

LETTER

**X-ray diffraction and Mössbauer spectroscopy of Fe<sup>3+</sup>-bearing Mg-silicate post-perovskite at 128–138 GPa**

**K. CATALLI,<sup>1,\*</sup> S.-H. SHIM,<sup>1</sup> V.B. PRAKAPENKA,<sup>2</sup> J. ZHAO,<sup>2</sup> AND W. STURHAHN<sup>3</sup>**

<sup>1</sup>Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, U.S.A.

<sup>2</sup>Consortium for Advanced Radiation Sources, University of Chicago, 5640 South Ellis Avenue, Chicago, Illinois 60637, U.S.A.

<sup>3</sup>Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, U.S.A.

ABSTRACT

The effect of ferric iron on the properties of Mg-silicate post-perovskite (PPv) were studied up to 138 GPa using synchrotron X-ray diffraction and Mössbauer spectroscopy. Our diffraction measurements revealed that the incorporation of Fe<sup>3+</sup> has virtually no effect on the volume of PPv, in contrast to Fe<sup>2+</sup>, which increases the volume. Therefore, incorporation of Fe<sup>3+</sup> increases the density of PPv much more effectively than Fe<sup>2+</sup>. Mössbauer spectroscopy suggests that Fe<sup>3+</sup> enters PPv through charge-coupled substitution and is high spin in the bipolar prismatic site and low spin in the octahedral site (i.e., mixed spin state). Our results may have important implications for the gravitational stability of lower-mantle heterogeneities.

**Keywords:** Post-perovskite, spin state of iron, ferric iron, X-ray diffraction, Mössbauer spectroscopy