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How large are departures from lithostatic pressure? Constraints from host--inclusion elasticity

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ABSTRACT

Minerals trapped as inclusions within other host minerals will develop non-lithostatic pressures during both prograde and retrograde metamorphism because of the differences between the thermoelastic properties of the host and inclusion phases. There is only a single possible path in *P--T* space, the entrapment isomeke, along which no residual pressure would be developed in a host--inclusion system; non-lithostatic pressures are developed in inclusions as a result of the external pressure and temperature deviating from the isomeke that passes through the entrapment conditions. With modern equation of state and elasticity data for minerals now available it is possible to perform precise calculations of the isomekes for mineral pairs. These show that isomeke lines are not straight lines in *P--T* space at metamorphic conditions. We show that silicate inclusions in silicate hosts tend to have flat isomekes, with small values of $\left(\partial P/\partial T\right)_{\text{isomeke}}$, because of the small range of thermal expansion coefficients of silicate minerals. As a consequence, the general behaviour under decompression is for soft silicate inclusions in stiffer hosts to develop excess pressures, whereas a stiff silicate inclusion in a softer matrix will experience lower pressures than lithostatic pressure. The opposite effects occur for compression after entrapment on the prograde path. The excess pressures in inclusions, including allowance for mutual elastic relaxation of the host and inclusion, are most easily calculated by using the isomeke as a basis. Analysis of the simplest possible model of a host--inclusion system indicates that deviations from lithostatic pressure in excess of 1 GPa can be readily produced in quartz inclusions within garnet in metamorphic rocks. For softer host minerals such as feldspar the pressure deviations are smaller, because of greater elastic relaxation of the host. The maximum pressure deviation from lithostatic pressure in the host phase around the inclusion is one--third of the pressure deviation in the inclusion. Routines for performing these calculations have been added to the EosFit7c software package.

Keywords: non-lithostatic pressures; inclusions; elasticity; isomekes.

INTRODUCTION

Non-lithostatic pressures can arise from two general types of mechanism, kinematic non-elastic processes such as plate motion or local deformation, and elastic interactions between different minerals. Physical constraint in the form of physical confinement often plays a key role in generating non-lithostatic stress states. At large scales, it has been suggested that constriction of subduction channels of variable width can generate over- or under-pressures on subducting sediments (e.g. Mancktelow, 1995, 2008; Raimbourg & Kimura, 2008). At the grain or sub-grain scale elastic interactions between minerals can also generate very significant non-lithostatic pressures. In this case the confinement can be simply provided by one mineral completely enclosing an inclusion of a different phase (e.g. Moulas *et al.*, 2013). Or, two phases of related structures (e.g. exsolution lamellae in alkali feldspar) can be coherently intergrown so that the bonded interfaces of the two phases are each constrained by the partner phase (e.g. Salje *et al.*, 1985; Scheidl *et al.*, 2014). Because the compressibilities and thermal expansion of the two phases will differ, a change in pressure and temperature would lead to free grains of the free phases undergoing different amounts of strain. However, the mutual confinement of the two phases constrains the strains that can occur. Therefore instead of the stress inside the grains following the external pressure, additional non-uniform stress fields are developed within the constrained two phase system. Note that this occurs as a purely elastic phenomenon, and no plastic deformation or brittle failure is required. Such stress fields can give rise to either over- or under-pressure with respect to the external pressure, whether or not the external pressure is lithostatic. Thus quartz inclusions trapped in the cores of garnet during the early stages of metamorphism (e.g. Parkinson, 2000) experience pressures less than the external pressure during subsequent prograde subduction to higher pressures which may be sufficient to prevent them entering the stability field of coesite (e.g. Guiraud & Powell, 2006; Angel *et al.*, 2014b). Over-pressure is well established in diamond, where the residual over-pressure in silicate inclusions measured at room conditions is used to constrain the conditions of entrapment (e.g. Izraeli *et al.*, 1999; Nestola *et al.*, 2011; Howell *et al.*, 2012). These elastic stresses can also be the driving force for plastic deformation of the host minerals or their brittle fracture (e.g. van der Molen & van Roermund, 1986).

In this paper we try to answer the question as to how big can the deviations from lithostatic pressure become when they are generated by microstructural constraints such as coherent interfaces or enclosure of inclusions, even when the external pressure is purely lithostatic. In order to address this question we focus on the simplest case, that of single isolated spherical isotropic inclusions in an elastically isotropic host, because this is one of the few cases that can provide exact solutions for geologically relevant ranges of pressure and temperature (e.g. Angel *et al.*, 2014b). We proceed by first calculating how the pressure in an inclusion, completely trapped and isolated by a host phase, changes as the temperature and the external pressure changes. We make use of the concept of the thermodynamic isomeke (Rosenfeld & Chase, 1961) to first determine the sense of the over- or under-pressure developed in the inclusion at various *P* and *T* conditions. Then the isomeke is used as a basis for calculating the elastic interaction between the host and inclusion; it thus allows the final inclusion pressure to be calculated. This approach provides a realistic calculation of the deviations from lithostatic pressures that can be developed through elastic interactions between elastically isotropic minerals under metamorphic conditions. It thus provides an estimate of the maximum deviations from lithostatic pressure that can arise from elastic effects due to mutual physical confinement of mineral grains in general. In the last section we then consider the stress fields induced in the host by the difference between the inclusion pressure and the external pressure.

INCLUSION PRESSURES

General considerations

Consider a mineral grain that grows and entraps another mineral (or grows together with it) and then continues to grow to the point at which the inclusion is elastically isolated by the host. At this stage no significant stress or temperature gradients exist across the host grain. Under these conditions, the host and inclusion are at the same P--T and the inclusion fits perfectly within the cavity of the host (Fig. 1). While these P--T conditions are maintained, and there is no change in the external stress field, there is no development of stress gradients across the host and inclusion, and both phases continue to experience the external pressure whether or not that is lithostatic. It is only when the pressure and/or temperature subsequently change that non-lithostatic pressures can be generated in the inclusion (Fig. 1). Non-lithostatic pressures arise because the inclusion is physically constrained by the host. To illustrate the principles, consider the case of a relatively soft inclusion (e.g. quartz) in a stiffer host (e.g. garnet) undergoing an isothermal decompression. If the quartz inclusion was not constrained by the garnet host it would expand more than the garnet because it is softer. Instead, being trapped inside the host, the quartz inclusion is constrained to expand only by the same amount as the garnet. After decompression the quartz inclusion therefore has a smaller volume than expected for a free quartz crystal at the external pressure and a non-lithostatic pressure is therefore developed in the inclusion.

The details of the elastic stress field in the host and the inclusion, and thus the deviation from lithostatic pressure, depend not only upon the volume elasticity of the two phases but also on their anisotropic elastic properties, their mutual orientation, the shape of the inclusion, and whether the inclusion is elastically isolated or, as is often the case, close enough to other inclusions or the surface of the host grain for these to exert an influence on the resulting stress fields. These effects can only be evaluated algebraically for a few simple specific cases and geometries (Eshelby, 1957). In general they have to be addressed by numerical calculations or use of approximations on a case by case basis. As a first step, one can obtain an analytical solution for the pressure generated in the inclusion in the simplified system of a small isolated spherical inclusion trapped within a large host grain, with both phases being elastically isotropic (Fig. 1). Classical analysis (e.g. Goodier, 1933; Eshelby, 1957) shows that after a change in pressure or temperature such an inclusion has a uniform pressure while the host develops a deviatoric stress field but the pressure remains equal to the external pressure. Note the common convention that compressional stresses are negative is used, and that the pressure in a system under non-uniform stress is defined as the negative of the average of the three principal stresses.

