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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Keywords: ab initio calculation, electronic structure, phase stability, magnetic properties, chemical disorder

MS26. Modulated, modular and composite materials

Chairs: Luis Elcoro, John Claridge

MS26-P1 Systematical study of the structure of Ni_2MnGa single crystals by high-resolution x-ray diffraction reciprocal space mapping

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Ni_2MnGa is nominally cubic, however small deviations from exact 2:1:1 stoichiometry give rise to structural changes, leading to tetragonal or even monoclinic lattices. Up to now, the structure of Ni_2MnGa has been studied mostly by means of powder diffraction; in our work we performed a detailed study of the structure of Ni_2MnGa single crystals using high-resolution x-ray diffraction and reciprocal space mapping. Our samples were found monoclinic at room temperature and they exhibit large twinning domains detected from splitting of diffraction peaks in reciprocal space. Moreover, we found distinct satellite peaks at non-integer HKL positions demonstrating that the lattice structure is self-modulated along [110]. This modulation can be described by a harmonic displacement wave, the coefficients of which have been obtained from a numerical analysis of the integrated intensities of the satellite peaks. We performed an annealing study and found martensitic (monoclinic)/austenitic(cubic) phase transition at approx. 60°C with the hysteresis of about 10°C; the twinning and modulation peaks disappeared in the cubic (high-temperature) phase.

Keywords: shape memory alloy, reciprocal space mapping, twinning, modulated structure, high-temperature diffraction