

# Modified dislocation model of tilt grain boundaries in high- $T_c$ superconductors

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The stress fields near grain boundaries of two types, viz., symmetric tilt boundaries (having a misorientation angle  $\theta$ ) with a periodic system of edge dislocations and similar boundaries with irregular periodicity in the arrangement of the dislocations, are calculated. The angular dependence  $J_c(\theta)$  of the critical current of grain boundaries in superconductors is found on the basis of these calculations under the assumption that the order parameter is reduced in regions of increased stress. In the former case  $J_c(\theta)$  drops at small values of  $\theta$ , but then increases and approaches the bulk value. This is attributed to the almost complete balancing of the stresses in the regular system of edge dislocations. In the latter case such composition does not occur, and the critical current  $J_c(\theta)$  decreases over the entire range of values of  $\theta$ . The corresponding dependence is nearly exponential:  $J_c(\theta) = J_c(0)\exp(-\theta/\theta_0)$ , where  $\theta_0 \sim 10^\circ$ . The calculation results are consistent with experiments involving measurement of the critical currents of Josephson junctions in superconducting films on bicrystal substrates and with the experimental magnetic-field dependence of these currents. © 1996 American Institute of Physics. [S1063-7761(96)02110-5]

## 1. INTRODUCTION

The influence of dislocations on the superconducting properties of various materials has been discussed and studied for many years. In particular, it has been known for a long time that dislocations promote vortex pinning in the mixed state, and this applies not only to low-temperature,<sup>1</sup> but also to high-temperature<sup>2</sup> superconductors. It has been established that the main role in this phenomenon is played not by the dislocations themselves, but by the stress fields they create (which extend over comparatively large distances). However, the specific mechanism which links the parameters of a material that are important for superconductors to stresses is not entirely clear. Nevertheless, it was postulated in Ref. 2 that in high- $T_c$  superconductors the main effect is associated with a decrease in the electron mean free path  $l$ , which leads to a decrease in the coherence length  $\xi$  and an increase in the magnetic-field penetration depth  $\lambda$  [in the “dirty” limit  $\xi \propto l^{1/2}$  and  $\lambda \propto l^{-1/2}$  (Ref. 3)].

High-temperature oxide superconductors are very sensitive to irregularities in the crystal structure and especially to variations in the oxygen concentration. Therefore, it is believed that dislocations (more precisely, the stresses they create) can produce another significant effect, viz., reduction of the order parameter in regions where these stresses are fairly great. Just this can account for the formation of regions of weak superconductivity on grain boundaries of various types in high-temperature superconductors.<sup>4–6</sup> The tilt boundaries in thin high- $T_c$  superconducting films on bi-crystal substrates have been investigated to the greatest extent. Numerous experiments with different high- $T_c$  superconducting materials have shown that a Josephson-type weak link forms on such a boundary. The critical current  $J_c$  of such a Josephson junction decreases monotonically and rapidly with increasing values of the tilt angle  $\theta$  (i.e., the misorientation angle of the

portions of the film located on opposite sides of the boundary).<sup>1)</sup>

The specific mechanism for suppressing superconductivity at sites of increased stress has not yet been established. At the same time, experiments show that the spatial distribution of the oxygen concentration in  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  films has a minimum near a grain boundary.<sup>7</sup> Far from a boundary  $\delta \approx 0.05$  holds, and on a boundary  $\delta \sim 0.3$  and  $\delta \sim 0.5–0.6$  hold for  $\theta = 7^\circ$  and  $\theta = 31^\circ$ , respectively.<sup>2)</sup> Restoration of the oxygen concentration to the bulk value occurs at a distance of only  $\sim 20$  nm from the boundary. Therefore, it is perfectly likely that the lowering of the oxygen concentration is due to stresses concentrated near the grain boundary.

The angular dependence of  $J_c(\theta)$  mentioned above is associated with the increase in the density of edge dislocations on the tilt boundary as the angle  $\theta$  increases. The quantification of this qualitative idea is based on the simplifying assumption that the superconducting state is totally destroyed in regions where the stress exceeds a certain critical value  $\sigma_c$ . There is basis to assume (see below)  $\sigma_c \sim 0.01G$ , where  $G$  is the shear modulus of the high- $T_c$  superconducting material.

