Flux Pinning in a Slab Model of Grain and Twin Boundaries

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The flux pinning potential and critical current of a grain and a twin boundary are evaluated for a S-S′-S junction model and a configuration of parallel magnetic field and junction plane. In the grain boundary model, the S′ domain is assumed to be disordered, to mimic oxygen disorder. Large critical currents $\approx O(10^6$ amp/cm$^2)$ are estimated for both models. The grain boundary model exhibits a "nonweak" link behavior and moderate critical current dependence on the grain misalignment angle. We briefly dicuss an approach to enhance critical currents based on our grain boundary model.

Key words: Critical currents, flux pinning, grain boundary, S-S′-S junction, superconductivity, twin boundary

INTRODUCTION

In a type II superconductor and magnetic field above the lower critical field, the motion of penetrating flux lines, or vortices, is impeded (pinned) by defects in the sample and the vortex-vortex interactions. The response of this motion to external perturbations, such as a transport current, is scientifically intriguing and of great practical importance in conjunction with superconductor magnetic applications, such as wires.[1] The latter follows since a high critical current is prerequisite for a viable large scale superconductor material. The critical current, in turn, is determined by the strength of vortex pinning and its sustainment in the presence of transport currents, magnetic fields, and temperatures in the respective commercially relevant regimes. All the above implies that flux dynamics is a subject of many facets. In this paper, we focus on a particular one, the modeling of static flux pinning by two ubiquitous defect types in $YBa_2Cu_3O_{7-\delta}$ (YBCO), namely, grain boundaries (GB) and twin boundaries (TB).[2]

The extensive research effort on GB pinning properties is motivated by the relatively poor critical current (J_c) of YBCO ceramics.[1] The importance of high temperature superconductor ceramics is that the magnitude of J_c limits their applicability for large scale applications. This deficiency is believed to be caused by the low current-carrying capacity of GB. Obviously, to devise a remedial ceramics processing method, insight into the factors controlling the GB current carrying-capacity is highly desirable. As for pinning by TB, our motivation is their demonstrated pinning properties[3] and their unavoidable presence at an "optimal" density for $B \approx O$ (1 Tesla), i.e. when the inter-TB and inter-vortex spacings are approximately equal. As will become clearer below, TB and GB are akin in the context of electromagnetic coupling.

To model flux pinning of these defects, we are guided by several pertinent experiments. Consider first the TB. The measurement of the magnetic susceptibility hysteresis of a high quality single crystal before and after forced detwinning, has recently established that TB provide pinning.[3] These measurements were carried out for low, medium, and high temperatures; two magnetic field configurations; and magnetic fields up to 5 Tesla. For most cases, and in

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particular at low fields and temperatures, the TB contribution is substantial (≈40%). This data is consistent with earlier decoration experiments,[4] which demonstrate flux pinning at or near TB. Another experiment, indicating pinning along the TB plane, suggests the presence of disorder in the TB domain.[5] Structurally, TEM studies reveal a finite width of TB, on the order of magnitude O(10Å),[6] which seems to depend on the oxygenation level and quality of the sample. Since the constituency of the TB slab has not been reported, it is suggestive to assume it be a degraded phase of the "host" superconductor, i.e. to model it by a S-S′-S junction.[2]

For GB, their characteristics depend on the processing method. The pioneering study of Dimos et al.[7] considered epitaxial thin film bicrystals of several orientations. The bicrystal interface served as a GB model, and the bicrystal misalignment was varied in a controlled manner. The results demonstrated a strong J_c dependence on the GB misalignment angle. At small angles (<< 10°), J_c was found to be comparable to that of each grain, and dropped exponentially with an increase in angle. At larger misalignment angles, the GB behaved as a Josephson junction.

However, other studies on flux grown bicrystals[8] and {103} sputtered thin films[9] observe GB which are characterized as flux-pinners ("nonweak" links), Josephson, and resistive junctions. Moreover, the above strong J_c dependence on the misalignment angle is absent. Flux pinning and Josephson junction GB are observed at relatively large and small angles, respectively. The origin of the difference between flux grown GB and bicrystal GB is not fully understood at present. A possible factor may be the local oxygenation level, which has an effect on the GB properties.[9] In addition, localized electron energy loss spectrometry (EELS) and parallel electron energy loss spectrometry (PEELS)[10] studies show that domains of certain GB entail a reduced oxygen profile (and Cu abundance), extending <100Å. Since a reduced local oxygenation level degrades local superconductivity, and oxygen atoms in YBCO are notoriously mobile, it is suggestive to assume that the slab constituting a flux-pinning GB is a *disordered*[11] and degraded phase of the host superconductor. This type of junction is denoted by $S\text{-}S'_D\text{-}S$.[12] Thus, both the TB and GB models share the S-S′-S junction structure and slab geometry, with the important difference of disorder (or, amount of) in the GB slab domain.

