American Mineralogist, Volume 85, pages 1497–1502, 2000

Cation distribution in synthetic zinc ferrite ($Zn_{0.97}Fe_{2.02}O_4$) from in situ high-temperature neutron powder diffraction

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ABSTRACT

Neutron powder diffraction experiments at high temperature (300–1600 K) were performed at BENSC (Berlin, D), on synthetic $Zn_{0.97}Fe_{2.02}O_4$, to investigate the cation partitioning of Zn and Fe over the tetrahedral and octahedral sites as a function of *T*. The data analysis combined Rietveld structure refinements with minimization techniques. The thermodynamic behavior of the thermally activated order-disorder transformation occurring in Zn-ferrite was interpreted by the O'Neill-Navrotsky model ($\alpha = 49.3 \pm 0.4$ and $\beta = -31.6 \pm 2.0$ kJ/mol) and by the equilibrium Landau theory. We obtain $\lambda_2 = 2.813 \pm 0.002$/K, $T_c = 1022 \pm 37$ K using a "pure" Landau approach, and h = –1.164 ± 0.002 kJ/mol, c = 9.868 ± 0.06 kJ/mol, $T_c = -742 \pm 10$ K, if the configurational contribution to entropy is explicitly accounted. The results are in agreement with the earlier powder XRD work of O'Neill (1992) on quenched specimens, but extend the temperature over which measurements were obtained to 1600 K.