**Simultaneously ferromagnetic and antiferromagnetic MnAs layer**

1. A. Pandey, B. G. Ueland, S. Yeninas, A. Kreyssig, A. Sapkota, Yang Zhao, J. S. Helton, J.W. Lynn, R. J. McQueeney, Y. Furukawa, A. I. Goldman, and D. C. Johnston, Coexistence of half-metallic itinerant ferromagnetism with local-moment antiferromagnetism in $Ba_{0.60}K_{0.40}Mn_2As_2$, Phys. Rev. Lett. **111**, 047001 (2013)..
2. B. G. Ueland, A. Pandey, Y. Lee, A. Sapkota, Y. Choi, D. Haskel, R. A. Rosenberg, J. C. Lang, B. N. Harmon, D. C. Johnston, A. Kreyssig, and A. I. Goldman, Itinerant ferromagnetism in the As $4p$ conduction band of $Ba_{0.6}K_{0.4}Mn_2As_2$ identified by x-ray magnetic circular dichroism, Phys, Rev. Lett. **114**, 217001 (2015).

Recommended with a Commentary by Atsushi Fujimori, University of Tokyo

Ferromagnetic (FM) and antiferromagnetic (AFM) orders are considered as distinct states of matter. In the former, macroscopic (i.e., uniform) magnetization appears due to time reversal symmetry breaking while the periodicity of the lattice is maintained. In the latter, time reversal symmetry breaking occurs in the form of staggered magnetization on the atomic scale, and leads to a lattice periodicity longer than that of the original lattice. In principle, however, one can conceive a superposition of these two orders, namely, a state where both the uniform magnetization and the staggered magnetization with the longer periodicity coexist. A canted antiferromagnet is the simplest realization of such a coexistence state. Alternatively, one can consider a system consisting of FM and AFM subsystems like an alternating stack of FM and AFM atomic layers with negligible coupling between them. Such a system may be realized in artificial multilayers by inserting non-magnetic layers between the FM and AFM layers, but is trivial and would not be interesting. (If there is finite magnetic coupling between the FM and AFM layers, complex phenomena such as magnetic frustration and exchange bias effect will take place.)

Under the above circumstance, it would be amazing and highly intriguing if FM order and AFM order coexist in the same atomic layer in the absence of canting of the AFM moments. In fact, in the recommended papers, Pandy *et al.* and Ueland *et al.* have reported that the MnAs layer in the layered compound $Ba_{1-x}K_xMn_2As_2$ (BKMA) is both FM and AFM and that there is no spin canting. BKMA is isostructural to the so-called 122-type Fe-based superconductors such as $Ba_{1-x}K_xFe_2As_2$, as shown in Fig. 1. The parent compound of BKMA, $BaMn_2As_2$, is an AFM insulator with a high Néel temperature ($T_N = 625$ K) and a large Mn $3d$ magnetic moment (3.9 $\mu_B$) aligned parallel to the *c*-axis [1], suggesting strong superexchange coupling between the Mn spins through the filled As $4p$ orbitals. Hole doping through K substitution for Ba makes the system an AFM metal, where the $T_N$ remains rather high (480 K for $x \sim 0.4$) and the Mn moment remains large. Further application of high pressure up to ~20 GPa does not reduce $T_N$ appreciably [2]. More surprisingly, in BKMA ($x \sim 0.4$), FM order develops below $T_C \approx 100$ K with the magnetic moment lying in the *ab* plane. NMR, x-ray magnetic circular dichroism (XMCD), and x-ray and neutron diffraction studies reported in the recommended papers have all excluded the possibility of the Mn spin canting (the upper limit of the *ab* component of Mn spin being 0.01 $\mu_B$), and indicated that holes doped into the As $4p$ band are fully FM (i.e., half-metallic).

