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Theory of the electrical transport in tilted layered superconducting Josephson junctions

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We present a theory of the Josephson effect in a twofold-tilted Josephson junction made by d-wave anisotropic layered superconductors. We find the appearance of an intrinsic electrical resistance that arises from the misalignment of the superconductive planes (the CuO_2 planes in YBCO) in the two electrodes. This intrinsic contribution to the tunnel barrier has several nontrivial consequences. The result is relevant for understanding the electric transport properties of [100] tilt and [100] tilt-tilt Josephson junctions based on d-wave superconductors.

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I. INTRODUCTION

Grain boundary Josephson junctions (GBJs) have been fabricated and studied immediately after the discovery of high Tc superconductors.[1] Nonetheless, the mechanism of the supercurrent transport in these devices is still matter of scientific investigation and argument of general physical interest.[2,3] It is well known that the dc Josephson effect can be described by means of a scattering theory using the Bogoliubov-de Gennes (BdG) equations.[4] Characteristic localized states of quasiparticles, known as Andreev bound states, are found in the superconductive energy gap region through which the Josephson supercurrent flows between the two electrodes.[5] This kind of theoretical approach has been successfully used in describing analytically the physics of in-plane grain boundary cuprate Josephson junctions ([001] tilt) where a two-dimensional scattering theory[6–8] finely incorporates both the propagation of the quasiparticles along the Cu-O planes and the anisotropic d-wave-induced symmetry of the pair potential.[9] Moreover, in Ref. 2, a numerical approach, also based on the BdG equations, has enriched the understanding of the role of charge inhomogeneities in limiting supercurrents in [001] GBJs.

However, a number of experiments have been carried out on [100] YBCO GBJs,[10–12] where the Cu-O planes of one or both electrodes are tilted by an arbitrary angle (ϕ_1 and ϕ_2 in Fig. 1) with respect the substrate surface, implying that the relevant geometry of the junction is no longer in-plane. In particular, relatively high values of the $I_c R_n$ products[12–14] have been observed in such YBCO GBJs. [100] junctions seem to be very promising for developing new sensors of radiation in the terahertz band[15,16] and observing macroscopic quantum properties.[17] Indeed Kawabata *et al.*[18] have pointed out that macroscopic quantum effects in YBCO devices may be better observed in junctions showing electrodes with pair potential lobes aligned each other (d_0/d_0 junctions). This configuration can be obtained with out-of-plane [100] GBJs geometries, whereas [001] GBJs are not suitable for fabricating d_0/d_0 junctions.[9]

In spite of all these circumstances, as of today, and differently from the [001] tilt junction case, a specific theoretical treatment of the transport properties in [100] junctions is lacking.[19] One can probably individuate emblematically the obstacle of developing a model theory for this case in the nontrivial modification suffered by the quasiclassical trajectories of the excitations. Indeed, such trajectories are no longer confined to a single plane as in [001] layered junctions[2,6–8] but lay in planes tilted with respect to the substrate plane by the misorientation angles ϕ_1,ϕ_2; see Fig. 1.

In this work we take a step toward the effective evaluation of the peculiar transport properties of YBCO [100] tilt junction ($\alpha_L = \alpha_R = 0$ in Fig. 1) and [100] tilt-tilt junctions (junctions in which one or both angles α_L, α_R differ from zero).

We focus on the dc Josephson effect and find that the influence of the different tilting of the conduction planes with respect to the barrier plane (on passing from one electrode to the others) brings about an enhanced normal state electric resistance of the junction. The key result is an analytical expression for the Andreev spectrum for the quasiparticles, which retains the influence of the tilting of the Cu-O planes as well as the effects of the d-wave anisotropic symmetry of the pair potential.

