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Water effects on the anharmonic properties of forsterite

YAN YANG^{1,*}, ZHONGPING WANG², JOSEPH R. SMYTH³, JIA LIU¹ AND QUNKE XIA¹

¹CAS Key Laboratory of Crust-Mantle Materials and Environments, School of Earth and Space Sciences, University of Science and Technology of China, Hefei 230026, China

²Physics Experiment Teaching Centers, University of Science and Technology of China, Hefei 230026, China ³Department of Geological Sciences, University of Colorado, Boulder, Colorado 80309, U.S.A.

ABSTRACT

To quantify the effects of hydration on anharmonicity of olivine thermodynamics, we have measured in situ Raman spectra of an extremely hydrous forsterite with 4500 ppm (wt) H₂O at temperatures up to 1273 K. All the Raman modes in hydrous forsterite shift linearly to lower wavenumbers with increasing temperature. The calculated isobaric mode Grünesien parameters related to SiO₄ internal stretching and bending vibrations are much lower than lattice vibrations. Additionally, compared with anhydrous forsterite, except for the modes at 919, 858, and 227 cm⁻¹, water greatly reduces the isobaric mode Grüneisen parameters of the Raman modes in forsterite. Water also has a large effect on the anharmonic parameters related to lattice vibrations, whereas it has little effect on the anharmonic parameters related to SiO₄ internal stretching and bending vibrations. Those results have the implications to the variations of local structure with temperature and estimation of water effects on the thermodynamics of forsterite.

Keywords: Water, anharmonic properties, Raman mode, forsterite