Anisotropic elasticity of jarosite: A high-P synchrotron XRD study

HONGWU XU,^{1,*} YUSHENG ZHAO,² JIANZHONG ZHANG,² YUEJIAN WANG,² DONALD D. HICKMOTT,¹ LUKE L. DAEMEN,² MONIKA A. HARTL,² AND LIPING WANG³

¹Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, U.S.A. ²Los Alamos Neutron Science Center, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, U.S.A. ³Department of Geosciences, State University of New York at Stony Brook, Stony Brook, New York 11794, U.S.A.

ABSTRACT

The elastic properties of jarosite were investigated using synchrotron X-ray diffraction coupled with a multi-anvil apparatus at pressures up to 8.1 GPa. With increasing pressure, the *c* dimension contracts much more rapidly than *a*, resulting in a large anisotropy in compression. This behavior is consistent with the layered nature of the jarosite structure, in which the (001) [Fe(O,OH)₆]/[SO₄] sheets are held together via relatively weak K-O and hydrogen bonds. Fitting of the measured unit-cell parameters to the second-order Birch-Murnaghan equation of state yielded a bulk modulus of 55.7 ± 1.4 GPa and zero-pressure linear compressibilities of 3.2×10^{-3} GPa⁻¹ for the *a* axis and 13.6×10^{-3} GPa⁻¹ for the *c* axis. These parameters represent the first experimental determination of the elastic properties of jarosite.

Keywords: Jarosite, elastic properties, compressibility, bulk modulus, equation of state, synchrotron X-ray diffraction