

MS.96.4

Acta Cryst. (2011) A67, C208

Iron vacancy superstructure and room temperature anti-ferromagnetic order in superconducting $X_2\text{Fe}_{2-x}\text{Se}_2$ ($X=\text{K}, \text{Cs}, \text{Rb}$)
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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

complicated, like determining the electron density of states from the band structure, instructors tend to skip the long tedious calculations needed since there is not enough time for this during lectures. The online student presentations have no such limitation and can explain how to do a long calculation step-by-step. This can be a valuable resource for those trying to perform similar calculations but for whom the scientific literature is still difficult to digest. Students teach at the right level for their fellow students to understand. The production of a collection of long and detailed calculations that go into more detail than the lectures but are written in a style that is accessible to students was an unexpected outcome of this experiment. An important factor for the success of this model is the sheer volume of material produced. The students produce much more material than a single instructor could. The students are also more likely to try new approaches. Not all material that the students produce is useful but the less useful material gets displaced by other student projects as the students continuously try to improve the course. The students of our solid state physics course have created some wonderful material that has enriched the course. The biggest challenge for the instructor is managing the influx of material that is produced.

Keywords: education, solid-state physics

MS.97.2

Acta Cryst. (2011) A67, C209

WebCSD: bringing the Cambridge Structural Database to undergraduate teaching

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The Cambridge Structural Database (CSD) represents a vast and ever growing compendium of accurate 3D structures that has massive chemical diversity across organic and metal-organic compounds. For these reasons, the CSD is finding increasing application in chemical education.

WebCSD is a web-based search engine for interrogating the CSD and displaying CSD information content. Requiring just a standard web-browser, and without the need for any local software installations, WebCSD is designed for use in classroom and computational teaching laboratory environments. This ease of access makes the online version of the CSD the ideal platform for furthering students' understanding of 3D chemistry, and introducing them to the 3D realities of the chemical world.

This talk will showcase examples of how WebCSD is currently being used to enhance student learning across the entire span of the chemistry curriculum. We will also introduce a teaching subset of more than 500 CSD structures created specifically to illustrate key chemical concepts, and a number of teaching modules that make use of this subset in a teaching environment.

[1] G.M. Battle, F.H. Allen, G.M. Ferrence, *J.Chem.Educ.* **2010**, *87*, 809-812 and *87*, 813-818. [2] G.M. Battle, G.M. Ferrence, F.H. Allen, *J.Appl.Cryst.*, **2010**, *43*, 1208-1223.

Keywords: database, teaching

MS.97.3

Acta Cryst. (2011) A67, C209

Remote access to SSRL crystallography beamlines: Tools for education and training

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For the last six years, the Structural Molecular Biology (SMB) group at the Stanford Synchrotron Radiation Lightsource (SSRL) has provided general users of the facility fully remote access to their macromolecular crystallography beam lines. This was made possible by implementing fully automated beam lines with a flexible control system and an intuitive user interface (Blu-Ice) [1], and by the development of the robust and efficient Stanford Automated Mounting (SAM) robotic sample changing system [2]. The ability to control a synchrotron beam line remotely from the comfort of the home laboratory has set a new paradigm for the collection of high-quality X-ray diffraction data [3] and has fostered new collaborative research whereby a number of remote users from different institutions can be connected at the same time to the SSRL beam lines. The use of remote access has revolutionized the way in which scientists interact with synchrotron beam lines and collect diffraction data, providing a true high-throughput crystal screening and collection system at a significantly reduced cost to researchers. Moreover, it has also triggered a shift in the way crystallography students are introduced to synchrotron data collection and are trained in the best methods to collect high quality data and make the best possible use of these facilities. SSRL provides expert crystallographic and engineering staff, state-of-the-art crystallography beam lines and X-ray detector technology, and a number of accessibility tools to facilitate data collection and in-house "remote training". The use of these facilities at SSRL for education, training, outreach and collaborative research [4] is strongly encouraged.

[1] T.M. McPhillips, S.E. McPhillips, H.-J. Chiu, A.E. Cohen, A.M. Deacon, P.J. Ellis, E. Garman, A. González, N.K. Sauter, R.P. Phizackerley, S.M. Soltis, P. Kuhn, *J. Synchrotron Rad.* **2002**, *9*, 401-406. [2] A.E. Cohen, P.J. Ellis, M.D. Miller, A.M. Deacon, R.P. Phizackerley, *J Appl Cryst* **2002**, *35*, 720-726. [3] S.M. Soltis, A.E. Cohen, A. Deacon, T. Eriksson, A. González, S. McPhillips, H.-J. Chui, P. Dunten, M. Hollenbeck, I.I. Mathews, M. Miller, P. Moorhead, R.P. Phizackerley, C. Smith, J. Song, H. van dem Bedem, P. Ellis, P. Kuhn, T. McPhillips, N. Sauter, K. Sharp, I. Tsyba, G. Wolf, *Acta Cryst.* **2008**, *D64*, 1210-1221. [4] C.A. Smith, G.L. Card, A.E. Cohen, T.I. Doukov, T. Eriksson, A.M. Gonzalez, S.E. McPhillips, P.W. Dunten, I.I. Mathews, J. Song, S.M. Soltis, *J. Appl. Cryst.* **2010**, *43*, 1261-1270.

Keywords: synchrotron, remote access, education

MS.97.4

Acta Cryst. (2011) A67, C209-C210

Structure utilities hosted by the Bilbao crystallographic server

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The experimental procedures (such as scattering and powder diffraction) and computational methods (such as ab-initio calculations and Monte-Carlo simulations) reveal the information on the lattice parameters and the atomic positions but since there is no unique way to describe a structure, in order to correctly classify and further compare it with other similar types of structures, it is necessary, in general, to take the equivalent descriptions into account. For the determination of a compatible orientation and/or origin shift, it is thus necessary to specify the transformation between different settings, followed by a systematic comparison of the corresponding descriptions.

Various tools are offered by the Bilbao Crystallographic Server for such purposes (<http://www.cryst.ehu.es>) [1]. CELLTRAN and TRANSTRU transform unit cell parameters or atomic coordinates into