According to the standard dislocation model, there is a periodic system of edge dislocations on a tilt boundary.<sup>9</sup> Calculations performed on the basis of this model show<sup>5</sup> that the fraction of the boundary with  $\sigma > \sigma_c$  increases with increasing  $\theta$  and that  $\sigma > \sigma_c$  holds almost everywhere on the boundary when  $\theta \gtrsim 10^\circ$ . It is concluded on this basis that the fraction of sites with weak coupling on a boundary should increase with increasing  $\theta$ , leading to a monotonically decreasing dependence of the grain-boundary critical current  $J_c$  on  $\theta$ . However, this does not reflect that the critical current of a weak link is determined not only by its presence, but also and mainly by the thickness  $d$  of the region of weak coupling separating the “banks” with strong coupling<sup>10</sup> [for example, for an SNS Josephson junction having a thickness

$d$  that exceeds the normal-metal coherence length  $\xi_N$  of electrons,  $J_c \propto \exp(-d/\xi_N)$ . Therefore, it is not enough to calculate the stresses on the grain boundary itself, but it is also necessary to find the width of the near-boundary region in which these stresses are sufficiently great. The corresponding calculation shows (see Sec. 2) that at large values of  $\theta$ , at which the dislocation density increases, the stresses they create are mutually compensated, so that the thickness of the "bad" near-boundary region decreases, rather than increases, with increasing  $\theta$ , beginning at  $\theta \approx 5^\circ$ . Thus, the standard dislocation model of a tilt boundary cannot account for the angular dependence of the grain-boundary critical current.

The present work examines a modified dislocation model of a tilt grain boundary: a boundary with irregular periodicity in the arrangement of the edge dislocations. A calculation of the stress fields on such boundaries makes it possible to find the angular dependence of the grain-boundary critical current. It turns out that a faithful description of such superconducting properties of grain boundaries as the angular and magnetic-field dependence of their critical current can be attained on the basis of the latter model.

## 2. SYMMETRIC TILT BOUNDARY WITH A PERIODIC SYSTEM OF DISLOCATIONS

Below we shall start out from known expressions<sup>9</sup> for the components of the stress tensor created by a single edge dislocation that is located at the origin of coordinates and characterized by a Burgers vector  $\mathbf{b}$  parallel to the  $x$  axis (since such a dislocation corresponds to an extra half-plane parallel to the  $y$  axis, we call it a  $Y$  dislocation):

$$\begin{aligned} \sigma_{xx}^Y &= -\sigma_0 \frac{y(3x^2 + y^2)}{(x^2 + y^2)^2}, & \sigma_{yy}^Y &= \sigma_0 \frac{y(x^2 - y^2)}{(x^2 + y^2)^2}, \\ \sigma_{xy}^Y &= \sigma_0 \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}, \end{aligned} \quad (1)$$

where  $G$  is the shear modulus,  $\mu$  is Poisson's ratio, and  $\sigma_0 = Gb[2\pi(1-\mu)]^{-1}$ .

This is a so-called Volterra equation, which was obtained in the model of a continuous medium. It ignores the atomic structure of the crystal and, in particular, does not take into account the details in the layout of the dislocation core. The latter could be taken into account by employing the physically more correct Peierls equation;<sup>9</sup> however, the resultant corrections to the stress are significant only at distances of the order of the lattice constant  $a$ . They do not have any appreciable influence on the superconducting properties of the near-boundary region, since the width of the latter is determined by the normal-metal coherence length  $\xi_N$  of electrons, which significantly exceeds  $a$ . [We also note that  $b \approx a$  in (1)].

A simple (symmetric) tilt grain boundary parallel to the  $y$  axis is a set of  $Y$  dislocations positioned at equal distances  $D_y = a[2 \sin(\theta/2)]^{-1}$  from one another, where  $\theta$  is the misorientation angle of the neighboring crystallites (grains). The total stresses created by a row of such dislocations can be calculated using the known expressions<sup>9</sup>

$$\begin{aligned} \frac{\sigma_{xx}}{\sigma_0} &= -\frac{\pi b}{D_y} \\ &\times \frac{\sin(2\pi Y)[\cosh(2\pi X) - \cos(2\pi Y) + 2\pi X \sinh(2\pi X)]}{[\cosh(2\pi X) - \cos(2\pi Y)]^2}, \\ \frac{\sigma_{yy}}{\sigma_0} &= -\frac{\pi b}{D_y} \\ &\times \frac{\sin(2\pi Y)[\cosh(2\pi X) - \cos(2\pi Y) - 2\pi X \sinh(2\pi X)]}{[\cosh(2\pi X) - \cos(2\pi Y)]^2}, \end{aligned} \quad (2)$$

$$\frac{\sigma_{xy}}{\sigma_0} = \frac{\pi b}{D_y} \frac{2\pi X[\cosh(2\pi X)\cos(2\pi Y) - 1]}{[\cosh(2\pi X) - \cos(2\pi Y)]^2},$$

in which  $X = x/D_y$  and  $Y = y/D_y$ .

