

## Structure and titanium distribution of feiite characterized using synchrotron single-crystal X-ray diffraction techniques

CLAIRE ZURKOWSKI<sup>1,\*</sup>, BARBARA LAVINA<sup>2,3</sup>, KELSEY PRISSEL<sup>1,†</sup>, STELLA CHARITON<sup>2</sup>,  
VITALI B. PRAKAPENKA<sup>2</sup>, AND YINGWEI FEI<sup>1,‡</sup>

<sup>1</sup>Earth and Planets Laboratory, Carnegie Institution for Science, 5241 Broad, Branch Road NW, Washington, D.C. 20015, U.S.A.

<sup>2</sup>Center for Advanced Radiation Sources, University of Chicago, 9700 South Cass Avenue, Building 434A, Argonne, Illinois 60439, U.S.A.

<sup>3</sup>X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, U.S.A.

### ABSTRACT

A solid solution of the mineral feiite ( $\text{Fe}_3\text{TiO}_5$ ) was recently discovered in a shock-induced melt pocket of the Shergotty martian shergottite. It is particularly interesting for its potential as an indicator of pressure-temperature ( $P$ - $T$ ) and oxygen fugacity in martian crustal and mantle material. To date, complete crystallographic analysis of feiite has not been conducted, as the mineral was previously analyzed by electron backscatter diffraction on micrometer-size grains (Ma et al. 2021). Here we report a convergent crystal-structure model for feiite based on synchrotron single-crystal X-ray diffraction data collected on three grains of feiite synthesized at 12 GPa and 1200 °C. Feiite adopts the  $\text{CaFe}_3\text{O}_5$  structure type ( $Cmcm$ ,  $Z = 4$ ), which is composed of two octahedral  $M1$  and  $M2$  sites and one trigonal prismatic  $M3$  site ( $M = \text{metal}$ ) in a ratio of 1:2:1. The three feiite grains with composition  $\text{Ti}_{0.46-0.60}\text{Fe}_{3.54-3.40}\text{O}_5$  were best modeled by substituting  $\text{Ti}^{4+}$  into only the octahedral  $M2$  site, accounting for 30% of this site. Comparisons of the measured average bond lengths in the coordination polyhedra with the optimized  $\text{Ti}^{4+}\text{-O}$ ,  $\text{Fe}^{2+}\text{-O}$ , and  $\text{Fe}^{3+}\text{-O}$  bond lengths suggest that ferrous iron occupies the trigonal  $M3$  site, while iron is mixed valence in the octahedral  $M1$  and  $M2$  sites. The  $\text{Ti}^{4+}$  and  $\text{Fe}^{3+}$  content constrained by our crystal-chemical analyses suggests that at least ~30% of the available iron must be ferric (i.e.,  $\text{Fe}^{3+}/\text{Fe}_{\text{total}} = 0.3$ ) for the sample synthesized at 12 GPa and 1200 °C and higher  $P$ - $T$  conditions may be needed to form the end-member feiite ( $\text{Fe}_3^{2+}\text{TiO}_5$ ).

**Keywords:** Feiite, crystal structure, iron oxides, Shergotty, mixed valence, titanium oxide