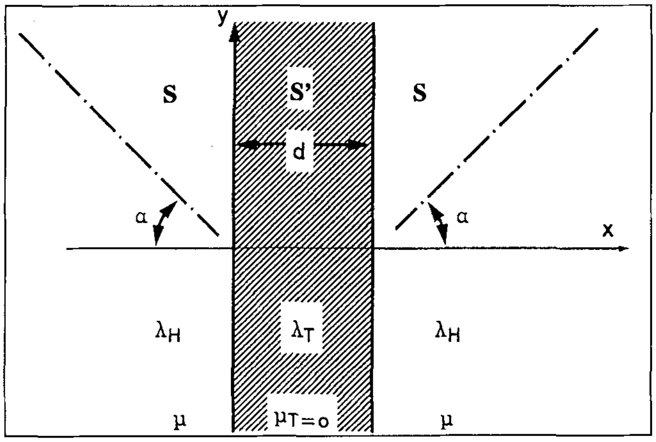


Fig. 1. The geometry and parameters of the S-S′-S junction. The hatched area marks the TB domain for the TB model and the disordered superconductor domain for the GB model. The dashed-broken lines delineate the Cu-O chains and misalignment angle in the two S banks. The penetration depths λ and mass anisotropy μ parameters pertaining to each domain are indicated. For the TB model, the μ parameters in both S banks are of opposite sign (not as depicted), see text.

TWIN BOUNDARY SLAB MODEL

In this section, we introduce the twin boundary S-S′-S slab model, which also provides the framework for the corresponding GB model in next section. The model's basic premises are

- validity of the London limit for which the London equation describes the pertinent phenomenology,
- the presence of a single, rigid, and fixed flux line, and
- the superconducting domains in the model are treated as continuous anisotropic superconductors.

The second and third assumptions correspond to the regime of small field and low temperatures (see Discussion section). The chosen geometry and notations are depicted in Fig. 1. Since TB run parallel to the [110] plane, the slab's plane is chosen parallel to the ĉ axis and α ≈ 45°. In order to simplify the analysis, the London equation is rendered two dimensional by choosing the flux to run parallel to the TB plane.

Using the coordinate system of Fig. 1, the London equation in each of the domains has the form:

$$B - \lambda^2\left[\frac{\partial^2}{\partial x^2} - 2\mu\frac{\partial^2}{\partial x \partial y} + \frac{\partial^2}{\partial y^2}\right]B = \Phi_0\delta(\vec{r} - \vec{r}_0) \quad (1)$$

$$\mu < 1, \quad \Phi_0 = \frac{\pi\hbar c}{|e|}$$

where the constant parameters λ and μ are the penetration depth and mass anisotropy, respectively, and the vortex position is at $\vec{r}_0$. For TB, the μ parameters of the left and right S banks (Fig. 1) are equal in magnitude and opposite in sign. Inside the TB domain S′, we choose μ = 0 to describe a situation where the YBCO copper-oxygen chains are badly broken so that the resulting small a^b anisotropy is reduced.

The pinning potential per unit vortex line length is obtained from the solution of Eq. (1) according to

$$\frac{U_L(\vec{r}_0)}{L} = \frac{\Phi_0}{8\pi}B_{IND}(\vec{r}_0;\vec{r}_0) \quad (2)$$

where L is the vortex line length, and the induced field $B_{IND}(\vec{r};\vec{r}_0)$ is the total magnetic field excess over that of the vortex, evaluated at point $\vec{r}$ for a vortex located at $\vec{r}_0$. The induced field is the field emanating from the vortex and reflected back from inhomogeneities in the system. Equation (2) can be interpreted as follows. When B_{IND} impinges on the "normal" vortex core at $\vec{r}_0$ in the presence of an external current, a Lorentz force is generated which represents the pull of the defect on the vortex. Thus, the pinning force calculated here is analogous to the image (polarization) force encountered in electrostatics[13] and, correspondingly, the London equation is analogous to the Poisson equation. For the configuration in Fig. 1, the pinning potential [Eq. (2)] depends *only* on the x coordinate since the model is invariant under y-axis translations.

