

CHEMISTRY AND MINERALOGY OF EARTH'S MANTLE

Identifying the spin transition in Fe²⁺-rich MgSiO₃ perovskite from X-ray diffraction and vibrational spectroscopy

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ABSTRACT

Based on numerical results from density-functional perturbation theory calculations, we show that the magnetic spin transition in Fe²⁺-rich MgSiO₃ 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})SiO₃ 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, diffraction, Raman, Earth's lower mantle