

Critical Current of Low-Angle Grain Boundaries in High- T_c Superconductors

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Abstract Dependence of the critical current on the misorientation angle in high-temperature superconductor [001] tilt bicrystal is theoretically examined. We suppose that in the case of relatively small values of the bicrystal misorientation angle θ ($\theta \leq 10\div 15^\circ$) the critical current is determined by depinning of vortices, which are locked by edge dislocations aligned along the bicrystal grain boundary. Dependence of the depinning critical current on the misorientation angle is calculated for this case and it reveals a good agreement with experimental data obtained on Y-Ba-Cu-O bicrystals with [001] tilt low-angle grain boundaries.

Keywords Superconductor, Bicrystal, Grain Boundary, Abrikosov Vortex, Dislocation, Pinning, Critical Current

1. Introduction

High-temperature superconducting (HTS) materials produced on the base of 'cuprate' compounds (RE)-Ba-Cu-O (RE – is the rare-earth element: Y, Gd, Nd) are of great practical interest for electrical engineering and electronics [1]. First of all it concerns the possibility of large-scale applications, such as: superconducting electric power cables, high-field magnets, motors, energy storage devices, etc. This interest is caused by a large current carrying ability of HTS materials, allowing dissipation-free current flow with densities more than 10^6 A/cm² at liquid nitrogen temperature (77K) and magnetic fields up to 10 T, obtained for HTS (RE)Ba₂Cu₃O_{7- δ} ((RE)BCO) films and coatings. Now significant efforts are aimed to improve production technology and current carrying characteristics of practically valuable HTS conductors - preferably in form of HTS tapes, deposited (over the special buffer layers) on flexible metallic substrates - so called 'second generation of HTS conductors' [2-3]. The most important task (both for physics and applications of superconductivity), which arises in these researches is enlargement of the critical current density j_c (maximal dissipation-free current density) and elimination

of its dependence on magnetic field value and orientation, as well as on the HTS specimen thickness.

Numerous studies performed on different HTS films and coatings with regard to their possible large-scale applications have unambiguously demonstrated that one of the most important structural features of these superconductors, which provides limitations on their current-carrying capability, is existence of grain boundaries (GB) within the material, playing the role of a strong barriers for supercurrent flow [1,4,5]. This evidence comes, first of all, from the studies on a single grain boundary in HTS bicrystals, usually obtained by deposition of HTS films on bicrystalline substrates [6,7]. For HTS epitaxial thin films and highly textured coatings, which possess the highest j_c values and are mostly interesting for applications, the main type of GB, affecting the critical current value, are [001] – tilt grain boundaries, which correspond to rotation of neighbouring crystalline grains on the both sides of GB around the c -axis, which is perpendicular to the superconducting Cu-O plains (ab -planes) of anisotropic (layered) HTS material and film/coating substrate. Experiments performed on [001]-tilt YBCO bicrystals [6-10] have demonstrated that the critical current density across the grain boundary depends strongly on the misorientation angle θ of grains, and drops nearly exponentially when θ increases: $j_c(\theta) \sim \exp(-\theta/\theta_c)$ where $\theta_c \approx 1 - 3^\circ$. The low-angle tilt [001] GB in YBCO bicrystals and c -oriented epitaxial films (coatings) may be considered as rows parallel to the c -axis edge dislocations [6]. The average distance between neighbouring dislocations in the row, according to Franck's relation, depends strongly on the misorientation angle θ of neighbouring grains in the (ab)-plane: $d(\theta) \sim \theta^{-1}$, and by the order of magnitude usually is about $3\div 10$ nm. At small θ values ($\theta \leq 10^\circ$), the dislocations which form the GB are well separated. Therefore, in this case the current passes the GB through the nano-sized channels between dislocation cores (Fig.1).

