Influence of the Fermi surface geometry on a Josephson effect between an iron-pnictide and conventional superconductors

A. A. Kalenyuk\textsuperscript{1,2}, E. A. Borodianskyi\textsuperscript{1}, A. A. Kordyuk\textsuperscript{2,3}, and V. M. Krasnov\textsuperscript{1,4}

\textsuperscript{1}Department of Physics, Stockholm University, AlbaNova University Center, SE-10691 Stockholm, Sweden;
\textsuperscript{2}Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine;
\textsuperscript{3}Kyiv Academic University, 03142 Kyiv, Ukraine; and
\textsuperscript{4}Moscow Institute of Physics and Technology, State University, 141700 Dolgoprudny Russia.

We study Josephson junctions between a multi-band iron-pnictide Ba\textsubscript{1−x}Na\textsubscript{x}Fe\textsubscript{2}As\textsubscript{2} and conventional s-wave superconductors Nb and Cu/Nb bilayer. We observe that junctions with a Cu interlayer exhibit much larger $I_c R_n$ despite a weaker proximity-induced superconductivity. This counterintuitive result is attributed to the difference in Fermi surface geometries of Nb and Cu, which leads to a selective one-band tunneling from Cu and a non-selective multi-band tunneling from Nb. The latter leads to a mutual cancellation of supercurrents due to the sign-reversal $s_\pm$ symmetry of the order parameter in the pnictide. Our results indicate that Fermi surface geometries play a crucial role for pnictide-based junctions. This provides a new tool for phase sensitive studies and paves a way to a conscious engineering of such junctions.

Electronic structure of superconductors is usually quite complicated, even for low-$T_c$ materials, such as the transition metal Nb. Nevertheless, a simple description of Josephson effects, which does not take into account complex Fermi surface (FS) geometry, works remarkably well for conventional superconductors \cite{1,2}. This happens because probabilities of electron and Cooper-pair tunneling are similar \cite{3}. Together with a momentum-independent s-wave energy gap, $\Delta$, it leads to the inverse relationship between the normal resistance, $R_n$, and the critical current, $I_c$. Thus, the $I_c R_n$ product becomes a universal function of $\Delta$, independent of FS geometry \cite{4}.

This universality, however, breaks for unconventional multi-band superconductors. A particularly drastic deviation should occur in the case of sign-reversal order parameter $s_\pm$ \cite{5,8}. This occurs in cuprate and iron-based superconductors, which are believed to have d-wave \cite{9,10} and $s_\pm$ \cite{11,13} symmetries, respectively. In this case, $I_c$ depends on gap values in each band, and the $I_c R_n$ is bandstructure-sensitive and not universal \cite{5,8,15}.

In this work we fabricate and study high-quality Josephson junctions (JJ’s) between single crystals of an iron-pnictide Ba\textsubscript{1−x}Na\textsubscript{x}Fe\textsubscript{2}As\textsubscript{2} (BNFA) and conventional low-$T_c$ superconductors made of either Nb film or Cu/Nb bilayer. Both types of JJ’s exhibit clean and clear Josephson phenomena. However, JJ’s with a Cu interlayer exhibit almost two orders of magnitude larger $I_c R_n$, despite a weaker proximity-induced superconductivity in Cu. This counterintuitive result is attributed to the difference in FS geometries of Nb [multiple FS’s at various parts of the Brillouin zone (BZ)] and Cu [a single quasi-spherical FS]. Therefore, tunneling from Nb takes place into all bands of BNFA. Due to the sign-reversal $s_\pm$ order parameter in BNFA, this leads to a mutual cancellation of supercurrents and a very small $I_c R_n \sim 3 \mu$V. To the contrary, tunneling from Cu occurs predominantly into one sub-band avoiding such cancellation and leading to a significantly larger $I_c R_n \sim 200 \mu$V. Our results indicate that FS geometries play a crucial role for JJ’s with multi-band, sign-reversal superconductors. This provides a new tool for fundamental studies of unconventional superconductivity and opens a possibility for optimization and adjustment of junction characteristics.

