Order parameter behavior at the structural phase transition in cummingtonite from Mössbauer spectroscopy

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ABSTRACT

The microscopic behavior of the $C2/m \leftrightarrow P2_1/m$ phase transition occurring in cummingtonite (36 mol% Fe) as a function of temperature has been investigated using Mössbauer spectroscopy performed in the temperature range 100–550 K. The quadrupole splitting (ΔE_Q) of the M4 doublet shows a change in slope at the critical temperature of the phase transition. The difference between ΔE_Q of the low-symmetry phase and the values obtained at the same temperatures by extrapolating ΔE_Q of the C2/m phase has been used as a measure proportional to the local order parameter associated with the phase transition. The Mössbauer data, which provide a measure of the local microscopic order parameter, scale in an identical manner to the macroscopic properties, indicating that the sub-unit scale structure of cummingtonite evolves in a parallel manner with the macroscopic average structure on a much longer length scale.