These dislocation cores are nonsuperconducting (dielectric or normal-metal cylindrical regions) owing to strain fields around them [11]. On the other hand, at high θ values, a transition from strong to weak (Josephson) coupling of grains takes place. The Josephson properties of

GB junctions in bicrystals with a high misorientation angle values have been widely studied (both experimentally and theoretically) [6,7]. In the present work we concentrate mostly on the behavior of GB junctions with a small misorientation angle, providing the bulk current flow through the narrow channels between dislocation cores. One of the most interesting features of low-angle [001]-tilt GB in HTS films and bicrystals is the exponential type of $j_c(\theta)$ dependence for this kind of grain boundaries, as it was mentioned above. There are several theoretical models which try to relate this type of $j_c(\theta)$ dependence with electron transparency of GB, which can drastically decrease with increase of the misorientation angle θ [11-13]. Nevertheless, there is a strong experimental evidence that the critical current value through the GBs of this type, followed by simultaneous onset of the resistive state of superconductor, is tightly related with the start of vortex motion along the GB under the Lorentz force influence [14-18]. These vortices (Abrikosov, or mixed type – Abrikosov-Josephson (AJ) vortices [19]), which are locked within the [001]-tilt GB and pinned by dislocations, forming it, arise due to applied magnetic field, or can be self-induced by transport current flow. As a rule, the critical current for depinning of such kind vortices and onset of their motion under the Lorentz force action, is essentially less than the depinning critical current for vortices, locked within grains. Thus, the GBs can form easy vortex flow channels in HTS films and bicrystals [14-18]

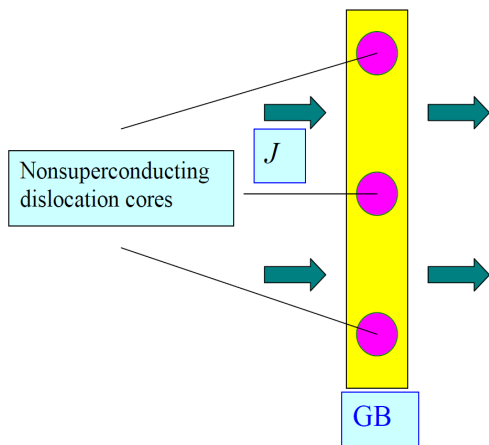


Figure 1. Current flow through the [001]-tilt grain boundary in HTS

In the present work the depinning critical current for periodic pinning potential created by a dislocation row along the [001]-tilt GB in HTS bicrystal is calculated. The strong exponential $j_c(\theta)$ dependence for the critical current density is obtained for $\theta \geq 5^\circ$ at low magnetic field values (e.g., those induced by a transport current). The calculated $j_c(\theta)$ dependence matches quantitatively well with the corresponding experimental data, obtained for YBCO bicrystals [1,6,8-10], when the coherence length and the Burgers vector values determined from experiments [1,6]

are used as a fitting parameters of the model. In the framework of suggested model the main features of experimentally observed $j_c(\theta)$ dependence, such as plateau at low angles and exponential decrease at higher angle values, follow from the specific form of periodic vortex pinning potential, created by the equidistant edge dislocations row, which forms the [001] tilt low-angle grain boundary in HTS bicrystal.

2. Model and Results

In this section the depinning critical current value is calculated for the case of periodic pinning potential $U_p(\mathbf{s})$, created by a linear row of parallel equidistant c -oriented edge dislocations, forming the low-angle [001] tilt grain boundary along the x – axis in HTS film or bicrystal. Following the works [20,2], the general expression for the pinning potential $U_p(\mathbf{s})$ in the framework of

Ginzburg-Landau theory can be written in form:

$$U_p(\mathbf{s}) = -\int V_p(\mathbf{r}) \left[1 - \left| \frac{\psi(\mathbf{r}-\mathbf{s})}{\psi_\infty} \right|^2 \right] d^2\mathbf{r} \quad (1)$$

Here $\psi(\mathbf{r})$ – is the order parameter of superconductor; $V_p(\mathbf{r})$ – is the depairing potential for electrons, which characterizes the materials inhomogeneity, leading to the local suppression of superconductivity. Within the model of (δT_c) –pinning an expression for $V_p(\mathbf{r})$ can be written in form [20]:

$V_p(\mathbf{r}) = |\psi_\infty|^2 \delta\alpha(\mathbf{r})$, where $\alpha \equiv \alpha'(T - T_c)$ - is the parameter of the Ginzburg-Landau theory. In the case of periodic potential $V_p(\mathbf{r})$, produced by dislocation row along the grain boundary, we will use an approximation:

$$V_p(\mathbf{r}) = \sum_n V_{p0}(\mathbf{r} - n\mathbf{d}); V_{p0}(\mathbf{r}) = V_0 \pi r_p^2 \delta_2(\mathbf{r});$$