II. THEORY

In order to describe charge transport in a mesoscopic [100] YBCO grain boundary Josephson junction, we assume a superconductor-normal-insulator-normal-superconductor (SNINS) model.[8,20–22] The superconductive material considered is a d-wave anisotropic layered cuprate. The presence of normal regions of the order $\sim\xi_0 = \hbar v_F/\pi\Delta_0$, the ballistic coherence length,[23] is introduced for modeling the mechanism of the Andreev reflection and a possible suppression of the order parameter near the junction.

Furthermore, we suppose that the quasiparticles are constrained to move exclusively along the Cu-O planes of the two electrodes. This last assumption is based on the fact that the normal conductivity in c-axis direction in YBCO is about 100 times smaller than that along the ab plane. In the superconducting state this strong anisotropy persists in the supercurrent distribution due to a large ratio $\lambda_c^2/\lambda_{ab}^2$, where λ_c (λ_{ab}) is the London penetration depth across the planes (in the planes).[3,24]

The junction barrier, the plane $x = 0$ in the frame xyz indicated in Fig. 1, is assumed to be normal to the substrate and considered perfectly flat. This assumption reflects schematically the fact that in a "valley"-type morphology junction, like the one represented in Figs. 1(b) and 1(c), there is almost perfect matching of the conducting planes at the grain boundary and the planes themselves face each other

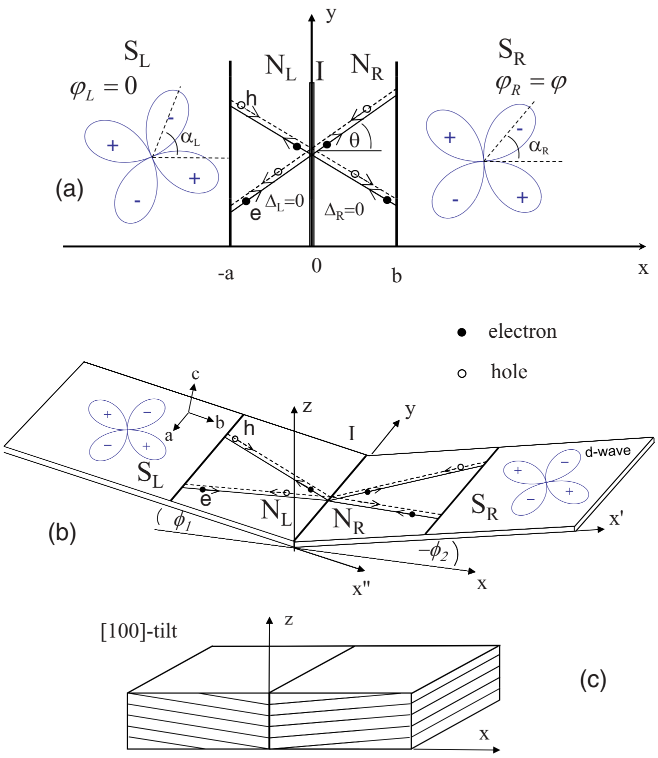

FIG. 1. (Color online) (a) z-axis view of a layered SNINS [100] tilt-tilt junction. The thickness of the normal region is a+b, the d-wave superconducting regions occupy the space defined by $x < -a$ and $x > b$. The insulating barrier (I) is represented by the plane $x = 0$. (b) 3D view of the conducting planes with the indicated tilt angles ϕ_1 and ϕ_2. The d-symmetry pair potential is represented by $\Delta^L(\theta) = \Delta_0 \cos(2\theta - 2\alpha_L)$; $\Delta^R(\theta) = e^{i\varphi}\Delta_0 \cos(2\theta - 2\alpha_R)$, $\varphi = \varphi_R - \varphi_L$ is the global phase difference between the two superconducting regions. The solid and dashed lines represent the electron-like and the holelike elementary excitation trajectories extending over the two planes, respectively. (c) Schematic crystallography of the entire [100] tilt junction.

along a nearly flat surface which is normal to the substrate.[25] The conduction planes are tilted with respect the substrate plane $z = 0$, by the angles ϕ_1 and $-\phi_2$ in the left ($x < 0$) and in the right ($x > 0$) electrode and parallel to the x''-y plane or to the x'-y plane, respectively. The propagation coordinates x', x'' in the left and right electrode are given by $x' = x\cos\phi_1 + z\sin\phi_1, x'' = x\cos\phi_2 - z\sin\phi_2$. The two SN interfaces are planes parallel to the junction barrier and normal to the x axis, as indicated in Fig. 1.

