^i_{Ptrap}}{V^i_{Pfoot}}\left[\frac{V^i_{Pinc}}{V^i_{Ptrap}}-\frac{V^h_{Pend}}{V^h_{Ptrap}}\right] \quad \text{(A5)}$$

And rearrange the expression to give the P_{inc}:

$$P_{inc}=P_{end}+\frac{4G_H}{3}\frac{V^i_{Ptrap}}{V^i_{Pfoot}}\left[\frac{V^i_{Pinc}}{V^i_{Ptrap}}-\frac{V^h_{Pend}}{V^h_{Ptrap}}\right]$$

$$\text{which is the same as:} \quad \text{(A6)}$$

$$P_{inc}=P_{end}-\frac{4G_H}{3}\frac{V^i_{Ptrap}}{V^i_{Pfoot}}\left[\frac{V^h_{Pend}}{V^h_{Ptrap}}-\frac{V^i_{Pinc}}{V^i_{Ptrap}}\right]$$

Compare this last equation to that given in Kohn (2014), which is the expression of Guiraud and Powell (2006) written for P_{inc} measured in bars when the host is at room conditions:

$$P_{incl}=1-\frac{4\mu}{3}\left[\frac{V^{298,1bar}_{host}}{V^{T,P}_{host}}-\frac{V^{298,P_{incl}}_{incl}}{V^{T,P}_{incl}}\right] \quad \text{(A7)}$$

In A7 from Kohn (2014), the notation used is related to ours by:

$$\begin{aligned} 1bar &\equiv P_{end} \\ \mu &= G_H \\ V^{298,1bar}_{host} &= V^h_{Pend} \\ V^{298,Pincl}_{incl} &= V^i_{Pinc} \\ V^{T,P}_{host} &= V^h_{Ptrap} \\ V^{T,P}_{incl} &= V^i_{Ptrap} \end{aligned} \quad \text{(A8)}$$

Thus the expression given in Kohn (2014) and Guiraud and Powell (2006) translated to our notation is:

$$P_{inc}=P_{end}-\frac{4G_H}{3}\left[\frac{V^h_{Pend}}{V^h_{Ptrap}}-\frac{V^i_{Pinc}}{V^i_{Ptrap}}\right] \quad \text{(A9)}$$

The difference in A9 from Equation A6 is the factor $\frac{V^i_{Ptrap}}{V^i_{Pfoot}}$, which is the volume change of the two phases along the entrapment isomeke. Thus, our approach and that of Guiraud and Powell (2006) agree on the value of P_{foot}, which is the entrapment pressure when the entrapment temperature is equal to the final temperature, because then $\frac{V^i_{Ptrap}}{V^i_{Pfoot}} = 1.000$. This indicates the problem in Guiraud and Powell (2006); they forgot that the relaxation term is explicitly derived for an isothermal pressure change. Instead, their approach calculates the volume change due to the relaxation along a generic P-T path, and this leads to their calculated entrapment conditions not lying on a single isomeke.

Another way of looking at this issue is as follows; to obtain the equation given by Guiraud and Powell (2006) or Kohn (2014) one has to substitute the following expressions into Eqn. A1:

$$\begin{aligned} \varepsilon_{inc} &= \frac{V^i_{Pinc}}{V^i_{Ptrap}} - 1 \\ \varepsilon_{host} &= \frac{V^h_{Pend}}{V^h_{Ptrap}} - 1 \end{aligned} \qquad (10)$$

But these substitutions are not valid because the reference state for the relaxation term as used, $\frac{3}{4G_H}\left(P_{inc} - P_{end}\right)$, is still P_{foot}, so they have mixed two different sets of strains referenced to different starting points.

References

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Kohn, M.J. (2014) “Thermoba-Raman-try”: Calibration of spectroscopic barometers and thermometers for mineral inclusions. Earth and Planetary Science Letters, 388, 187-196.
Rosenfeld, J.L., and Chase, A.B. (1961) Pressure and temperature of crystallization from elastic effects around solid inclusion minerals? American Journal of Science, 259, 519-541.