Iron vacancy superstructure and room temperature antiferromagnetic order in superconducting $\text{XFe}_2\text{Se}_2$ ($\text{X}=\text{K}, \text{Cs}, \text{Rb}$)
Laboratory for Neutron Scattering, Paul Scherrer Institute, 5232 Villigen (Switzerland).
Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, CH-5322 Villigen PSI, (Switzerland).
Swiss-Norwegian Beam Lines at ESRF, BP220, 38043 Grenoble, (France).
Laboratory for Neutron Scattering, Paul Scherrer Institute, 5232 Villigen (Switzerland).

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 as well. All crystals show an ordered iron vacancy pattern and the crystal structure is well described by the $I4/mmm$ (no. 139) with $a=4$, $c=15\AA$. The propagation vector star corresponds to the 5 times bigger unit cell given by transformation $A'=2a-b$, $B'=-a+2b$, $C'=c$. The twin domain corresponding to the star {1/5,2/5,1} is observed in the single crystal experiment as well. For the Cs-crystal the solutions space is highly degenerate whether random atomic substitutions could produce such remarkable magnetic behaviour. Interestingly the lowest energy configuration, and the τ7 structure is called “zig-zag calculation” [4], where the τ2 structure is called “block spin” and is allows two different magnetic moments in the structure. Interestingly the magnetic moments amounted to $m_{\text{Fe}}=2.15(3)$ μB, 2.55(3) μB for τ2 and 2.08(6) μB, 2.57(3) μB for τ7 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 τ2 and τ7 are one of the best fit solutions with $m_{\text{Fe}}=2\mu$B. Irrep τ2 corresponds to the Shubnikov group $I4/m$ and gives a constant moment antiferromagnetic magnetic structure variants include ferromagnetic (f), collinear & non-collinear antiferromagnetic (a/f), mixed axial f + planar a/f, and even incommensurate a/f structures. This remarkable magnetic behaviour is symmetrical 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 a/f). Such behaviour is most clearly seen in PrMn$_2$Ge$_2$Si compounds where x = 1.

We report a combined neutron and synchrotron X-ray diffraction study of the PrMn$_2$Ge$_2$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

**Microsymposia**

**MS.96.4** *Acta Cryst. (2011) A67, C208*

**Iron vacancy superstructure and room temperature antiferromagnetic order in superconducting $\text{XFe}_2\text{Se}_2$ ($\text{X}=\text{K}, \text{Cs}, \text{Rb}$)**

Laboratory for Neutron Scattering, Paul Scherrer Institute, 5232 Villigen (Switzerland).
Swiss-Norwegian Beam Lines at ESRF, BP220, 38043 Grenoble, (France).
Laboratory for Neutron Scattering, Paul Scherrer Institute, CH-5322 Villigen PSI, (Switzerland).
E-mail: vladimir.pomjakushin@psi.ch

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 as well. All crystals show an ordered iron vacancy pattern and the crystal structure is well described by the $I4/mmm$ (no. 139) with $a=4$, $c=15\AA$. The propagation vector star corresponds to the 5 times bigger unit cell given by transformation $A'=2a-b$, $B'=-a+2b$, $C'=c$. The twin domain corresponding to the star {1/5,2/5,1} is observed in the single crystal experiment as well. For the Cs-crystal the solutions space is highly degenerate whether random atomic substitutions could produce such remarkable magnetic behaviour. Interestingly the lowest energy configuration, and the τ7 structure is called “zig-zag calculation” [4], where the τ2 structure is called “block spin” and is allows two different magnetic moments in the structure. Interestingly the magnetic moments amounted to $m_{\text{Fe}}=2.15(3)$ μB, 2.55(3) μB for τ2 and 2.08(6) μB, 2.57(3) μB for τ7 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 τ2 and τ7 are one of the best fit solutions with $m_{\text{Fe}}=2\mu$B. Irrep τ2 corresponds to the Shubnikov group $I4/m$ and gives a constant moment antiferromagnetic magnetic structure variants include ferromagnetic (f), collinear & non-collinear antiferromagnetic (a/f), mixed axial f + planar a/f, and even incommensurate a/f structures. This remarkable magnetic behaviour is symmetrical 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 a/f). Such behaviour is most clearly seen in PrMn$_2$Ge$_2$Si compounds where x = 1.

We report a combined neutron and synchrotron X-ray diffraction study of the PrMn$_2$Ge$_2$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


**Harnessing students to advance e-learning**
Roland Resel, Peter Hadley, Institute of Solid State Physics, Graz University of Technology, Graz (Austria). E-mail: p.hadley@ugraz.at

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 form 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