The coupled motion of holelike (v) and electron-like (u) components of the wave function Ψ in the Cu-O planes is described by the 2D quasiclassical BdG equations.[26] For the x'-y plane and $x' > 0$ the BdG equations are

$$\begin{cases} Eu(x',y) = \hat{h}(x',y)u(x',y) + \Delta_R(\hat{k})\Theta(x'-b)v(x',y) \\ Ev(x',y) = -\hat{h}(x',y)v(x',y) + \Delta_R(\hat{k})\Theta(x'-b)u(x',y) \end{cases} \tag{1}$$

and, analogously, for the x''-y plane and $x'' < 0$ we have

$$\begin{cases} Eu(x'',y) = \hat{h}(x'',y)u(x'',y) + \Delta_R(\hat{k})\Theta(x''-b)v(x'',y) \\ Ev(x'',y) = -\hat{h}(x'',y)v(x'',y) + \Delta_R(\hat{k})\Theta(x''-b)u(x'',y) \end{cases} \tag{2}$$

where $\hat{h}(x',y) = -\hbar^2(\partial^2/\partial x'^2 + \partial^2/\partial y^2)/2m + V(x',y) - E_F$ and $\hat{h}(x'',y) = -\hbar^2(\partial^2/\partial x''^2 + \partial^2/\partial y^2)/2m + V(x'',y) - E_F$, are the Hamiltonian operators. $V(x',y)$ and $V(x'',y)$ are the potential energies in the right and left electrodes, respectively, $\Theta(z)$ is the Heaviside step function and $E_F = \hbar^2 k_F^2/2m$ is the Fermi energy. In the following we assume that the two interfaces SN and NS are perfectly clean, the only potential being the one associated with a thin insulating barrier at $x = 0$. Hence, $V(x',y) = V(x'',y) = 0$, and we model such a barrier by a δ function potential $V(x,y) = U_0\delta(x)$. Here U_0, the Hartree potential, is taken to be a constant independent from ϕ_1 and ϕ_2.

The spatial dependence of the pair potential is assumed to have a step-functional form described by $\Delta(\hat{k},\mathbf{r}) = \Theta(-a-x)\Delta_L(\hat{k}) + \Theta(x-b)\Delta_R(\hat{k})$. The bound states solutions of Eqs. (1) for $\Psi(x')$ and $\Psi(x'')$ [$\Psi(x',y) = \Psi(x')\exp(ik_y y), \Psi(x'',y) = \Psi(x'')\exp(ik_y y)$] in the S_L, N_L, N_R, and S_R regions, including normal and Andreev reflections of holes and electrons, then are, respectively,

$$\begin{aligned} \Psi^{S_L}(x'') &= a_B(E)\begin{pmatrix} u_0^{L,-} \\ v_0^{L,-}e^{-i\varphi_-^L} \end{pmatrix} e^{-ik_-^{L,e}x''} \\ &\quad + b_B(E)\begin{pmatrix} v_0^{L,+} \\ u_0^{L,+}e^{-i\varphi_+^L} \end{pmatrix} e^{ik_+^{L,h}x''} \\ \Psi^{N_L}(x'') &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}\left(U_1 e^{ik_1^e x''} + U_2 e^{-ik_1^e x''}\right) \\ &\quad + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\left(V_1 e^{ik_1^h x''} + V_2 e^{-ik_1^h x''}\right) \\ \Psi^{N_R}(x') &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}\left(U_3 e^{ik_1^e x'} + U_4 e^{-ik_1^e x'}\right) \\ &\quad + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\left(V_3 e^{ik_1^h x'} + V_4 e^{-ik_1^h x'}\right) \\ \Psi^{S_R}(x') &= c_B(E)\begin{pmatrix} u_0^{R,+} \\ v_0^{R,+}e^{-i(\varphi_+^R+\varphi)} \end{pmatrix} e^{ik_+^{R,e}x'} \\ &\quad + d_B(E)\begin{pmatrix} v_0^{R,-} \\ u_0^{R,-}e^{-i(\varphi_-^R+\varphi)} \end{pmatrix} e^{-ik_-^{R,h}x'} \end{aligned} \tag{3}$$