For the row of c -oriented edge dislocations with a Burgers vector \mathbf{b} , which form a low-angle [001] tilt grain boundary in HTS film or bicrystal, the distance between neighboring dislocations is determined by the Franck's relation:

$$d = \frac{b}{2 \sin \frac{\theta}{2}}; \quad \mathbf{d} = d \cdot \hat{\mathbf{x}}; \quad b = |\mathbf{b}|; \quad (2)$$

Besides that, in (1) we will use a well known relation for the local change of the order parameter $\psi(\mathbf{r})$ in vicinity of the Abrikosov vortex core on the scale of the coherence length ξ [20]:

$$f(r) = \left| \frac{\psi(r)}{\psi_\infty} \right| \cong \frac{r}{\sqrt{r^2 + 2\xi^2}}$$

Using these assumptions one can obtain for the pinning potential $U_p(\mathbf{s})$, given by (1):

$$\begin{aligned}
U_p(s) &= -V_0 \pi r_p^2 \times \\
&\times \int d^2 r \sum_n \delta_2(r - nd) \left[1 - \frac{(r-s)^2}{(r-s)^2 + 2\xi^2} \right] = \\
&= -V_0 \pi r_p^2 \sum_n \frac{2\xi^2}{(nd + s_x)^2 + s_y^2 + 2\xi^2} ; \\
d \equiv d(\theta) &= \frac{b}{2 \sin \frac{\theta}{2}}
\end{aligned} \tag{3}$$

Performance of summation in (3) using expression for the sum of series: $\sum_{k=-\infty}^{\infty} \frac{1}{k+a} = \pi \operatorname{ctg}(\pi a)$ gives the following result for the periodic pinning potential $U_p(s)$ determined by (3) [21] and shown in Fig.2:

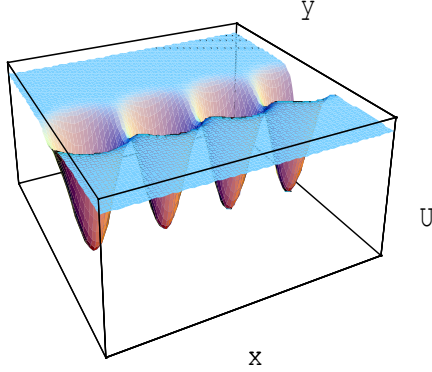


Figure 2. Pinning potential $U_p(s)$ calculated from Eq.(4)

$$\begin{aligned}
U_p(s) &= -V_0 \pi r_p^2 \frac{2\pi\xi^2}{d\sqrt{s_y^2 + 2\xi^2}} \times \\
&\times \frac{\operatorname{sh}\left(\frac{2\pi\sqrt{s_y^2 + 2\xi^2}}{d}\right)}{\operatorname{ch}\left(\frac{2\pi\sqrt{s_y^2 + 2\xi^2}}{d}\right) - \cos\left(\frac{2\pi s_x}{d}\right)}
\end{aligned} \tag{4}$$

From (4) it follows, that the periodic pinning potential in the plane of grain boundary $U_p(s_x)$ has the form:

$$\begin{aligned}
U_p(s_x) &= -V_0 \pi r_p^2 \frac{\sqrt{2}\pi\xi}{d} \times \\
&\times \frac{\operatorname{sh}\left(\frac{2\sqrt{2}\pi\xi}{d}\right)}{\operatorname{ch}\left(\frac{2\sqrt{2}\pi\xi}{d}\right) - \cos\left(\frac{2\pi s_x}{d}\right)}
\end{aligned} \tag{5}$$

The pinning potential determined by (4), (5) depends on

the misorientation angle θ of neighboring crystalline blocks, separated by grain boundary. The latter is determined by the dependence $d(\theta)$ given in (2). This allows to find an angular dependence of the critical current density $j_c(\theta)$, which is determined by depinning of vortices, locked within the grain boundary:

$$j_c(\theta) = \frac{1}{\varphi_0} \max\left(\frac{\partial U_p}{\partial s_x}\right) ; \tag{6}$$

(here $\varphi_0 = \frac{\pi\hbar}{e}$ - is the flux quantum).