The dislocation model of a weak superconducting link on a boundary between superconducting grains is based on the assumption that the superconducting order parameter is reduced in regions subjected to strong mechanical stresses. Without going into the specific mechanism of this phenomenon, we note that it is associated with the appearance of an electric potential when a lattice undergoes strain, i.e., the so-called deformation potential  $\varphi \sim \Xi \varepsilon$ , where  $\Xi \sim 10$  eV is the deformation potential constant and  $\varepsilon \sim \sigma/\sigma_0$  is the strain of the lattice. When the displacement of the electronic energy levels  $\sim e\varphi$  becomes comparable to the Fermi energy  $\varepsilon_F \sim 0.1$  eV (for high- $T_c$  superconductors), the electronic spectrum undergoes radical reorganization, which results in suppression of the superconducting state. Thus, a stress  $\sigma_c \sim (\varepsilon_F/\Xi)\sigma_0 \sim 0.01\sigma_0$ , under which the relative strain of the lattice amounts to  $\sim 1\%$  (Ref. 5), can be considered strong. For simplicity we assume that the order parameter vanishes in regions where  $\sigma_{ik} \geq \sigma_c$  and remains unchanged wherever  $\sigma_{ik} < \sigma_c$ . Then the effective local thickness  $d_{\text{eff}}$  of the near-boundary layer, in which the superconductivity is destroyed by the stress, varies along the boundary and can be calculated using the relation

$$\langle d_{\text{eff}}^{ik} \rangle = 2 \int_0^\infty h(\sigma_{ik}(x, y) - \sigma_c) dx, \quad (3)$$

where  $h(s)$  is a Heaviside function [ $h(s > 0) = 1$ ,  $h(s \leq 0) = 0$ ],  $\langle d_{\text{eff}}^{ik} \rangle$  is the local thickness (which depends on the coordinate  $y$  along the boundary) of the nonsuperconducting near-boundary layer calculated from the stress  $\sigma_{ik}$ , and the factor 2 takes into account the fact that the superconductivity is destroyed on both sides of the boundary.

It is not known which of the stress components, i.e., the compression (expansion) or the shear, more effectively destroys superconductivity. Therefore, in this paper we shall consider their effects equivalent, assuming that the magnitude of the critical stress  $\sigma_c$  is identical for all the components  $\sigma_{ik}$ .

The local critical current density of a weak link is determined by the local value of  $\langle d_{\text{eff}}^{ik} \rangle$  and can be written in the form<sup>10</sup>

$$j_c^i(y) \approx j_c^0 \exp(-\langle d_{\text{eff}}^{ik} \rangle / \xi_N), \quad (4)$$

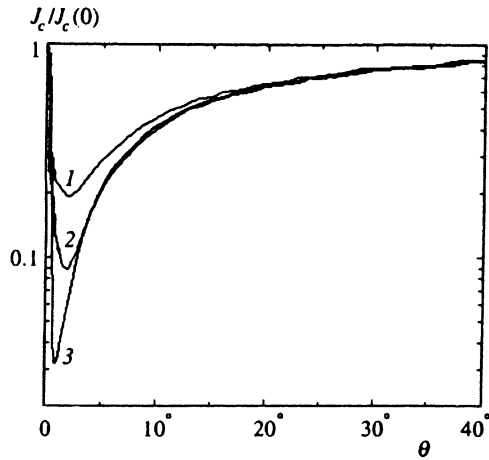


FIG. 1. Dependence of the average critical current density of a simple (symmetric) tilt grain boundary on the misorientation angle  $\theta$  for  $\xi_N/a=10$ . The critical stress  $\sigma_c=0.01\sigma_0$ : 1 —  $ik=xx$ , 2 —  $ik=yy$ , 3 —  $ik=xy$ .

where  $j_c^0$  is the critical current density in the bulk of the grain.

Finally, the critical current density  $J_c$  of a grain boundary is obtained by averaging the local current density and is defined by the relation

$$J_c = \frac{1}{L} \int_0^L j_c(y) dy \approx j_c^0 \left( \frac{1}{L} \int_0^L \exp\left(-\frac{\langle d_{\text{eff}}^{ik} \rangle}{\xi_N}\right) dy \right), \quad (5)$$

where  $L$  is the length of the boundary.

