Simultaneously ferromagnetic and antiferromagnetic MnAs layer


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, Pandey et al. and Ueland et al. have reported that the MnAs layer in the layered compound Ba1−xKxMn2As2 (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 Ba1−xKxFe2As2, as shown in Fig. 1. The parent compound of BKMA, BaMn2As2, is an AFM insulator with a high Neel temperature (TN = 625 K) and a large Mn 3d magnetic moment (3.9 µB) 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 TN remains rather high (480 K for x ∼ 0.4) and the Mn moment remains large. Further application of high pressure up to ~20 GPa does not reduce TN appreciably [2]. More surprisingly, in BKMA (x ∼ 0.4), FM order develops below TC ∼ 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 µB), 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 Ba1−xKx(Zn1−xMnx)2As2 having the same crystal structure as BKMA (Fig. 1) was recently synthesized, and its TC was found to exceed 100 K [4]. Since Ba1−xKx(Zn1−xMnx)2As2 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.


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Fig. 1. Common crystal structures of the superconducting $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, antiferromagnetic $\text{Ba}_{1-x}\text{K}_x\text{Mn}_2\text{As}_2$, and ferromagnetic $\text{Ba}_{1-x}\text{K}_x(\text{Zn}_{1-y}\text{Mn}_y)\text{As}_2$ (reproduced from [4] with modification).