Highlights

Novel superconducting and functional materials for energy and environment - 2019

The huge effect of Mn substitution on the structural and magnetic properties of LaFeAsO: the La(Fe,Mn)AsO system

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The substitution of Mn for Fe in the sub-structure of La($Fe_{1-x}As_x$)O has a remarkable impact on both structural and magnetic properties. For example, the structural and magnetic transition temperatures decrease of ~ 20 K in samples with a Mn-content as low as x = 0.01. Such a dramatic effect results from the high stability of the substituting Mn2$^+$ ion (3d^5) in its high-spin state, which opposes any variation to its electronic state (configuration), perturbing thereby interactions within the transition metal sub-structure between the Fe ions surrounding the Mn substituent. Several investigations ascertained that the structural transition in *Ln*FeAsO compounds (*Ln*: lanthanide) cannot be ascribed to structural degrees of freedom, but rather to electronic or spin ones. In this context, even an extremely low concentration of Mn^{2+} ions diluted in the Fe sub-structure produces a reduction of the electronic degree of freedom of the system, thus hindering both the structural and the magnetic transitions. Remarkably, we recently detected the development of a static incommensurate modulated structure across the low-temperature orthorhombic phase in the La($Fe_{1-x}Mn_x$)AsO system, revealing a possible major role of charge density wave in Fe-based SC materials. The structural transition is also accompanied by an anomalous increase of the structural strain parallel to the Fermi surface nesting wave-vector just above the desymmetrization (Fig. 1). The phase diagram of the La($Fe_{1-x}Mn_x$)AsO system has been drawn for the Mn-poor side on the basis of structural and magnetic data obtained by synchrotron X-ray and neutron powder diffraction (Fig. 2).

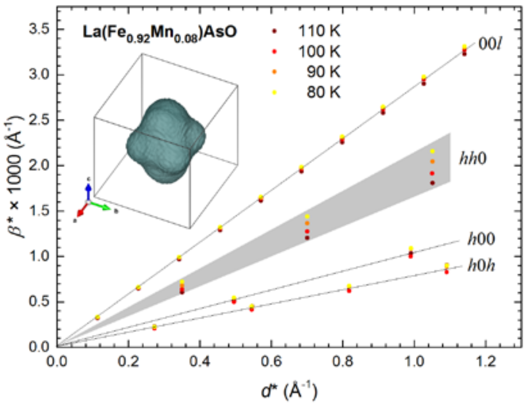

Fig. 1: Superposition of Williamson-Hall plots showing the evolution of the lattice microstrains in the tetragonal phase on cooling. The inset shows the observed tensor isosurface representing the microstrain broadening characterizing the sample as the structural transition is approached.

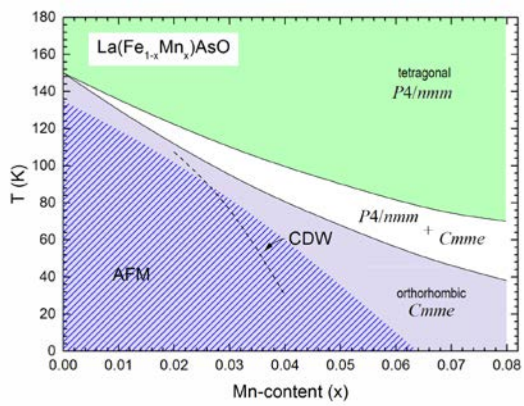

Fig. 2: Phase diagram of the La($Fe_{1-x}Mn_x$)AsO system (Mn-poor side); the hatched area represents the region of the phase diagram where long-range magnetic ordering takes place; the dotted line defines the region where a static CDW state was detected.