Intergrain Josephson Currents in Multigap Superconductors: Microscopic Origin of Low Intergrain Critical Current and Its Recovery Potential in Iron-Pnictide Materials

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We microscopically examine the intergrain Josephson current in iron-pnictide superconductors in order to solve the puzzle of why the intergrain current is much lower than the intragrain one. The theory predicts that the intergrain Josephson current is significantly reduced by the ±s-wave symmetry when the incoherent tunneling becomes predominant and the density of states and the gap amplitude between two bands are identical. We find in such a situation that the temperature dependence of the intergrain Josephson current shows an anomalously flat curve over a wide temperature range. Finally, we suggest important points for increasing the intergrain current.

Since the discovery of iron-pnictide superconductors, their application potential has been intensively argued. It is now widely accepted that they have several advantages as superconducting wires, tapes, and cables due to high transition temperature, rich material varieties, and weak anisotropy. However, an issue crucial for the transport applications of iron-pnictide superconductors has been reported by several groups. In polycrystalline samples, although the superconductivity is sufficiently strong inside each grain, the bulk critical current is unexpectedly small. This experimental finding indicates that the bulk critical current is limited by intergrain currents over the grain boundaries in polycrystalline samples.

In polycrystalline samples of high-$T_c$ cuprates and conventional superconductors, the intergrain coupling at the grain boundaries has been a key topic in assessing their transport applicability. Hence, it is also important in iron-pnictide superconductors to examine the intergrain coupling and understand their own physics.

In this study, we investigate the superconducting tunneling current at the grain boundaries in polycrystalline samples of two-band superconductors described by the two-band BCS Hamiltonian. We show that the intergrain Josephson current is largely suppressed when the Cooper pair symmetry is ±s-wave, together with some conditions. On the basis of this result, we propose that the bulk critical current is limited by the reduction mechanism due to the ±s-wave symmetry in iron-pnictide superconductors. The limitation is significant when polycrystalline samples are regarded as a Josephson-coupled assembly of superconducting grains. In addition, we discuss strategies for increasing the intergrain critical current.

Throughout this study, we concentrate on a weak-link formed between two grains and evaluate its intergrain current, assuming the ±s-wave gap symmetry. As shown in Fig. 1, the weak-link is regarded as a one-dimensional Josephson junction sandwiched by two superconducting plates. We microscopically calculate the Josephson critical current density $J_c$. Such a basic study is necessary prior to examining an ensemble of weak-links.

It is known that in Josephson junctions there are two tunneling processes depending on junction quality. One is incoherent tunneling, which does not conserve the momentum of quasi-particles at the tunneling process. This process takes place in junctions with diffusive interfaces. The other is coherent tunneling, in which the momentum of the quasi-particles is conserved. In most artificially made Josephson junctions, the incoherent tunneling is predominant, while in high-$T_c$ intrinsic Josephson junctions such as Bi$_2$Sr$_2$CaCu$_2$O$_{8+}$, the coherent tunneling should be considered as a relevant process in the c-axis transport. In this study, we calculate the intergrain Josephson current by taking account of both the processes.

In a Josephson junction between multigap (typically two-gap) superconductors, two channels are possible in the incoherent tunneling, i.e., intra- and inter-band tunneling channels. In the intra (inter)-band tunneling, Cooper pairs can tunnel between identical (different)

![FIG. 1: (Color online) Schematic figure of a polycrystalline sample (left-hand side) and focus of an intergrain Josephson junction between two-gap superconducting grains (right-hand side), in which two incoherent tunneling channels are schematically depicted.](image-url)
bands in the left and right superconductors, as seen in Fig.1, in which the solid (dashed) arrows indicate the intra (inter)-band Cooper pair tunneling. On the other hand, we note that no interband channel exist in the coherent tunneling.

