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Highlights and Breakthroughs

How to apply elastic geobarometry in geology

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Pressure and temperature estimates of rocks provide the fundamental data for the investigation of many geological processes such as subduction and exhumation, and yet their determination remains extremely challenging (Tajcmanova et al. 2020). A wide variety of methods are constantly being developed to tackle the ambitious objective of pinpointing the geological history of rocks through the many complex processes often interacting with one another at depth in our planet. Analytical advances are being pushed to the limit of conventional methods, allowing information preserved by mineral, fluid, and solid inclusions to be used for high spatial resolution determinations that can unravel a large variety of processes occurring at the micro- to the nano-scale. Among these, chemical geothermobarometry that is often challenging in many rock types due to alteration processes, chemical re-equilibration, diffusion, and kinetic limitations has been increasingly coupled with elastic geothermobarometry (e.g., Anzolini et al. 2019; Gonzalez et al. 2019). Elastic geothermobarometry of host-inclusion systems, in paper Mazzucchelli et al. 2021, this issue, is a new and complementary non-destructive method (see Fig. 1 for an example) to determine the pressures (*P*) and temperatures (*T*) of inclusion entrapment (i.e., the *P*-*T* conditions attained by rocks and minerals at depth in the Earth) from the remnant stress or strain measured in inclusions still trapped in their host mineral at room conditions (e.g., Nestola et al. 2011; Howell et al. 2012; Alvaro et al. 2020).

This method underwent significant developments in the past decade aimed at overcoming several serious restrictions to previously available models and methodologies, which led to questions being raised about the general validity of the method. Most of the recent developments have been focused on enhancing the method to allow its application to a broader variety of scenarios, overcoming the three major assumptions (1) linear elasticity (Angel et al. 2014); (2) spherical shape (Campomenosi et al. 2018; Mazzucchelli et al. 2018); and (3) isotropic elastic properties for the host and the inclusion, allowing its application to an increasing number of host inclusion pairs with a variety of analytical techniques (e.g., micro-Raman spectroscopy, Murri et al. 2018) and calculation methods (e.g., nonlinear elasticity and numerical modeling, Anzolini et al. 2019; Mazzucchelli et al. 2019; Morganti et al. 2020).

This first part of the development essentially concerned the calculation of the mutual elastic relaxation of the host and inclusion, for which initial estimates have relied on the assumption of linear elasticity theory. Angel et al. (2014) presented a new formulation of the problem that avoids this assumption and incorporates full nonlinear elastic behavior for the host and the inclusion and has been enhanced with the progressive implementation of carefully validated equations of state for several host and inclusion phases (e.g., Angel et al. 2017a, 2020; Mihailova et al. 2019; Milani et al. 2015, 2017; Murri et al. 2019; Zaffiro et al. 2019). This finally allowed analyses incorporating the accurate behavior of quartz inclusions in garnet over a large *P* and *T* interval (Angel et al. 2017a; Morana et al. 2020). The methods and the calculation algorithm have been included in the freely available EoSFit-Pinc software (Angel et al. 2017b). The availability of the new software and algorithm strongly promoted the use of this methodology, enabling several researchers to perform their measurements and calculations independently (Anzolini et al. 2019, 2018; Nestola et al. 2016, 2018a, 2018b; Nimis et al. 2016, 2019).

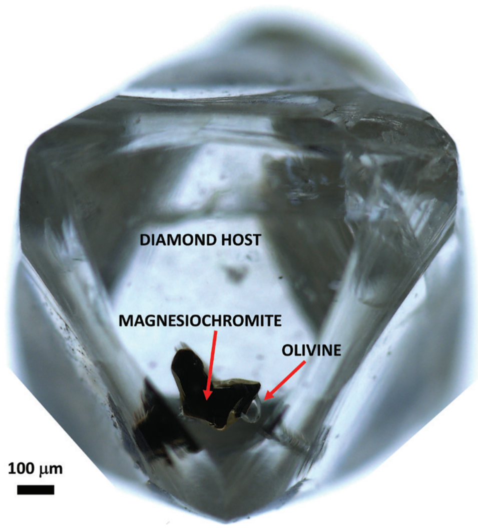

Figure 1. An example of a host-inclusion system. In this specific case, the transparent host is a natural diamond from Udachnaya (Siberia, Russia), whereas the black inclusion is a magnesiochromite spinel [~$(Mg,Fe)(Cr,Al)_2O_4$]. Magnesiochromite, in turn, has in contact a second transparent inclusion, which is an olivine [~$(Mg,Fe)_2SiO_4$)] (the diamond was provided by J.W. Harris, University of Glasgow; photo: Caterina Canovaro, University of Padova). (Color online.)

