Elasticity of hydrous aluminosilicate mineral- topaz ($Al_2SiO_4(OH)_2$)

MAINAK MOOKHERJEE[1], JUN TSUCHIYA[23] AND ANANT HARIHARAN[1]

[1]Earth and Atmospheric Sciences, Cornell University, Ithaca, NY 14853, USA, mm2457@cornell.edu
[2]Geodynamics Research Center, Ehime University, 2-5 Bunkyo-cho, Matsuyama, Ehime 790-8577, Japan.
[3]Earth-Life Science Institute, Ehime Satellite, 2-5 Bunkyo-cho, Matsuyama, Ehime 790-8577, Japan

We examine high-pressure elasticity of hydrous phases relevant to the Al_2O_3-SiO_2-H_2O ternary system relevant for the subducted sedimentary layer. In particular, we have used *first principles* simulation based on density functional theory to calculate the equation of state and elasticity of hydrous aluminosilicate mineral, topaz, $Al_2SiO_4(OH)_2$. The pressure-volume results for topaz is well represented by a third order Birch-Murnaghan formulation, with K_0 = 166.4 (±0.6) GPa and K'_0 = 4.03 (±0.04). The calculated full elastic tensor at 0 GPa is in good agreement with experimental results on fluorine end member of topaz. There are nine independent components to the full elastic constant tensor with the compressional elastic constants: c_{11} = 285.6 GPa, c_{22} = 357.3 GPa, c_{33} = 289.2 GPa, the shear elastic constants- c_{44} = 105.4 GPa, c_{55} = 114.6 GPa, and c_{66} = 122.5 Ga; the off-diagonal elastic constants c_{12} = 121.9 GPa, c_{13} = 76.9 GPa, and c_{23} = 87.9 GPa. Topaz exhibits moderate single-crystal elastic anisotropy with $AV_P \sim$ 11.3 % and $AV_S \sim$ 8.4 % at 0 GPa. The compressional wave anisotropy, AV_P decreases with pressure, whereas the shear wave anisotropy increases upon compression.

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