In-plane electronic anisotropy in underdoped Ba(Fe_{1-x}Co_x)As_2 revealed by detwinning in a magnetic field

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We present results of angle-dependent magnetoresistance measurements and direct optical images of underdoped Ba(Fe_{1-x}Co_x)As_2 which reveal partial detwinning by action of a 14T magnetic field. Driven by a substantial magneto-elastic coupling, this result provides evidence for an electronic origin of the lattice distortion in underdoped iron pnictides. The observed anisotropy in these partially detwinned samples implies a substantial in-plane electronic anisotropy in the broken symmetry state, with a smaller resistivity along the antiferromagnetic ordering direction.

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High temperature superconductivity emerges in the proximity of an antiferromagnetic(AF) ground state in several closely related families of iron-pnictides[1]. Interestingly, the AF transition in most of these materials is either precede by or coincident with a structural transition, which lowers the system’s symmetry from tetragonal to orthorhombic[2]. It is generally believed that insights into the physics of this antiferromagnetism will lead to a better understanding of the origin of high temperature superconductivity in this family of compounds. To fully understand the magnetic ground state, it is crucial to measure the intrinsic in-plane anisotropy. However, the formation of structural twins in the orthorhombic crystals[3,4], makes such a measurement very challenging, and one would ideally like to find a simple method to detwin these materials and hence reveal the underlying in-plane anisotropy.

In 2002, Lavrov and coworkers performed a series of magnetotransport measurements accompanied by direct optical imaging on lightly doped La_{2-x}Sr_xCuO_4 which has an orthorhombic transition around 450K, showing that it can be detwinned by a 14T magnetic field [5]. Encouraged by this result, we have explored the possibility of affecting the structural/magnetic domains of iron pnictides in a similar manner, choosing Co-doped BaFe_2As_2 as a starting point. By doping with cobalt the single structural/magnetic transition of the undoped parent compound splits into two: the system first undergoes a tetragonal to orthorhombic structural transition(T_{ortho}), then enters a collinear AF state at a lower temperature(T_N) [6,7,8,9,10]. Homogeneous doping and large single crystals, combined with the small temperature difference between T_{ortho} and T_N, makes this an ideal material for such study.

In this Letter, we show via a combination of angle-dependent magnetoresistance(MR) measurements and direct optical images how magnetic fields can be used to detwin underdoped Ba(Fe_{1-x}Co_x)As_2. Our observations imply a surprisingly large in-plane electronic anisotropy below T_N with a smaller resistivity along the AF ordering direction (\rho_a < \rho_b). This result has important consequences for our understanding of the reconstructed Fermi surfaces of underdoped iron pnictides, and for the driving force behind the structural transition.

Single crystals of Ba(Fe_{1-x}Co_x)As_2 were grown from a self flux, as described previously [6]. Electrical contacts were made using sputtered gold pads in a standard four-point configuration, with typical contact resistance of 1–2 Ohms. Angle-dependent magnetotransport measurements were made in fields up to 14T. All the measurements were performed with both current and field parallel to the FeAs plane. Samples were cut into bar shapes of typical dimension 1mm×0.2mm×0.05mm and the crystal axes determined by x-ray diffraction. Except for the first set of experiments shown in Fig 1 for which we deliberately varied the current orientation, all the measurements were taken with current along the orthorhombic a/b direction. Optical measurements were performed in a superconducting magnet cryostat, in which the field could be varied between 0 and 10T. The sample was illuminated with linearly polarized light, and viewed through an almost fully crossed polarizer in order to maximize the contrast of birefringence between neighboring domains. Crystals were mounted in an identical manner for both transport and optical measurements in such a way as to minimize external stress.

For the first set of experiments, samples of Ba(Fe_{1-x}Co_x)As_2 were cut such that the direction of the current varied with respect to the crystal axes. Representative data are shown in fig. 1 for x=2.5%
FIG. 1: (Color online) The in-plane magnetoresistance $\Delta \rho_{ab}/\rho_{ab}$ (%) of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ for $x = 2.5\%$ for two specific current orientations (sample A and B). The angle independent part of the magnetoresistance for sample B has been subtracted for clarity. The data were taken at 84K, below both $T_{ortho}$ and $T_N$ for this cobalt concentration. The geometry of the measurement is indicated below each panel. Both current and field are in the ab-plane, and the angle of the magnetic field is measured relative to the current direction. For sample A current is applied parallel to the orthorhombic a/b axis, whereas for sample B current is applied at 45 degree to the orthorhombic a/b axis.