Let us now investigate the Josephson coupling between the two-gap superconductors as depicted in Fig.1. We calculate the Josephson critical current $J_c$ in two cases of the gap symmetry, i.e., $\pm s$-wave and $s$-wave with no sign change, to show the significant reduction in $J_c$ in the $\pm s$-wave case. The tunneling Hamiltonian in the present system is written as

$$\hat{H}_T = \sum_{a,b,\sigma} \int d^3r \int d^3r' [T_{r,r'}^{(ab)} \hat{\psi}_{\sigma 1}^\dagger (r) \hat{\psi}_{\sigma 2} (r') + \text{h.c.}],$$

(1)

where $\hat{\psi}_{\sigma 1}$ is the field operator for electrons with spin $\sigma (\pm 1, 1)$ in the $a$-th band in the $\ell$-th grain ($\ell = 1, 2$). We assume that the tunneling matrix element $T_{r,r'}^{(ab)}$ is real. To describe the tunneling processes explicitly, we introduce the momentum representation of $T_{r,r'}^{(ab)}$. The Fourier component $T_{k,k'}^{(ab)}$ is expressed as $T_{k,k'}^{(ab)} = \delta_{ab} \delta_{kk'} T_k^{(aa)} + T_{k,k'}^{(ab)}$. The first (second) term corresponds to the coherent (incoherent) tunneling. The incoherent tunneling usually gives a principal contribution in conventional Josephson junctions. In iron-pnictide polycrystalline systems composed of randomly oriented grains with rough boundaries, one expects a similar situation, i.e., the incoherent tunneling is predominant. We examine just such a case, in which a tiny coherent tunneling in addition to a predominant incoherent tunneling exists. As shown below, the coherent tunneling alters not only the critical current but also its temperature dependence.

Josephson coupling energy is derived on the basis of the second order perturbation theory with respect to $\hat{H}_T$. In this study, we assume for simplicity that $(T_{k,k'}^{(ab)})^2$ is expressed as

$$(T_{k,k'}^{(ab)})^2 \approx T^2 [w \delta_{ab} \delta_{kk'} + (1-w)] \quad (0 \leq w < 1).$$

(2)

In the following, we examine the dependence of intergrain critical current on the nature of the grain boundary interface, i.e., $w$ (ratio of the coherent tunneling to incoherent tunneling) dependence.

On the basis of the standard method employed in several studies, the Josephson coupling energy between the two grains is given by

$$E_J = -\sum_{a,b} (\delta_{ab} J_{\text{coh}}^{(ab)} + J_{\text{incoh}}^{(ab)}) \cos (\varphi_2^{(b)} - \varphi_1^{(a)}),$$

(3)

where

$$J_{\text{coh}}^{(ab)} = w T^2 N_a^2 2 \pi \epsilon_F L (\beta \Delta_a),$$

$$J_{\text{incoh}}^{(ab)} = (1-w) T^2 N_a N_b \pi^2 \Delta_b^{ab} K (k; \beta \Delta_b^{ab}),$$

$\Delta_b^{ab}$ is the density of states (DOS) on the Fermi surface for the electron of the $a(b)$-th band, $\epsilon_F$ is the Fermi energy, and $\beta = (1/k_B T)$ is the inverse temperature. The amplitude of the $a(b)$-th order parameter is written as $\Delta_a (\Delta_b) > 0$. We define $\Delta_b^a (\Delta_b)$ as $\Delta_b^{ab} = \min (\Delta_a, \Delta_b)$ ($\Delta_b^a = \max (\Delta_a, \Delta_b)$).

Clearly, $\Delta_b^a = \Delta_b^a$. The $a$-th superconducting phase in the $\ell$-th grain is expressed as $\varphi_\ell^{(a)}$. The functions $L(\nu)$ and $K(k; \nu)$ are, respectively, defined as

$$L(\nu) = \int_0^{\pi/2} du \ln \left( \frac{\nu}{2 \cos u} \right),$$

$$K(k; \nu) = \frac{2}{\pi} \int_0^1 \frac{1}{\sqrt{(1-k^2 u^2)(1-u^2)}} \tanh \left( \frac{\nu \sqrt{1-k^2 u^2}}{2} \right).$$

(6)

(7)

Here, we note that the difference of chemical potentials between the grains is assumed to be zero as deriving Eq. (4).

Let us evaluate the intergrain critical current from $E_J$. First, we define the $a$-th band superconducting phase difference between the two grains as

$$\gamma^{(a)} = \varphi_2^{(a)} - \varphi_1^{(a)}.$$  

(8)

In term of $\gamma^{(a)}$, we find that

$$\varphi_2^{(1)} - \varphi_2^{(2)} = \gamma^{(1)} + \chi_1,$$

$$\varphi_2^{(2)} - \varphi_1^{(1)} = \gamma^{(2)} - \chi_1,$$

(9)

