Magnetic and superconducting structures near twin boundaries in low doped Fe-pnictides

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The effects of twin boundaries (TBs) on the complex interaction between magnetism and superconductivity in slightly electron-doped Ba(Ca)(FeAs)$_2$ superconductors are investigated. The spatial distributions of the magnetic, superconducting and charge density orders near two different types of TBs are calculated. We find that TBs corresponding to a 90° lattice rotation in the a-b plane enable magnetic domain walls to form with only a small effective Coulomb interaction between valance electrons, and that superconductivity is enhanced at such TBs. Contrasting, we find that superconductivity is suppressed at TBs corresponding to an asymmetrical placement of As atoms with respect to the Fe atoms in the a-b plane.

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The recent discovery of Fe-pnictide based superconductors offers an alternative avenue to explore the physics of high temperature superconductors [1–3]. Similar to the cuprates, the parent compounds of the FeAs-based superconductors also possess antiferromagnetic (AF) ground states [4, 5]. With increasing electron or hole doping, the AF order is suppressed and superconductivity (SC) appears in both the cuprates and the Fe-pnictides. However, different from the cuprates, SC and a (SC) appears in both the cuprates and the Fe-pnictides.

In the cuprates, the parent compounds of the FeAs-based superconductors, the magnetic and superconducting structures near twin boundaries in low doped Fe-pnictides.

Recently, twin boundaries (TBs) oriented 45° from the x(a)-axis were observed in the normal state of Ca(Fe$_{1-x}$Co$_x$As)$_2$ [10]. Across these TBs, the a-axis of the crystal rotates by 90°, and the modulation direction of AF order that exists is rotated by 90° as well. That is, 90° magnetic domain walls (DWs) are formed at the TBs. Also, in the SC state of underdoped Ba(Fe$_{1-x}$Co$_x$As)$_2$ with x < 0.07, it has been found that the diamagnetic susceptibility is increased and that the superfluid density is enhanced on the same type of TB [11]. Consistent with these experiments, a theoretical study [12] found that 90° DWs can be formed at low doping levels and that SC is enhanced on them. However, the DWs considered in that study formed in the absence of TBs, being induced instead by a strong effective Coulomb interaction between valance electrons, while in the experiments [10, 11], the DWs were pinned at TBs. In this letter, in order to better understand the effects that TBs have on the development of magnetic and superconducting order, we investigate the magnetic, SC and charge density orders near 4 different TB configurations using the Bogoliubov-de-Gennes (BdG) equations for very under-doped Ca(or Ba)(FeAs)$_2$ compounds. Among these TBs are ones involving assymetric placement of the As atoms above and below the Fe plane. This type of TB has not been previously studied. This study is based upon the band model [13] and the phase diagram for electron doped Ba(Fe$_{1-x}$Co$_x$As)$_2$ [14]. We predict that the enhancement or suppression of SC, the location of DWs and the electron-density distributions are largely dependent on the nature of TBs. Our results provide a theoretical explanation for the relationship between TBs and enhanced SC order observed in experiments.

Consider a Hamiltonian $H = H_0 + H_{SC} + H_{int}$, that describes the energy of valance electrons. $H_0$ is a non-interacting energy from a two-orbital tight-banding model, the detailed form of which can be found in Ref. [13, 14]. The pairing interaction energy of the electrons is

$$H_{SC} = \sum_{i,j,\nu,\sigma} \Delta_{ij\nu} c_{i\nu\sigma}^{\dagger} c_{j\nu\bar{\sigma}} + H.c.$$ 

where $\Delta_{ij\nu}$ is the pairing parameter between two electrons, one at position $i$ with orbital $\mu$ and the other at position $j$ with orbital $\nu$, and $c_{i\nu\sigma}$ is the creation operator of an electron with spin $\sigma$ at position $i$ with orbital $\mu$. Here $\bar{\sigma}$ denotes the opposite spin of $\sigma$. The mean-field magnetic interaction energy is [14]

$$H_{int} = (U - 3J_H) \sum_{i,\mu \neq \nu, \sigma} \langle n_{i\mu\sigma} \rangle n_{i\nu\sigma} + (U - 2J_H) \times \sum_{i,\mu \neq \nu, \sigma \neq \bar{\sigma}} \langle n_{i\mu\sigma} \rangle n_{i\nu\sigma} + U \sum_{i,\mu, \sigma \neq \bar{\sigma}} \langle n_{i\mu\sigma} \rangle n_{i\nu\sigma}$$

