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Short range order in ferroelectric triglycine sulphate

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Triglycine sulphate (TGS) $[(NH_2CH_2COOH)_3H_2SO_4]$ is a hydrogen-bonded ferroelectric with a phase transition temperature of 322K [1]. The phase transition is reversible and second-order, order disorder type, making TGS of fundamental interest in the field of phase transitions [2]. Above the critical temperature, one of the glycine molecules is disordered across a mirror plane and below the critical temperature, it chooses a side, breaking the symmetry. The ferroelectric state is obtained through the ordering of the glycine orientations on neighbouring sites, but the mechanism for the phase transition is not well understood.

We have investigated the short range order in TGS by collecting single crystal diffuse scattering data on TGS (x-ray) and fully deuterated TGS (neutron). We have also developed a model of the short-range order using the program ZMC [3] by creating a model crystal in which the molecules can interact and bringing it to equilibrium using a Monte Carlo algorithm. The validity of the model crystal was assessed by calculating the x-ray and neutron diffuse scattering patterns and comparing them with the experimental data.

This approach has yielded new insights into the behaviour of the disordered glycine molecule. For example, above the critical temperature, the correlations in the orientation of the disordered glycine molecule persist over short range rather than being completely random as suggested by the average structure. This is important information because understanding the behaviour of the disordered glycine molecule is crucial to understanding the phase transition and influences the ferroelectric properties of TGS.

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Diffuse scattering and superstructures in brownmillerites and related materials

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Brownmillerite-type materials exhibit a wide range of structures, which vary in the arrangement of tetrahedral chains. In brownmillerites perovskite-like layers of octahedra alternate with layers of tetrahedral chains. The tetrahedral chains can adopt two mirror-related configurations, which allow different inter- and intra-layer ordering patterns to form. The simplest of which result in space groups *Pnma* and *I2mb*. More complicated ordering patterns show commensurate or incommensurate intra-layer ordering sequences. Variants with alternating intra-layer order exhibit stacking faults [1] and commensurate or incommensurate stacking sequences. Apart from that, domain structures (anti-phase and twin domains) are possible and cause diffuse scattering to appear.

Diffuse scattering related to stacking faults is observed in layered brownmillerites $Ca_4(Fe,Al)_2(Mn,Ti)O_9$, which exhibit separated blocks (OTO) of the brownmillerite structure. Similar to $Sr_2Fe_2O_5$ [1], the layered brownmillerites show a certain degree of order according to superstructures with different stacking sequences, as evident by electron diffraction experiments. All possible superstructures can be described in superspace group $A2_1/m(0\beta\gamma)0s$ utilising different modulation wave vectors.

In order to explain the observed diffuse scattering intensities, computer simulations were performed. For example, Fig. 1 shows the (3kl) layer of the reciprocal space of a layered brownmillerite. Experimental data is displayed on the right, whereas the left side shows diffuse scattering calculated [2] from a computer model with random stacking faults. The scattering of the average structure (Bragg peaks) is removed from the calculated pattern.

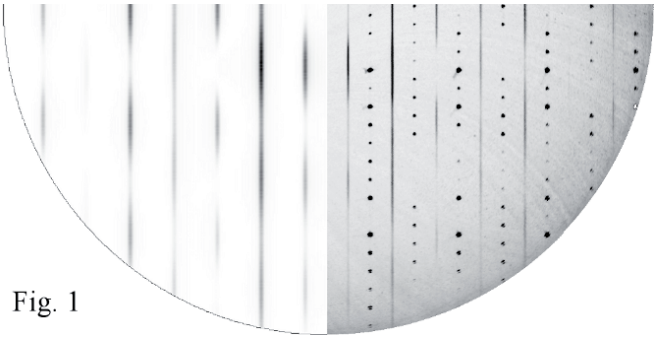

Fig. 1

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Hydrogen storage characteristics of melt spun $Ti_{45}Zr_{38}Ni_{17}$ nano-quasicrystalline alloys

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The present study describes the microstructural changes with respect to the quenching rate and their correlation with hydrogen storage characteristics of $Ti_{45}Zr_{38}Ni_{17}$ quasicrystalline alloys. The ribbons of the alloy have been synthesized at different quenching rates obtained through different wheel's surface speeds (35, 40, 45 and 50