Thermoelastic properties of zircon: Implications for geothermobarometry

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ABSTRACT

A thermal-pressure equation of state has been determined for zircon (ZrSiO₄) that characterizes its thermoelastic behavior at metamorphic conditions. New pressure-volume (P-V) data from a “Mud Tank” zircon have been collected from 1 bar to 8.47(1) GPa using X-ray diffraction, and elastic moduli were measured from room temperature up to 1172 K by resonance ultrasound spectroscopy. These data were fitted simultaneously with temperature-volume (T-V) data from the literature in EosFit7c using a new scaling technique. The parameters of a third-order Birch-Murnaghan EoS with a Mie-Grüneisen-Debye model for thermal pressure have compressional EoS parameters K₀ = 224.5 (1.2) GPa, K″₀ = 4.90 (31) with a fixed initial molar volume V₀ = 39.26 cm³/mol and thermal parameters γ₀ = 0.868 (15), q = 2.37 (80), and Θ₀ = 848 (38) K. EoS parameters that describe the variation of unit-cell parameters with pressure and temperature were determined using an isothermal-type EoS. This new EoS confirms that zircons are stiffer than garnets and exhibit a much lower thermal expansion. This results in steep isomekes between zircon and garnets, which makes zircon trapped as inclusions in garnets at metamorphic conditions a good piezothermometer.

Keywords: Zircon, equation of state, piezobarometry, EosFit

INTRODUCTION

Zircon (ZrSiO₄) is an important and widespread mineral in the Earth’s crust and upper mantle, commonly used to date geologic events using the U-Th-Pb geochronometer (e.g., Hanchar and Hoskin 2003). Because it is highly refractory, zircon is a common detrital component in many sedimentary deposits (e.g., Fedo et al. 2003) and can also be found as an accessory mineral in sedimentary, metamorphic, and igneous rocks (e.g., Finch and Hanchar 2003). Zircon can also be produced during prograde metamorphism as a result of the breakdown of minerals bearing Zr as a minor or trace component. It is, therefore, common for zircon crystals to be found trapped as inclusions, frequently within garnet hosts, as a result of garnet growth during prograde metamorphism. Zircon inclusions in garnet therefore have the potential to be used in piezobarometry in which the residual stress or pressure in the inclusions, arising from the contrast in the elastic properties of garnet and zircon, can be inferred from the adiabatic bulk modulus, K₀, were obtained from the elastic tensor of a non-metamict zircon at high temperatures determined using resonant ultrasound spectroscopy (RUS). A Mie-Grüneisen-Debye (MGD) thermal-pressure EoS was determined from this new data plus literature data using a new scaling method in the fitting to remove bias and ensure consistency. The moduli values determined from the fitting and discussed in this paper are Reuss bound values, appropriate for describing the properties of zircon under adiabatic pressure. In this paper, we show that not only does our thermal-pressure EoS for zircon fit these data well, but the isobaric heat capacity Cᵥ calculated from our EoS closely matches the experimentally determined Cᵥ values from the literature.

EXPERIMENTAL METHODS

P-V study

A portion of the standard sample UWZ-1, originating from the Mud Tank carbonatite near Alice Springs, Australia, was kindly provided by John Valley (University of Wisconsin). This sample is characterized by very low-U/Th substitution and low amorphization and has an estimated age of 732 Ma (e.g., Jackson et al. 2004; Yuan et al. 2008). Samples from the UWZ-1 bulk crystal...