MS26-P5 When alternative layer stackings cause commensurate structures to co-exist the interpretation of the diffraction data need not be unique.

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Refinements of crystal structures with commensurate stacking faults should recognize that the structure is not everywhere the same and the structure can change coherently from one structure to another across an interface between adjacent layers. Assumptions are commonly used to constrain a refinement by placing the structure in a particular category consistent with the capabilities of a particular program. However this categorization can restrict the success of a refinement. The first assumption is that the options for a layer can be constructed using a symmetry operation commensurate with the crystal lattice and either a single reference layer or a single commensurately modulated structure. The second is that a clear distinction can be made between twinning and disorder. The twinning concept can include allo twins, ie the diffraction pattern has independent intensity contributions from different selections of layers corresponding to different ordered structures. Problems associated with these constraints are minimized when a single orientation of a single component structure dominates the diffraction data. However a systematic error still remains. Pseudo equivalent reflections of a disordered structure containing the various packing options can be used to project out the contributions to the scattering density from different irreducible representations of a commensurate parent structure and hence refine a correlation coefficient (range 0 to 1) between the component structures. Recent structure determinations will be used to illustrate this.

Keywords: polymorphs, stacking faults, refinement

MS26-P6 Influence of the oxygen concentration on crystal growth and structure of the $BaCuSi_2O_{6\pm\delta}$ and $Ba_{1-x}Sr_xCuSi_2O_{6\pm\delta}$ spin dimer compounds

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By using the crystal growth method with O_2-partial pressure the new $Ba_{1-x}Sr_xCuSi_2O_{6\pm\delta}$ mixed system can be prepared for $x \leq 0.3$. The crystal growth of $BaCuSi_2O_{6\pm\delta}$ is also possible at a temperature of 1150°C by using an oxygen pressure of around 1 bar. The particular challenge of crystal growth of this material is that for the existing oxygen networks oxygen partial pressure operates as control parameter. $BaCuSi_2O_{6\pm\delta}$ and $Ba_{1-x}Sr_xCuSi_2O_{6\pm\delta}$ mixed crystals have the same tetragonal structure type $I4_1/acd$ down to low temperature, which has only one type of dimer layers. First results from single crystal structure diffraction of the new $BaCuSi_2O_{6\pm\delta}$ show that, in contrast to Sr doped crystals of this mixed system, the incommensurate structure is present at low temperature (see Fig. 1). $BaCuSi_2O_6$ is a model material for studying Bose-Einstein condensation (BEC) of magnons in high magnetic fields. It is also a quasi-two dimensional spin dimer system. The material is observed to have a singlet ground state in zero magnetic field with a large gap to the lowest excited triplet states [1, 2]. The quantum critical point at around 23 T and T=0 K separates the quantum paramagnetic regime from the ordered state [3, 4]. The investigation of the proportions of oxygen in the compounds shows a variation of the imbedded oxygen content (±δ). A detailed understanding of the crystal structure, the incommensurately modulated structure depending on the oxygen content will enable studying the spin dynamics of field-induced order states in this model magnetic compound of high current interest with only one type of dimer layers, showing the same distance between the Cu atoms, in the structure.

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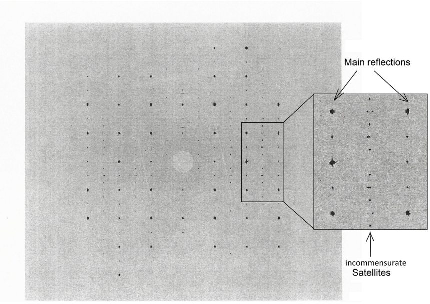

Figure 1. The first experimental (*0kl*) reciprocal space plane of $BaCuSi_2O_{6\pm\delta}$ (1bar) at 4.3K.

Keywords: growth with oxygen partial pressure, phase transition, spin dimer compounds

MS26-P7 Complete decoupling of magnetic order and superconducitvity in a conventional superconductor

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Conflicting electron states at the Fermi surface usually prevent a harmonic coexistence of superconductivity and magnetism in conventional superconductors. In order to improve the understanding of the interaction between superconductivity and magnetism a model material with missing competition between the two phenomena is required. In $Pr_2Pt_3Ge_5$ we discovered a system, in which multiple magnetic orders and superconductivity not only coexist, but do not compete [1]. The systems displays a relatively high transition temperature T_c = 7.8 K and two antigerromagnetic transitions T_{N1} = 3.4 and T_{N2} = 4.1 K with a commensurate and an incommensurate canted structure [1, 2]. We studied the superconducting and magnetic properties of he compound by means of neutron diffraction, magnetization and transport measurements. The interpenetrating *HT*-phase diagrams, representing the refined magnetic structures, preclude any direct competition between the superconducting and magnetic phases. We propose that different sheets oft he Fermi surface are involved in the magnetic and superconducting exchange interactions.

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