with current running along the orthorhombic [100] and [010] direction (sample A) and along the orthorhombic [110] direction (sample B). The configuration is illustrated schematically below each panel. At 84K, which is below both the structural and magnetic transitions for this cobalt concentration ($T_{ortho} = 99\pm0.5K$ and $T_N = 93\pm0.5K$ respectively), we applied 14T and rotated the field within the FeAs plane to measure the resistivity as a function of angle. The angle-dependent MR of sample A is shown in the polar plot fig. (a). It has a two-fold symmetry (as reported previously by Wang et al.[11]), with a positive MR for fields aligned parallel to the current, and negative when the field is perpendicular to the current. The angle dependent MR of sample B is shown in the polar plot fig. (b). It also has a two-fold symmetry, but the magnitude is much smaller and the angle is shifted by 45 degrees. Clearly the two-fold MR is tied to the crystal axes and not to the current orientation.

To investigate the origin of this angle-dependent MR, we performed a detailed temperature dependent map close to the magnetic and structural transition temperatures. Representative data for $x = 2.5\%$ and $3.6\%$, in a 14T magnetic field and using the “Sample A” configuration ( i.e. current along orthorhombic a/b axis) are shown in Fig 2. These data are shown together with the temperature derivative of resistivity, which can be used to determine the two transition temperatures [8][9][6].
FIG. 3: (Color online) Representative magnetoresistance data for Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ as a function of field and angle for $x = 1.6\%$ at $T = 80K$ (panels (a) and (b)) and $T = 20K$ (panels (c) and (d)). For all cases the current is aligned parallel to the orthorhombic $a/b$ axes and field is applied parallel to the $ab$ plane (i.e. sample A configuration). For field sweeps, the magnetic field was swept from 0 to 14T, then 14 to -14T, then back to 0T following an initial zero-field cool. Data were taken for fields aligned parallel (red) and perpendicular (green) to the current. Angle sweeps were performed in a field of 14T following an initial zero-field cool. Data were taken continuously as the angle was increased from 0 to 360 degrees and then back to zero.

FIG. 4: (Color online) Temperature dependence of the resistivity for representative samples with $x = 1.6\%$ (panels (a) and (b)) and $x = 2.5\%$ (panels (c) and (d)). Data were taken during an initial field cool (FC) in 14T, after which the field was cycled to zero and the resistivity measured in zero field while warming (ZFW). The current is aligned parallel to the $a/b$ orthorhombic axes, and the field applied either parallel (red) or perpendicular (green) to the current. For comparison, data are also shown for the same samples while cooled in zero field (ZFC). The FC MR ($\rho_{FC} - \rho_{ZFC}$) and ZFW resistivity difference induced by FC ($\rho_{ZFW} - \rho_{ZFC}$) for the two field configurations are also plotted in (b) for $x = 1.6\%$ and (d) for $x = 2.5\%$.

slower (essentially frozen on laboratory time scales) at lower temperatures, resulting in a larger hysteresis. The angle dependence implies that the projection of the applied field on to specific crystal orientations must exceed a specific threshold value to induce these changes at low temperatures.

In order to maximize this effect, samples can be cooled through the structural/magnetic transitions in an applied magnetic field. Representative data are shown in Fig. 4 for $x = 1.6\%$ and 2.5% for fields applied both parallel and perpendicular to the current (still employing the Sample A configuration). Measurements were taken while cooling in an applied field of 14 T (field cool FC), and then while warming in zero field (zero field warm, ZFW) after cycling the field to zero at base temperature. The resistivity difference induced by field cooling along one orientation can be as large as 5% at low temperature, even after the field is cycled to zero. The FC MR and ZFW resistivity difference for the two field configurations are also plotted in (b) and (d) for the two cobalt concentrations. The sign of MR for the two field orientations is opposite, and the absolute value appears to follow the magnetic order parameter, developing rapidly below $T_N$. A positive background in the FC MR data can be observed for both orientations, the magnitude of which increases as temperature is decreased, which is likely due to the ordinary metallic MR. In contrast, the resistivity difference of ZFW cycles appears to be rather symmetric. Its magnitude converges rapidly as the temperature is increased, consistent with thermally assisted relaxation, and with the hysteresis effect observed in field sweeps as a function of temperature.