The key assumption (e.g. Goodier, 1933; Eshelby, 1957) is that after trapping by the host, the inclusion completely fills the hole in the host and continues to do so at all subsequent pressures and temperatures. This is certainly true for changes in P—T, which lead to the pressure of the inclusion being greater than zero (c.f. Kouketsu *et al.*, 2014). Under these conditions, and if we ignore mutual elastic relaxation which is addressed below, after a change in external pressure and temperature the inclusion pressure $P*$ can be calculated directly from thermodynamics. The change in the volume of the cavity in the host containing the inclusion is determined from the change in external P--T and the equation of state (EoS) of the host. Because the inclusion is constrained by the host to fit the volume of the cavity in the host, the inclusion pressure $P*$ is determined entirely by the volume change of the host and the external temperature, and the EoS of the inclusion. In the absence of further elastic, plastic or other relaxation, this calculation is exact, and can be used to follow the evolution of the differences between the inclusion pressure and the external pressure during metamorphism and subsequent exhumation (e.g. Guiraud & Powell, 2006). However, as shown by Angel *et al.* (2014b), this approach leads to problems in calculating the effects of

the mutual elastic relaxation of the host and the inclusion because the elastic properties of both phases can change considerably from entrapment to the final P--T conditions of interest. An alternative approach is to split the calculation of inclusion pressures into two sequential steps along a P--T path to final conditions (Fig. 2). The first step is to consider a temperature change from the initial temperature of entrapment T_{trap} to the final T_{end} accompanied by a simultaneous change in external pressure such that the pressures in the host and inclusion remain equal to each other and equal to the external pressure. The second step is to calculate the pressure change in the inclusion during an isothermal change in the external pressure to the final P_{ext}. This is possible because the system is being considered as being purely elastic, and elasticity is by definition reversible. Thus the final pressure in the inclusion is independent of the path taken in P--T space from entrapment to any other final pressure and temperature, but the use of this two-step path makes the calculation of the elastic relaxation of the system easier.

Isomekes

The first step in the calculation of inclusion pressures, which assumes a P--T path along which no over- or under-pressure is developed, corresponds to the thermodynamic definition of an isomeke (Rosenfeld & Chase, 1961; Adams et $al.$, 1975), for the following reasons. The fractional volume change $\dfrac{\partial V}{V}$ of a single unconstrained phase, such as the host (H), as a result of a change in pressure and temperature is defined by its volume thermal expansion coefficient α and its volume compressibility β:

$$\frac{\partial V_H}{V_H} = \alpha_H \partial T - \beta_H \partial P \tag{1}$$

From this one obtains the definition of the isochor, or constant volume line, of the free host phase as:

$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{\alpha_H}{\beta_H} \tag{2}$$

This is not the condition that is applied to the first step of calculation of the host-inclusion problem because the volumes of the hole in the host V_H and the volume of the inclusion V_I do change with pressure and temperature even though they remain equal to one another. The initial volumes V_{H0} and V_{I0} are also equal, so it follows that:

$$V_H - V_{H0} = V_I - V_{I0} \tag{3}$$

And thus:

$$\frac{V_H - V_{H0}}{V_H} = \frac{\partial V_H}{V_H} = \frac{\partial V_I}{V_I} = \frac{V_I - V_{I0}}{V_I} \tag{4}$$

It then follows from Eq. (1) that the P--T path for the first step of the calculation is defined by $\alpha_H \partial T - \beta_H \partial P = \alpha_I \partial T - \beta_I \partial P$ (Rosenfeld & Chase, 1961). This constrains the changes in pressure and temperature along the path to be:

$$\left(\frac{\partial P}{\partial T}\right)_{(V_I - V_H)} = \frac{\alpha_I - \alpha_H}{\beta_I - \beta_H} \tag{5}$$

These ideas were introduced by Rosenfeld & Chase (1961) and the path was subsequently named an isomeke (Adams et $al.$, 1975). It is a path that is dependent upon the contrast in thermoelastic properties between the host and inclusion phases. It is never a straight line in P--T space for several reasons. First, the slope of the isomeke is $\left(\dfrac{\partial P}{\partial T}\right)_{isomeke} = 0$ at absolute zero in temperature, as indicated by Rosenfeld & Chase (1961), because the thermal expansion coefficients are zero. But at finite temperatures the slope of the

isomeke will be non-zero unless the thermal expansion coefficients of the two phases are identical. Second, the change in α and β of the host and inclusion phases with pressure and temperature will be significantly different. For example, the value of α of quartz changes by a factor of more than 3 from room temperature to 500°C while that of garnet only increases by a factor of 1.7 (Table 1). Over the same temperature range, the volume compressibility of quartz increases by a factor of 1.7, whereas that of garnet by only a factor of 1.1. Therefore calculations of isomekes with physically realistic EoS (i.e. with α and β that vary with P--T) have to be performed numerically. Routines for performing these calculations have been added to the EosFit7 software package (Angel *et al.*, 2014a). All of the calculations described in this paper were performed with the EosFit7c program using thermal-pressure equations of state with the EoS parameters listed in Table 1.

Note that isomekes defined by Eq. (5) are generally very different from isochors (Eq. 2) because the volumes of the two phases change equally along an isomeke line, whereas along an isochor a single phase keeps exactly the same volume. The isochors of diamond, for example, show strong curvature at low temperatures because the regime of very low thermal expansion in diamond extends to above room temperature (Fig. 3a), whereas the isochors of garnet exhibit less curvature at geologically relevant temperatures. Because isomekes of diamond with garnet are derived from the differences in thermoelastic properties, the isomeke lines are only parallel to the isochors when the isochors of both phases have the same slope, for example around 300°C in the example shown in Fig. 3a,b. At such points there is no change in volume of either phase along the isomeke. At other pressures and temperatures the slope of the isomeke is related to the divergence of the two isochors, and the fractional changes of the volumes of the two phases are equal to one another from one point to another along the isomeke (Eq. 4). Note that the only situation in which the pressure in an inclusion would follow its own isochor is when the host is infinitely rigid with $\alpha_H = \beta_H = 0$, a situation never met in reality.

As envisaged by Rosenfeld & Chase (1961), the concept of the isomeke first provides the basis for determining whether over- or under-pressures are developed in inclusions. Consider a garnet inclusion trapped in a diamond at mantle conditions of 5.7 GPa and 1175°C (Howell *et al.*, 2010, Milani *et al.*, 2015). If the diamond was exhumed along the isomeke passing through the entrapment conditions (Fig. 3c), corresponding initially to a rate of 0.3 GPa per 100°C, then the fractional volume change, or volume strain of both the diamond host and garnet inclusion would be the same, and the pressure inside the inclusion would remain equal to the external pressure, and there would be no stress gradients. Such an exhumation path is, of course, unrealistic for diamond; its eruption in kimberlites involves rapid decompression at high temperatures. The diamond/garnet pair therefore moves off the isomeke line towards the lower-pressure side during eruption. In this case the garnet is constrained by the diamond and experiences over-pressure with respect to the external pressure. Conversely, were the diamond/garnet pair to be taken to higher pressures after entrapment, the diamond would not compress as much as a free crystal of garnet would compress. In this case, the stiff diamond host in some sense would protect the soft inclusion and the inclusion pressure would then be less than the external pressure (Fig. 3c).

The qualitative result, which can be extended to any host--inclusion system, is that the isomeke line passing through the entrapment conditions divides P--T space into two regimes; when the host--inclusion system moves to one side of the entrapment isomeke the inclusion pressures exceed the external pressure, to the other side the inclusion is under-pressured (Rosenfeld & Chase, 1961). When the host and inclusion phases are exchanged, for example a diamond inclusion entrapped in a garnet, the sense of over- or under-pressure is reversed (Fig. 2d).

