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Coupling between non-convergent ordering and transition temperature in the $C2/c \leftrightarrow P2_1/c$ phase transition in pigeonite

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ABSTRACT

A Landau potential with linear-quadratic coupling has been developed to describe interactions between a non-convergent order parameter, Q_{OD}, for Fe/Mg ordering, and the order parameter, Q_D, for the $C2/c$-$P2_1/c$ phase transition in pigeonite. Spontaneous strain relationships, and expressions for the effect of ordering on the transition temperature derived from this expansion, have been tested by single crystal X-ray diffraction methods. Lattice parameters collected from a natural pigeonite crystal with composition $En_{47}Fs_{44}Wo_9$, in situ at temperatures up to 1050 °C, reveal that increasing Q_{OD} could act to suppress Q_D by a mechanism which includes overlapping and opposing strain fields. In a second experiment, the intensities of superlattice reflections ($h + k = 2n + 1$) were followed in situ at temperatures up to 500 °C. The crystal was heated ex situ successively at 700, 750, 800, and 850 °C between repeated in situ measurements in order to produce changes in the degree of cation order. The resulting data sets, giving the temperature dependence of Q_D^2 for different fixed values of Q_{OD}, are consistent with the initial Landau model. In particular, they show a strong and linear dependence of transition temperature on Q_{OD}. The fourth order coefficient of the expansion describing the phase transition is perhaps also renormalized by changes in Q_{OD}. It is suggested that the influence of Q_{OD} on the phase transition could be greater than the influence of the phase transition on the equilibrium variation of Q_{OD}.