We also performed direct optical measurements to observe the twinning domains on the surface of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$. Representative images of a 2.5% sample at $T = 40K$ are shown in Fig. 5. Data were taken in zero field, and also after sweeping to 10 T. The presence of vertical stripes in both images indicates that the sample was twinned in zero and 10 T field. However, the relative density of the two domains is changed by application of the magnetic field. To track the difference of domain distributions, we plot the intensity profile across the boundaries, since the intensity depends on the crystal axes’ orientation with respect to the light polarization. The twinning boundaries between two adjacent domains can then be determined from the maximum of the derivative of the intensity, from which we calculate the
(a) T = 40K H = 0T  
(b) T = 40K H = 10T

FIG. 5: (color online) Representative optical images of a Ba(Fe1−xCo2)xAs2 sample for x = 2.5%. The images (obtained as described in the main text) were taken at T = 40K below both T_{c1} and T_N. The initial image (a) was taken in zero field, following a zero field cool from above T_N. The field was then swept to 10T, at which field the second image (b) was taken. Horizontal intensity profiles, shown below each image, were calculated by integrating vertically over the image area after background subtraction and noise filtering. Boundaries between domains were estimated as described in the main text, resulting in an estimate of the relative fraction of the two domains indicated by black and white stripes below the figures. The field was oriented along the orthorhombic a/b axes.

percentage of the volume of the domains of high intensity (f = V_b/(V_a + V_b)). For the two images shown in Fig.5, f increases from 54 ± 1% to 61 ± 1% a difference Δf = 7% upon application of 10 T. Several regions in the optical images were analyzed, yielding percentage differences Δf ranging from 5% to 15%. Despite the large range in Δf, which is due to the spatial variation of domain distribution, it is always positive, providing convincing evidence for partial field-induced detwinning.[15]

The origin of this detwinning effect is presumably related to the anisotropic in-plane susceptibility (χ_a ≠ χ_b) that must develop below T_N. Since the magnetic structure is collinear, with moments oriented along the long a-axis (referred to the orthorhombic unit cell)[2], we can anticipate that χ_b > χ_a. In this case, fields oriented along the a/b axis of a twinned crystal will favor domains with the b-axis oriented along the field direction. Therefore for currents applied along the a/b axis and fields parallel to the current, the resistivity comprises a larger component of ρ_b than ρ_a. For fields aligned perpendicular to the current the opposite is true. The effect clearly indicates the presence of a strong magneto-elastic coupling, suggestive of an electronic origin of the lattice distortion in these materials. Since the crystals are only partially detwinned, the observation of a positive MR for fields aligned parallel to the current implies a substantial anisotropy below T_N with ρ_a < ρ_b. [16]

This result has some important consequences. Intuitively one might expect to find that ρ_a > ρ_b, both because the a-axis lattice constant is larger than the b-axis lattice constant, and also because the spin-density wave(SDW) wave-vector is directed along the a-axis. Indeed, local-density approximation (LDA) calculations of the reconstructed Fermi surface for BaFe2As2 (incorporating a negative U to reduce the moment to the observed value)[13] indicate a larger plasma frequency for the b-axis relative to the a-axis.[14], consistent with this expectation in the limit of isotropic scattering. The observed anisotropy points towards either an unanticipated k-dependence of the scattering rate, or a stronger variation in the orbital character around the Fermi surface than is predicted by LDA.

In summary, we have shown how magnetic field can be used to detwin underdoped iron pnictides, opening a new avenue for research into their anisotropic electronic properties. Our initial experiments have focused on the electron-doped system Ba(Fe1−xCo2)xAs2, but given the generic collinear AF structure found in this family of compounds, it is likely that the effect is quite general, limited only by details of the twin-boundary pinning and the strength of field available. Our experiments reveal a surprisingly large in-plane anisotropy, with a smaller resistivity along the AF ordering direction. Understanding the source of this anisotropy will be a key step towards establishing the origin of superconductivity in these materials.

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An alternative explanation for the origin of the dark stripes in the images shown in Fig. 5 is that these regions consist of densely twinned domains. Such regions would be optically isotropic if the domain size is much smaller than the incident light’s wavelength, giving rise to low intensity in the nearly crossed polarized configuration. Although we cannot rule out this possibility from the current measurements, nevertheless it is clear from the effect of magnetic field on the relative areas of light and dark regions in the optical images that the magnetic field detwins the sample. Partial detwinning reduces the twin boundary density, and therefore presumably decreases the contribution to the overall scattering rate from twin boundary scattering. However this effect cannot explain the permanent increase of resistivity for fields parallel to the current at low temperature. Moreover the twin boundaries extend along orthorhombic [110] direction, hence any scattering process would contribute equally to the resistivity along a and b-axis, inconsistent with the observed anisotropy.