where $U$ is the on-site Coulomb interaction, $J_H$ is the Hund’s coupling, $n_{i\mu\sigma}$ is the electron number operator, and $\langle n_{i\mu\sigma} \rangle$ is the local electron density. The eigenvalues and eigenfunctions of the total Hamiltonian $H$ can be obtained by self-consistently solving the BdG equations

$$\sum_{j,\nu} \left( \begin{array}{c} H_{ij\nu} - \Delta_{ij\nu} \Delta_{ij\nu}^{*} \end{array} \right) \begin{bmatrix} c_{j\nu\sigma}^{\dagger} \\ n_{j\nu\sigma}^{\dagger} \end{bmatrix} = E_n \begin{bmatrix} c_{i\nu\sigma} \\ n_{i\nu\sigma} \end{bmatrix}$$
where

\[ H_{ij\mu\sigma} = -t_{ij\mu} + [U(n_{i\mu\sigma}) + (U - 2J_H)(n_{i\mu\bar{\sigma}}) + (U - 3J_H)(n_{i\bar{\mu}\sigma}) - t_0] \delta_{\mu\nu} \]

is the matrix element of \( H \) with the same spin \( \sigma \) between the orbital \( \mu \) at position \( i \) and the orbital \( \nu \) at position \( j \), and \( t_0 \) is the chemical potential. The pairing parameter \( \Delta_{ij\mu} \) and the local electron densities \( \langle n_{i\mu\sigma} \rangle \) and \( \langle n_{i\bar{\mu}\bar{\sigma}} \rangle \) satisfy the following self-consistent conditions

\[ \Delta_{ij\mu} = \frac{V_{ij\mu}}{4} \sum_n \left( u_{i\mu\sigma}^n u_{j\nu\sigma}^n + u_{j\nu\sigma}^n u_{i\mu\sigma}^n \right) \tanh(\frac{E_n}{2k_B T}) \]

\[ \langle n_{i\mu\sigma} \rangle = \sum_n |u_{i\mu\sigma}^n|^2 f(E_n) \]

\[ \langle n_{i\bar{\mu}\bar{\sigma}} \rangle = \sum_n |u_{i\bar{\mu}\bar{\sigma}}^n|^2 [1 - f(E_n)] \]

where \( V_{ij\mu} \) is the pairing strength and \( f(x) \) is the Fermi-Dirac distribution function. The SC order parameter at position \( i \) is defined as \( \Delta_i \equiv \frac{1}{4} (\Delta_{i+1} + \Delta_{i-1} + \Delta_{i+\bar{\mu}} + \Delta_{i+\bar{\mu}} - 2 \Delta_{i+\bar{\mu}} + \Delta_{i+\bar{\mu}}) \), the local magnetic moment at position \( i \) is defined as \( m_i \equiv \frac{1}{2} \sum_{\mu}(\langle n_{i\mu\sigma} \rangle - \langle n_{i\bar{\mu}\bar{\sigma}} \rangle) \), and the total charge density at position \( i \) is defined as \( \langle n \rangle_i \equiv \sum_{\mu}(\langle n_{i\mu\sigma} \rangle + \langle n_{i\bar{\mu}\bar{\sigma}} \rangle) \). The chemical potential \( t_0 \) is determined by the electron filling per site \( n \) (\( n = 2 + x \)), and for the value of the hopping terms \( t_{ij\mu} \), are assumed to be \( t_{1-4} = 1.0, 4, -2.0, 0.04 \) \([13, 14]\). Only the electron pairings of the same orbital between the nearest-neighbor Fe sites are considered. For example, we choose \( V_{ij\mu} = 1.4 \) for \( \mu = \nu \) and \( |i - j| = 1 \), and zero for all other cases. This choice of the pairing potential implies that the SC order has \( s_\pm \)-wave symmetry \([15, 16]\).

