

MS.96.4

Acta Cryst. (2011) A67, C208

Iron vacancy superstructure and room temperature anti-ferromagnetic order in superconducting $X_n\text{Fe}_{2-x}\text{Se}_2$ ($X=\text{K}, \text{Cs}, \text{Rb}$)
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Neutron and x-ray powder and single crystal synchrotron diffraction [1], [2] show the presence of superstructure reflections with propagation vector star $\{2/5, 1/5, 1\}$ with respect to the average crystal structure $I4/mmm$ (no. 139) with $a \approx 4$, $c \approx 15 \text{ \AA}$. The propagation vector star corresponds to the 5 times bigger unit cell given by transformation $\mathbf{A}=2\mathbf{a}+\mathbf{b}$, $\mathbf{B}=-\mathbf{a}+2\mathbf{b}$, $\mathbf{C}=\mathbf{c}$. The twin domain corresponding to the star $\{1/5, 2/5, 1\}$ is observed in the single crystal experiment as well. All crystals show an ordered iron vacancy pattern and the crystal structure is well described by the $I4/m$ (no. 87) space group with the lattice constants $a = 8.799$, $c = 14.576$; $a = 8.730$, $c = 14.115 \text{ \AA}$ and $a = 8.8582(3)$, $c = 15.2873(9) \text{ \AA}$ and the refined stoichiometry $x = 0.30(1)$, $y = 0.83(2)$; $x = 0.34(1)$, $y = 0.83(1)$ and $x = 0.29(1)$, $y = 0.83(1)$ for Rb, K and Cs crystals, respectively. The structure contains one fully occupied iron position (16i) and one almost empty vacancy position (4d). Assuming that the iron moment is ordered only on the fully occupied site we have sorted out all eight irreducible representations (irreps) of $I4/m$ for the propagation vector $k = 0$ and have found that irreps τ_2 and τ_7/τ_3 ($k=k14$, Table T121 [3]) well fit the experimental data with the moments along the c axis. The moment amplitudes amounted to $m_{\text{Fe}} = 2.15(3) \mu\text{B}$, $2.55(3) \mu\text{B}$ for τ_2 and $2.08(6) \mu\text{B}$, $2.57(3) \mu\text{B}$ for τ_7/τ_3 for Rb and K crystals, respectively. For the Cs-crystal the solutions space is highly degenerate and we cannot choose a specific solution. However both τ_2 and τ_7 are one of the best fit solutions with $m_{\text{Fe}} = 2 \mu\text{B}$. Irrep τ_2 corresponds to the Shubnikov group $I4/m'$ and gives a constant moment antiferromagnetic configuration, whereas τ_7 does not have a Shubnikov counterpart and allows two different magnetic moments in the structure. Interestingly to note that τ_7 and τ_2 solutions are predicted by recent first-principles calculation [4], where the τ_2 structure is called “block spin” and is the lowest energy configuration, and the τ_7 structure is called “zig-zag collinear” and is the second lowest energy configuration.

[1] V. Yu. Pomjakushin, D.V. Sheptyakov, E.V. Pomjakushina, A. Krzton-Maziopa, K. Conder, D. Chernyshov, V. Svitlyk, Z. Shermadini, *Physical Review* **2011**, B83, 144410, arXiv:1102.1919. [2] V. Yu. Pomjakushin, E.V. Pomjakushina, A. Krzton-Maziopa, K. Conder, Z. Shermadini, *J. Phys.: Condens. Matter* **2011**, 23, 156003, arXiv:1102.3380. [3] O.V. Kovalev, *Representations of the Crystallographic Space Groups* (Gordon and Breach Science Publishers, 1993), 2nd ed. [4] C. Cao, J. Dai, **2011**, arXiv:1102.1344.

Keywords: iron superconductors, magnetism, neutron diffraction

MS.96.5

Acta Cryst. (2011) A67, C208

Magnetostriction and phase separation in $\text{PrMn}_2\text{Ge}_{2-x}\text{Si}_x$ compounds

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Ternary intermetallic compounds of RMn_2X_2 (where R = rare earth or Yttrium and X = Si or Ge) are tetragonal layered compounds with sequencing of -R-X-Mn-X- planes along the unique c -axis. These compounds display a rich variety of magnetic structures due to changes in magnetic exchange interaction between neighbouring manganese atoms, resulting from changes in chemical pressure. Magnetic structure variants include ferromagnetic (f), collinear & non-collinear antiferromagnetic (af), mixed axial $f +$ planar af , and even incommensurate af structures. This remarkable magnetic behaviour is symptomatic of subtle changes in interatomic bond lengths, differentiated at sub-picometre length scales. Transformation between magnetic variants is often accompanied by structural distortions due to magnetoelastic coupling. Furthermore pseudoternary compounds, in which one or more sites has mixed occupancy (e.g. La & Y on the R site or Si & Ge on the X site), sometimes separate into two coexistent structural variants with differing axial magnetic order (f or af). Such behaviour is most clearly seen in $\text{PrMn}_2\text{Ge}_{2-x}\text{Si}_x$ compounds where $x \approx 1$.

We report a combined neutron and synchrotron X-ray diffraction study of the $\text{PrMn}_2\text{Ge}_{2-x}\text{Si}_x$ system, through which we gain new insights into the magnetic and structural origins of the curious behaviour of these compounds. Phase separation (both structural and magnetic) is clearly seen over a certain range of concentration and temperature, prompting us to propose a two-phase structural model driven by changes in the Mn-Mn magnetic exchange energy. Our evidence suggests that the phase separation derives from variations in local strain originating at the shared crystallographic sites. Our interpretation brings into question whether random atomic substitutions could produce such remarkable magnetoelastic phenomena or whether site-specific local atomic order prevails in the family of mixed 122 compounds. A tendency towards site ordering also raises the possibility of a miscibility gap.

Keywords: magnetism, ternary_compounds, diffraction

MS.97.1

Acta Cryst. (2011) A67, C208-C209

Harnessing students to advance e-learning

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Science is typically advanced by teams which make small improvements to the state-of-the-art. Teamwork is important because the collective knowledge and skill set of the team is greater than that of any individual in the team. We have been experimenting with applying a similar model to e-learning development. In a solid state physics course that consists of lectures and a weekly exercise session, the students were asked to evaluate the e-learning components of the course and propose ways to improve it. They implemented their ideas in small teams. Collectively, a class of university students usually has a broad knowledge of web development tools. The students have produced simulations in Java and Javascript, written lecture notes, Matlab template files, solutions to exam questions, and videos. Having the same material presented in a written document and in a video file can be useful because different students learn better from different media. Some of this material is in English and some is in German (the local language). We strive to have all important material available in both languages so that both local and international students do not experience a language barrier. When a topic is intrinsically