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LETTER

Crystal structure of a new spinelloid with the wadsleyite structure in the system Fe_2SiO_4-Fe_3O_4 and implications for the Earth's mantle

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ABSTRACT

A new spinelloid polytype with a composition $Fe_{2.45}Si_{0.55}O_4$ has been synthesized at 1100 °C and 5.6 GPa that is isostructural with wadsleyite [β–$(Mg,Fe)_2SiO_4$]. The refined parameters (space group *Imma*) are: a = 5.8559(2) Å, b = 11.8936(4) Å, c = 8.3684(2) Å, V = 582.84(2) Å^3. Tetrahedrally coordinated Fe^{3+} and Si are completely disordered and the substitution of Fe^{3+} for nearly one-half of the Si results in a significant expansion of the tetrahedra. This is the first direct evidence that significant amounts of Fe^{3+} can be incorporated into the wadsleyite-type structure. Because the β form of Fe_2SiO_4 is unstable, the implication is that Fe^{3+}, by the substitution mechanism: $2Fe^{3+} = Si^{4+} + Fe^{2+}$, acts to stabilize the wadsleyite structure. It is possible that the addition of Fe^{3+} could stabilize $(Mg,Fe)_2SiO_4$ wadsleyites to lower pressures, which would influence the exact position of the ''410 km'' discontinuity. The apparent compatibility of Fe^{3+} in the wadsleyite structure, suggests that available Fe^{3+} will be readily incorporated in the modally dominant phase in the upper parts of the transition zone, thereby leading to a low f_{O_2} in this region of the mantle.