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Critical Current in High-Temperature Superconductors with Disordered Tilt Grain Boundaries

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Abstract—A model is suggested to describe the effect of tilt grain boundaries with partly random dislocation distribution on the critical current value in high-temperature superconductors. Within this model, the field of grain-boundary stresses $\sigma_{\alpha\beta}$ acquires a much more pronounced long-range character than in the case of a periodic dislocation arrangement. At large distances x from a tilt grain boundary, $\sigma_{\alpha\beta} \propto x^{-3/2}$ (which corresponds to the quasi-equidistant dislocation walls), whereas at small x, we have $\sigma_{\alpha\beta} \propto x^{-1/2}$ (which corresponds to randomly arranged dislocation walls). A region with stresses exceeding a certain critical value is treated as the region of normal metal, and, therefore, the critical current passing through this region decreases exponentially. It is shown that the model suggested satisfactorily agrees with experimental data. *© 2000 MAIK "Nauka/Interperiodica".*

Almost immediately upon the discovery of high-temperature superconductivity, it was established that grain boundaries strongly reduce the critical current value in high-temperature superconductors (HTSCs) [1]. In particular, the presence of grain boundaries with the misorientation angle $\Theta < 15°$ in $YBa_2Cu_3O_{7-\delta}$ bicrystals results in an exponential decrease in the critical current j_c depending on Θ in accordance with the approximate expression $j_c(\Theta) \sim j_c(0)\exp(-\Theta/8°)$ [1]. With a further increase in the misorientation angle Θ, the critical current exhibits saturation at a level of about $0.02J_c(0)$ [1].

Numerous attempts were made at interpreting this phenomenon [2–6]. In particular, several models were suggested to explain the observed decrease in the critical current in polycrystalline superconductors by various factors, such as a decrease in the free path of electrons in the vicinity of grain boundaries [2], vortex pinning [3], the formation of an antiferromagnetic phase [4], the effect of *d*-electrons [5], inhomogeneous chemical composition, etc. Unfortunately, none of these models can be recognized as satisfactory. However, most of them have one common feature—the stress fields generated by grain-boundary dislocations in HTSCs "suppress" the order in the vicinity of grain boundaries [2–4]. No detailed mechanism of this suppression has been suggested as yet, but it is frequently assumed that there exists a definite critical value of the stress field, σ_c, above which the superconducting phase undergoes transition into a nonsuperconducting state [3, 4, 6]. However, this leads to another problem. The point is that at the periodic arrangement of dislocations forming small-angle grain boundaries, the thickness of the nonsuperconducting phase (which is close to the period of a dislocation ensemble) starts decreasing with an increase in the misorientation angle Θ. This, in turn, should result in an increase in the critical current, which contradicts the known experimental data [1]. Therefore, it was assumed [4] that the nonsuperconducting phase has a dual nature, being partly a normal metal and partly an antiferromagnetic dielectric destroying the Cooper pairs.

Below, we propose a new approach to the problem. Since polycrystalline high-temperature superconductors are obtained under nonequilibrium conditions, the grain-boundary dislocations usually form nonequilibrium (nonperiodical) structures such as partly relaxed disordered walls [7, 8]. In this case, the stress fields have a more pronounced long-range nature. The law describing the stress decrease becomes power rather than exponential. At small distances x from grain boundaries, it has the form $\sigma_{\alpha\beta} \sim x^{-1/2}$, whereas at large distances x it is described as $\sigma_{\alpha\beta} \sim x^{-3/2}$ [7]. This approach provides for a sufficiently adequate description of the known experimental data on the critical current in HTSCs [1].

Consider first an infinite periodic small-angle tilt boundary in the plane yz of a coordinate system with the dislocation ordinates $y_n = nh_0$ ($n = 0, \pm 1, \pm 2, \ldots$), where $h_0 = b/2\sin(\Theta/2)$ is the dislocation spacing, Θ is the misorientation angle of grain boundaries, and $\mathbf{b} = (b, 0, 0)$ is the Burgers vector. In "nonequilibrium" grain boundaries, dislocations are randomly displaced by the distances $h_0\delta_n$ from their equilibrium positions, where δ_n are random numbers uniformly distributed over a certain interval $(-a, a)$. Then, for a "nonequilibrium" small-angle tilt boundary, the ordinates of dislocations are given by the formula

$$y_n = \frac{b}{2\sin(\Theta/2)}(n + \delta_n), \quad (1)$$

where

$$\langle \delta_n \rangle = 0, \quad \langle \delta_n^2 \rangle = a^2/3, \quad \langle \delta_m \delta_n \rangle = 0, \quad (2)$$

and the dispersion of the stress field of the boundary equals the sum of the dispersions of stresses due to individual dislocations:

$$D\sigma_{\alpha,\beta}(x, y) = \sum_{n=-\infty}^{\infty} \{\langle [\sigma_{\alpha,\beta}(x, y)]^2 \rangle - \langle [\sigma_{\alpha,\beta}(x, y)] \rangle^2\}. \quad (3)$$

Here, $\sigma_{\alpha\beta}^{(n)}$ is the stress field of the nth dislocation ($\alpha, \beta = (x, y)$) [9]:

$$\frac{\sigma_{xx}^{(n)}}{G} = \frac{b}{2\pi(1-\mu)} \frac{(y - y_n)[3x^2 + (y - y_n)^2]}{[x^2 + (y - y_n)^2]^2}, \quad (4)$$

$$\frac{\sigma_{yy}^{(n)}}{G} = \frac{b}{2\pi(1-\mu)} \frac{(y - y_n)[x^2 - (y - y_n)^2]}{[x^2 + (y - y_n)^2]^2}, \quad (5)$$

$$\frac{\sigma_{xy}^{(n)}}{G} = \frac{b}{2\pi(1-\mu)} \frac{x[x^2 - (y - y_n)^2]}{[x^2 + (y - y_n)^2]^2}, \quad (6)$$

$$\frac{\sigma_{zz}^{(n)}}{G} = \frac{\mu}{G}(\sigma_{xx}^{(n)} + \sigma_{yy}^{(n)}), \quad (7)$$

where G is the shear modulus and μ is Poisson's ratio.