with

$$\begin{aligned} u_0^{\beta,\pm} &= \left[\frac{1}{2}\left(1 + i\frac{\Omega_\pm^\beta}{E}\right)\right]^{1/2} \\ v_0^{\beta,\pm} &= \left[\frac{1}{2}\left(1 - i\frac{\Omega_\pm^\beta}{E}\right)\right]^{1/2} \\ k_\pm^{\beta,e} &= \left(k_F^2 - k_y^2 + i\frac{2m\Omega_\pm^\beta}{\hbar^2}\right)^{1/2} \\ k_\pm^{\beta,h} &= \left(k_F^2 - k_y^2 - i\frac{2m\Omega_\pm^\beta}{\hbar^2}\right)^{1/2} \end{aligned}$$

$$\Omega_\pm^\beta = (|\Delta_\pm^\beta|^2 - E^2)^{1/2}$$
$$k_1^e = \left(k_F^2 - k_y^2 + \frac{2mE}{\hbar^2}\right)^{1/2}$$
$$k_1^h = \left(k_F^2 - k_y^2 - \frac{2mE}{\hbar^2}\right)^{1/2} \quad (4)$$

with β denoting right (R) or left (L), $k_\pm^{\beta,e}$, $k_\pm^{\beta,h}$ are the wave numbers of the electron-like and hole-like quasiparticles, respectively, see Fig. 1(a), that move in the superconducting regions, with k_1^e, k_1^h the wave numbers of the electrons and holes in the normal regions, respectively, and $E \leqslant |\Delta_\pm^\beta|$. For d-wave symmetry the effective pair potential is modeled as $\Delta_\pm^L = \Delta_0|\cos[2(\theta \mp \alpha_L)]|e^{i\varphi_\pm^L}, \Delta_\pm^R = \Delta_0|\cos[2(\theta \mp \alpha_R)]|e^{i(\varphi+\varphi_\pm^R)}$,[6,7] where $\varphi_\pm^\beta$ are the phases as felt in a normal reflection by the electrons $(+)$ and holes $(-)$, φ is the global phase difference between the two superconducting regions, and α_L, α_R are the angles between the crystallographic a axis of the left and right superconductors and the normal to the y axis. θ is the incident angle of the quasiparticle trajectories to the y axis.

Boundary conditions have to be specified at the three different interfaces, $x = -a$, $x = 0$, and $x = b$, to determine the 12 unknown coefficients in $\Psi(x')$ and $\Psi(x'')$. These conditions are the continuity of the function Ψ and its derivatives, $d\Psi/dx'$ and $d\Psi/dx''$, across the clean interfaces $x = -a$, $x = b$, respectively. Moreover, at the normal-insulator-normal interface (plane $x = 0$) where the change in the propagation direction from x'' to x' occurs, boundary conditions are the continuity of Ψ and the discontinuity of $d\Psi/dx$ imposed by the presence of the δ-function barrier insulator. Then, since $d/dx = \cos\phi_1 d/dx'$ and $d/dx = \cos\phi_2 d/dx''$, we write the matching conditions at $x = 0$ as

$$\Psi_{N_L}(0) = \Psi_{N_R}(0)\cos\phi_2 \frac{d\Psi_{N_R}(0)}{dx''} - \cos\phi_1 \frac{d\Psi_{N_L}(0)}{dx'} = \frac{2mU_0}{\hbar^2}\Psi_{N_L}(0). \quad (5)$$