(10)

where $\chi_\ell$ is the relative phase difference between the two order parameters in the $\ell$-th grain. The pairing symmetry in iron-pnictide superconductors is presently expected to be the $\pm s$-wave symmetry. In addition, the recent experiments of the magneto optical images...
show that superconductivity grows inside each grain. Thus, we can naturally assume that $\chi_\ell$ should be rigidly fixed as $\pi$. This indicates that $\varphi_2^{(1)} - \varphi_1^{(2)} = \gamma^{(2)} + \pi$, $\varphi_2^{(1)} - \varphi_1^{(1)} = \gamma^{(1)} - \pi$, and $\gamma^{(1)} = \gamma^{(2)}$ up to modulo $2\pi$. Then, we have $E_3 = -J_c \cos \gamma^{(1)}$, where

$$J_c = \sum_a \left( J^{(aa)}_{\text{coh}} + J^{(aa)}_{\text{incoh}} \right) + \left( -1 \right)^\eta \left( J^{(11)}_{\text{coh}} + J^{(21)}_{\text{incoh}} \right),$$

and $\eta = 1$ for the $\pm s$-wave symmetry. In Eq. (11), we find a cancellation mechanism between the currents in the incoherent tunneling channels, i.e., a cancellation between $J^{(aa)}_{\text{incoh}}$ and $J^{(ab)}_{\text{incoh}}$ ($a \neq b$) [Fig. 2] for the $\pm s$-wave symmetry. We remark that for the $s$-wave with no sign change, we have $\eta = 0$ and no cancellation. At $T = 0$, we have an explicit formula for $J_c(T = 0)$ as a function of $w$,

$$J_c(T = 0) = (1-w) J_0 \frac{1 - (-1)^\eta r}{1 + r} + w\sigma_n \frac{3\hbar e^2}{4c^2},$$

where

$$J_0 = \frac{\sigma_n \pi \hbar}{4c^2} N_1^2 \Delta_1 + N_2^2 \Delta_2 + 2\kappa N_1 N_2 \Delta_1^{1/2},$$

$$\sigma_n = \frac{4\pi e^2}{\hbar} T^2 (N_1 + N_2)^2,$$

$$r = \frac{2\kappa N_1 N_2 \Delta_1^{1/2}}{(N_1^2 \Delta_1 + N_2^2 \Delta_2)},$$

and $e$ is the charge of an electron. The positive number $\kappa (\leq 1)$ is given by $\kappa = 2K(k)/\pi$, where $K(k)$ is the complete elliptic integral of the first kind. The factor $J_0$ is the intergrain critical current for $w = 0$ (i.e., incoherent tunneling only), and $\sigma_n$ is the normal electron conductivity determined by the incoherent tunneling.

Here, let us evaluate $J_c$ in the limiting case, i.e., $w = 0$ and $T = 0$, in more detail. Figure 3 shows that the $\pm s$-wave symmetry leads to the significant suppression of $J_c$ compared with the $s$-wave symmetry. The suppression ratio of the critical current to $J_c(=\sigma_n \pi \hbar \Delta_1(0)/4c^2)$, which corresponds to the intergrain $J_c$ in the single-gap ($\Delta_1$) superconducting case, strongly depends on the differences between the DOS and the gap magnitudes of the two bands. The theory predicts that the perfect identity of the superconducting and normal properties between the two different bands (i.e., $N_1 = N_2$ or $\Delta_1 = \Delta_2$) leads to a great suppression for the $\pm s$-wave.