Elastic relaxation

While the host and inclusion remain at P--T conditions on the entrapment isomeke, the inclusion pressure remains equal to the external pressure. At P--T conditions away from the entrapment isomeke the pressure P^* in the inclusion differs from the external pressure but remains uniform and hydrostatic (Goodier, 1933). The stress is also uniform and hydrostatic in the host, but equal to the external pressure P_{ext}. This however is a virtual state because there is a jump in radial stress at the inclusion wall of P^* - P_{ext} (Fig. 4a). Therefore the host--inclusion system is not in mechanical equilibrium. If the host has been moved off the entrapment isomeke to the side where the inclusion pressure P^* exceeds the external pressure, then the stress difference P^* - P_{ext} will force the inclusion wall outwards. The inclusion will expand and so the pressure (and radial stress) in the inclusion will decrease. The expansion of the inclusion will compress the surrounding host, developing a radial stress gradient in the host adjacent to the inclusion. This expansion will stop when the radial stress in the host and the inclusion are equal (Fig. 4b). Conversely, if the host and inclusion are moved to a P--T on the opposite side of the entrapment isomeke where $P_{ext} > P^*$, the inclusion will be compressed by the elastic relaxation and the pressure in the inclusion will be increased. This change in inclusion pressure is an elastic relaxation, and it modifies the pressure of the inclusion from the thermodynamic calculation of P^* to the true final pressure P_{inc}. The final inclusion pressure is equal to P^* only when the host--inclusion pair remains at a P--T on the entrapment isomeke, in which case $P^* = P_{ext}$.

The final inclusion pressure P_{inc}, and thus the deviation from external pressure, at any P--T away from the entrapment isomeke is therefore comprised of two parts; the pressure P^* derived directly from the EoS of the two phases, and the adjustment in the inclusion pressure due to the mutual elastic relaxation. The calculation of the pressure change in the inclusion due to relaxation is not trivial because the changes in inclusion pressure during relaxation are accompanied by simultaneous changes in elastic properties. A correct, but numerically complex, approach is to apply this correction in step-wise iterative calculations to determine the mechanical equilibrium of the host and inclusion at infinitesimal increments in pressure and temperature from entrapment to the final P--T conditions using the full variation of elasticity with pressure and temperature (e.g. Gillet *et al.*, 1984; van der Molen & van Roermund, 1986). Simpler approaches invoke some approximation to the full EoS of the inclusion and provide approximate results. The most widely used method (e.g. Zhang, 1998; Izraeli *et al.*, 1999; Guiraud & Powell, 2006; Howell *et al.*, 2012; Kohn, 2014; Kouketsu *et al.*, 2014) was originally derived (Zhang, 1998) by assuming that the elastic properties of the host and the inclusion do not change over the full range of P--T from entrapment to final conditions, which is clearly not valid for changes in pressure and temperature that are geologically relevant.

The two step approach via the entrapment isomeke simplifies the relaxation problem to that accompanying an isothermal pressure change from the pressure on the isomeke to the final external pressure. The volume strain $\frac{\partial V_H}{V_H}$ of the host in this step is calculated directly from its EoS. Because this second step starts from a state without stress gradients and is isothermal, the final volume of the inclusion can be derived from the result of Goodier (1933) as the volume of the inclusion phase on the entrapment isomeke at T_{end} multiplied by the factor $\left(1 + (1 - K_{21})\frac{\partial V_H}{V_H}\right)$ (Torquato, 2002; Angel *et al.*, 2014b). The corresponding relaxed inclusion pressure can then be calculated from this volume change and the full EoS of the inclusion (Angel *et al.*, 2014b). The parameter K_{21} is an elastic interaction parameter whose value is dependent on the elastic properties of both the host and inclusion (Torquato, 2002):

$$K_{21} = \frac{K_I - K_H}{K_I + \frac{4}{3}G_H}$$ (6)

The values of the bulk (K_H) and shear (G_H) moduli of the host are the values at the external pressure, because the pressure in the host remains equal to the external pressure (e.g. Zhang, 1998; Tajcmanova *et al.*, 2014, and see discussion below). The appropriate value of the bulk modulus of the inclusion (K_I) is the effective value of the inclusion bulk modulus over the interval of relaxation. When the relaxation is small, the value at *P** can be used as a good approximation, as can be seen from consideration of the elastic hollow sphere problem (e.g. Bower, 2010).

Elastic relaxation always reduces the difference between the inclusion pressure and the external pressure. The amount of elastic relaxation depends on the factor K_{21}. Although this varies with temperature and pressure for all host--inclusion pairs, one can draw some general conclusions about the magnitude of the relaxation effects. For stiff hosts such as diamond, the factor is dominated by the moduli of the host material and, as expected, relaxation is small. For garnet inclusions in diamond recovered from upper mantle to room conditions, the relaxation is 0.16 GPa. If the host is significantly softer than the inclusion phase then the factor K_{21} becomes large and the relaxation is proportionately larger. For some metamorphic inclusion pairs (e.g. kyanite in feldspar) the relaxation can exceed 50% of the difference between the unrelaxed inclusion pressure *P** and the external pressure.

Metamorphic inclusions
The amount of over- or under-pressure in the inclusion depends on the difference between the external pressure and the pressure on the entrapment isomeke at the same temperature (e.g. Fig. 2). Therefore the greatest deviations from lithostatic pressures will be generated in host inclusion pairs in which the *P*--*T* path following entrapment is perpendicular to the isomeke lines for the mineral pair. This is common in metamorphic rocks in which the early low-*P* and low-*T* stages of prograde metamorphism frequently generate trapped inclusions of silicates in newly grown silicate host grains whose thermal expansion coefficients are similar to one another. These host--inclusion pairs therefore tend to have shallow isomekes (c.f. Eq. 5), while prograde paths in typical subduction metamorphism are steep in *P*--*T* space and cross the isomekes at high angles. We take as an example the quartz inclusions originally entrapped in garnet cores on the prograde path of the Kulet whiteschist (Parkinson, 2000). The isomekes for garnet and quartz (Fig. 5a) are strongly curved at metamorphic conditions because of the volume effects of the alpha--beta transition in quartz. We have modelled the transition with a Landau formalism equivalent to that used by Holland & Powell (2011) but with slightly modified coefficients (Table 1) to provide better agreement with the published *P*--*V*--*T* and elasticity data. However, because the *P*--*T* path does not pass through the boundary, the same residual pressures within uncertainties can be obtained by just fitting the *P*--*V*--*T* data with a single--phase EoS (Angel *et al.*, 2014b).

Consider a quartz inclusion trapped and isolated within the garnet at 0.7 GPa and 380°C. At these conditions the garnet--quartz isomeke is almost horizontal (Fig. 5b) with $\left(\frac{\partial P}{\partial T}\right)_{isomeke} \approx 0$ because the thermal expansion coefficients of the two phases are almost identical at these conditions. Therefore almost isobaric heating or cooling would move the garnet and quartz along the isomeke and produce no internal stress fields and no deviation from the external pressure. By contrast a small increase in pressure will develop a significant under-pressure in the quartz inclusion because the compressibility of the garnet is substantially less than that of the quartz; the volume of the quartz inclusion would not decrease as much with an increase in pressure as would be expected for a free quartz crystal

subject to the same external pressure. Therefore, for all P--T conditions above the entrapment isomeke the quartz inclusion will exhibit an under-pressure. Conversely, at external pressures below the entrapment isomeke the quartz inclusion will exhibit an over-pressure with respect to the external pressure. Figure 5b shows these deviations from external pressure as contours in terms of the temperature and external pressure without allowing for elastic relaxation. It shows that along the prograde path of this whiteschist (Parkinson, 2000) there is a rapid increase in difference between the external pressure and the unrelaxed inclusion pressure $P*$ (Fig. 5b). By peak conditions of ~3.5 GPa and ~780°C the unrelaxed pressure $P*$ of the quartz inclusion would be only ~1.4 GPa, a deviation of more than 2 GPa from the external pressure. Elastic relaxation leads to additional compression of the inclusion because $P_{ext} > P*$, and it raises the final pressure of the inclusion to ~1.9 GPa (Fig. 5c). Note that in order for the pressures in these quartz inclusions to reach pressures in the stability field of coesite, it would be necessary for the peak external pressure to reach in excess of 5.8 GPa at 780°C, once elastic relaxation is accounted for.

