American Mineralogist, Volume 99, pages 1270–1276, 2014

CHEMISTRY AND MINERALOGY OF EARTH'S MANTLE

Identifying the spin transition in Fe^{2+}-rich $MgSiO_3$ perovskite from X-ray diffraction and vibrational spectroscopy

RAZVAN CARACAS[1,*], HARUKA OZAWA[2,3], KEI HIROSE[2,3], HIROFUMI ISHII[4], NOZOMU HIRAOKA[4], YASUO OHISHI[5] AND NAOHISA HIRAO[5]

[1]CNRS, Laboratoire de Géologie de Lyon, Université Claude-Bernard Lyon 1, Ecole Normale Supérieure de Lyon, Site Monod, 15 parvis René Descartes, 69342 Lyon, France
[2]Institute for Research on Earth Evolution, Japan Agency for Marine-Earth Science and Technology, Yokosuka, Kanagawa 237-0061, Japan
[3]Earth-Life Science Institute, Tokyo Institute of Technology, Meguro, Tokyo 152-8551, Japan
[4]National Synchrotron Radiation Research Center, Hsinchu Science Park, Hsinchu 30076, Taiwan
[5]Japan Synchrotron Radiation Research Institute, Sayo, Hyogo 679-5198, Japan

ABSTRACT

Based on numerical results from density-functional perturbation theory calculations, we show that the magnetic spin transition in Fe^{2+}-rich $MgSiO_3$ perovskite can be identified as changes in the powder X-ray diffraction (XRD) pattern and the vibrational spectra. In particular theory predicts how the symmetry breaking and the volume reduction associated with the spin transition affects both structural and vibrational properties. The XRD measurements of $(Mg_{0.5}Fe_{0.5})SiO_3$ perovskite indeed demonstrated that the new diffraction peaks and the peak broadening formed during the spin transition can be explained by the associated symmetry breaking. We also show computationally that certain vibrational peaks exhibit a shift at the transition; the Grüneisen parameters of certain modes are affected by the transition, thus bearing on the thermodynamical properties. Raman and/or infrared measurements before and after the spin transition could identify these changes.

Keywords: Spin transition, perovskite, diffration, Raman, Earth's lower mantle