III. RESULTS AND DISCUSSION

Using Eq. (3) and imposing the above conditions, under the assumption of perfect retro-reflectivity ($E_F \gg E, |\Delta_\pm^\beta|$) of the Andreev reflections,[27] we derive an homogeneous linear system of equations for the the 12 unknown coefficients. The condition of existence of solutions, in addition to the trivial one, provides the following spectral equation:

$$[\Gamma_-^L\Gamma_-^R - e^{-i(\gamma_- + \varphi)}e^{-iDr}][\Gamma_+^L\Gamma_+^R - e^{i(\gamma_+ + \varphi)}e^{-iDr}] + Z_{\text{eff}}^2(\Gamma_-^L\Gamma_+^L - e^{-i\gamma_L}e^{-2iAr})(\Gamma_-^R\Gamma_+^R - e^{i\gamma_R}e^{-2iBr}) = 0 \quad (6)$$

with

$$\Gamma_\pm^\beta = \frac{E - i\Omega_\pm^\beta}{|\Delta_\pm^\beta|}, \quad \gamma_\beta = \varphi_+^\beta - \varphi_-^\beta, \quad \gamma_\pm = \varphi_\pm^R - \varphi_\pm^L$$
$$r = \frac{k_F}{\cos\theta}\frac{E}{E_F}, \quad A = \frac{a}{\cos\phi_2}, \quad B = \frac{b}{\cos\phi_1}, \quad D = A + B \quad (7)$$

and where the effective barrier parameter Z_{eff}, defining the electrical transparency of the junction $T_{\text{eff}} = 1/(1 + Z_{\text{eff}}^2)$, appears as

$$Z_{\text{eff}}(\theta,\phi_1,\phi_2) = \sqrt{\frac{4Z(\theta)^2 + (\cos\phi_1 - \cos\phi_2)^2}{4\cos\phi_1\cos\phi_2}} \quad (8)$$

with $Z(\theta) = Z_0/\cos\theta$ and $Z_0 = k_F U_0/2E_F$ the usual barrier parameters. With the definition Eq. (8) we may write the spectral equation in the same form which holds for the [001] case described in Refs. 27 and 22. However, Eq. (8) shows a new contribution to the barrier, coming from the specific geometrical configuration depending on the angles ϕ_1 and ϕ_2.

Equation (6) provides the quasiparticle energy levels as a function of the superconducting phase difference φ for the case of layered SNINS d-wave [100] tilt-tilt junctions and other limits (SIS, SNS, INS). When the junction is in the clean limit ($Z_0 = 0$), the transparency of [100] junctions does not reach the unitary value but it is still limited to

$$T_{\text{eff}}^0 = \frac{4\cos\phi_1\cos\phi_2}{(\cos\phi_1 + \cos\phi_2)^2}, \quad (9)$$

which is θ independent. Equation (9) embodies the pure effect on the junction transparency of the misalignment of the conducting planes between the two electrodes. The zero-temperature normal-state conductance G_n is evidently also affected by the angles ϕ_1 and ϕ_2 and can be written, in terms of the average transparency $\langle T_{\text{eff}}\rangle$, as

$$G_n = 2\frac{e^2 k_F L_y}{h}\langle T_{\text{eff}}\rangle$$
$$\langle T_{\text{eff}}\rangle = T_{\text{eff}}^0\left[1 - \frac{C^2\coth^{-1}(\sqrt{1+C^2})}{\sqrt{1+C^2}}\right], \quad (10)$$

where $C = 2Z_0/(\cos\phi_1 + \cos\phi_2)$ and $2\langle T_{\text{eff}}\rangle = \int_{-\pi/2}^{\pi/2} d\theta \cos(\theta) T_{\text{eff}}(\theta,\phi_1,\phi_2)$. Therefore, the effect of the tilting of the planes in SNINS junction manifests as *an excess of electrical resistance in the normal state*. This effect persists also in the limit of zero size normal regions ($a = b = 0$).