The amount of relaxation also increases with the difference between external pressure and the isomeke pressure; compare the contours in Fig. 5c with those in Fig 5b. As a consequence both the prograde and retrograde paths of the inclusion deviate significantly from that predicted without relaxation (Fig. 5, and see also Guiraud & Powell, 2006), so the correct form of elastic relaxation is important for calculating non-lithostatic pressures at all P--T points except those on the entrapment isomeke. When the retrograde path of the host crosses the entrapment isomeke, the system is returned to a state without stress gradients and both the host and inclusion will experience a uniform pressure, unaffected by the model for relaxation (Fig. 5b,c). As exhumation subsequently proceeds beyond the isomeke the deviation from the external pressure will increase again, with the inclusion pressure being higher than the external pressure. At room conditions this remnant over-pressure can be used, along with the elastic properties of the two phases, to infer the entrapment isomeke and thus constrain the conditions of entrapment and elastic isolation of the inclusion.

The general conclusions drawn for the quartz--in--garnet system also apply to other soft and, respectively, stiff phases of silicate minerals, because of their common property of having flat isomekes (Eq. 5) due to the similarity of thermal expansion coefficients. Obviously, as we have discussed for garnet with diamond, the sense of over- or under-pressure in the inclusion generated by the host--inclusion system moving off the entrapment isomeke is reversed when the host and inclusion phases are swapped. Thus, the stiffer garnet host and softer quartz inclusion generates excess inclusion pressures at external pressures below the entrapment isomeke. For a host--inclusion system in which, instead, the inclusion is stiffer than the host, the opposite occurs. Thus, for example, inclusions of stiff kyanite ($K_0 \sim$ 160 GPa, Table 1) in relatively compressible alkali feldspar ($K_0 \sim$ 55 GPa) will exhibit excess inclusion pressures at external pressures above the entrapment isomeke (Fig. 6). The over-pressure in the inclusion arises because the hole in the host containing the inclusion compresses following the equation of state of the host. Since the host is more compressible than the inclusion, the inclusion will be constrained to have a smaller volume than it would have as a free phase, and hence be over-pressured with respect to the external pressure. Exactly the converse occurs on decompression; the hole in the host containing the inclusion expands more than a free inclusion phase would expand under the external pressure, thus allowing the inclusion to expand more than a free phase at the external pressure. Therefore the inclusion has a pressure less than the external pressure.

This has important implications for the interpretation of the zoned rims of plagioclase around kyanite within alkali feldspar in felsic granulites (e.g. Tajcmanova *et al.*, 2011). The rims are typically zoned in anorthite (An) content, with the denser An--rich plagioclase being adjacent to the kyanite. In one example, the rims were developed during approximately isothermal decompression from 1.6 -- 1.8 GPa and 850 -- 1000°C to pressures of 0.4 -- 0.6

GPa. It has been suggested (Tajcmanova *et al.*, 2014) that the preservation of the rims indicates that a pressure gradient was developed around the inclusion due to it being trapped by the alkali feldspar, with higher pressures in the parts of the rims adjacent to the inclusion. However, if the kyanite is part of the peak metamorphic assemblage as indicated by the presence of garnet inclusions in the feldspar (Tajcmanova *et al.*, 2011), then the isomekes (Fig. 6) show that the kyanite would exhibit lower pressures than the external pressure during decompression because the kyanite inclusion is stiffer than the feldspar host. The contrast in compressibilities of kyanite and feldspar is so great that isothermal decompression of the feldspar from 1.8 GPa to 1.0 GPa is sufficient to reduce the unrelaxed inclusion pressure to ambient pressure. Inwards elastic relaxation of the soft feldspar actually maintains a significant residual pressure on the inclusion of 0.7 GPa, still leading to a reduction in pressure relative to external pressure of ~0.3 GPa. Simple decompression of a kyanite inclusion within a feldspar host cannot therefore generate excess pressures in the inclusion. The sign and magnitude of the calculated inclusion pressures are insensitive to which feldspar (alkali feldspar or the plagioclase rim) is considered as the host phase, because the difference in thermal expansion coefficients for feldspar is small (e.g. Hovis *et al.*, 1999; Tribaudino *et al.*, 2010) and the contrast in compressibility between kyanite and all feldspar is much greater than the difference in compressibility between feldspar (e.g. Angel, 2004; Ross *et al.*, unpublished data; Friedrich *et al.*, 2004). Because the isomekes are flat, the calculated inclusion pressures are also insensitive to the difference between entrapment and final temperatures. The only way in which the simple host--inclusion elastic mechanism can generate over-pressures in these kyanite inclusions during the retrograde decompression is for the inclusions to have been formed and elastically isolated at pressures significantly lower than the recorded peak pressures. Entrapment at ~1 GPa, for example, would result in calculated relaxed inclusion pressures of ~2.1 GPa at the reported peak pressure of 1.8 GPa, an over-pressure of just 0.3 GPa. The consequences of this result require examination of the stress state in the host surrounding the inclusion.

PRESSURE IN THE HOST

To this point we have been calculating the pressures in the inclusion generated by the host--inclusion system moving off the entrapment isomeke, and we have noted that classical analysis shows that the stress field in an isotropic spherical inclusion is uniform, isotropic and can be described as a hydrostatic pressure. The stress field in the host is more complex than that in the inclusion, as can be understood by considering the expansion of the inclusion from the virtual state (Fig. 4a) to the relaxed final state (Fig. 4b). The change in the size of the inclusion not only changes the radial stress in the host, but also changes the two tangential stresses in the host; an expanding inclusion (when $P^* > P_{ext}$) compresses the host in a radial direction but leads to tension in the tangential directions. The classic elasticity solutions (Goodier, 1933; Eshelby, 1957) show that, relative to the external pressure, the two tangential stresses are exactly equal to one half of the radial stress but, being in tension instead of compression, are of opposite sign (Fig. 7a). The counter--intuitive result is that while the normal stresses in the host have changed after elastic relaxation, the pressure, equal to the average of the three normal stresses, remains equal to the external pressure at all points (e.g. Zhang, 1998; Tajcmanova *et al.*, 2014). Because thermodynamic properties are primarily dependent on the pressure and, with the exception of materials close to structural phase transitions, much more weakly dependent on deviatoric stresses, there will be no significant effect of the presence of the inclusion and its stress field on the thermodynamic properties of the host. Thus the properties of the host under these conditions essentially remain those of the host under hydrostatic pressure. The deviatoric stress field, not just the pressure step (Whitney *et al.*, 2000), developed in the host around the inclusion will tend to promote cracking of the host when the tangential stress becomes purely tensional (van der Molen & van Roermund,

1986). Tajcmanova *et al.* (2014) pointed out that the host can be cracked in such a way that the inclusion pressure is not released at all; they drew an excellent analogy with a multi-anvil press which maintains the sample pressure even though the strong anvils are not in direct contact with one another and the tangential stresses in the anvils are partly relaxed. Applied to the inclusion model, such cracking could, at most, fully relax the two tangential stress components in the host so that they become equal to the external pressure (Fig. 7b). If the inclusion pressure is maintained completely then the radial stress component adjacent to the inclusion wall remains equal to P_{inc} (see also fig. 3 of Tacjmanova *et al.,* 2014). Then the average of the three normal stresses (one radial, two tangential) in the host adjacent to the inclusion will be $(P_{inc} + 2P_{ext})/3$, which is $(P_{inc} - P_{ext})/3$ above the external pressure (van der Molen & van Roermund, 1986). This gradient in the average normal stress is, by definition, a gradient in pressure. Because the fully relaxed multi-anvil model is the limiting case, the pressure in the host adjacent to the inclusion will always lie between P_{ext} (when there are no cracks) and $(P_{inc} + 2P_{ext})/3$ when the system is fully relaxed from cracking.