The solution of Eq. (1) for the configuration of Fig. 1 is given elsewhere.[2] Here we quote just the ensuing TB parallel critical current, $J_c(||)$. In proximity to the slab interface, the expression is (in cgs units)

$$J_c(||) \sim \frac{c\Phi_o}{16\pi^2\lambda_H^3} * \frac{|\Delta\lambda|}{<\lambda>} * \frac{1}{\sqrt{1-\mu^2}} * |\ln\left(\frac{2\xi(0)}{\lambda_H}\right)| \quad (3)$$

where $\xi(0)$ is the coherence length at T = 0K, $\Delta\lambda = \lambda_H - \lambda_T$ and $<\lambda> = 0.5*(\lambda_H + \lambda_T)$. To estimate Eq. (3), the assumptions $|\Delta\lambda|/<\lambda> \approx 0.01$, $\xi(0) \approx 15Å$, $\lambda(0) \approx 900Å$, and $\mu \approx 0$ give $J_c(||) \approx 4. * 10^5$ amp/cm^2. This estimate may be compared to the critical current extracted from the magnetic susceptibility hysteresis via the Bean model. At H = 1 Tesla, $\vec{H} || \hat{c}$, and T = 10K, the data[3] yields $\Delta M \approx 2000$ emu/cm^3. Insertion of $D \approx 0.2$ cm for the sample dimension in Bean model one obtains $J_c(||) \approx 3*10^5$ amp/cm^2, which is of the same order of magnitude as the above estimate.

GRAIN BOUNDARY SLAB MODEL

As discussed in the Introduction, the adaptation of the S-S′-S slab model to describe a GB is obtained by assuming the S′ domain to be a disordered superconductor. Also, the μ parameters of the two S banks (Fig. 1) are chosen equal to minimize the number of phenomenological parameters, and the misalignment angle α is arbitrary.

Disorder in the present context is embodied by a spatially random penetration length λ. Specifically, denoting $\lambda^2(\vec{r}) = <\lambda^2(\vec{r})> + \delta[\lambda^2(\vec{r})]$ where the mean and fluctuations of the squared penetration depth are denoted by $<\lambda^2(\vec{r})>$ and $\delta[\lambda^2(\vec{r})]$, respectively, and defining the convenient random variable $\varphi(\vec{r}) = \delta[\lambda^2(\vec{r})]/(\phi_0 <\lambda^2(\vec{r})>)$, the statistical assumptions are[12]

$$<\lambda^2(\vec{r})> = \lambda^2$$
$$<\varphi(\vec{r})> = 0 \quad (4)$$
$$<\varphi(\vec{r})\varphi(\vec{r}')> = \frac{2\pi\varepsilon^2\sigma^2}{\phi_0^2}\delta(\vec{r}-\vec{r}')$$

In Eq. (4) σ and ε, which characterize the disorder in S′, denote the correlation length and relative strength of the penetration depth fluctuations, respectively. It can be shown[12] that the London Eq. (1) with the proper $\lambda^2(\vec{r})$ is valid provided $\xi(0) < |\vec{r} - \vec{r}_0| \leq \sigma << \lambda$.

As a consequence of disorder in the S′ domain, the pinning potential in the "regular" S banks acquires a spatially random component which is superimposed on the spatially smooth mean pinning potential. Underlying this effect are the *supercurrents* circulating around the vortex, which carry the disorder over a distance (from S′ interface) of the order of the penetration depth. The situation of a regular superconductor, which exhibits disorder features as a consequence of its proximity to a disordered superconductor, is referred to as disorder proximity effect. Thus, in addition to pinning by the mean pinning potential, pinning from vortices trapped in local minima of the pinning potential fluctuations must be considered. The corresponding potential barrier is the mean squared deviation of the pinning potential fluctuations. Since in the present model the sole mechanism for breaking translational invariance in the y direction is disorder, *all* pinning in that direction is the result of disorder. This component of the pinning determines J_c normal to the slab. Note that the above disorder proximity effect is analogous to the pairing proximity effect, yet is different in that it is a consequence of electromagnetic coupling and not electron pairing.