It is worth to notice that in thick superconducting films or plates with a thickness $d > \lambda$ (λ - is the London penetration depth) (6) determines the critical current density on the specimen surface: when the surface current density reaches the critical value, the instability of vortex pinning state emerges and process of vortex escape from linear defect (dislocation) under the Lorentz force influence starts at the surface and subsequently propagates inside the specimen [22,23] (see Fig.3).

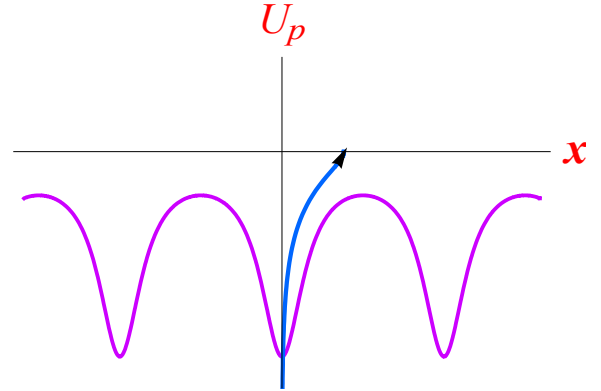


Figure 3. Lorentz force induced vortex transfer in a periodic pinning potential of dislocation [001]-tilt grain boundary in HTS bicrystal

Numerical calculation of $j_c(\theta)$ dependence from (2), (5), (6) leads to results presented in Fig.4(a),(b) in a semi-log scale for different values of relevant parameters – the coherence length ξ and modulus of the Burgers vector b . In Fig.4(a) this dependence is shown for the fixed value b (0,4 nm) and a set of different ξ values, while Fig.4 (b) demonstrates dependencies $j_c(\theta)$ for the fixed value ξ (2 nm) and a set of different b values. The dotted curve (curve 3) both in 4(a) and 4(b) figures corresponds to the parameters values: $b = 0,4$ nm, $\xi = 2$ nm, which seem to be quite relevant for the case of YBCO bicrystals (see, e.g. [1,6,8]). In accordance to experimental data, the most specific features of $j_c(\theta)$ dependence, which are common for HTS [001] tilt bicrystals, are following: (a) - existence of a plateau region at small misorientation angles, and (b) - exponential decrease of $j_c(\theta)$ value with increase of θ at higher angles: $j_c(\theta) \sim \exp(-\theta/\theta_0)$. Typically for YBCO [001] tilt bicrystals the plateau region is observed at $\theta < 2 \div 4^\circ$ and exponential decrease at higher angles is characterized by $\theta_0 = 2 \div 5^\circ$

[1,6-10]. As one can see from the Fig.4(a),(b), the calculated $j_c(\theta)$ dependence reveals both these features. The plateau width and the exponential slope angle depend on ξ and b values: decrease of ξ value or alternatively increase of b value leads to spreading of the small angle plateau region and increase of the exponential slope angle θ_0 at higher angles. For the selected dotted curve 3 in Fig.4(a),(b) the plateau width is about 3° and the slope angle $\theta_0 \approx 1,7^\circ$. Thus, one can conclude that obtained results for $j_c(\theta)$ dependence agree well with experimental data for YBCO bicrystals with low-angle [001] tilt grain boundaries.

