Ferric iron and water incorporation in wadsleyite under hydrous and oxidizing conditions: a XANES and SIMS study

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Wadsleyites with varying iron contents were synthesized at about 13 GPa and 1400°C under oxidizing and hydrous conditions in coexistence with enstatite. The recovered samples were studied using micro-XANES (X-ray Absorption Near Edge Structure) to determine the ferric iron contents in polyphasic samples and SIMS (Secondary Ion Mass Spectrometry) to determine the water concentrations. XANES analyses show that ferric iron content increases with increasing total iron content, and reaches a maximum of 30-40 mole percent of the total iron. The divalent cation concentrations (i.e., $Mg^{2+} + Fe^{2+}$) and the Si content in wadsleyite decrease with increasing Fe^{3+} content, indicating an incorporation mechanism via substitution into the metal (Me) sites. In such a reaction, a substantial part of the hydrogen is replaced by ferric iron in the octahedral site which is charge compensated by vacancies in the metal and silicon sites.