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Trapped minerals under stress

Paolo Nimis

Dipartimento di Geoscienze, Università di Padova, via G. Gradenigo 6, 35131 Padua, Italy

Learning how to read in rocks the record of the physical conditions in which they formed has allowed earth scientists to address important geological questions, which can be as diverse as, say, the conditions of crystallization of phenocrysts in a lava, the pressure-temperature (*P*-*T*) path of a tectonic unit in an orogen, the stratigraphy and thermal state of a mantle section represented by a xenolith suite, or the depth of origin of a diamond found in a placer. This has been essential to our understanding of, for instance, plumbing systems beneath volcanos (e.g., Dahren et al., 2012), the processes of subduction–exhumation at convergent margins (e.g., Platt, 1986), the geochemical heterogeneity of the lithospheric mantle (O'Reilly and Griffin, 2006), or the deep carbon cycle (Shirey et al., 2013). Several thermobarometric tools have been developed to estimate *P* and *T* for a variety of geological materials. However, some materials are more challenging than others: high-variance mineral assemblages may be stable over large ranges of *P*-*T* conditions; suitable geothermobarometers based on chemical equilibria may not be available for some mineral associations; mineralogical resetting during, for instance, metamorphism may obliterate earlier assemblages and, consequently, part of the *P*-*T* record; and incomplete equilibration and overstepping of reactions (Spear et al., 2014) may limit the reliability of *P*-*T* estimates.

In some cases, mineral inclusions in other minerals can be used to obtain thermobarometric information that would not be retrieved otherwise. Significant examples are inclusions of mantle minerals in kimberlite-borne diamonds (Stachel and Harris, 2008) and relicts of ultrahigh-*P* minerals such as coesite or diamond in other metamorphic minerals (e.g., Smith, 1984; Sobolev and Shatsky, 1990). However, using inclusions as petrologic markers is not free from ambiguities. In fact, because the inclusion and host have different compressibilities and thermal expansions, after the entrapment the two minerals will follow distinct *P-T* paths, causing departures from the lithostatic pressures of up to several gigapascals at the mineral grain scale (Gillet et al., 1984; Van der Molen and van Roermund, 1986; Guiraud and Powell, 2006; Angel et al., 2015).

Although non-lithostatic pressures may complicate the thermobarometric analysis of rocks, they may also become a resource to petrologists. When a host-inclusion pair formed at high *P-T* is exhumed to the surface, a residual *P*, P_{inc}, may develop on the inclusion as a result of the two minerals having different elastic properties (Rosenfeld and Chase, 1961). The P_{inc} can be measured by determining the shift of Raman peaks (Kohn, 2014), by measuring birefringence changes in the host around the inclusion (Howell et al., 2010), by comparing *in situ* X-ray diffraction data (unit cell volume) on the inclusion with data obtained in air (Harris et al., 1970), or by combining *in situ* X-ray diffraction data (unit cell volume and chemistry) with the appropriate elastic properties at high *P* of the same mineral (Nestola et al., 2011). If the elastic properties of the inclusion and host are known, and the entrapment *T* is also known (or the thermal expansions are similar), then the *P* at entrapment, P_{trap}, can be calculated back from P_{inc} using elasticity theory.

On this basis, a method of ‘elastic thermobarometry’ has been developed for some specific and more general cases (Adams et al., 1975; Cohen and Rosenfeld, 1979; Gillet et al., 1984; Zhang, 1998). A strength of this method is that it is totally independent of chemical equilibrium. However, it requires several assumptions to be satisfied: (1) interactions between inclusion and host are purely elastic; (2) host and inclusion are elastically isotropic; (3) the inclusion is spherical and elastically isolated from any other inclusion or host surface; and (4) on entrapment, the inclusion fits the host cavity perfectly. Many of these requirements are not generally met in rocks. Brittle or plastic deformation in the host after entrapment may lead to non-elastic relaxation of P_{inc}, causing underestimation of P_{trap}. Although a few minerals can be treated as being elastically isotropic (e.g., garnet is practically so, diamond is so stiff that its moderate anisotropy can generally be neglected), many others are strongly anisotropic and will develop deviatoric stresses during their route to the surface. This may be a particularly serious problem if P_{inc} is derived by using techniques that are sensitive to anisotropic stress, such as Raman spectroscopy (e.g., Briggs and Ramdas, 1977). Finally, the geometry and distribution of the inclusions are often far from ideal.