The thermodynamic properties of a cracked host phase within the stress field around an inclusion will therefore be different from those for an uncracked host phase that is at the external pressure. It has been suggested that such pressure gradients are responsible for the preservation of compositional gradients in plagioclase rims around kyanite inclusions in felsic granulites (Tajcmanova *et al.*, 2014). As described above, and shown in Fig. 6, the kyanite inclusion could be over-pressured if it was elastically isolated in the ternary feldspar host at pressures significantly below the pressures inferred for growth of the plagioclase rims. In order to generate the 0.6 GPa gradient in pressure in the host inferred from the zoning of the plagioclase rim (Tajcmanova *et al.*, 2014), the inclusion pressure would have to be 1.8 GPa above the external pressure. To achieve this excess pressure in the inclusion, the system would have to experience an increase in external pressure of at least 4 GPa after entrapment of the kyanite by the feldspar. Therefore, if the zoned plagioclase rims truly indicate a pressure gradient existed in the host, the calculations show this could not have been developed during exhumation as a result of the differences in thermoelastic properties of the kyanite inclusion and feldspar host. We emphasise that these calculations apply to an isolated host and inclusion system with the host subject to the lithostatic pressure. Other boundary conditions may be more appropriate, but can generally be considered in terms of the pressure applied to the host by the external microstructure. Then it is clear that over-pressure may be generated on decompression were the feldspar host to be in turn completely encapsulated in a stiffer third mineral, even though the current microstructure of the felsic granulites described by Tajcmanova *et al*. (2014) does not appear to have evidence of such a phase.

CONCLUSIONS

Pressures in inclusions can deviate significantly from the external pressure applied to their hosts, even if the external pressure is lithostatic. Such pressure deviations will always occur during the metamorphic evolution of a rock whenever one mineral is mechanically constrained by another, and the pressure and/or temperature conditions change away from the entrapment isomeke. Deviations from external pressure of the order of 1.5 GPa can be readily developed in common mineral assemblages such as quartz within garnet during prograde and peak metamorphism of continental rocks (Fig. 5c), even without bulk plastic deformation of the rock and even in the presence of fluids to ensure hydrostatic lithostatic pressures. The deviations from lithostatic pressure within the inclusion are greater when the contrast in compressibilities between host and inclusion is large. The deviations are less when the host phase is softer because of the elastic relaxation of the host around the inclusion (Eq. 6).

The pressure and stress differences that are generated during the metamorphic history are not by themselves preserved in rocks recovered to room conditions because the mechanism that generates the excess pressure is purely elastic, and thus completely reversible.

When the external pressure and temperature returns to the entrapment isomeke, for example, there is no remnant excess pressure in the inclusion (e.g. Fig. 5) and there is no elastic record of the system having been to higher *P--T*. However, provided the entrapment isomeke does not pass through room conditions, the inclusion in the recovered sample will exhibit a pressure different from room pressure.

Mechanical or thermodynamic effects may however provide evidence of excess inclusion pressures during metamorphism. The most obvious and direct type of mechanical evidence is brittle fracturing (cracking) of the host grain due to the combination of pressure deviation from lithostatic pressures in the inclusion, and the deviatoric stresses developed in the host. Even if such cracks develop on decompression below the entrapment isomeke, their presence indicates that the elastic stresses were not released during the previous metamorphic history of the rock to that point. Second, the difference between inclusion pressures and external pressure may have driven plastic deformation of the host mineral, evidence for which will be preserved in the deformation microstructure of the host grain around the inclusion. Plastic deformation and brittle fracture cannot change the inclusion pressure beyond the value of the external pressure at which they occur; they can only promote full or partial relaxation of the stress gradients and thus reset the inclusion pressure. If the system subsequently remains elastically isolated, the pressure of the recovered inclusion will then reflect the conditions of this resetting, and not the original entrapment. The elastic signal from host--inclusion systems therefore needs to be considered carefully just as isotopic or chemical systems need interpretation in the context of possible re-equilibration.

Thermodynamic evidence of non-lithostatic pressures can be provided by the host and the inclusion separately. After entrapment the inclusion is not only isolated chemically, but it is also protected from lithostatic pressure. Thus the quartz in the garnet cores of the Kulet whiteschist did not transform to coesite at peak conditions because it was never subjected to pressures in the coesite stability field even though the host garnet was (Fig. 5c); the quartz did not transform because it was elastically isolated, not because it was chemically isolated from fluids. More generally, preservation of apparently metastable inclusion phases through peak conditions may be, in some cases, evidence of non-lithostatic pressures. Similarly, the preservation of apparent non-equilibrium assemblages or compositional profiles in the host adjacent to inclusions may also indicate that significant non-lithostatic pressures were generated during metamorphism by elastic interactions although the maximum excess pressure that can be generated within the host is only one--third of that generated in the inclusion.

In summary, the calculation of elastically generated stresses in simple constrained systems such as a single isolated inclusion is useful because it provides an indication of the sign and magnitude of the non-lithostatic stress gradients that can be generated by mechanical constraints between two minerals and the nature of the controlling factors. The concept of the isomeke (Rosenfeld & Chase, 1961) provides a basis for both the qualitative and quantitative evaluation of the development of non-lithostatic pressure gradients in host--inclusion systems due to elastic interactions. First, as a qualitative tool, the entrapment isomeke divides *P--T* space in to two regions in which the inclusion will exhibit respectively over- or under-pressures with respect to external pressure. Thus soft silicate inclusions in stiffer silicate hosts will exhibit over-pressures after decompression. Stiffer silicate inclusions in softer hosts will exhibit under-pressures after decompression. As a quantitative tool, the isomeke provides the basis for calculating the magnitude of deviations from external pressure. The deviation depends on the difference between the external (lithostatic) pressure and the pressure on the entrapment isomeke at the same temperature. Non-lithostatic pressure in the inclusion therefore depends on the entrapment conditions, the external *P--T* and the thermoelastic properties of the host and inclusion phases.

Extension to more realistic physical systems involving elastic anisotropy and non-spherical inclusions can proceed by treating the anisotropy as a deviatoric effect relative to the isotropic case that we have described here. Because deviatoric stresses are self-relaxing, in the sense that the directions of higher stress undergo greater stress relaxation, and deviatoric stresses do not, to first order, change the volume and hence the thermodynamic properties of minerals, the magnitudes of non-lithostatic pressures calculated for the single inclusion problem remain relevant for real systems. When inclusions are not isolated elastically the overlap of their stress fields allows for further mutual elastic relaxation beyond that calculated here. Provided that the inclusions are of the same phase, and entrapped at the same time, this further relaxation means that the single inclusion model provides realistic estimates of the maximum deviations from lithostatic pressure.

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FIGURE CAPTIONS

Fig. 1: The basic concepts of inclusion entrapment and isolation leading to non-lithostatic pressures. During entrapment and subsequent growth of the host the pressure in both the host and the inclusion remains equal to the external lithostatic pressure. The inclusion pressure can only deviate from the external pressure after elastic isolation followed by a change in external P--T.

