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Anti-phase boundaries and phase transitions in titanite: An X-ray diffraction study

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ABSTRACT

X-ray diffraction rocking curves of titanite, $CaTiSiO_5$, were measured using a novel high-resolution diffractometer. Three Bragg reflections were recorded as a function of temperature and their profiles analyzed in terms of a Gaussian Bragg peak and a diffuse scattering component with an overall Lorentzian shape. The temperature dependence of the Gaussian intensities of the rocking peaks of superstructure reflections, *hkl* with $k + l$ odd, scale with the long-range order parameter as $I \propto Q^2 \propto |T - T_c|^{2\beta}$, where $\beta = 0.14(1)$ is the effective order parameter exponent.

The diffuse scattering intensity changes little with temperature at $T < T_c - 20$ K. Strong diffuse scattering is found at $T > T_c$ with centers of their Lorentzian diffraction profiles shifted by $\Delta\omega \approx 0.5°$ with respect to the position of the equivalent Bragg peak. A second phase transition at 825 K is confirmed and the possibility of a third transition at ~1150 K is discussed.