Figure 1 presents plots of the dependence of the average critical current density of a simple tilt phase boundary thus calculated on the misorientation angle  $\theta$ . It was assumed in these calculations that  $\xi_N/a=10$ , which corresponds to  $\xi_N \sim 40 \text{ \AA}$ , if we assume that  $a \sim 4 \text{ \AA}$ .<sup>3)</sup> It is seen that the critical current  $J_c$  drops sharply already at small values of  $\theta \sim 1^\circ - 2^\circ$ ; however, as  $Y$  increases further, it begins to increase, and it no longer differs much from the bulk value when  $\theta \approx 30^\circ - 40^\circ$ . This is a consequence of the almost complete balancing of the stresses created by numerous dislocations at distances exceeding the period  $D_y$ . Since  $D_y$  approaches  $a$  at large misorientation angles, only a comparatively narrow band of bad (strongly stressed) material with a width  $\sim a$  remains along the boundary, and it lowers the grain-boundary critical current only slightly when  $\xi_N \gg a$ .

The result obtained is consistent with experiment in only one respect: it predicts a sharp drop in  $J_c$  at small values of  $\theta$ . At the same time, the dependence of  $J_c$  on  $\theta$  obtained deviates sharply from the experimental dependence, which exhibits a monotonic decrease in  $J_c$  with increasing  $\theta$ . Thus, it is clear that the simple model used becomes invalid at large misorientation angles and must be revised.

We also note that, according to Fig. 1, the most effective suppression of the grain-boundary critical current occurs over the entire range of values of  $\theta$  due to the shear stress  $\sigma_{xy}$  of the edge dislocations. This can apparently account for the experimental fact that the current-carrying properties of twist boundaries (where there is only a shear stress of screw

dislocations) differ only slightly from the properties of tilt boundaries. However, we recall, first, that this conclusion is based on an assumption that the critical values for all the stress components are equal and, second, that it refers only to the periodic system of edge dislocations considered here, which incorrectly predicts the angular dependence of the grain-boundary current.

### 3. SYMMETRIC TILT BOUNDARY WITH A PERIODIC SYSTEM OF DISLOCATIONS

Within the model considered above the system of dislocations on the grain boundary was considered periodic, since just such a system should (all other conditions being equal) have the smallest energy. This is the standard approach used in practically all studies devoted to the influence of boundary dislocations on the electrophysical properties of grain-boundary junctions in superconductors. Nevertheless, there are various factors that destroy the periodicity in a system of edge dislocations. The first of these is associated with the incommensurate relationship between the period  $D_y$  and the lattice constant  $a$ . It leads to random displacement of the dislocations relative to their regular positions, the typical value of such displacements being of order  $a$ . However, even in the case of a commensurate relationship, the thermodynamic-equilibrium state of a system of dislocations at room temperature contains excitations of various types, which cause bending of the dislocations and their displacement from the positions corresponding to the smallest energy.

The dispersion or the characteristic value of such displacements can be calculated on the basis of thermodynamic arguments, for example, by treating a dislocation as an elastic string:<sup>9</sup>

$$\Delta \sim \frac{1}{\pi} \left( \frac{2LkT}{\Phi} \right)^{1/2}, \quad \Phi \approx \frac{Gb^2}{4\pi} \ln\left(\frac{L}{b}\right), \quad (6)$$

where  $\Phi$  is the so-called linear stress of the dislocation,  $L$  is its length, and  $T$  is the temperature. In our case  $L$  is the dimension of the grain boundary along the rotation axis of one grain relative to the other (in the case of a superconducting film deposited on a bicrystal substrate,  $L$  is simply the thickness of the film).

To evaluate  $\Delta$  we note that  $Gb^3 \sim 5 \text{ eV}$ . For  $kT \sim 0.05 \text{ eV}$  (the temperature at which grain-boundary junctions or films are created on bicrystal substrates) and  $L = 0.1 - 1 \mu\text{m} \sim 10^3 b$ , this gives  $\Delta \sim b$ .

Thus, it is physically more correct to take into account the destruction of the periodicity in a system of edge dislocations by assuming that under typical conditions the dislocations are randomly displaced relative to their equilibrium positions by a distance of the order of the lattice constant. The problem is to understand whether such displacements influence the field of dislocation stresses in the near-boundary region, which determines the critical current of the weak link formed.

To take into account this circumstance in an approximation, we consider a simple model, in which the edge dislocations on a symmetric tilt boundary are randomly displaced

relative to their equilibrium periodic positions. In addition, we further simplify the problem by assuming that such random displacements occur only along the tilt boundary. The period of the dislocation structure then becomes a random quantity, which is centered relative to the former value  $D_y = b/2 \sin(\theta/2)$  with a spread  $\Delta$ .