Fig. 2: The use of the isomeke concept to calculate in two steps the pressure in an inclusion entrapped at P_{trap} and T_{trap}, using the example of quartz trapped in garnet on the prograde path. The calculation first considers moving the host and inclusion along the entrapment isomeke to the final temperature T_{end} where the stress in both the inclusion and the host is uniform and equal to the pressure P_{foot} defined by the isomeke. At this temperature T_{end} the volume change of the host garnet due to isothermal compression from P_{foot} to the external pressure can be calculated from the EoS of the host garnet. The final pressure of the quartz inclusion P_{inc} can be calculated directly from this volume change and the elastic parameters of the host and inclusion. It is comprised of two parts, the unrelaxed inclusion pressure P^* determined solely by the equations of state of the host and inclusion, plus the pressure change on relaxation ΔP_{relax}.

Fig. 3: (a) The isochors for diamond and an eclogitic garnet as calculated from their EoS (Table 1). The diamond isochors are curved because of the strong variation in thermal expansion coefficient below 400°C. (b) The isomekes of garnet with diamond are only parallel to the isochors when the isochors of the two phases are parallel to one another, for example around 300°C. (c,d) Entrapment conditions for garnet in diamond (Howell *et al.*, 2010) and diamond in garnet (Zhang *et al.*, 2012) are shown as grey ellipses. The isomekes through entrapment conditions divide P--T space. On one side of the entrapment isomeke the inclusion has a higher pressure than the external pressure, on the other side an under-pressure. The sense of over- or under-pressure is reversed if the host and inclusion phases are exchanged as can be seen by comparing (c) and (d).

Fig. 4: Sketches of the radial stress against radius in an ideal host--inclusion system. (a) Prior to relaxation the radial stress in the host is equal to the external pressure P_{ext}, but the radial stress in the inclusion is P^* due to the constriction of the inclusion phase to the final volume of the host. There is therefore a step in stress at the inclusion--host boundary. (b) As a consequence, the inclusion expands until the internal stress becomes equal and opposite to the radial stress in the host. A radial stress gradient is therefore developed in the host, and the inclusion is at the final pressure P_{inc}.

Fig. 5: The relationship between isomekes and deviations of inclusion pressures from external pressure, as illustrated for quartz trapped in a garnet (Parkinson, 2000). (a) Isomekes of α--quartz and garnet calculated from their EoS parameters (Table 1). (b) Contours of the deviation of unrelaxed inclusion pressures P^* from the external pressure for a quartz trapped at 0.7 GPa and 380 °C (Parkinson, 2000) plotted in terms of the temperature and external pressure. The contour values are given in the white boxes on the left-hand side of the diagram. Note that the contours of excess pressure are only parallel to the isomekes along the entrapment isomeke (black line). (c) The deviation of relaxed inclusion pressures P_{inc} (grey

contours) from the external pressure for the same inclusion. The real P--T of the inclusion during burial and exhumation shown in (c) differs significantly from the un-relaxed calculation shown in (b), except at the point that the retrograde P--T path for the inclusion crosses the entrapment isomeke at the same point and time as the host.

Fig. 6: Isomekes calculated for kyanite and an average alkali feldspar (Table 1). Because kyanite is stiffer, kyanite inclusions trapped in feldspar at estimated peak conditions will always exhibit under-pressures during the retrograde decompression. The entrapment conditions and retrograde path shown are for the felsic granulites described by Tajcmanova *et al.* (2011).

Fig. 7: Radial and tangential normal stress components around an inclusion after elastic relaxation of an inclusion with $P_{inc} > P_{ext}$ (after Tajcmanova *et al.*, 2014). (a) In an un-cracked host the radial stress at the inclusion wall is equal to the inclusion pressure (c.f. Fig 6b), and the two normal tangential stresses are tensional and equal to $(3P_{ext} - P_{inc})/2$. As a consequence there is no gradient in pressure in the host (e.g. Zhang, 1998). (b) If cracking of the host around the inclusion releases the tangential stresses without releasing the inclusion pressure (multi-anvil model) then the pressure in the host at the inclusion wall becomes $(2P_{ext} + P_{inc})/3$ and there is a pressure gradient in the host (Tajcmanova *et al.*, 2014).
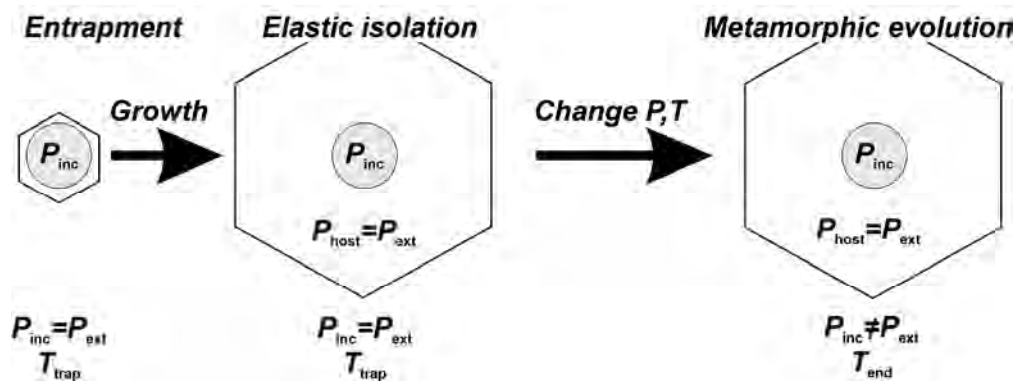
TABLE CAPTION

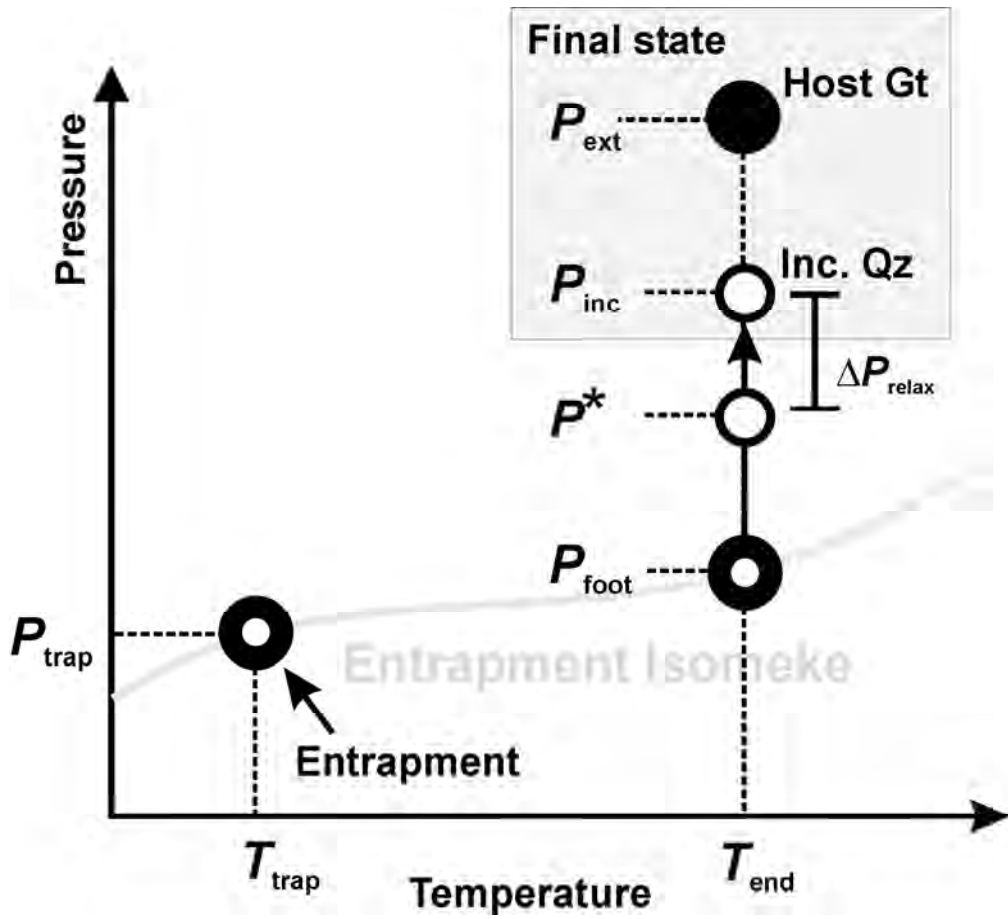**Table 1:** EoS Parameters used in example calculations.

