The influence of OH content on elastic constants of topaz [Al$_2$SiO$_4$(F,OH)$_2$]

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ABSTRACT

Topaz, Al$_2$SiO$_4$(OH)$_2$, F$_{0.27-0.72}$, may play a significant role in transporting water and fluorine into the Earth’s interior at subduction zones. Seismological detection of topaz gives us insights into the transport mechanisms of water and fluorine but requires a thorough understanding of its elastic properties. The influence of OH content on elastic constants of topaz has not been fully understood, though experimental and theoretical studies have been done on topaz with various OH contents. We thus determined elastic constants of topaz for five natural single-crystal specimens with different OH contents ($x=0.28$–$0.72$) via the sphere resonance method at an ambient condition. Our determined $C_{11}$, $C_{22}$, $C_{44}$, $C_{66}$, $C_{12}$, $C_{33}$, and $C_{13}$ increase with OH content while $C_{33}$ and $C_{55}$ decrease. For the change in OH molar content from 0.0 to 1.0, relatively large changes (>3.0%) are seen in $C_{11}$ [8.0(6)%], $C_{55}$ [4.9(6)%], and $C_{22}$ [3.1(7)%]. The OH content dependence of elastic constants is qualitatively similar to that of theoretically determined values except for $C_{11}$. The theoretical value of $C_{11}$ decreases as the OH molar content increases from 0.0 to 1.0, whereas the experimental value of $C_{11}$ slightly increases. Our elastic constants are significantly higher (>3%) than theoretically determined values, especially in diagonal components ($C_{ii}$). The theoretical lower values must be related to the used lattice parameters, which are systematically larger than the measured lattice parameters. The theoretical approach should be modified to reproduce measured lattice parameters and lead to the agreement of theoretical and experimental elastic constants. Our results provide a clue to a better understanding of the elasticity of topaz and a basis for the seismological detection of subducted oceanic sediments.

Keywords: Topaz, elastic constants, sphere resonance method, OH content dependence

INTRODUCTION

Topaz is an orthosilicate mineral with the ideal formula Al$_2$SiO$_4$(OH)$_2$. It is usually found as an accessory mineral in fluoride-rich granitic rocks related to the formation of pneumatolitic/hydrothermal deposits (Pichavant and Manning 1984; Taylor 1992; Taylor and Fallick 2003) or in rock formations that experience ultrahigh-pressure metamorphism (Zhang et al. 2002; Alberico et al. 2003). High-pressure and high-temperature experiments on the Al$_2$O$_3$-SiO$_2$-H$_2$O ternary system, which represents subducted oceanic sediments, showed hydrous aluminosilicate minerals like phase $\pi$ [Al$_2$SiO$_4$(OH)$_3$] and topaz-OH can retain water up to ~8 GPa (Wunder et al. 1993a, 1993b; Schreyer 1995). Later, high-pressure experiments on synthetic oceanic sediment revealed that topaz-OH is stable at pressures from 8 to 12 GPa and transforms to another hydrous aluminosilicate mineral phase Egg [AlSiO$_3$(OH)] at pressures beyond 12 GPa, which can carry water into the mantle transition zone (Ono 1998). The difference in the stability field of topaz-OH reflects the difference in the chemical composition of their starting materials. The hydroxy-rich topaz, thus, might play a significant role in transporting water into the Earth’s interior (Mookherjee et al. 2016; Ulian and Valdré 2017; Sema and Watanabe 2017; Tennakoon et al. 2018).

Topaz might also be a major carrier of fluorine into the Earth’s interior (Ulian and Valdré 2017; Sema and Watanabe 2017). Halogens, especially fluorine (320 ppm) and chlorine (850 ppm) are relatively abundant in oceanic sediments (Carpenter 1969; Muramatsu and Wedepohl 1998). Fluorine ions can substitute for hydroxy groups in many hydrous minerals because of their same ionic charge and similar radii (Pyle and Mather 2009). Although seismological detection of topaz gives us insights into the transport processes of water and fluorine in subduction zones, it requires a thorough understanding of elastic properties of topaz with a wide range of OH contents.

Elastic constants of topaz were first determined by Voigt (1888) through bending and twisting of single-crystal prisms. Later, Haussühl (1993), Sema and Watanabe (2017), and Tennakoon et al. (2018) determined elastic constants of topaz with various chemical compositions through the resonance method. Though the temperature dependence of elastic constants was investigated by Sema and Watanabe (2017) and Tennakoon et al. (2018), these measurements have been conducted only at atmospheric pressure. The pressure dependence of elastic constants has been studied through the first-principles calculation