In solving this problem we can regard the resultant stress field as result of the superposition of the random perturbations associated with the displacements of the dislocations from their equilibrium positions on the periodic background (which corresponds to their equilibrium periodic configuration). Such perturbations are created by dislocation dipoles located on the grain boundary, which have a characteristic dimension (the distance between dislocations of opposite sign)  $\sim \Delta$ . If the spread  $\Delta$  of the values is great, compensation of the stresses due to the dipoles occurs only at a large distance from the boundary ( $x \gg \Delta$ ). At such distances the weak periodic background can be neglected, and only the stresses due to the system of dipoles need be taken into account.

The largest contribution to the stress at a given point is made, of course, by the dipoles nearest to it, whose number increases as  $\theta$  increases. Their contribution coincides in order of magnitude with the contribution of the single dipole closest to the particular point. The latter (for example,  $\delta\sigma_{xx}$ ) can be evaluated easily using the corresponding relation (1):  $\delta\sigma_{xx} \approx 3\sigma_0 b \Delta / x^2$  ( $x$  is the distance from the point under consideration to the boundary). The analogous contribution associated with the displacement of dislocations by a distance  $\sim \Delta$  in the direction perpendicular to the boundary is  $\delta_{\perp}\sigma_{xx} \approx 2\sigma_0(y/x)b\Delta/x^2$ , i.e., it is significantly smaller. The same conclusion also applies to  $\sigma_{yy}$ . Conversely, the displacements of dislocations perpendicular to the boundary are most significant for  $\sigma_{xy}$ .

In the region where the magnitude of the stress created by the nearest dislocation dipole is greater than the critical value  $\sigma_c$ , superconductivity is absent. The thickness  $d$  of this region is specified by the equality  $\delta\sigma_{xx} \approx \sigma_c$ , from which follows the relation

$$d \approx 2 \left( \frac{3b\Delta}{\sigma_c/\sigma_0} \right)^{1/2}. \quad (7)$$

(The factor 2, as above, takes into account the formation of bad material on both sides of the boundary.) The critical current of the weak link formed can be evaluated using the relation

$$\frac{j_c}{j_c(0)} \sim \exp\left(-\frac{d}{\xi_N}\right) \sim \exp\left[-\left(\frac{12b\Delta/\xi_N^2}{\sigma_c/\sigma_0}\right)^{1/2}\right]. \quad (8)$$

If  $b \approx \Delta \approx a$  and  $\sigma_c/\sigma_0 = 0.01$ , it hence follows that  $j_c/j_c(0) \sim \exp(-35a/\xi_N)$ , which gives  $j_c/j_c(0) \sim 0.03$  when  $\xi_N \approx 10a$ . This result, of course, applies to the situation in which the critical current is determined not by the background stress of the periodic system of edge dislocations, but by the random system of dislocation dipoles. This corresponds to  $\theta \gtrsim 5^\circ$  (see Fig. 2).

Numerical calculations of the stresses in the model under consideration were performed using the relations<sup>4)</sup>

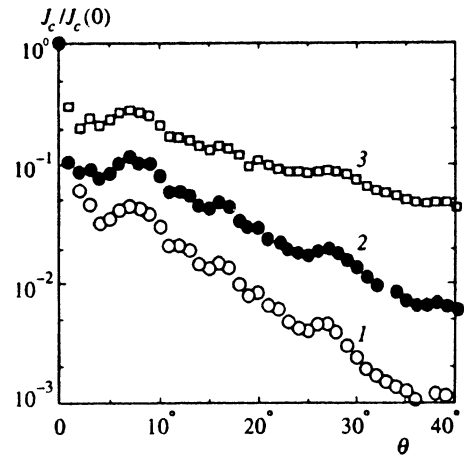


FIG. 2. Dependence of the average critical current density of a symmetric tilt boundary with randomly displaced dislocations on the misorientation angle  $\theta$  for  $\xi_N/a = 6$  (1), 10 (2), and 20 (3). The critical stress  $\sigma_c = 0.01\sigma_0$ ;  $\Delta = 2a$ .

$$\sigma_{xx} = \sigma_{xx}^0 + \delta\sigma_{xx}, \quad \delta\sigma_{xx} = \sum_{n=-\infty}^{\infty} \sigma_{xx}^y(x, y_n + \Delta_n(y_n)) - \sum_{n=-\infty}^{\infty} \sigma_{xx}^y(x, y_n), \quad (9)$$

$$\sigma_{xy} = \sigma_{xy}^0 + \delta\sigma_{xy}, \quad \delta\sigma_{xy} = \sum_{n=-\infty}^{\infty} \sigma_{xy}^y(x + \Delta_n(y_n), y_n) - \sum_{n=-\infty}^{\infty} \sigma_{xy}^y(x, y_n),$$

where  $\sigma_{ik}^0$  is the background stress created by the periodic system of dislocations [it is defined by (2)] and  $\Delta_n(y_n)$  is a random function with a zero mean value. When the calculations were performed, the random values of this function were distributed uniformly in the range  $-\Delta < \Delta_n$  for  $\Delta = a, 2a$  (the root-mean-square displacements of the dislocations from their equilibrium positions equal  $a/\sqrt{3} \approx a/2$  and  $2a/\sqrt{3} \approx a$ , respectively).

