LETTER

EosFit-Pinc: A simple GUI for host-inclusion elastic thermobarometry

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ABSTRACT

Elastic geothermobarometry is a method of determining metamorphic conditions from the excess pressures exhibited by mineral inclusions trapped inside host minerals. An exact solution to the problem of combining non-linear Equations of State (EoS) with the elastic relaxation problem for elastically isotropic spherical host-inclusion systems without any approximations of linear elasticity is presented. The solution is encoded into a Windows GUI program EosFit-Pinc. The program performs host-inclusion calculations for spherical inclusions in elastically isotropic systems with full P-T-EoS for both phases, with a wide variety of EoS types. The EoS values of any minerals can be loaded into the program for calculations. EosFit-Pinc calculates the isomeke of possible entrapment conditions from the pressure of an inclusion measured when the host is at any external pressure and temperature (including room conditions), and it can calculate final inclusion pressures from known entrapment conditions. It also calculates isochors and isomekes of the two phases.

Keywords: Geobarometry, inclusion, Equations of State, elasticity

INTRODUCTION

The determination of the remnant pressures in inclusions, as measured by X-ray diffractometry, birefringence analysis, or Raman spectroscopy, provides an alternative and complementary method to conventional geothermobarometry by using elasticity theory. A remnant pressure in an inclusion is developed because the inclusion and the host have different thermal expansions and compressibilities, and therefore the inclusion does not expand in response to P and T as would a free crystal. Instead it is restricted by the host mineral, and this confinement can result in inclusions exhibiting over-pressures, or under-pressures, when the host is studied at room conditions. By measuring the remnant pressure the possible temperatures and pressures of entrapment can be calculated by using the elastic properties of the host and inclusion minerals. This basic concept has been known for a long time (Rosenfeld and Chase 1961). Difficulties arise because the classic solutions for the stress distribution in host-inclusion systems (e.g., Goodier 1933, Eshelby 1957) are derived for linear elasticity, which assumes that the stresses and strains are small, and that the elastic properties do not change with pressure or temperature. However, minerals are subject to large changes in pressure and temperature from formation to room conditions, so their elastic properties are not constant but are described by non-linear Equations of State (EoS).

Several approaches have been used to apply the classic host-inclusion elastic solutions to mineral systems. All of them assume that the two minerals are elastically isotropic, and that the inclusion is spherical and isolated from the host surface and any other inclusions or defects in the host mineral. The simplest approach has been to ignore the variation of the elastic properties of minerals with pressure and temperature (e.g., Zhang 1998). This leads to errors in inclusion pressures, especially when they are calculated for prograde metamorphic conditions following entrapment (e.g., Angel et al. 2014b). A second approach has been to calculate the evolution of the inclusion pressure in a series of small steps from entrapment conditions by adjusting the elastic properties of the host and inclusion at each step according to either a full or approximate EoS, and then using the linear solution at each step to calculate mechanical equilibrium (Gillet et al. 1984; van der Molen and van Roermund 1986; d’Arco and Wendt 1994). A third approach is to consider the “thermodynamic pressure”, $P_{\text{thermo}}$, in the inclusion when it is constrained to have the same volume change as the host crystal from entrapment $P_{\text{trap}}$ and $T_{\text{trap}}$ to the final external $P_{\text{end}}$ and $T_{\text{end}}$ (Fig. 1). $P_{\text{thermo}}$ is different from the final external pressure on the host, and this drives a further mutual elastic relaxation that reduces the difference between the inclusion pressure and $P_{\text{end}}$. This relaxation must be calculated in a second step. The advantages of this approach are that the calculation of $P_{\text{thermo}}$ can be exact by using appropriate non-linear EoS, and the only linear elasticity approximation is in the relaxation term. However, the correct solution for the pressure in the spherical inclusion requires that the relaxation is evaluated during isothermal decompression from a state of uniform stress (Goodier 1933), and not along any P-T path as often incorrectly assumed (e.g., Guiraud and Powell 2006). The first step is therefore to consider a temperature change from $T_{\text{trap}}$ to $T_{\text{end}}$ and to calculate the change in external pressure required to induce an equal pressure change in the inclusion (Fig. 1). This thermodynamic path is an isomeke of the host and inclusion phases (Rosenfeld and Chase 1961; Adams et al. 1975). The pressure, $P_{\text{thermo}}$, on the entrapment isomeke at $T_{\text{end}}$ can be deter-