The model yields explicit expressions for the critical currents parallel and normal to the slab interface and their dependence on the misalignment angle α. The critical current is calculated here by equating the maximum Lorenz force to an average pinning force. The latter is extracted from the calculated pinning potential. For lack of space only some of these are quoted:[12]

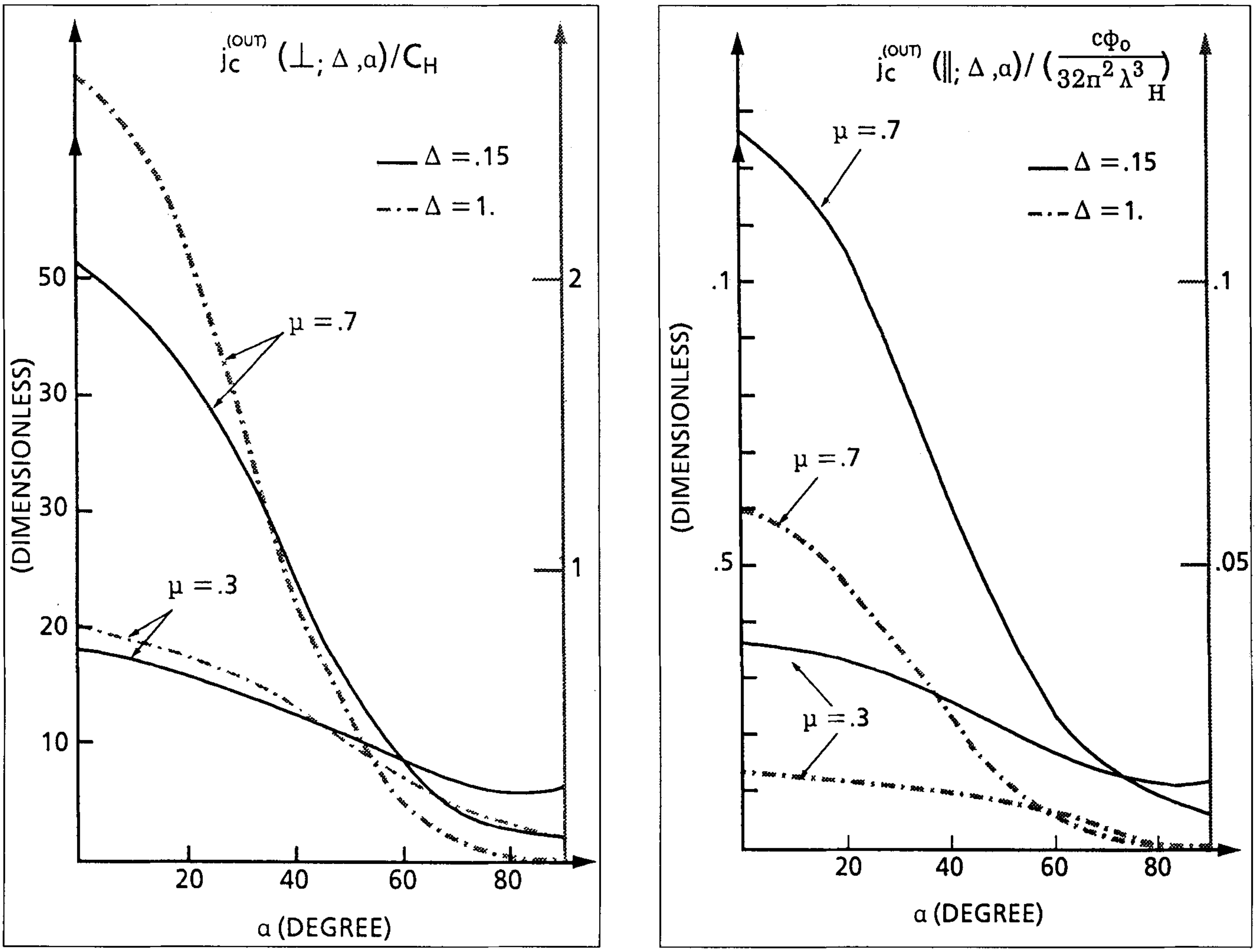
$$J_c^{(S)}(\perp;\xi-\delta,\alpha) = C_H f_B(\xi-\delta,\alpha),$$