The calculations show that among the restrictions imposed on the critical current by the different stress components ( $\sigma_{xx}$ ,  $\sigma_{yy}$ ,  $\sigma_{xy}$ ), the one associated with the stress field  $\sigma_{xx}$  is the most significant. The random field  $\sigma_{xx}$  has the most long-range influence, and therefore the critical current calculated from  $\sigma_{xx}$  is several times smaller than the values calculated from  $\sigma_{yy}$  and  $\sigma_{xy}$ .

Figure 2 presents calculated plots of the dependence of the critical current on the misorientation angle  $\theta$ , which were obtained within the stochastic dislocation model considered here. At small misorientation angles ( $\theta \leq 5^\circ$ ), at which the distance between the dislocations is great ( $D_y \gg a$ ), the stress field they create is weakly sensitive to the random displacements of the dislocations by distances of order  $a$ . Therefore, the critical current has the same behavior as in the model of regularly distributed dislocations. As  $\theta$  increases, the average distance between the dislocations becomes comparable to their random displacement, and the system becomes com-

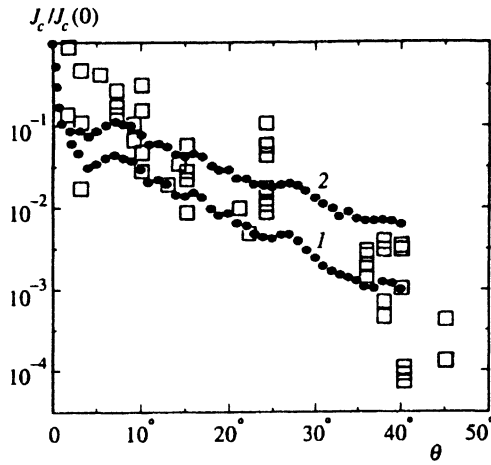


FIG. 3. Comparison of calculated angular dependences of the critical current of a symmetric tilt grain boundary [model of randomly distributed edge dislocations,  $\Delta=2a$ ,  $\sigma_c=0.01$ ,  $\xi_N/a=6$  (1) and 10 (2)] with experimental data pertaining to tilt grain boundaries in YBCO films on bicrystal substrates.<sup>12</sup>

pletely irregular. In this case the stresses of the individual dislocations becomes unbalanced, and the thickness of the layer of bad material near the boundary increases. This results in a rapid decrease in the critical current with increasing  $\theta$ . As is seen from Fig. 2, the dependence of  $j_c$  on  $\theta$  in this case is nearly exponential, i.e.,  $j_c(\theta) \propto \exp(-\theta/\theta_0)$ , where  $\theta_0 \sim 10^\circ$ , and depends on the set of parameters chosen.

How well the proposed model agrees with experiment can be seen from Fig. 3, which presents experimental data on the critical currents of tilt grain boundaries in YBCO films on bicrystal substrates<sup>12</sup> and calculated plots for randomly distributed edge dislocations.

#### 4. MAGNETIC-FIELD DEPENDENCE OF THE GRAIN-BOUNDARY CRITICAL CURRENT

The magnetic-field dependence  $J_c(H)$  of the critical current of a Josephson junction is determined, as we know, by the spatial dependence  $j_c(y)$  of the local critical current density:<sup>10</sup>

$$J_c(H) \propto \left| \int j_c(y) \exp\left(\frac{i\Phi}{\Phi_0} \frac{dy}{L}\right) \right|, \quad (10)$$

where the integration is carried out over the entire length  $L$  of the junction,  $\Phi$  is the magnetic flux in the junction, and  $\Phi_0$  is the magnetic flux quantum.