Figure 1(a) represents a scanning electron microscope (SEM) image of the BNFA-Cu/Nb sample. Our samples contain six junctions made on a freshly cleaved BNFA single crystal. Fig. 1(b) shows a closeup of the junction. Here the vertical strip represents the window in SiO\textsubscript{2} isolation layer and the horizontal strip - the top contact electrode. Micrometer-size JJ’s are formed at the overlap between the two strips. As the top electrode we use either pure Nb film ($\sim 200$ nm thick) or Cu(15 nm)/Nb(180 nm) bilayer deposited by magnetron sputtering in a single cycle without breaking vacuum. Details of sample fabrication, experimental setup and a list of JJ parameters can be found in the Supplementary.

Multiterminal configuration of our samples allows simultaneous measurements of junction and crystal characteristics \cite{23,24}. The blue line in Fig. 4(c) shows the in-plane resistive transition of BNFA. At $T \sim 150$ K there is a kink in $R(T)$, corresponding to a structural transition and spin-density-wave (SDW) ordering \cite{12,14}. The superconducting transition occurs at $T_c$ (BNFA) $\sim 30$ K. Observation of the SDW state and the slightly sub-optimal $T_c$ indicate that the BNFA crystal is moderately underdoped. The red line in Fig. 4(e) shows a simultaneously measured resistive transition of a junction. It has two steps, first at $T_c$ (BNFA) and the second at $T_c$(Nb) $\sim 9$ K.

Figs. 1(d) and (e) show current-voltage (I-V) characteristics at different $T$ for (d) BNFA-Nb and (e) BNFA-Cu/Nb JJ’s. In both cases the I-V’s have the shape typical for resistively shunted JJ’s \cite{11,2} with a well defined $I_c$ and $R_n$. Green, blue and red curves are measured at zero field. The wine-color line in Fig. 1(d) shows the I-V at $T \sim 0.3$ K, measured at in-plane magnetic field of...
$B_0 = 15 \text{ mT}$. It is seen that $I_c$ is completely suppressed by a small parallel field, much smaller than the upper critical fields of BNFA $^{[23, 25]}$ and Nb $^{[26]}$. Therefore, in such a field we can carefully measure temperature dependence $R_n(T)$, as shown in Fig. 1 (f). The modest upturn of $R_n$ with decreasing $T$ is quite common for c-axis characteristics of high-$T_c$ superconductors, commonly associated with a pseudogap $^{[27]}$.

Suppression of $I_c$ by small parallel field is caused by flux quantization in the junction. Figure 2 (a) shows $I_c(H_{\parallel})$ modulations at different temperatures for a BNFA-Cu/Nb JJ. Fig. 2 (b) represents normalized $I_c/I_c(0)$ versus flux curves for BNFA-Nb (blue) and BNFA-Cu/Nb (red) JJ’s at low $T$. Both types of JJ’s exhibit clear Fraunhofer modulation depicted by the black line. This is a figure of merit indicating good uniformity of JJ’s $^{[1, 2]}$.

Figure 2 (c) shows $I$-$V$ curves of a BNFA-Cu/Nb JJ without (black) and with (red) applied high-frequency electromagnetic radiation at $f \approx 74 \text{ GHz}$ at $H = 0$ and $T \approx 0.4 \text{ K}$. A clear Shapiro step is seen at $V_1 = hf/2e$. Fig. 2 (d) shows the normalized differential conductance for this $I$-$V$ as a function of $V_1/V$. It reveals numerous subharmonic Shapiro steps. This indicates the strongly non-sinusoidal current-phase relation in the JJ $^{[28]}$, which is indeed anticipated for s-s$_{\pm}$ JJ’s $^{[7, 8]}$. On the other hand, the non-sinusoidality may also be caused by the proximity effect in the Cu/Nb bilayer $^{[29]}$.

Thus, our JJ’s exhibit clean and clear dc- and ac-Josephson effects. The high quality of the JJ’s together with a good reproducibility of junction parameters (see the Supplementary $^{[15]}$) allows us to investigate genuine characteristics of composing them superconductors (as opposed to interface defects). Figs. 2 (e) and (f) show temperature dependencies of (e) the critical current density $J_c$ and (f) the $I_cR_n$ product for both types of junctions. Despite similarities in behavior, the same BNFA crystal $^{[15]}$ and fabrication procedure, the two types of JJ’s exhibit largely (almost by two orders of magnitude) different $I_cR_n$ values. BNFA-Nb JJ’s have a very small $I_cR_n \approx 3 \mu \text{V}$ $^{[24]}$, much smaller than $\Delta/e > 1 \text{ mV}$ in both superconductors, while for BNFA-Cu/Nb JJ’s $I_cR_n \approx 200 \mu \text{V}$. The difference can be clearly seen in the $I$-$V$ curves from Figs. 1 (d) and (e). The reported remarkable influence of the thin Cu interlayer is the key observation of this work.
The increase of $I_cR_n$ in BNFA-Cu/Nb JJ’s is associated with the increase of $R_n$. The latter indicates that the interface transparency, $\beta$, between BNFA and Cu is reduced compared to BNFA-Nb. Yet, as mentioned above, this does not explain the increase of $I_cR_n$ because usually $I_c \propto 1/R_n$, and $I_cR_n$ is independent of $\beta$.