The phase diagram of the electron-doped Ba(Fe\(_{1-x}\)Co\(_x\)As\(_2\)) \(_2\) compounds as a function of temperature \( T \) and doping \( x \) has been qualitatively mapped out with \( U = 3.4 \) and \( J_H = 1.3 \) \([14]\). When both \( T \) and \( x \) are small, 2x1 collinear AF order is found, with SC order uniformly distributed over the sample. However, this AF order is unstable against the formation of the 90° magnetic DWs oriented 45° from the x-axis as the strength of \( U \) is increased to \( U = 4.8 \) for small \( x \) at \( T = 0 \) \([12]\). In the following, the spatial profiles of the magnetic, SC and charge density order near four different types of TB at \( T = 0 \) will be investigated. Throughout this work, we set \( x = 0.04 \), \( U = 3.8 \) and \( J_H = 1.3 \). Note that DWs do not form spontaneously in the absence of TBs at these parameter values, instead the superconducting and charge density orders are uniform and AF order exists.

### A. Diagonal TB of the Lattice

The lattice in the Fe-plane of these compounds is almost square, having slightly different lattice constants \( a \) and \( b \) along \( x \)- and \( y \)-directions \([17]\). TBs can thus be formed by exchanging the lattice constants \( a \) and \( b \) on the opposite side of the TB. Figure 1(a) shows the structure of a single such TB oriented at 45° with respect to the x-axis. Since there is only a small difference in the magnitudes of \( a \) and \( b \), this TB can be accounted for by assuming slightly different nearest neighbor hopping terms \( t_a = 1.0 \) and \( t_b = 1.2 \). To analyze the effects of this type of TB, we considered a 28x28 lattice with periodic boundary conditions divided into 4 different domains separated by three parallel TBs (not shown) along the lines \( y = x + 14 \), \( y = x \) and \( y = x - 14 \). As shown in Fig.1(b), there are three 90° DWs formed and pinned on the TBs. The patterns of these quantities are very similar to those found in \([12]\) without the TBs (see Fig.2(a) to 2(c) in \([12]\)). However, in this case, the DW forms with a smaller value of the effective Coulomb interaction \( U \), indicating that the existence of this type of TB is beneficial to the formation of the 90° DWs. The solutions presented in Fig.1 are always stable against the uniform 2 \( \times \) 1 collinear AF order \([14]\).

Similar to the results without TBs \([12]\), the SC as well as the charge density get significantly enhanced on the DWs, which occur at the TBs, and suppressed in the middle of the magnetic domains (see Fig.1(c) and 1(d)). All of this is in good agreement with experiments \([14, 11]\). It is important to note that the lattices on both sides of the TB should be well matched at the TB, and that each of the unit cells along the TB is only slightly deformed from the square shape. Thus, we do not expect that scattering of the electrons from any disorder due to the TB would be strong.
B. Parallel TB of the Lattice- A TB formed by exchanging the $a$ and $b$ lattice constants can also be oriented parallel to the $x$- or $y$-axis (as shown in Fig.2(a)). We studied this case by considering a a $28 \times 28$ lattice with periodic boundary conditions divided into 3 different domains separated by two TBs (not shown) along the lines $x = 7$ and $x = 20$.

Here the magnetic DWs are pinned at the TBs (see Fig.2(b)) on which weak local ferromagnetic order appears. The SC has a periodic modulation and is enhanced on the DWs, but suppressed in the middle of the magnetic domains (see Fig.2(c)). A charge density wave appears near the DWs (see Fig.2(d)) while the electron density gets suppressed in the middle of the magnetic domains. It is important to point out that in this case, the lattices on the opposite sides of a TB are not well matched. Therefore, there may be considerable scattering of the electrons due to the disorder near these TBs. If this effect is included, we expect that the SC would get suppressed, instead of being enhanced, on the DWs and the TBs.

C. Parallel twin boundary due to the asymmetry of As atoms- Another possible TB can be generated by slipping the lattice constant along the $y$-direction with respect on the lattice on the left of the TB. There are two different types of As atoms in our model, we label them as As(up) and As(down) atoms relative to the Fe plane. This can be clearly seen from Fig.3(a), in which the TB is represented by the red-dashed line. The crystal lattice for the FeAs layer has $D_{2d}$ symmetry, namely the 4 nearest neighboring As atoms of a "down" As atom should be all "up". The hopping terms between the next-nearest-neighbor Fe ions via the hybridization of the 4p orbital with the As atom in the middle should have different values depending on whether the As atom is above ($t_2$) or below ($t_3$) the Fe plane. The $D_{2d}$ symmetry is broken by the presence of the TB. We considered a $28 \times 28$ lattice with periodic boundary conditions divided into three domains by two TBs located at $x = 7$ and $x = 20$ (not shown). The lattice constants are both $a$ along $x$- and $y$-axis. Figure 3(b) shows the magnetic order is enhanced near the TBs. Defining the magnetic DWs to be where the magnetic order is suppressed, that is, near the middle between two TBs, then, clearly, the DWs are not located at the TBs. On the opposite sides of a DW, there is no change in the magnetic phase, thus we could label the DWs as the 0° DWs. Figure 3(c) shows that the SC is enhanced along the DWs, and that it is suppressed near the TBs. Figure 3(d) shows that the electron density is depleted near the TBs. Apparently, the depleted electron density leads to strong magnetic order that suppresses the SC order. On the DWs, the electron density appears to be close to optimal doping and thus SC gets enhanced.