The random character of the distribution of the boundary dislocations leads to a random distribution of the local critical current density  $j_c(y)$  along a grain boundary. An example of such a distribution for a  $15^\circ$  symmetric grain boundary, which was obtained using (4), is presented in Fig. 4.<sup>5)</sup> It is known<sup>10</sup> that the magnetic-field dependence of the total critical current of a Josephson junction with a random distribution of the local critical current should have a plateau at fairly strong magnetic fields, which corresponds to the so-called residual critical current  $J_{c,\text{res}}$ . The relative magnitude  $\gamma = J_{c,\text{res}}/J_c(H=0)$  of this current is defined by the relation

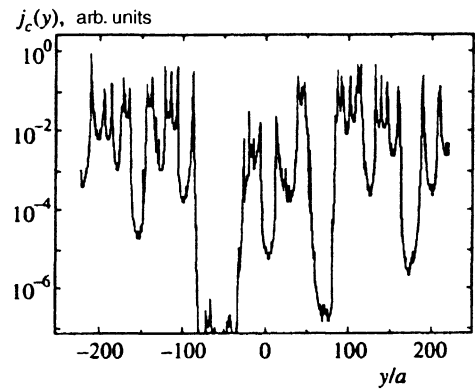


FIG. 4. Fragment of the distribution of the local critical current density along a  $15^\circ$  symmetric tilt grain boundary ( $\xi=6a$ ,  $\Delta=2a$ ).

$$\gamma^2 = \frac{\langle (j_c - \bar{j}_c)^2 \rangle}{\bar{j}_c^2} \frac{2R}{L}, \quad (11)$$

and the right-hand boundary of the plateau corresponds to the magnetic field at which  $\Phi/\Phi_0 \approx L/2R$ . Using the numerical values of the corresponding parameters presented in the last footnote, we find  $J_{c,\text{res}}/J_c(H=0) \approx 0.05$  for a junction with  $L=3 \times 10^4 a \approx 10 \mu\text{m}$ . The value found is in good agreement with the experimentally determined values of the residual current of grain-boundary Josephson junctions in YBCO films on bicrystal substrates.<sup>13</sup>

A distinct plateau appears on the plot of  $J_c(H)$  only in the limit  $L \rightarrow \infty$ . For a junction of finite length we should expect only that the average value  $\langle J_c \rangle$  of the critical current would remain more or less constant in the region of the postulated plateau. A calculation of  $J_c(H)$  using Eq. (10) confirms this conclusion: instead of the Fraunhofer dependence  $J_c(H) \propto |\sin(\pi\Phi/\Phi_0)(\pi\Phi/\Phi_0)^{-1}|$ , typical of a junction with a constant local critical current density (which is characteristic of  $\theta=0$ ), the calculated plot of  $J_c(H)$  is far less regular, and in the range of magnetic fields indicated the average value  $\langle J_c \rangle$  does not, in fact, tend to zero with increasing  $H$  (see Fig. 5). This dependence is often observed both in experiments with Josephson junctions in superconducting films on bicrystal substrates<sup>14,15</sup> and in experiments with grain-boundary junctions in polycrystalline superconductors.<sup>16</sup>

Figure 6 presents the calculated magnetic-field dependence of the critical current of a  $20^\circ$  junction over a far broader range of magnetic fields than in Fig. 5. It is clearly seen that the plateau on the plot of  $J_c(H)$  gives way to a power-law decrease in the average critical current. The estimate of the position of the right-hand boundary of the plateau given above ( $\Phi/\Phi_0 \approx 15$  for  $L=440a$  and  $R \approx 15a$ ) agrees well with the calculation, and the exponent of the power-law decrease in  $\langle J_c \rangle$ , which equals  $\approx (2/3)$ , coincides with the experimentally measured value.<sup>15</sup>

#### 5. CONCLUSIONS

We have shown that the model of a tilt grain boundary with a periodic system of edge dislocations cannot correctly describe the angular dependence of the critical current of

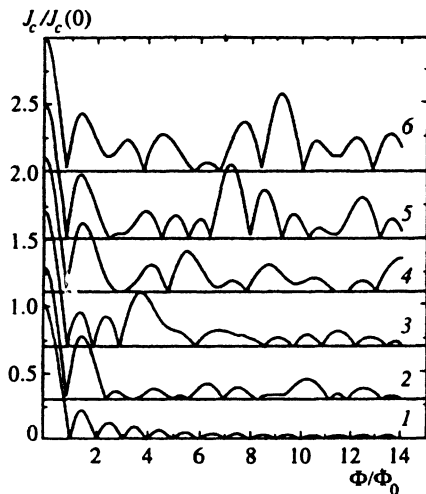


FIG. 5. Magnetic-field dependence of the critical current of symmetric tilt grain boundaries with a random local critical current density ( $\xi=6a$ ,  $\Delta=2a$ ,  $L=440a$ ) for various values of the misorientation angle  $\theta$  (in degrees): 1 — 0, 2 — 5, 3 — 10, 4 — 15, 5 — 20, 6 — 25. Curve 4 corresponds to the plot of  $j_c(y)$  in Fig. 4.

such a boundary. Conversely, the model of a boundary with irregular periodicity in the arrangement of the edge dislocations is perfectly consistent with experiment.