One of the consequences is that the Andreev level spectra are strongly modified. Indeed, in Fig. 2 the Andreev spectra for two different GBJ configurations are reported. In particular, we have considered, most representatively, the case of a [100] tilt-tilt mirror ($\alpha_L = -\alpha_R = \alpha$) GBJ, with $\phi_1 = 0$, $\phi_2 = \pi/4$, and $\alpha = \pi/8$ (dashed line), and the analogous mirror [001] junction (solid line) both in the clean limit ($Z_0 = 0$). As is well known, in mirror junctions, for a given symmetric rotation α ($0 < \alpha < 45^\circ$) around the c axes, depending on the quasiparticle incidence angle $\theta(-\pi/2 < \theta < \pi/2)$, two kinds of bound levels exist:[21,28] midgaplike states, for $\pm\pi/4 - |\alpha| < \theta < \pm\pi/4 + |\alpha|$ and edgegaplike states in the complementary intervals. The formation of midgap states, i.e., the formation of zero energy states when the phase difference across the junction is zero is characteristic of d-wave Josephson junction.[29] Both kinds of levels determine the magnitude of the Josephson current as well as the dependence of the maximum Josephson current on the temperature.[7] The two kinds of Andreev levels, selected for two illustrative θ values, have been derived according to Eq. (6). In particular, when the levels are degenerate in energy, i.e., at $\phi = \pi$, an asymmetric

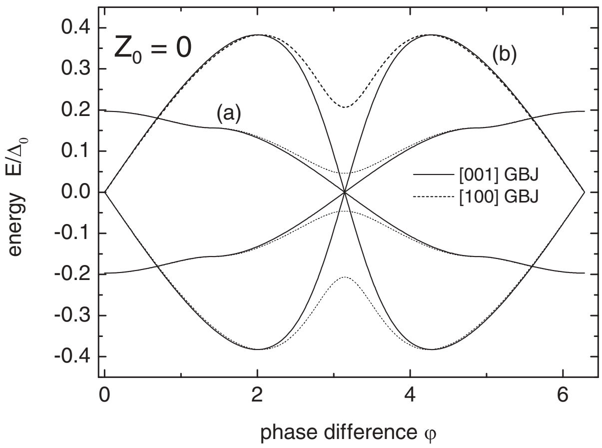

FIG. 2. Comparison between Andreev level spectra of d-wave SNS 45° mirror ($\alpha_L = -\alpha_R = 22.5°$) grain boundary junctions calculated in the clean limit ($Z_0 = 0$) for [001] and [100] configurations, respectively. Solid and dashed curves refer to [001] GBJs with $\phi_1 = \phi_2 = 0$ and [100] GBJs ($\phi_1 = 0$ and $\phi_2 = 45°$), respectively. (a) edgegaplike state Andreev levels for a trajectory with quasiparticle incidence angle $\theta = \pi/10$; (b) midgaplike state Andreev levels with $\theta = 3\pi/16$.

tilt of [100] junctions ($\phi_1 \neq \phi_2$) opens up an energy gap (E_{gap}) in both kinds of Andreev level spectra, similarly to what happens in the presence of impurities. For selected trajectories ($\theta = 0$ and $\theta = \pi/4$), the entity of this band gap may be simply expressed as $E_{\text{gap}}/\Delta_0 = 2\sqrt{1 - T^0_{\text{eff}}}|\sin 2\alpha|$ for edgelike energy states and $E_{\text{gap}}/\Delta_0 = 2\sqrt{T^0_{\text{eff}}}|\cos 2\alpha|$ for midgaplike states, respectively.

