REPORT OF THE ESRF EXPERIMENT HC-2646

Thermal dependence of the structural and microstructural properties of $La(Fe_{1-x}Mn_x)As(O_{0.89}F_{0.11})$ samples

Selected members of the $La(Fe,Mn)As(O_{0.89}F_{0.11})$ system were analysed using high resolution synchrotron X-ray powder diffraction data. As a result, the tetragonal-to-orthorhombic structural transition is progressively recovered in the optimally electron-doped $LaFeAs(O_{0.89}F_{0.11})$ phase by very light Mn-substitution; at the same time, superconductivity is suppressed whereas magnetic ordering is restored. Distinct incommensurate satellite peaks develops within different thermal ranges and mark the occurrence of charge density waves; in particular, some of them arise in conjunction with the structural transformation process. The thermal evolution of the satellite reflections indicates a strong competition between the charge density waves and the superconductive state.

X-ray powder diffraction (XRPD) data (λ = 0.400020 Å) were collected between 5 K and 295 K (on warming) at the ID22 high-resolution powder diffraction beamline of the European Synchrotron Radiation Facility (ESRF).

Mn-substitution progressively recovers the symmetry breaking that is suppressed in optimally F-doped compounds (Figure 1). As a rule, the structural transition in these compounds is marked by a selective peak splitting of the tetragonal *hhl* reflections; nonetheless, in some cases only a selective peak broadening of the same tetragonal *hhl* diffraction lines can be detected, depending on the amplitude of the orthorhombic distortion and/or the instrumental resolution.

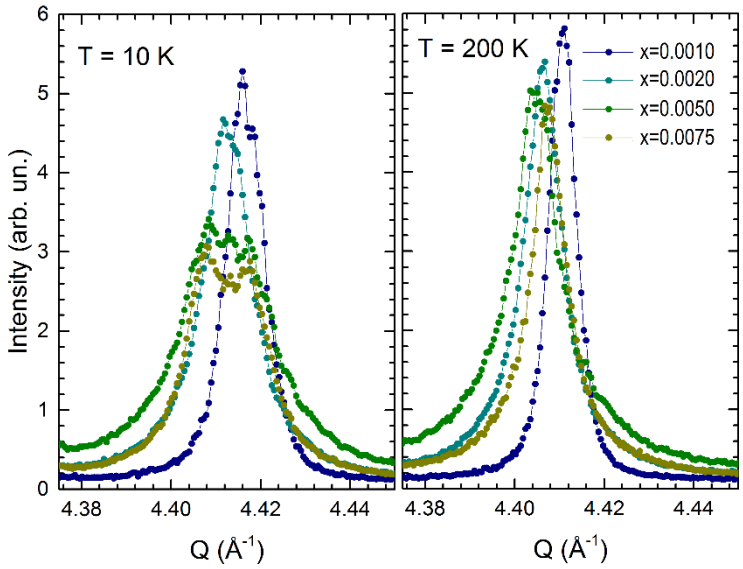

Figure 1: Evolution of the 220 diffraction line (tetragonal indexing) as a function of Mn-content at 200 K and 10 K.

A closer inspection of the XRPD patterns reveals the presence of some extremely weak Bragg reflections that cannot be indexed by three-integer indices, possibly marking the occurrence of an incommensurate modulated structure involving a CDW state. In particular, these satellite reflections are observed at **Q** ~ 1.93 $Å^{-1}$, ~ 1.975 $Å^{-1}$, ~ 2.00 $Å^{-1}$ and ~ 2.36 $Å^{-1}$, but their intensities differently evolve in the different samples, pointing to distinct incommensurate periodicities depending on temperature (Figure 2.

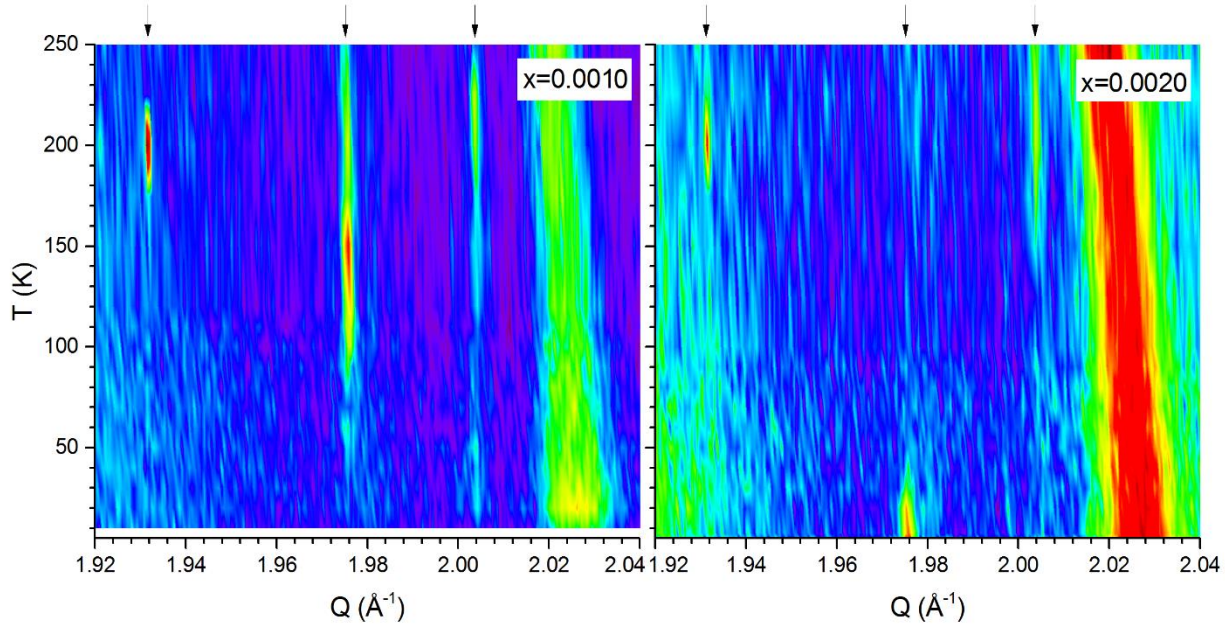

Figure 2: Enlarged view of the thermodiffractograms for the samples with x = 0.0010 and 0.0020 showing the thermal dependence of the intensity of the satellite peaks located at **Q** ~ 1.93 $Å^{-1}$, ~ 1.975 $Å^{-1}$ and ~ 2.00 $Å^{-1}$ (arrowed).

In conclusion, our analysis confirmed the occurrence of incommensurate structures in Fe-based superconductors, as already detected in the homologous La(Fe,Mn)AsO system [1].

[1] A. Martinelli et al., Phys Rev. Lett. 118 (2017) 055701