Since the calculation of the critical current was performed on the basis of approximate relations, the results obtained should be regarded as semiquantitative. A more exact scheme based on a numerical solution of the Ginzburg-Landau equation in the near-boundary region with a nonuniform temperature in the superconducting junction was used in Ref. 17. The spatial dependence  $T_c(x)$  for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  films was determined from experimental data taken from  $\delta(x)$  profiles of the oxygen concentration near boundaries<sup>7</sup> using the known relation  $T_c = T_c(\delta)$ . However,

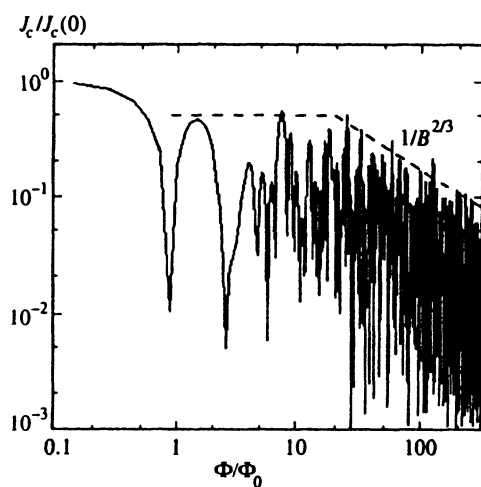


FIG. 6. Magnetic-field dependence of the critical current of a symmetric 20° tilt grain boundary with a random local critical current density ( $\xi=6a$ ,  $\Delta=2a$ ,  $L=440a$ ). The dashed lines correspond to the plateau and the region of the power-law decrease in the critical current ( $J_c \propto B^{-m}$ ,  $m=2/3$ ). The autocorrelation function of the local current density for this boundary is nearly exponential and has a correlation radius  $R \approx 15a$ .

such an approach cannot yield the angular dependence of the grain-boundary critical current  $J_c(\theta)$ . At the same time, the current-carrying ability of polycrystalline systems of practical importance is associated with the passage of current through a large number of differently oriented grain boundaries, and, therefore, the angular dependence of the critical currents of such boundaries must be known for calculations. In Ref. 18 a simplified calculation of this kind was based on the introduction of a certain critical angle  $\theta_c$ , such that  $J_c(\theta < \theta_c) = \text{const}$  and  $J_c(\theta > \theta_c) = 0$ . Although interesting results were obtained, it is clear that such an approximation is fairly rough, and the calculation requires a refinement based on the use of more exact angular dependences of the ground-boundary critical currents.

<sup>1</sup>There are indications of the existence of special tilt boundaries with strong coupling.<sup>6</sup> However, such boundaries, which are apparently associated with specific features of the crystal structure, are not typical and are not considered in the present work.

<sup>2</sup>We recall that the superconducting transition temperature in  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  depends strongly on the value of  $\delta$ :  $T_c \approx 92$  K for  $\delta=0.05$ ,  $T_c \approx 60$  K for  $\delta=0.4$ , and  $T_c=0$  for  $\delta \geq 0.6$  (Ref. 8).

<sup>3</sup>The values of  $\xi_N$  for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  crystals with different values of the resistivity  $\rho_N$  were presented in Ref. 11. For the case in which the near-boundary region behaves like a normal metal with  $\rho_N = 10^{-4} \Omega \cdot \text{cm}$ , we find  $\xi_N(50 \text{ K}) \approx 20 \text{ \AA}$ , which gives  $\xi/a \approx 5$  for  $a \approx 4 \text{ \AA}$ . The main results presented below were obtained during calculations in which it was assumed that  $\xi/a = 6$ .

<sup>4</sup>The expression for  $\sigma_{yy}$  is analogous to the relation for  $\sigma_{xx}$  presented in the text.

<sup>5</sup>The autocorrelation function of this distribution is nearly exponential and has a correlation radius  $R \approx 10a$  and a standard deviation  $\langle (j_c - \bar{j}_c)^2 \rangle / \bar{j}_c^2 \approx 6$ , where  $\bar{j}_c$  is the average value of  $j_c$  (the averaging is performed along the grain boundary). The numerical values of these parameters are used to evaluate the residual critical current of a Josephson junction (see below).

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