Thus, the single MnAs layer in the BKMA crystal would be divided into the two, magnetically decoupled subsystems: the Mn sublattice and the As sublattice. Strictly speaking, as the Mn layer and the two adjacent As layers are at different heights (Fig. 1), it may not be fair to refer to the MnAs layer as a single atomic layer. Nevertheless, as each Mn atom is tetrahedrally coordinated by four As atoms in the MnAs layer, it is non-trivial to explain why the Mn $3d$ and As $4p$ appear to be magnetically decoupled. Notably, in diluted FM semiconductors such as Mn-doped GaAs, holes doped into the As $4p$ band are believed to induce FM coupling between the Mn spins [3]. Furthermore, a new diluted FM semiconductor $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$ having the same crystal structure as BKMA (Fig. 1) was recently synthesized, and its $T_C$ was found to exceed 100 K [4]. Since $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$ can be derived from BKMA by diluting Mn atoms by Zn and this dilution recovers the Mn-As magnetic coupling, the apparent magnetic decoupling between Mn and As in BKMA may be a result of cancellation of different magnetic interactions. While spin-orbit coupling does not lead to Dzyaloshinskii-Moriya interaction and hence no spin canting in BKMA, it might be responsible for the formation of the mutually perpendicular Mn and As magnetic moments. If the Mn $3d$ and As $4p$ subsystems were indeed decoupled, the As $4p$ band itself must have inherent

FM instability. Such instabilities have been discussed for the relatively compact oxygen, nitrogen, and carbon $2p$ electrons, but are less likely for the much more extended pnictogen and chalcogen $4p$ orbitals. The interesting problems raised by the recommended papers obviously need and are worthwhile for further systematic investigations in the present Mn arsenide and related pnictides.

[1] A. Pandey, R. S. Dhaka, J. Lamsal, Y. Lee, V. K. Anand, A. Kreyssig, T. W. Heitmann, R. J. McQueeney, A. I. Goldman, B. N. Harmon, A. Kaminski, and D. C. Johnston, Phys. Rev. Lett. **108**, 087005 (2012).

[2] D. Gu, X. Dai, C. Le, L. Sun, Q. Wu, B. Saparov, J. Guo, P. Gao, S. Zhang, Y. Zhou, C. Zhang, S. Jin, L. Xiong, R. Li, Y. Li, X. Li, J. Liu, A. S. Sefat, J. P. Hu and Z.-X. Zhao, Sci. Rep. **4**, 7342 (2014).

[3] See, e.g., A. Chattopadhyay, S. Das Sarma, and A. J. Millis, Phys. Rev. Lett. **87**, 227202 (2001).

[4] K. Zhao, Z. Deng, X. C. Wang, W. Han, J. L. Zhu, X. Li, Q. Q. Liu, R. C. Yu, T. Goko, B. Frandsen, L. Liu, F. Ning, Y. J. Uemura, H. Dabkowska, G. M. Luke, H. Luetkens, E. Morenzoni, S. R. Dunsiger, A. Senyshyn, P. Bni, and C. Q. Jin, Nat. Commun. **4**, 1442 (2013).

[5] For a recent review, O. Volnianska and P. Boguslawski, J. Phys.: Condens. Matter **22,** 073202 (2010).

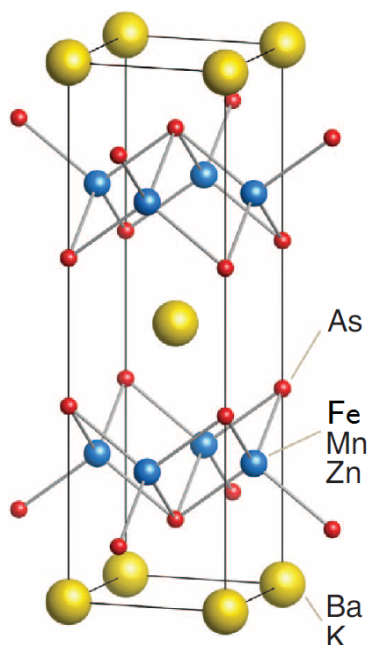Fig. 1. Common crystal structures of the superconducting $Ba_{1-x}K_xFe_2As_2$, antiferromagnetic $Ba_{1-x}K_xMn_2As_2$, and ferromagnetic $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$ (reproduced from [4] with modification).