A numerical model for steady-state temperature distributions in solid-medium high-pressure cell assemblies

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ABSTRACT

We present a numerical model for calculating the temperature distribution inside resistance-heated high-pressure solid-medium axi-symmetric cell assemblies that incorporates both composition- and temperature-dependent thermal conductivity. The code was validated using both analytic solutions of simplified thermal diffusion problems and comparisons to actual laboratory experiments and was found to be reliable in matching the temperature characteristics of multi-anvil experiments. Calculations for various cell assembly designs resulted in temperature fields that are consistent with experimental measurements of thermal gradients. These calculations also illustrated the influence of temperature-dependence of thermal conductivity, an important and often-overlooked property, on the thermal profiles. This model may be used to fine-tune the design of cell assemblies, either to minimize thermal gradients or to produce a desired temperature distribution. The four “typical” multi-anvil cells that we used to demonstrate this technique have temperature profiles across the sample that range from 25 to 75 °C when the thermocouple temperature is 1200 °C. The thermocouple in all four is in a region where the temperature gradient is on the order of 100 °C per millimeter, which could lead to experimental temperature uncertainties that are correlated with the thermocouple location.

Keywords: Multi-anvil, high pressure, thermal gradients, temperature, numerical modeling

INTRODUCTION

Solid-medium high-pressure devices are in widespread use for the replication of conditions that exist in the Earth’s interior, or for the synthesis and study of materials at high pressures and temperatures. The typical solid-medium device consists of a ram that exerts a force on an arrangement of anvils, which in turn exert forces on a solid but ductile container for the sample. An electrically heated resistance furnace may be placed inside the container, with a thermocouple and a sample. Due to practical fabrication considerations, the geometry of the innermost parts of the sample assembly is often (but not always) cylindrical, or can be closely approximated as cylindrical.

The primary advantages of solid-medium high-pressure techniques include a relatively large sample volume, stable temperature control, and the ability to perform long duration experiments. Further advantage could be obtained by controlling the temperature distribution using carefully designed assemblies. Uncontrolled thermal gradients, on the other hand, not only decrease the temperature resolution of experiments, but may also lead to anomalous effects in the chemistry of the sample (Schmidt and Ulmer 2004).

Thermal gradients in solid samples are the result of heat transport by conduction. Because it is seated inside a cylindrical furnace, the temperature inside a sample tends to increase radially from its center. Also, the furnace has a finite axial extent, inducing heat conduction along the assembly axis and causing cooler temperatures to prevail away from the center of a sample in the axial direction. Thus a simple assembly consisting of a uniform thickness furnace and solid-medium materials produces roughly paraboloid isotherms (opening in the axial direction away from the sample center) with temperature variations sometimes exceeding 100 °C across the sample. This gives rise to the hourglass-shaped compositional or phase layering frequently observed in high-pressure samples. The problem is exacerbated when the furnaces are short relative to their radii, decreasing the axial extent and enhancing axial conduction. Examples of high-pressure experiments where this is the case are multi-anvil experiments (Kawai and Endo 1970; Walker et al. 1990) with assembly sizes on the order of a few millimeters, and experiments using opposed-anvil presses such as the Bridgman device (cf. Ringwood and Major 1966) and the Drickamer cell (Funamori and Yagi 1993; Yamazaki and Karato 2001).

Several types of measurements can be made to estimate or calibrate the thermal gradients in high-pressure experiments. One such calibration would be measurement of a standard temperature relative to the temperature of the thermocouple; for example, determination of the melting front in a single component metal (e.g., gold) as a function of the temperature at a nearby thermocouple (Bertka, pers. comm.). Or, more than one thermocouple may be placed in selected locations in the