$$C_H = \frac{c\phi_0}{32\pi^3\lambda_H^3}\frac{(2\pi)^{3/4}}{4}\varepsilon\sqrt{\frac{\lambda_H}{\sigma}} \quad (5)$$

$$J_c^{(S')}(\perp;\xi;fl) \sim \frac{c\phi_0}{16\pi^2\sigma\lambda_H^2}\frac{\varepsilon}{R_T^2}\ln(\lambda_T/\xi(0))$$

where $J_c^{(S)}$ and $J_c^{(S')}$ denote the critical currents in S and S′ domains, respectively, $f_B(\xi-\delta,\alpha)$ is a dimensionless pinning potential correlation function and $\Delta = \xi - \delta = (x-d)/\lambda_H$, see Fig. 1. Note from Eq. (5) that the critical current in S′ is, to a very good approximation, α-independent.

The angular dependence of Eq. (5) is depicted in Fig. 2 for several parameter choices. Note first the moderate decrease of $J_c^{(S)}$ with increasing α. This behavior is quite different from the exponential falloff observed in epitaxial thin films bicrystals.[7] It originates from the dependence of f_B on α solely through a '$1 + \mu\cos(2\alpha)$' factor (not shown here). The magnitude of the critical current is obtained by estimating the prefactors in Eq. (5). Assuming the conservative values $\lambda_H/\sigma \approx 40$ ($\sigma \approx 35Å$), $\varepsilon \approx 0.01$, $R_T = 1.5$ (corresponding to a $T_c = 60K$



a b

Fig. 2. The misalignment angle and distance dependence of the perpendicular [$j_c(\perp)$] and parallel [$j_c(\|)$] critical currents in domain S. The expression for C_H is given in Eq. (5). The chosen parameters are: $\delta = d/\lambda_H = 0.06$ and $R_T = \lambda_T/\lambda_H = 1.5$.

in S′), and $\lambda_H = 1400$Å, Eq. (5) yields $J_c \approx 10^6$ amp/cm^2 for small angles, at $\Delta = 0.15$, *both* inside and outside the slab. Thus, the model predicts a "nonweak" link junction, and a moderate falloff of $J_c^{(S)}$ with increasing the misalignment angle. These features are qualitatively consistent with data on flux-pinning GB in flux-grown ceramics[8] and certain thin films.[9]

DISCUSSION

The S-S′$_D$-S slab model for GB predicts a high J_c and a moderate misalignment angle dependence, both of which are desirable GB attributes. The materials sciences implication of this result is that, provided a processing method which produces such junctions at GB can be devised, two important problems of YBCO ceramics can be overcome, i.e. the low J_c and the need for grain texturing. A possible approach to achieve this objective is by in-diffusing *metallic* atoms such as Cr, Ni, and Ti, hopefully via the sample's GB and TB. By strongly binding with the volatile oxygens which tend to out-diffuse primarily via the planer defects, these metallic atoms block their escape out of the sample. In addition, when substituted in YBCO, these metals do not excessively degrade superconductivity.[14] Hence, their in-diffusing into the grains has a minimal degrading effect. By the same token, an attempt should be made to transform the dense TB into flux pinning defects by an appropriate processing approach.

The parallel analysis of the GB and TB models above, as different versions of the same S-S′-S junction model, highlights their affinity in the context of electromagnetic coupling. The explicit expressions of the critical currents, Eqs. (3) and (5), offer insight into the dependence of J_c on defining parameters and provide an additional guideline to devising processing approaches.

The underlying simplifying assumptions of the models delineate their domain of validity. First, as a result of the short (atomic scale) coherence length in HTSC, these materials are extreme type II superconductors and, hence, the London limit is well satisfied. The adopted static limit implies a low temperature regime, when thermally activated flux motion can be disregarded.[15] The single vortex approximation implies a low magnetic field, when inter-vortex spacing is considerably larger than the penetration depth, so that each vortex can be considered individually. In the same vein, the calculated critical current pertains to a single flux line. Contributions from the presence of inter-vortex correlations are not included. For the GB model, the assumed "weak" and "short" range disorder are plausible, however, more studies are obviously needed.

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