Equation of state of brucite: Single-crystal Brillouin spectroscopy study and polycrystalline pressure-volume-temperature measurement

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ABSTRACT

Acoustic velocities of brucite were measured at room pressure in over 48 directions from Brillouin spectroscopy using a natural sample. These data are supplemented with volume measurements as a function of pressure and temperature that range from ambient conditions to 11 GPa and 873 K using synchrotron X-ray radiation at the National Synchrotron Light Source (NSLS) in a cubic-anvil apparatus (SAM-85) with a synthetic polycrystalline sample. The diffraction patterns are collected during cooling cycles to minimize the effect of deviatoric stress on the measurements. These data yield internally consistent thermoelastic parameters defining the equation of state of brucite along with the single-crystal elastic moduli. The Brillouin spectroscopy measurements are best fit with the following elastic model: \( C_{11} = 156.7(8), C_{33} = 46.3(8), C_{44} = 21.7(5), C_{13} = 44.4(10), C_{15} = 12.0(15), \) and \( C_{16} = 0.2(8) \) GPa. The resultant linear compressibilities of the \( a \) and \( c \) axes are \( 3.8(1) \times 10^{-3} \) and \( 19.6(6) \times 10^{-3} \) (GPa \(^{-1}\)), respectively, with the Reuss bound for the bulk modulus, \( K_R = 36.7(10) \) GPa and the Hill average, \( K_H = 46(1) \) GPa. The unit-cell parameters \((a, c, \text{and volume})\) determined from the diffraction measurements were fit with a Birch-Murnaghan equation of state, yielding \( K_0 = 39.6(14) \) Gpa, \( K' = 6.7(7), (\alpha K_0 / \alpha T)_p = -0.0114(16) \) GPa/K, and \( \alpha = 5.0(7) \times 10^{-4} / \text{K} \). The bulk modulus and linear compressibilities from X-ray diffraction are in agreement with those from Brillouin spectroscopy. The ratio of linear compressibility of the \( a \) to \( c \) axes is about five times at ambient conditions and reduces to almost unity by 10 GPa. The axial thermal expansions reflect a similar pressure dependence. The ambient shear anisotropy \((C_{44}/C_{11})\) is about 2.5.

INTRODUCTION

Brucite provides a particularly useful platform to study the effect of pressure on the manner that H affects physical properties of minerals. The brucite structure consists of layers with octahedrally coordinated Mg, separated by layers containing only H (Fig. 1). The crystal structure of brucite is trigonal and the space group is \( \text{P}3\text{m}1 \) (Zigan and Rothbauer 1967). Each O atom in the hexagonally closed-packed layers is bonded with H such that the O-H bond is perpendicular to the layers, with bond length close to 1 Å, while the distance between the layers of octahedra containing Mg is about 2.7 Å (Parise et al. 1994). Thus, thermal expansion and hydrostatic compression of the \( a \) axis (perpendicular to the layers) is dominated by the stronger of the two layers, whereas expansion and compression of the \( c \) axis (parallel to the layers) reflects the properties of the weaker layer. Because the linear compressibility and thermal expansion of the \( a \) axis are similar to MgO, the compressibility and expansion of the \( c \) axis reflects the interactions of the H and O atoms. Thus a detailed study including single-crystal elastic properties and high-pressure, high-temperature cell dimensions can provide some information for understanding the behavior of brucite at high pressure.

Recently brucite has been studied at high pressure using various techniques, such as powder X-ray diffraction (Fei and Mao 1993), single-crystal X-ray diffraction (Duffy et al. 1995), powder neutron diffraction (Parise et al. 1994; Catti et al. 1995), shock wave compression (Duffy et al. 1991), Raman spectra (Kruger et al. 1989), and theoretically (Sherman 1991; D’Arco et al. 1993). These studies showed that the linear compressibilities of the \( a \) and \( c \) axes are different and that the pressure dependence of these compressibilities is very different. Such behavior gives rise to deviatoric stresses under pressure that in turn can increase uncertainties in cell dimensions and induce errors in determinations of equations of state at pressure. Hence it is important to minimize the deviatoric stresses to get good data on bulk modulus. In the first part of this paper, we report the results of a single-crystal Brillouin spectroscopy study using a natural brucite sample. These data are sufficient to define all elastic properties at ambient conditions, including the aggregate bulk modulus and linear compressibilities that are appropriate to hydrostatic pressure conditions. In the second part of this paper, we report results from an X-ray power diffraction study using cubic-anvil apparatus (SAM-85) with in situ synchrotron X-ray along with the