The Josephson current may be derived directly from the energy spectrum. As a consequence it is sensitive to the modifications derived so far. In the short junction limit, for which $a + b \ll \xi_0$, the discrete Andreev levels determine all the Josephson current through the expression[8,30]

$$I_x(\varphi,\phi_1,\phi_2) = \frac{2e}{\hbar}\frac{k_F L_y}{2\pi}\sum_n \int_{-\pi/2}^{\pi/2} d\theta \cos(\theta)\frac{dE_n(\theta,\varphi)}{d\varphi} f[E_n(\theta)], \tag{11}$$

where the index n labels the bound Andreev energy levels and $f[E_n(\theta)]$ is the Fermi function.

As a matter of fact it turns out that the Josephson current shows a dependence on the angles ϕ_1 and ϕ_2 in [100] geometries. Figure 3 shows a comparison of the dependence on the temperature of the maximum Josephson current between asymmetric [100] and [001] mirror junctions. The current is normalized with respect to $I_0 = 2ek_F L_y \Delta_0/h$, which is the zero temperature maximum Josephson current through an s-wave SNS junction in the clean limit.[30] The superconductive gaps in the two electrodes are assumed to obey a Bardeen-Cooper-Schrieffer temperature dependence. It is well known that in this kind of junction the interplay between midgap and edgegap states may lead to a temperature sign inversion of the maximum Josephson current [Fig. 3(b)], i.e., to a temperature-dependent 0-π crossover[7,21] (arrow in Fig. 3). For the chosen value of the barrier strength parameter $Z_0 = 0.7$, the modifications for increasing values of the tilt angle ϕ_2 are evident, showing a shift toward higher temperatures of the 0-π crossover as ϕ_2 increases from 0° to 45°; see Fig. 3(b).

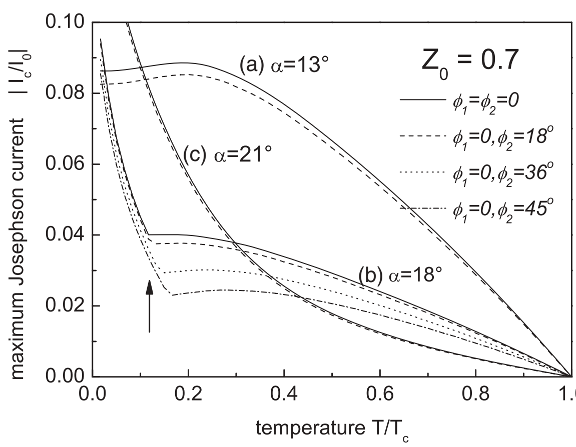

FIG. 3. Comparison of the temperature dependence of the absolute value of the Josephson critical current in d-wave [001] tilt (solid curves) and [100] tilt-tilt mirror ($\alpha_L = -\alpha_R = \alpha$) grain boundary junctions with barrier parameter $Z_0 = 0.7$ for three representative misorientation angles α. (a) $\alpha = 13°$, (b) $\alpha = 18°$, and (c) $\alpha = 21°$. For $\alpha = 18°$ arrow indicates the sign inversion of the critical current ($0 - \pi$ crossover) in [001] GBJs. The remaining curves in (b) show a shift of the crossover temperature with the tilt angle ϕ_2 in [100] GBJs. The sign of the critical current I_c is positive for curves (a), negative for curves (c).

IV. SUMMARY

We have presented a theoretical model for the description of electrical transport in YBCO [100] tilt "valley" type GBJs based on the quasiclassical BdG equations. We have compared our results with the well-studied [001] tilt case. We have derived the spectral relation in the case of [100] tilt-tilt junctions. The Andreev bound states calculated through this equation show modifications analogous to those caused by the presence of an insulating layer. However, the nature of this modifications differs: It depends on the geometrical mismatch between conducting planes. We have evaluated the temperature dependence of the maximum Josephson current in the case of [100] mirror junctions and found a dependence of the 0-to-π crossover temperature on the interelectrode misorientation angles.

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