The proximity induced superconducting order parameter in Cu at the junction interface is $\Phi_N = \beta \Psi_S \exp(d_N/\xi_N)$, where $\Psi_S$ is the order parameter in Nb, $d_N = 15$ nm is the Cu layer thickness and $\xi_N$ is the coherence length in Cu. According to Ref. [30], for thin sputtered Cu films $\xi_N \approx 18\sqrt{T_c(Nb)/T}$ (nm), where $T_c(Nb) \approx 9$ K. It gives $\xi_N(0.3K) \approx 100$ nm, $\xi_N(3K) \approx 30$ nm and $\xi_N(T_c(Nb)) \approx 18$ nm. Thus, our Cu interlayer is always thinner than $\xi_N$. Although Cu and Nb films are deposited without breaking vacuum, the Cu/Nb interface transparency is modest, $\beta \approx 0.4$ [30], predominantly due to the FS mismatch between Nb and Cu. Thus the proximity induced order parameter in Cu is smaller than in Nb. For SINS JJ’s (I-insulator, N-normal metal) made of s-wave superconductors, the proximity effect leads to the reduction of $I_cR_n$ [31]. This is opposite to our observation. This discrepancy points out that the unconventional (non-s-wave) symmetry of the order parameter in BNFA plays an essential role. In particular, the extremely small $I_cR_n$ of BNFA-Nb junctions provides evidence for the sign-reversal $s_{\pm}$ symmetry in BNFA, due to which supercurrents from bands with opposite signs of $\Delta$ cancel each other [24].

For a more quantitative understanding we consider FS geometries of involved metals. Figures 3 (a-c) show DFT calculated three-dimensional images of Fermi surfaces for Cu (a), Nb (b) [32, 33] and BNFA (c) [34]. FS of Cu is simple quasi-spherical. The transition metal Nb has a very complex FS with many small pockets spread over the BZ. BNFA has two bunches of the FS sheets, the three large quasi-cylinders in the center and the propeller-like FS’s at the corners of the BZ [35, 36]. Those bunches are believed to have opposite signs of $\Delta$ [12, 13].

Electron tunneling between two metals usually con-
FIG. 3. (Color online). (a-c) The Fermi surface topologies in the 1st Brillouin zone for (a) Cu, (b) Nb and (c) BNFA. (d) and (e) The $k_z$-integrated projections of Fermi surfaces on the (001) plane for Cu (d) and Nb (e). (f) and (g) The same projections averages over the in-plane momentum angle, representing the effective ($k_z$-integrated) density-of-states distribution for poly-crystalline Cu (f) and Nb (g) films. (h) and (i) Product of $k_z$-integrated Fermi surface projection of BNFA with effective density-of-states for Cu (h) and Nb (i). It can be seen that for BNFA-Cu junctions tunneling current flows predominantly into the propeller-like corner bands of BNFA (h). On the other hand, for BNFA-Nb junctions the tunneling current is distributed relatively uniformly between central and corner bands.

serves the in-plain momentum $k_\parallel = (k_x, k_y)$. Therefore, the total single-electron current can be written as

$$J \propto \oint T_{12}^2 A_1(k_{z1}, k_\parallel) A_2(k_{z2}, k_\parallel) (f_1 - f_2) dk_\parallel dk_{z1} dk_{z2},$$

where $T_{12}$ is the tunneling matrix element between initial and final states, $(k_{z1}, k_x, k_y)$ and $(k_{z2}, k_x, k_y)$, in the two electrodes, $A_{1,2}$ are the spectral functions (momentum-dependent density of states) and $f_{1,2}$ are the corresponding distribution functions. The key band-structure-dependent factor is the density of states projection on the junction plane, which can be integrated independently

$$N_i(k_\parallel) = \int A_i(k_{z1}, k_\parallel) dk_{z1},\ (i = 1, 2). \quad (1)$$

Figs. 3(d) and (e) show such projections for Cu and Nb. The corresponding projection for BNFA is pretty similar to the pattern, shown in Fig. 3(i).