Following the method suggested in [7], one can readily average $\sigma_{\alpha\beta}$ and $\sigma_{\alpha\beta}^2$ over y in the interval from $-a$ to a and then sum up the corresponding series in (3) to obtain the dispersions of the stress-tensor components averaged over y. The most pronounced dispersion is obtained for σ_{xx}:

$$D\sigma_{xx}(x) = \left(\frac{Gb}{2\pi h_0(1-\mu)}\right)^2 \frac{5\pi a^2}{4(x/h_0)[(x^2/h_0^2) + a^2]}. \quad (8)$$

The values of $D\sigma_{xy}$ and $D\sigma_{yy}$ are five times smaller than the value of $D\sigma_{xx}$, whereas $D\sigma_{zz}$ (at $\mu = 0.2$ [?]) is four times smaller than $D\sigma_{xx}$. Therefore, in what follows, we restrict our consideration to the component $D\sigma_{xx}$. Since $\langle \sigma_{xx} \rangle = 0$, the average value of the σ_{xx} modulus for an infinite grain boundary is

$$\langle |\sigma_{xx}| \rangle = \sqrt{\frac{D\sigma_{xx}}{\pi}}. \quad (9)$$

By a similar method, one can also calculate the dispersion of the stress field of partly relaxed dislocation walls. It was shown [8] that, in this case, dispersion decreases in the same way for all x and attains a value of $\Delta^2 D\sigma_{xx}$ in the range $0 < \Delta < 1$, where Δ is the relaxation coefficient. Thus, the average value of the stress-tensor modulus depends on the distance to the grain boundary in the following way:

$$\sigma(x) \equiv \langle |\sigma_{xx}| \rangle = \Delta \sqrt{\frac{D\sigma_{xx}}{\pi}} = \frac{G\Delta}{2\pi(1-\mu)} \sqrt{\frac{5\sin(\Theta/2)}{2(x/b)\left[1 + 4(x^2/a^2b^2)\sin^2\frac{\Theta}{2}\right]}}. \quad (10)$$

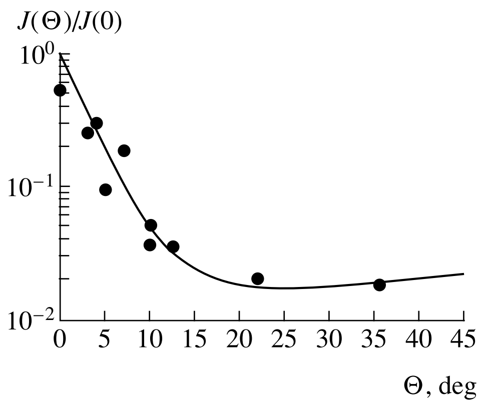
It is seen that the above dependence is determined by two dimensionless parameters a and Δ: $\sigma \sim x^{-3/2}$ for $x \gg ab/2\sin(\Theta/2)$, and $\sigma \sim x^{-1/2}$ for $x \ll ab/2\sin(\Theta/2)$ [7].

Now, assume that the stress field σ suppresses the superconducting order at $\sigma > \sigma_c = \alpha_c G$, where $\alpha_c \ll 1$ is the critical value of the ratio σ/G. According to the estimates [6], $\alpha_c \sim 10^{-2}$ and, if $-x_c < x < x_c$ (where x_c is the root of the equation $\sigma(x)/G = \alpha_c$), the superconducting phase passes into a nonsuperconducting state. In what follows, we will consider this state as a normal metal. The critical current through a $2x_c$-thick layer of a normal metal is known to decrease exponentially [9, 10] as

$$\frac{j_c(\Theta)}{j_{c0}} = \exp(-2x_c(\Theta)/\xi), \quad (11)$$

where ξ is the coherence length of electrons in a normal metal. Thus, once the dependence $x_c(\Theta)$ has been calculated from formula (10), one can also determine the dependence of the critical current on the misorientation angle.

The results calculated for the model suggested in this study were compared with the experiment according to the following scheme. First, the α_c and ξ/b values were set and the a and Δ values providing optimum correspondence to the experimental data were calculated. For example, at $\mu = 0.2$ (which corresponds to the values $\alpha_c = 10^{-2}$ and $\xi/b = 5$ for $YBa_2Cu_3O_{7-\delta}$), we obtain $a_{opt} \approx 4.13$ and $\Delta_{opt} = 0.313$. The theoretical curve $j_c(\Theta)/j_{c0}$ and the experimental data [1] corresponding to the above values are plotted in the figure to demonstrate a satisfactory coincidence. Our studies show that the shape of the calculated curve is almost independent of the choice of ξ/b and α_c, because $a_{opt} \approx 0.83\xi/b$ and, therefore, the value of Δ_{opt} at constant a is proportional



Average critical current as a function of the misorientation angle Θ. The solid line represents the theoretically calculated data and the filled circles represent the experimental data obtained in [1].

to the value of α_c. With an increase in ξ/b, the value of Δ_{opt} also slightly increases. In particular, at $\alpha_c = 0.01$ and $\xi/b = 50$, we obtain $a_{opt} \approx 41.2$ and $\Delta_{opt} = 0.989$.

This, the model of grain boundaries with randomly distributed dislocations in high-temperature superconductors qualitatively agrees with experimental data on the dependence of the critical current on the misorientation angle (see figure).

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