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Nanoscale probe of magnetism, orbital occupation, and structural distortions in iron-based superconductors[1]

CLAUDIA CANTONI, Oak Ridge National Lab

Local probes of atomic and electronic structures with sub-nanometer spatial resolution can provide additional insights into the physics of iron-based superconductors (FBS) by resolving the influence of inhomogeneities that are typically averaged over by bulk-sensitive techniques. Here we apply aberration-corrected scanning transmission electron microscopy coupled with electron energy loss spectroscopy to a wide class of iron-based superconductors and parent compounds to decipher the interplay between crystal distortions, local magnetic moment, orbital occupancy, and charge doping in these complex materials. In addition to revealing universal trends for hole concentration and local magnetic moment across families of FBS, we directly observe the effects of magneto-elastic coupling in 122 arsenides at room temperature, well above the structural and antiferromagnetic transition. The presence of atomic displacements indicates that the C_4 tetragonal symmetry is already broken at room temperature in unstrained crystals, lowering the symmetry to orthorhombic (*I2mm*), and that all of the crystals are twinned with domains the size of a few nanometers. By tracking these local atomic displacements as a function of doping level x, in $Ba(Fe_{1-x}Co_x)_2As_2$, we find that the domain size correlates with the magnitude of the dynamic Fe moment, and both are enhanced near optimal doping where the ordered moment is suppressed. The non-monotonic behavior of the local Fe magnetic moment is linked to the strong coupling between lattice, spin, and orbital degrees of freedom.

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