For comparison with experiment we must take into account the polycrystalline structure of Cu and Nb ele-
todes and make an average with respect to random crystalline orientation. This is similar to averaging with respect to rotation of \( k_{x,y} \) axes. Figs. 3(f) and (g) show thus averaged projections, \(<N_{Cu}(k_x,k_y)>\) for polycrystalline Cu and Nb. The key difference is that due to the quasi-spherical FS of Cu, the polycrystalline density of states projection keeps the circular shape with the radius given by the Fermi momentum. To the contrary, averaging for multi-band polycrystalline Nb leads to a more uniform distribution of the density of states.

Figs. 3(h) and (i) show a product of the density of state projections \(<N_{Cu}(k_x,k_y)>N_{BNFA}(k_x,k_y)\) for BNFA-Cu/Nb and \(<N_{Nb}(k_x,k_y)>N_{BNFA}(k_x,k_y)\) for BNFA-Nb junctions. It gives a hint about contribution of the two BNFA bands in electrical current through the junction. For BNFA-Nb JJ’s both BNFA bands participate approximately equally due to fairly uniform distribution of \(<N_{Nb}(k_x,k_y)>\) in the BZ projection, Fig. 3(g). To the contrary, the highly non-uniform, circular-shape \(<N_{Cu}(k_x,k_y)>\), Fig. 3(f), blocks tunneling into the central band of BNFA.

For calculation of supercurrent, \( A_i \) should be replaced by \( A_i\Psi_i \), where \( \Psi_i \) is the superconducting order parameter in the corresponding metal. For Nb and Cu/Nb with s-wave order parameter \( \Psi \) is just a number. However, for the unconventional two-band superconductor BNFA, which likely has the \( s_{\pm} \) symmetry, \( \Psi \) changes sign between central and corner bands. For BNFA-Nb JJ’s with similar transport contribution of the two bands this leads to an almost complete cancellation of the total supercurrent [24]. However, for BNFA-Cu/Nb JJ’s the cancellation is much smaller because tunneling from central bands is suppressed. Therefore, such analysis qualitatively explains larger values of both \( R_n \) and \( I_cR_n \) in BNFA-Cu/Nb junctions.

To conclude, we fabricated and studied high-quality Josephson junctions between an iron-pnictide superconductor \( \text{Ba}_{1-x}\text{Na}_x\text{Fe}_2\text{As}_2 \) and either a conventional low-\( T_c \) superconductors Nb or a Cu/Nb bilayer. Remarkably, we observed that addition of a very thin (15 nm) Cu interlayer changes drastically junction properties and, in particular, increases the \( I_cR_n \) product by almost two orders of magnitude. The latter is opposite to expectations for proximity-coupled junctions made of conventional s-wave superconductors [31]. This counterintuitive result adds to evidence for the unconventional \( s_{\pm} \) symmetry of the order parameter in the pnictide. The phenomenon is explained qualitatively taking into account particular Fermi surface geometries of involved metals. It is shown that the multi-band structure of Nb leads to similar contributions of both pnictide bands into electron transport, which due to the sign-reversal \( s_{\pm} \) superconducting order parameter in the two electronic bands of the pnictide, leads to the cancellation of the total supercurrent and results in a very small \( I_cR_n \simeq 3 \, \mu \text{V} \) [24]. To the contrary, the simple quasi-spherical Fermi surface of Cu supports tunneling predominantly from only one band, avoiding the supercurrent cancellation and resulting in much larger \( I_cR_n \simeq 200 \, \mu \text{V} \). Our results indicate that unlike for junctions made of conventional s-wave superconductors, for junctions with unconventional sign-reversal superconductors the Fermi surface geometry plays a crucial role. This provides a new tool for phase sensitive studies of such materials and could probably explain some of reported variations of \( I_cR_n \) values in pnictide JJ’s [31][24][37]. The reported material-dependence of tunneling into pnictide superconductors can be used for optimization and conscious engineering of pnictide-based Josephson junctions.

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*Vladimir.Krasnov@fysik.su.se*

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