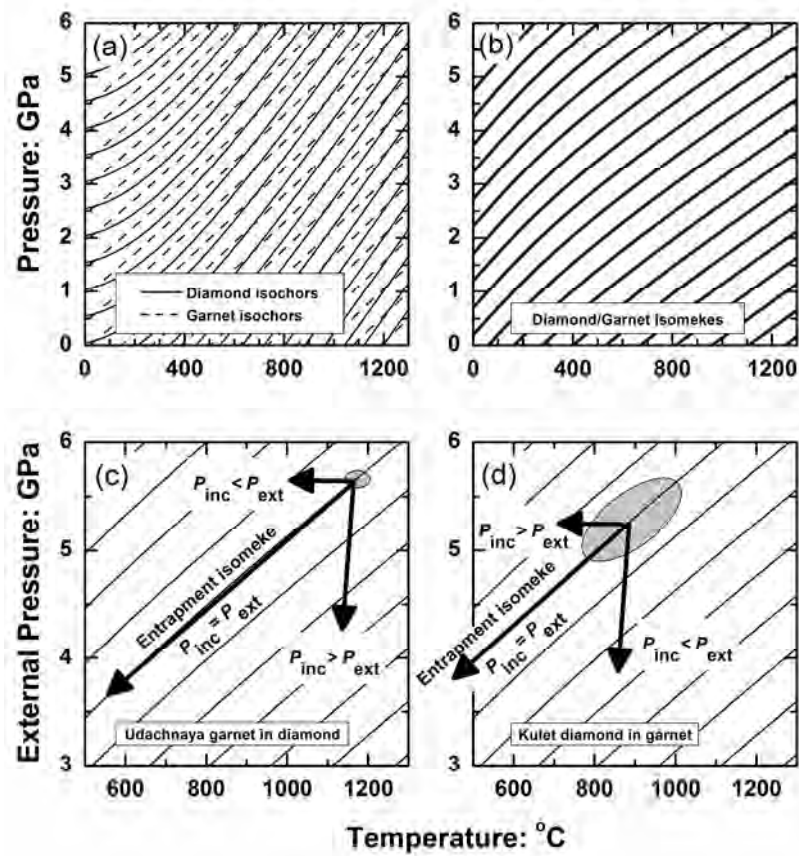Table 1: EoS Parameters used in example calculations

Phase	K_{0T}: GPa	K_0'	$\alpha_0 \times 10^{-5}$. K^{-1}	θ_E: K	Notes
Example 1					
diamond	444	4.0	0.2672(3)	1500	(Angel *et al.*, 2015)
garnet	169.2	5.88	2.135	477	Derived for an estimated average composition of eclogitic diamond inclusions of Py41Al33Gr26Sp1 by interpolation from properties of end-members.
Example 2					
garnet	174.7	5.3	2.748	757	Derived from the core composition of the garnet (Parkinson, 2000) by interpolation from properties of end-members.
α-quartz	37.12	5.99	3.64	-	These are room pressure and temperature values of parameters. Calculations were performed with a Landau model for the alpha--beta phase transition, fitted to the *P-V* data of Angel *et al.* (1997) the -*T-V* data of Carpenter *et al.* (1998) and the room-pressure bulk moduli (Ohno *et al.*, 2006). The room-pressure transition temperature of 574°C and the slope of the transition boundary $dT_r/dP = 255$ °C.GPa^{-1} were used as fixed constraints in the EoS model.
Example 3					
kyanite	160.1	4.05	1.92	630	Holland & Powell (2011)
feldspar	55	4.0	2.5	470	Average K_{0T} and K_0' from *PV* data (Ross *et al.*, unpublished data). Average thermal expansion coefficient from Hovis *et al.* (1999). Average θ_E from Holland & Powell (2011).

All parameters are for the Birch-Murnaghan EoS for the purely compressional part (K_{0T} and K_0') in combination with the thermal pressure EoS of Holland & Powell (2011). The reference pressure and temperature for the EoS are 0 GPa and 298 K. α_0 is the volume thermal expansion coefficient at the reference conditions, and θ_E is the Einstein temperature.
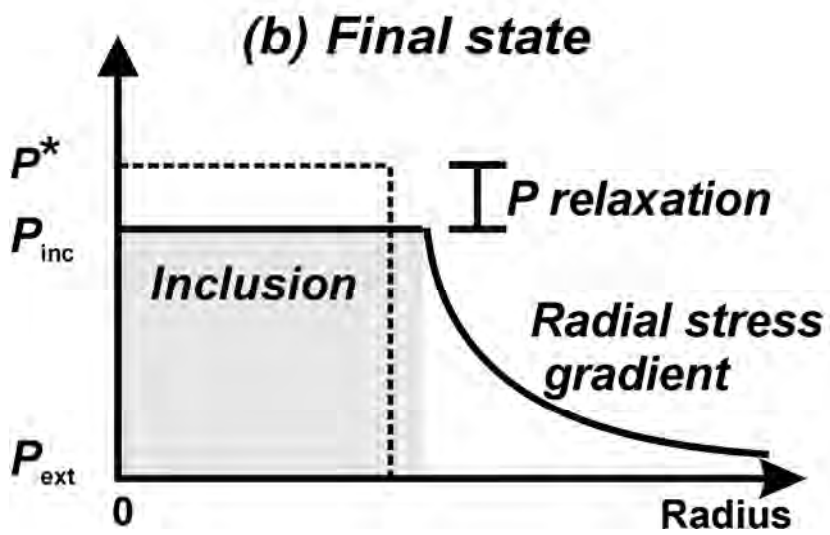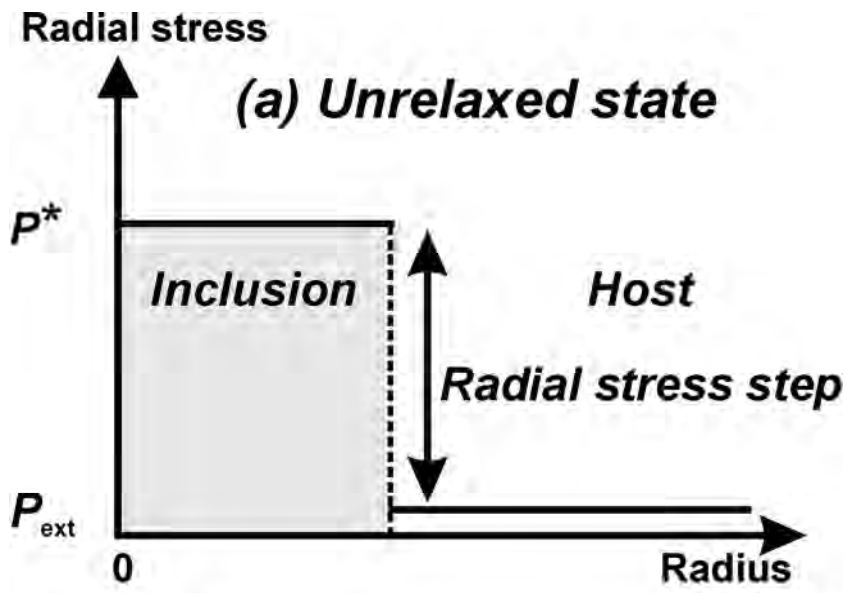
For relaxation calculations, the following shear moduli parameters were used. Diamond $G_0 = 535$ GPa; garnet $G_0 = 94$ GPa, $dG/dP = 1.3$, $dG/dT = -0.0135$ GPa.K^{-1}; feldspar $G_0 = 35$ GPa, the value for albite from Brown *et al.* (2006). The temperature and pressure derivatives of the shear moduli of feldspar are unknown.
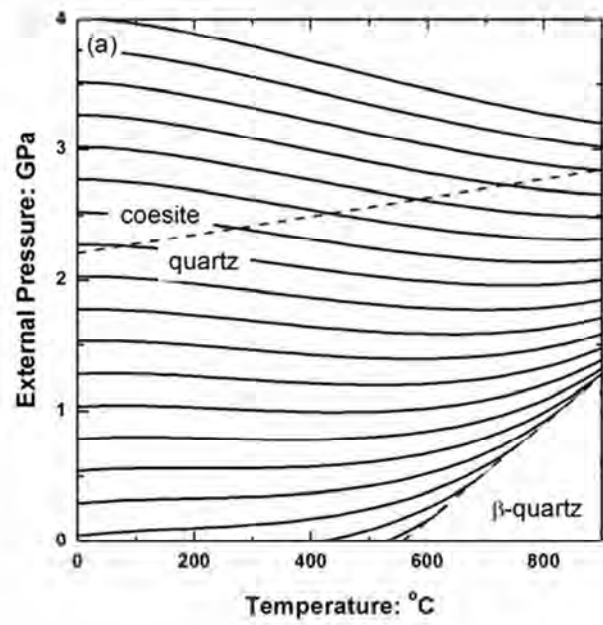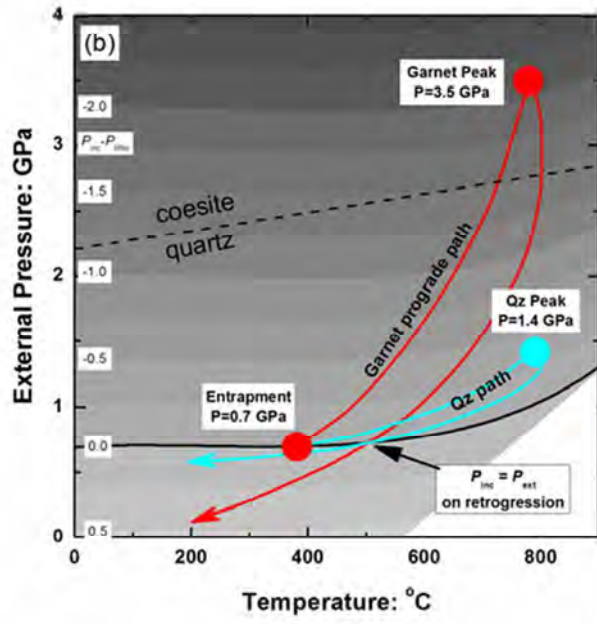
Entrapment   *Elastic isolation*   *Metamorphic evolution*

