Diffuse X-ray Scattering in Cadmium Pyroniobate

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Cadmium pyroniobate, $Cd_2Nb_2O_7$ (CNO), is known as a ferroelectric pyrochlore compound with interesting and unusual properties, as it exhibits behaviour similar to typical relaxor-ferroelectrics over a limited temperature range below 200K (Tachibana et al. 2004). CNO is cubic at ambient temperature, with a pyrochlore type structure (space group Fd-3m). Determination of the distorted crystal structures that occur for $T < 205K$ is hindered by their strongly pseudo-cubic nature (Weller et al. 2004). Recently the low temperature structure of CNO has been explored by all electron ab-initio calculations in the framework of density functional theory. According to these studies CNO distorts to monoclinic symmetry (space group Cc) at low temperatures via an intermediate orthorhombic phase (space group Ima2). The monoclinic structure is characterized by an ordered arrangement of short and long Nb-O-bonds. While these ab-initio structure calculations imply a purely displacive mechanism of the ferroelectric phase transition in CNO, anisotropic diffuse scattering intensity seen in X-ray diffraction studies suggests local deviations from cubic symmetry in the paraelectric phase (Malcherek 2007). The deviations correlate along $<110>$, giving rise to sheets of diffuse scattering normal to these directions. In order to investigate the possible order-disorder contributions to the ferroelectric phase transition of CNO, Monte Carlo simulations of a modified 12-state Potts-model on a pyrochlore lattice are being conducted. The equilibrated spin configurations of the model serve to generate supercells of CNO with local Nb-offsets from the center of their coordination polyhedra. Simulated diffraction images obtained from these structural models are compared with single crystal X-ray diffraction data measured at various temperatures.

References

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