The second part of the development has been focused on measurements and calculations of non-spherical inclusions in complex geometrical relationships with the host and/or other inclusions. Such issues have been addressed with several numerical models on a variety of shapes by Mazzucchelli et al. (2018), producing numerical correction factors to guide the readers toward estimating the uncertainties associated with shapes different from spheres, including the complex interplay of edges and corners for which only numerical solutions can be provided. In Mazzucchelli et al. (2018), the authors estimated

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the maximum discrepancies caused by geometry and shape and validated their estimations against simple experimental results obtained on mechanically polished host inclusion systems by Campomenosi et al. (2018).

The most complex portion of development dealt with elastic anisotropy of inclusions as this is also the largest source of uncertainties that cannot be evaluated a priori simply by looking at the sample under the optical microscope or with more complex techniques (e.g., Scanning Electron Microscopy, X-ray micro-Tomography, *inter alia*). The importance of elastic anisotropy essentially arises from the fact that an inclusion trapped in a host of any symmetry exhumed to the lower P and T conditions at the Earth surface is subject to the strain imposed by the host. The simplest, and yet still extremely complex, case that can be envisaged is that of a cubic host (e.g., diamond) that we will consider nearly isotropic. In this case, after exhumation, the inclusion is subject to isotropic strains imposed by the host. An anisotropic inclusion subject to isotropic strains must develop non-hydrostatic stresses (Angel et al. 2019; Murri et al. 2019, 2018). This observation is sufficient to demonstrate that whatever tentative interpretation of the measured state of stress for a non-isotropic inclusion in an isometric host using conventional equations of state (as currently determined under hydrostatic compression) is meaningless. However, several tentative steps have been made to try to estimate the effect of the elastic anisotropy on (1) the calculation of the residual strain, stress, and pressures; and (2) the calculation of the entrapment conditions. For the calculation of the residual pressure, the major issue arises from measurements performed via micro-Raman where most of the studies interpret the peak shift of Raman bands ($\Delta\omega$) as a pressure effect using an empirical calibration that relates Raman shift with P (e.g., Morana et al. 2020; Schmidt and Ziemann 2000). As already shown by Grüneisen (1926) and later confirmed by Angel et al. (2019) and Murri et al. (2018, 2019), this is physically incorrect as the Raman band shift depends upon the applied strains through the Grüneisen tensor rather than the applied stress through a $\Delta\omega$ vs. P calibration. This fact may appear to have small effects when dealing with cubic hosts, but as shown by Bonazzi et al. (2019), the effects become non-negligible at a few gigpascals of entrapment. There are several examples (Bonazzi et al. 2019; Gonzalez et al. 2019; Thomas and Spear 2018) of inclusions with 0 kbar of residual pressure calculated from the shift of the 464 cm^{-1} band that instead were apparently entrapped at several kilobars, if calculations are performed via the Grüneisen tensor approximation. These calculations from the Raman shift of multiple bands are now possible through the software "Strainman" (Angel et al. 2019). The second part of the elastic anisotropy contribution plays a crucial role in calculating the entrapment conditions starting from the strains determined either from the Raman shifts or from the lattice parameters measured via X-ray diffraction (e.g., Alvaro et al. 2020). This part has been addressed by the recent publication of numerical and analytical solutions for non-isotropic, host-inclusion pairs presented in Mazzucchelli et al. (2019) and Morganti et al. (2020).

The new EntraPT web application, published by Mazzucchelli et al. (2021) in *American Mineralogist*, provides a platform for elastic geobarometry that includes these recent advances. Thanks to this application, the user can interpret the residual strain of anisotropic inclusions in an intuitive and consistent manner. Moreover, EntraPT, that is built on the underlying code of Eosfit7c, provides the tools to perform calculations of the residual pressure and of the entrapment pressure and temperature of isotropic and anisotropic systems using a self-consistent set of thermoelastic properties (e.g., Alvaro et al. 2020; Gonzalez et al. 2019).

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