

EXPERIMENTAL AND THEORETICAL ANALYSIS OF CATION ORDERING IN THE ILMENITE-HEMATITE SOLID SOLUTION

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The solid solution between ilmenite (FeTiO_3) and hematite (Fe_2O_3) is an important system in both paleomagnetism and petrology. The fundamental magnetic and thermodynamic properties of this system are determined by the presence of a cation order-disorder phase transition in ilmenite-rich material, which involves the partitioning of Fe and Ti cations between alternating (001) layers. Here we present the results of a combined experimental and theoretical analysis of this transition. The equilibrium distribution of Fe and Ti in samples containing between 70% and 100% ilmenite has been determined up to 1350 °C using in-situ time-of-flight neutron powder diffraction. The combination of in-situ measurements with excellent neutron scattering contrast between Fe and Ti provides, for the first time, an accurate characterisation of the ordering transition over this region of temperature-composition space. The experimental results have been used to constrain both a macroscopic and microscopic thermodynamic description of the solid solution. In the microscopic description, the results are used to derive interaction parameters for Fe^{2+} -Ti, Fe^{3+} -Ti and Fe^{2+} - Fe^{3+} exchange. Monte Carlo simulations are then used to derive the equilibrium phase diagram, taking full account of short- and long-range cation order. Using insights gained from the Monte Carlo simulations, it is shown that a macroscopic mixing model of the solid solution can be developed, which although simple to apply, correctly accounts for the effects of short- and