Growth   *Change P,T*

P_{inc}

P_{inc}

$P_{host} = P_{ext}$

P_{inc}

$P_{host} = P_{ext}$

$P_{inc} = P_{est}$
T_{trap}

$P_{inc} = P_{ext}$
T_{trap}

$P_{inc} \neq P_{ext}$
T_{end}

226x319mm (300 x 300 DPI)

(a) Unrelaxed state

Radial stress

P^*

Inclusion

Host

Radial stress step

P_{ext}

0

Radius

(b) Final state

P^*

P_{inc}
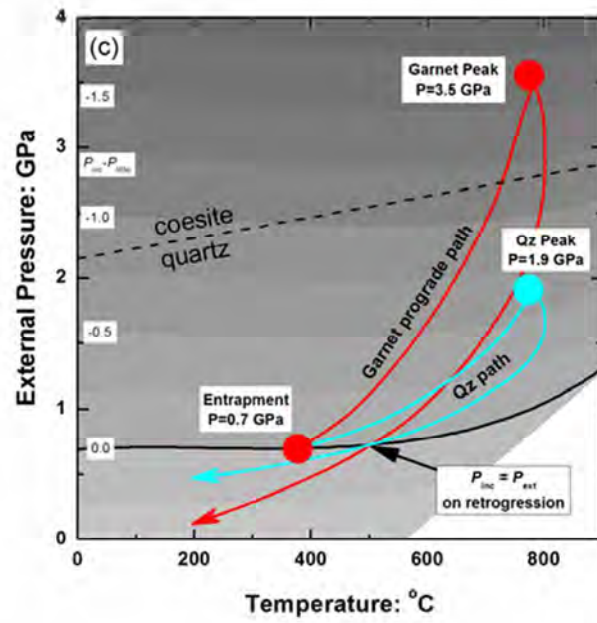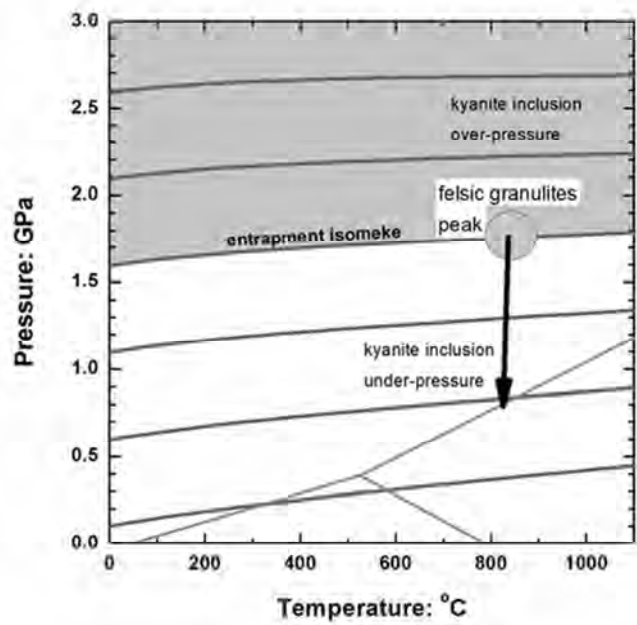
P relaxation

Inclusion

Radial stress gradient

P_{ext}

0
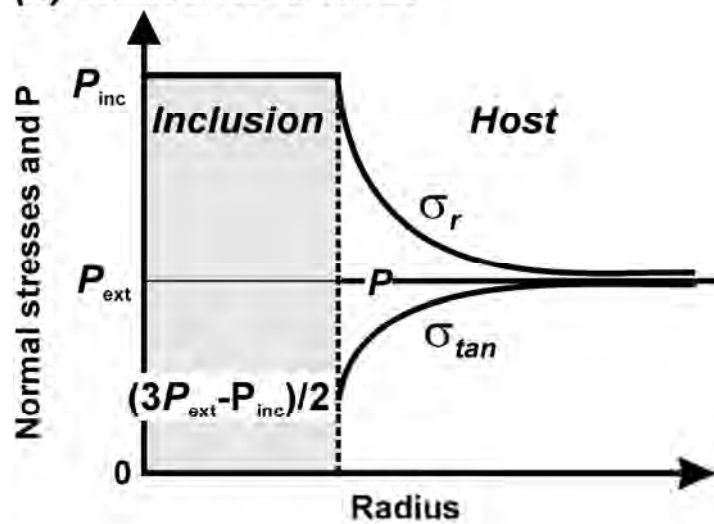
Radius

56x39mm (300 x 300 DPI)

56x39mm (300 x 300 DPI)

56x39mm (300 x 300 DPI)

56x39mm (300 x 300 DPI)

(a) Uncracked host

Normal stresses and P

P_{inc}

Inclusion

Host

σ_r

P_{ext} — P

σ_{tan}

$(3P_{ext}-P_{inc})/2$

0

Radius

(b) Multi-anvil model

Normal stresses and P

P_{inc}

Inclusion

Host

$(2P_{ext}+P_{inc})/3$

σ_r

P

P_{ext} — σ_{tan}

0

Radius