Finite element modeling of elastic volume changes in fluid inclusions:
Comparison with experiment

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ABSTRACT

We have used finite element modeling (FEM) to successfully reproduce elastic volume changes of synthetic fluid inclusions in quartz pressurized in a hydrothermal diamond-anvil cell (HDAC) at external pressures up to 250 MPa. At higher pressures, the synthetic inclusions are somewhat stiffer than would be predicted by linear elasticity due to the effect of pressure on the elastic moduli. The finite element models were created to reproduce the inclusion’s approximate shape, and crystallographic orientation within the host, which is elastically anisotropic. The models successfully predict changes in fluid inclusion volume measured using the HDAC, which gives us confidence that FEM may be used to predict the elastic behavior of inclusions in other situations.

Keywords: Mechanical properties, elastic volume change, high-pressure studies, hydrothermal diamond anvil cell, metamorphic petrology, fluid inclusion, finite element modeling, elastic deformation, volume change

INTRODUCTION

Inclusions within mineral grains are nearly ubiquitous in rocks of all types. Whether they are crystalline, glass, fluid, or gas, inclusions contain information about either the environment of formation of the host mineral grain or in the case of secondary fluid inclusions, conditions since the mineral grain was formed. If the temperature or pressure changes after the inclusion-host system forms, differences in thermal expansion or compressibility between the two will create differential stresses in the host and may cause it to permanently deform. In many situations, understanding the mechanics of the inclusion-host system is helpful for interpreting measurements made on the inclusion. For example, interpretation of homogenization temperatures of fluid inclusions is based on the assumption that the inclusion’s volume has not changed since trapping (Roedder 1984). For solid inclusions, patterns of cracks in the host or measurement of the internal pressure within the inclusion may be useful in deducing information about the geologic history of a sample (e.g., Kenkmann and Dresen 1998; Whitney et al. 2000). Fluid and melt inclusions can be studied using a hydrothermal diamond-anvil cell (HDAC) to prevent decrepitation and/or water loss. In such studies, elastic changes of the inclusion volume due to the application of high confining pressures can lead to significant changes in the measured phase transition temperature (Darling and Bassett 2002; Schmidt et al. 1998). The elastic volume change as a function of pressure depends on the inclusion geometry (Burnley and Davis 2004). Therefore, it must be determined for individual inclusions, either empirically or by modeling, to correct measured phase transition temperatures for the stress-related component of the volume change. In an effort to test the utility of finite element models for understanding the mechanical behavior of inclusions in minerals, we have compared measured elastic volume changes and deformation of synthetic pure water inclusions in quartz with finite element models of the individual inclusions. Such inclusions are ideal for this study. The internal pressure, as well as associated elastic and plastic volume changes of the inclusion can be determined accurately from the homogenization temperature because reliable data are available for the molar volume along the liquid-vapor curve of water. Therefore, all the mechanical boundary conditions as well as the resulting deformation are known and can be compared to those produced under the same conditions in the model. Finite element models are useful because they can be used to reproduce more complex shapes than can be modeled analytically and the elastic anisotropy of the host can be included.

METHOD

Hydrothermal diamond-anvil cell experiment

The experimental set-up for this study is shown schematically in Figure 1. We used an externally heated hydrothermal diamond-anvil cell (HDAC) (Bassett et al. 1993). The thermal gradients within the sample chamber are small, which permits accurate and reproducible temperature measurements. Slow heating rates and stability of the set point temperature to within ±0.2 °C were achieved by controlling the power input to the resistive heaters using Eurotherm 2408 temperature controllers. All experiments were conducted at a constant inert gas flow (controlled using a flow meter) to ensure reproducibility of temperature measurements. The temperature in the sample chamber of the HDAC was measured using NiCr-Ni thermocouples and calibrated before and after the experiments using the melting point of NaNO3, at 1 atm pressure (306.8 °C) and the ice I±L±V triple point of water (0.01 °C, 0.6 kPa). No shift of the temperature calibration was detected. The accuracy of the temperature measurements was better than ±1 °C and the reproducibility was better than ±0.5 °C.

The sample used in this study (sample 062895-IX) was a disk of Brazilian quartz that contained synthetic pure water inclusions. The inclusions were formed by healing fractures in a quartz core at about 580 °C and 300 MPa following the...