In recent years, attempts have been made to improve and extend the applicability of elastic thermobarometry. The main efforts have been aimed at reducing the number of assumptions or evaluating the effects of deviations from ideal cases. Angel et al. (2014) introduced a method to calculate P_{trap} that avoids the assumption of linear elasticity (i.e., that the elastic properties do not change with P or T), a common, but unwarranted pre-requisite in all previous studies. The paper by Mazzucchelli et al. (2018) in this issue of *Geology* addresses another critical issue: the *geometric effects*. As discussed in the paper, geometric effects are important because they affect the force balance at the interface between host and inclusion. This balance causes deformation in the host and partial relaxation of the *P* that has built up on the inclusion. Quantification of this relaxation is an essential part of elastic thermobarometry (cf. Zhang, 1998; Angel et al., 2014). By using finite-element modeling, Mazzucchelli et al. have quantified the magnitude of geometric effects on the final P_{inc} and, in turn, on the calculation of P_{trap}. Numerical simulations have been made for inclusions with various shapes, inclusion/host size ratios, and proximity to host external surfaces. The results indicate that for stiff inclusions in soft hosts (e.g., kyanite in feldspar, diamond in garnet), neglecting geometric effects may lead to significant overestimation of P_{trap}, but that for soft inclusions in stiff hosts (e.g., quartz in garnet or any mineral in diamond) these effects are often insignificant. Mazzucchelli et al. have provided practical guidelines that help one to decide whether this is the case for the particular inclusion-host system under study. In all other instances, reliable elastic thermobarometry can only be performed through numerical modeling on a case-by-case basis.

The work of Mazzucchelli et al. is a welcome advance toward a more robust application of elastic thermobarometry, but several aspects of the method still require investigation. For example, Mazzucchelli et al. still assume isotropic elasticity. This may be a reasonable approximation for some minerals, but what happens when the method is applied to elastically very anisotropic minerals such as olivine, feldspars, or coesite? Also, correct calculation of P_{trap} from P_{inc} strongly relies on the quality of the elastic parameters of the minerals involved (i.e., thermal expansion coefficients, bulk modulus and its *P-T* derivatives, and, for the host, shear modulus), which is the subject of ongoing research (e.g., Angel et al., 2017). The recent finding of fluids surrounding solid inclusions in diamonds (Nimis et al., 2016) even challenges the commonly accepted assumption that mineral inclusions completely fill the host cavity. These fluids are not easy to detect and have remained unnoticed for decades. Are these fluid rims solely present in inclusions in diamonds or do they occur also in other types of inclusion-host systems? And what is their ultimate effect on P_{inc}? Finally, the development of over-pressures in the inclusion during the exhumation path may lead to fracturing or plastic deformation in the host. Whereas fractures can generally be easily detected under an optical microscope, studying the effects of plastic deformation requires more sophisticated techniques such as transmission electron microscopy or electron backscatter diffraction (e.g., Cayzer et al., 2008). Plastic deformation is favored at high T, and some minerals are more resistant than others to this mechanism, but the times required to remove the inclusion stress are quite uncertain (Dabrowski et al., 2015); then for what conditions and for what types of inclusion-host systems can we reasonably ignore its effects on the final P_{inc}? One of the merits of Mazzucchelli et al.’s paper is that it finally defines the conditions under which geometric effects can safely be neglected. If these conditions are satisfied and discrepancies between elastic and conventional thermobarometry still occur, then the reason may indeed be found in some of the above questions. Further numerical modeling and dedicated experiments will hopefully provide solutions to some of these problems in the future.

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