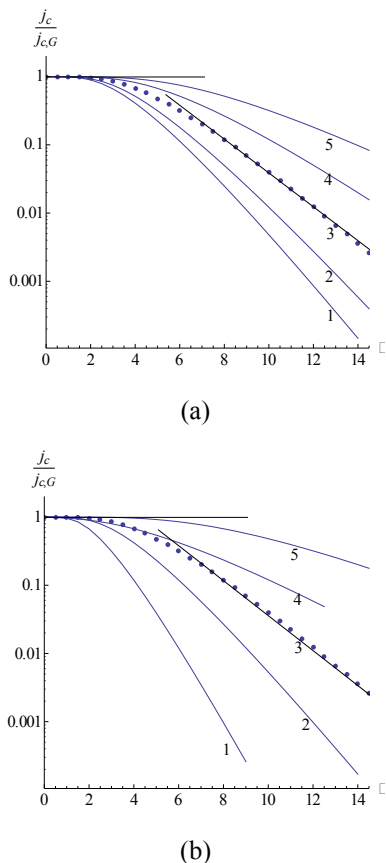


Figure 4. Dependence of the intergrain depinning critical current density $j_c(\theta)$ (normalized on the intragrain critical current density value) on the misorientation angle θ for [001]-tilt grain boundary in HTS bicrystal, calculated for different values of the relevant parameters ξ and b : (a) – fixed value $b = 0,4$ nm and different values ξ : 1- $\xi = 2,7$ nm; 2 - $\xi = 2,4$ nm; 3- $\xi = 2$ nm; 4 - $\xi = 1,6$ nm; 5 - $\xi = 1,2$ nm; (b) – fixed value $\xi = 2$ nm and different values b : 1- $b = 0,2$ nm; 2 - $b = 0,3$ nm; 3- $b = 0,4$ nm; 4 - $b = 0,6$ nm; 5 - $b = 0,8$ nm.

3. Conclusion

In the present work we examine dependence of the intergrain critical current density j_c on the misorientation angle θ in HTS [001] tilt bicrystals. As distinct from other theoretical models [11-13], relating j_c with electron transparency of this type grain boundaries, we consider j_c as a depinning critical current density for Abrikosov (or Abrikosov-Josephson) vortices, which are locked by nearly equidistant c -oriented edge dislocations, forming low-angle

[001] tilt grain boundaries in HTS films and bicrystals. It is shown, that specific form (5) of the periodic vortex pinning potential $U_p(s)$, created by dislocation rows along a such kind grain boundaries, allows to reproduce the main features of $j_c(\theta)$ dependence, experimentally observed in HTS [001] tilt bicrystals, namely: existence of plateau at small misorientation angles, and exponential decrease of $j_c(\theta)$ value with increase of θ at higher angles: $j_c(\theta) \sim \exp(-\theta/\theta_0)$. The results for $j_c(\theta)$ dependence, obtained in the present work, agree well with experimental data for YBCO [001] tilt bicrystals when suitable values for fitting parameters (coherence length ξ and modulus of the Burger vector b) are used for calculations. The width of the plateau region, as well as the slope angle θ_0 on the exponential part of $j_c(\theta)$ dependence, change with varying of fitting parameters ξ and b , as it is shown in Fig. 4(a),(b). Nevertheless, there are some experimental data, concerning $j_c(\theta)$ dependencies for [001] tilt grain boundaries in HTS and also Fe-based pnictides (e.g., those obtained on YBCO [001] tilt bicrystal films, grown by liquid epitaxy method [24], and Co-doped BaFe_2As_2 bicrystal films [25,26]) which differ noticeably from the previous results on $j_c(\theta)$ dependence in HTS [001] tilt bicrystals, which in most cases were obtained on YBCO thin film bicrystals produced by pulse laser deposition technique [1,6-10]. The main difference of results on $j_c(\theta)$ dependence presented in [24-26], comparatively to those obtained before for YBCO bicrystals [1,6], concerns large values of the plateau region (up to 10 - 12°) at small angles and gentle exponential slope of $j_c(\theta)$ dependence at higher angles, characterized by the slope angle values $\theta_0 \approx 9$ - 10° , which are 2-3 times larger than similar ones observed before for YBCO bicrystals. It seems rather difficult to obtain these values of the plateau width and θ_0 in the framework of presented model, using reasonable values of fitting parameters ξ and b . We suppose the following reasons, why suggested model of vortex depinning in a periodic pinning potential of dislocation row doesn't provide quantitative explanation of results, presented in [24-26]: a) inside the grain boundaries there are some other strong pinning sites besides dislocations, e.g., irregularities of grain boundaries, their meandering (both in (ab) plane and through the films thickness in the case of rather thick films [9]), nonsuperconducting inclusions, etc., providing strong vortex pinning which is weakly dependent on the misorientation angle; (b) we have used a simplified model for the pinning potential of dislocation row $U_p(s)$ which should be improved by account for strain fields and local compositional and carrier concentration variations in the vicinity of nonsuperconducting dislocation cores of finite radius. We also suppose, that the real insight in the nature of the critical current and the onset of resistivity in HTS grain boundaries can be founded on analysis and subsequent understanding of I-V characteristics, especially at very low dissipation levels [14].

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