D. Diagonal twin boundary due to the asymmetry of As atoms- A TB due to missing one line of the lattice contains of both Fe and As(down) atoms oriented along 45° from the x-axis is shown in Fig.4(a). The $D_{2d}$ sym-
Figure 4: (a) The lattice structure near a twin boundary (red dashed line) with misplacing the As atoms along diagonal (or 45°) direction. The open circles represent the positions of Fe atoms, and the red and blue dots respectively denote the As(up) and As(down) atoms. Corresponding spatial profiles of (b) the magnetic order, (c) the superconducting order, and (d) the charge density order are presented.

The symmetry of the lattice is also broken by the presence of this TB. Note that the geometry of this TB is fundamentally different from the one showed in Fig.3(a) since the TB does not pass through any of the Fe or As atoms. To study this case, we considered a 30×30 lattice with periodic boundary conditions and three identical TBs oriented 45° from the x-axis (not shown). The TBs are located along y = x − 15, y = x and y = x + 15.

Different from the case in Fig.3(b), the magnetic order shown in Fig.4(b) is suppressed along the TBs where DWs are located. The magnetic domain between the TBs still has the usual 2×1 collinear AF structure, except the magnetic moments are strongly and periodically modulated along the x-axis, which may be due to finite size effects of the TB and the distance between two nearest neighboring TBs. It also appears that the local 2×1 collinear AF structure is replaced by a stripe-like 2√2×2√2 AF structure oriented 45° from the x-axis. Furthermore, the SC is enhanced in these regions (see Fig.4(c)). From Fig.4(d), note that on the TBs or DWs the carrier density is corresponding to that in the overly hole-doped case \( x \approx -0.3 \), which explains why the magnetic and SC orders are both suppressed on both sides of the TB. Interestingly, stripe-like charge density waves oriented 45° from the x-axis occur on both sides of each TB.

Our work has considered the effects of TBs on the complex interaction of magnetism and superconductivity in Fe-pnictides. There are three points that need to be emphasized here. First, the formation and the location of the DWs are strongly related to the nature of TBs. For the four kinds of TBs studied here, the DWs in cases A, B and D are found to be pinned at the TBs, while in case C the DWs are separated from the TBs. Second, the formation of the DWs implies that the magnetism is inhomogeneous. This inhomogeneity strongly affects the SC and the electron density distribution. In cases of A, B and C, the SC is enhanced in the regions where \( m_i \) is suppressed and \( \langle n_i \rangle \) is enhanced. The reasons for the enhancement of SC are (i) the competition between the SC and magnetism, and (ii) the \( \langle n_i \rangle \) in the enhanced regions is close to the optimal doping level. However in case D, on the DWs where the \( m_i \) is suppressed, the electron density is close to over(hole)-doping level, which is unfavorable to SC. As a result, SC coexists with the magnetism in the middle of magnetic domains. Finally, we point out that our results on the diagonal TB of the lattice (see Fig.1) are in good agreement with experiments \[10, 11\]. In a very recent scanning tunneling microscopy (STM) experiment for FeSe \[20\] similar types of the TBs were detected but the SC was suppressed on the TBs. This may be caused by the differences in lattice structures and Fermi surface topologies of the two materials. We also find that the Coulomb-interaction-induced anti-phase DWs, as predicted in \[8\] and measured indirectly in nuclear magnetic resonance (NMR) experiments \[21\], always have higher ground energies than those of the 2x1 collinear AF order and the 90° DW structures. These anti-phase DWs could form metastable states and may occur under certain conditions. In the present work we assume the lattices are well matched at the TBs. In the case that the lattice on both sides of the TB are not well matched, the SC could be suppressed by disorder scattering along the TBs. This issue deserves further investigation.

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