The marked suppression due to the $\pm s$-wave symmetry requires equivalence between the corresponding two bands. However, the equivalence is not perfect in real iron-pnictide superconductors, since several experiments suggested that two (in reality more than two) different magnitude gaps coexist in such materials. As for Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$, one can find two gaps in hole-like bands, $\Delta_\alpha$ and $\Delta_\beta$, and one gap in an electron-like band, $\Delta_\gamma$, where $|\Delta_\alpha| \approx |\Delta_\beta| \approx |\Delta_\gamma| \approx 0.5$. One can find that SmFeAsO$_{1-x}$F$_x$ has two different-magnitude gaps, although their relevance to the band structure remains unclear. The value of $N_2/N_1$ is also not equal to 1. From the first-principles calculation of the electronic structures, we can find that, for LaFeAs (BaFe$_2$As$_2$), the DOS’s in the three hole-like bands are 0.24, 0.64, and 0.49 (0.39, 0.64, and 0.49), and the DOS’s in the two electron-like bands are 0.34 and 0.41 (0.42 and 0.38). Information on the gap amplitudes and band structure is crucial in evaluating the effect of the $\pm s$-wave symmetry. In particular, when the very low intergrain critical current density is measured like those in SmFeAsO$_{1-x}$F$_{3.456}$ and Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, it is important to examine the suppression ratio induced by the $\pm s$-wave symmetry.
In the presence of the coherent tunneling, the above situation is markedly altered even if the coherent component is tiny. From Eq. (12), one understands that the incoherent tunneling does not become predominant when \( \Delta_1, \Delta_2 \ll \hbar \omega_f \). We assume that \( \Delta_1(T = 0)/\epsilon_F = 10^{-2} \) and \( \Delta_1(T = 0) > \Delta_2(T = 0) \) hereafter. Figure 3 shows the increase in \( J_c \) by the inclusion of the coherent tunneling. It is clear that the suppressed \( J_c \) rapidly recovers by incorporating a small fraction of the coherent tunneling. We also find that the temperature dependence of \( J_c \) shows characteristic features. Here, we note that the temperature dependence of each superconducting gap is assumed to obey the weak coupling isotropic BCS-type theory. We use the approximate formula\(^2\), \( \Delta_n(T) = \Delta_n(0) \tanh \{1.82[1.018(T_c/T - 1)]^{0.51}\} \). When \( w = 0 \) and \( N_1 = N_2 \), the temperature dependence of \( J_c \) is almost constant over a wide range of temperature. This behavior arises from two facts. First, the incoherent inter-band Josephson currents obey almost equivalent temperature dependences over a wide temperature range when \( N_1 = N_2 \). This means that their rates of decrease with respect to temperature are almost equal. Secondly, the cancellation between them due to the \( \pm s \)-wave occurs in Eq. (11). Thus, as the two conditions are satisfied, such an anomalous temperature dependence becomes observable. Hence, one can roughly determine the gap symmetry (\( \pm s \) or \( s \)) and the incoherent tunneling ratio from the temperature dependence of \( J_c \).

When the incoherent tunneling is predominant, the suppression and temperature dependence of \( J_c \) strongly depend on \( \Delta_2/\Delta_1 \) and \( N_2/N_1 \). The suppression rate of \( J_c \) to \( J_s \) is 0.004 for \( N_2/N_1 = 1 \) and \( \Delta_2/\Delta_1 = 0.8 \) [Fig. 3(a)]. When \( \Delta_2/\Delta_1 = 0.8 \), we can find that \( J_c/J_s \) is the suppression of the \( \pm s \)-wave are 0.06, 0.19, and 0.39, respectively, for \( N_2/N_1 = 0.67, 0.42, \) and 0.25. The flat temperature dependence of \( J_c \) in Fig. 3(a) is observed when \( N_1 \sim N_2 \).

Finally, let us discuss important points to enhance the intergrain critical current. As shown above, the coherent tunneling induces a drastic enhancement of \( J_c \). We emphasize that even if the percentage of the coherent component in the tunneling process is only 0.5%, \( J_c \) becomes about fivefold larger. This can be achieved by improving the weak-link (junction) properties. On the other hand, in the case where no coherent tunneling exists the suppression of \( J_c \) strongly depends on the physical equivalence between the different bands. We have found that quite a large suppression in \( J_c \) occurs when \( \Delta_1 = \Delta_2 \) and \( N_1 = N_2 \) in the \( \pm s \)-wave case. Moreover, we point out that the suppression is not so sensitive to the misorientation angle between neighboring grains due to the full gap compared to the angle-sensitive cuprate-superconductors. This consideration simply indicates that materials with \( \Delta_1 \neq \Delta_2 \) and \( N_1 \neq N_2 \) are preferable in avoiding the large suppression of \( J_c \). Of course, \( J_c \) in real polycrystalline samples depends on the global network structure between grains, and an ultimate solution for solving the weak-link problem at grain boundaries is to grow a quasi-single crystal as large as possible.

In summary, we investigated the intergrain Josephson current in polycrystalline two-band superconductors with the \( \pm s \)-wave symmetry by microscopically deriving the Josephson coupling energy. The present theory reveals that the intergrain Josephson current is significantly reduced by the existence of inter-band tunneling channels when the incoherent tunneling is predominant. We also found the anomalous temperature dependence in the limit at which the incoherent tunneling is predominant. Finally, we discussed the important points for increasing the intergrain Josephson current.

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