Elasticity of single-crystal periclase at high pressure and temperature: The effect of iron on the elasticity and seismic parameters of ferropericlase in the lower mantle

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ABSTRACT

In this study, we measured the sound velocities of single-crystal periclase by Brillouin light scattering (BLS) combined with in situ synchrotron X-ray diffraction (XRD) up to ~30 GPa and 900 K in an externally heated diamond-anvil cell (EHDAC). Our experimental results were used to evaluate the combined effects of pressure and temperature on the elastic moduli of single-crystal periclase using third-order Eulerian finite-strain equations. All of the elastic moduli increased with increasing pressure but decreased with increasing temperature, except the off-diagonal modulus $C_{12}$, which remained almost constant up to ~30 GPa and 900 K. The derived aggregate adiabatic bulk and shear moduli ($K_{ag}$, $G_{ag}$) at ambient conditions were 162.8(±0.2) and 130.3(±0.2) GPa, respectively, consistent with literature results. The pressure derivatives of the bulk $[(\partial K/\partial P)_{300 K}]$ and shear moduli $[(\partial G/\partial P)_{300 K}]$ at ambient conditions were 3.94(±0.05) and 2.17(±0.02), respectively, whereas the temperature derivatives of these moduli $[(\partial K/\partial T)_T$ and $[(\partial G/\partial T)_T]$ at ambient conditions were −0.025(±0.001) and −0.020(±0.001) GPa/K, respectively. A comparison of our experimental results with the high-pressure ($P$) and high-temperature ($T$) elastic moduli of ferropericlase (Fp) in the literature showed that all the elastic moduli of Fp were linearly correlated with the FeO content up to approximately 20 mol%. These results allowed us to build a comprehensive thermoelastic model for Fp to evaluate the effect of Fe-Mg substitution on the elasticity and seismic parameters of Fp at the relevant $P$-$T$ conditions of the lower mantle. Our modeling results showed that both the increase of the Fe content in Fp and the increasing depth could change the compressional wave anisotropy ($V_P$) and shear wave splitting anisotropy ($V_S$) of Fp in the upper parts of the lower mantle. Furthermore, using our modeling results here, we also evaluated the contribution of Fp to seismic lateral heterogeneities of thermal or chemical origin in the lower mantle. Both the thermally induced and Fe-induced heterogeneities ratios ($R_{SP} = \partial n V_P/\partial n V_S$) of Fp from 670 to 1250 km along a representative lower mantle geotherm increased by ~2–5% and ~15%, respectively. The thermally induced $R_{SP}$ value of Fp20 is ~30% higher than Fp10, indicating that the Fe content has a significant effect on the thermally induced $R_{SP}$ of Fp. Compared to the seismic observation results ($R_{SP} = 1.7–2.0$) in the upper regions of the lower mantle, the Fe-induced $R_{SP}$ value of Fp is more compatible than the thermally induced $R_{SP}$ value of Fp20 (the expected composition of Fp in the lower mantle) within their uncertainties. Thus, we propose that Fe-induced lateral heterogeneities can significantly contribute to the observed seismic lateral heterogeneities in the Earth’s lower mantle (670–1250 km).

Keywords: Elasticity, periclase, Brillouin light scattering, lower mantle, diamond anvil cell

INTRODUCTION

Periclase (MgO) is a classic, simple oxide that crystallizes in the rock-salt structure with no known experimental phase transition up to 250 GPa at least (e.g., Dorfman et al. 2012; Duffy et al. 1995a; McWilliams et al. 2012). The rock-salt structured MgO also represents one of the most common yet simply structured materials in the deep Earth. The structure can potentially be stable up to approximately 400 GPa based on computational studies and laser shock experiments (e.g., Karki et al. 1997; Belonoshko et al. 2010; McWilliams et al. 2012; Coppari et al. 2013; Oganov et al. 2003). MgO also has very high melting temperatures compared to other mantle minerals (e.g., Zerr and Boehler 1994; Ito et al. 2004; McWilliams et al. 2012; Tateno et al. 2014; Kimura et al. 2017). The wide $P$-$T$ stability of MgO covers relevant high $P$-$T$ conditions of the deep earth (Duffy and Ahrens 1995) and possibly terrestrial planets or exoplanets (Coppari et al. 2013; Duffy et al. 2015; Bolis et al. 2016). Therefore, precise knowledge of the elastic properties of MgO under high $P$-$T$ conditions is crucial for constructing a reliable mineralogical model of the Earth’s lower mantle. There have been an increasing number of studies on the elastic behavior of MgO covering a range of high-pressure or high-temperature conditions using different techniques, including static XRD (e.g., Utsumi et al. 1998; Fei 1999; Dewaele et al. 2000; Speziale et