MS25-P10 Magnetic and crystal structures of the multiferroic $Ca_2CoSi_2O_7$ melilite at low temperatures

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The magnetic properties of $Ca_2CoSi_2O_7$ are often compared with those of other multiferroic compounds from the same family, such as $Ba_2CoGe_2O_7$. However, in contrast to $Ba_2CoGe_2O_7$, the crystal structure of $Ca_2CoSi_2O_7$ is described as a commensurate lock-in phase below approx. 150 K with a supercell tripled along the *a* and *b* axes related to the normal state above approx. 480 K. Thus, the magnetic structure of $Ca_2CoSi_2O_7$ is not necessarily the same as in other melilites. In order to characterise the magnetic order of $Ca_2CoSi_2O_7$, we performed a detailed crystallographic study at temperatures just above (10 K) and below (2.2 K) the antiferromagnetic phase transition (5.7 K) by neutron diffraction on single crystals. The results of the magnetic structure refinement are discussed and compared with those from $Ba_2CoGe_2O_7$.

Keywords: melilites, multiferroics, magnetic structure

MS25-P11 Theoretical study of complex relationships among chemical disorder, crystal stability, electronic and magnetic properties in Fe-based σ-phases and high entropy alloys

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Nowadays, *ab initio* calculations are well-adapted tools to investigate microscopic reasons for appearance of specific physical behaviours in ordered compounds and disordered alloys. The charge- and spin-selfconsistent Green function Korringa-Kohn-Rostoker method belongs to the well-established techniques to determine electronic band structure and relevant physical quantities such as density of states, magnetic moments, magnetic structure, hyperfine fields and total energy. Besides, the KKR combined with the coherent potential approximation (CPA) [1] allows for reliable treatement of chemical disorder in complex multicomponent systems [2].

In this work, the KKR-CPA methodology is applied to study two different groups of materials:

(i) Fe-based σ-compounds (space group P42/mnm), which belongs to the famous Frank-Kaspers phases, are characterised by high coordination numbers and lack of stoichiometry. Their topological and chemical complexity appears to determine particular relations among crystal stability, electronic structure features as well as magnetic properties and hyperfine interactions. Recent results of KKR-CPA calculations on Fe-*M* (*M*= V, Cr, Mo, W) [2-4] σ-phases will be presented in view of magnetisation, neutron diffraction and Mossbauer data.

(ii) High entropy alloys (HEA), which consist of at least five transition metal elements (sometimes also s, p element) with almost equal concentrations, crystallize in surprisingly simple structures (bcc, fcc or hcp). On the whole, the crystal stability of these highly disordered systems appear to be driven essentially by configuration entropy, but also by the magnetic entropy. Besides, the chemical disorder strongly affects the electronic and magnetic properties of HEA as well as the preference of the crystal structure (bcc vs. fcc). The KKR-CPA results obtained for the $Al_xCrFeNiCo$ [5] and $Pd_xCrFeNiCo$ HEA will be discussed in view of XRD and magnetisation data.

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