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CRITICAL CURRENT DENSITY IN POLYCRYSTALLINE HIGH-T_C SUPERCONDUCTORS WITH DISORDERED TILT BOUNDARIES

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Abstract. A theoretical model is suggested which describes the effect of tilt boundaries with chaotically arranged dislocations on the critical current density in high-transition-temperature (T_c) superconductors. Stress fields of such boundaries, that suppress high-T_c superconductivity, are revealed to be long-range as compared to those of tilt boundaries with periodically ordered grain boundary dislocations. With this factor taken into consideration, the dependence of the critical current density accross tilt boundaries on boundary misorientation θ is calculated and compared with the experimental data [1].

1. INTRODUCTION

The transport properties of grain boundaries in high - Tc superconducting materials are the subject of intensive theoretical and experimental studies (e.g., see [1-14]) motivated by extremely large interest to appllications of such materials. It has been experimentally revealed that grain boundaries drastically suppress the superconducting critical current [1-3]. In particular, the critical current density, j_c, across tilt boundaries in $YBa_2Cu_3O_{7-\delta}$ superconductors decreases with boundary misorientation angle θ as follows : $j_c(\theta)\approx j_c(0°)\exp(-\theta/8°)$, for θ ranging from 0° to 15°. The critical current density $\gamma_c(\theta)$ across high-angle tilt boundaries with θ > 15° is tentatively constant and low: $j_c(\theta > 15°) \approx 0.02\, j_c\,(0°)$ [1-3].

Microscopic mechanism of the grain boundary effect on high-T_c superconductivity is not understood yet, though several models of the effect in question have been suggested [5-14]. In particular, theoretical models have been elaborated describing the grain boundary effect as that related to the following factors : *(i)* a decrease of electron free path in vicinities of grain boundaries [6]; (*ii*) stress-field-induced structural disorder and pinning of magnetic vortices at grain boundaries [7-9]; (*iii*) formation of the antiferromagnetic phase within grain boundary cores [10]; (*iv*) faceting of grain boundaries and *d* -symmetry of the superconducting order parameter [11]; (*v*) deviations from bulk stoichiometry in vicinities of grain boundaries [12-14]. Most models discussed treat stress fields of grain boundary dislocations as those responsible for suppression of the superconducting order parameter in vicinities of grain boundaries in high-T_c superconductors [7-10]. Though the concrete mechanism of the suppression is not unambigiously recognized yet, many researchers assume the existence of a critical stress, σ_c, which characterizes superconductor-to-non-superconductor transition in stressed regions [7-10]. More precisely, superconductivity is supposed to be completely suppressed in regions where some component(s) of stress tensor is (are) larger than σ_c. However, this idea is in contradiction with experimental data in case of low-angle boundaries consisting of periodically arranged lattice dislocations (Fig.1a). Actually, for any value of σ_c, the volume fraction of "critically stressed" regions (regions where some component(s) of stress tensor is (are) larger than σ_c) in vicinities of such low-angle boundaries (that create short- or intermediate-range stress fields which drop as $exp(-x/h_0)$, where x denotes the distance from a boundary plane, and h_0 the interspacing (period) between periodically arranged dislocations, see (Figs. 1a and 2a) decreases with boundary misorientation θ.

This, in context of the idea on existence of the critical stress sc, results in increase of the critical current density, j_c, with boundary misorientation θ, while experiments [1-3] are indicative of the fact that j_c drastically decreases with θ in the range of θ from 0° to tentatively 15°. In order to avoid the contradiction dis-

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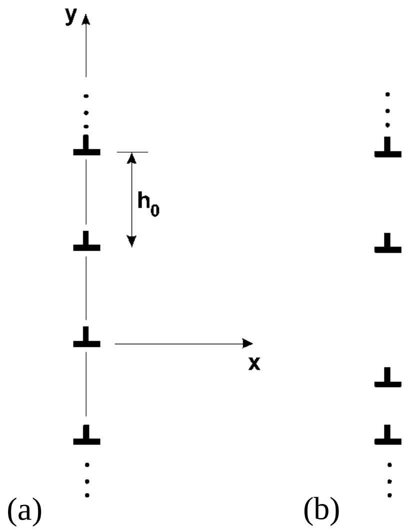

Fig. 1. Ordered and disordered, low-angle tilt boundaries are represented as (a) periodically ordered and (b) disordered walls of crystal lattice dislocations of the edge type, respectively.

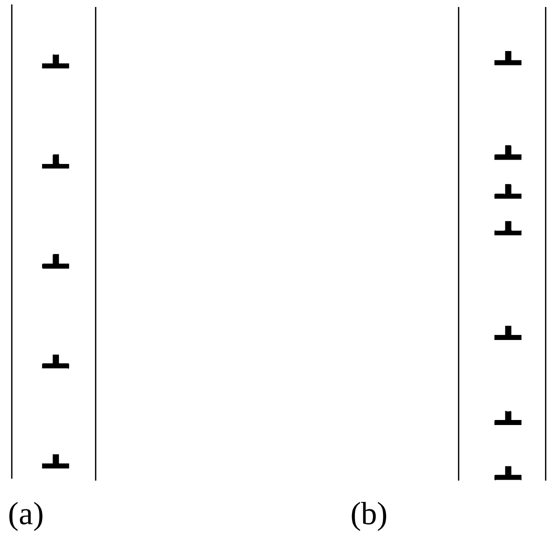

Fig. 2. High-angle tilt boundaries with (a) periodically ordered and (b) disordered ensembles of grain boundary dislocations.

cussed, Gurevich and Pashitskii [10] assume that the non-superconducting, critically stressed regions consist of two, normal metal and antiferromagnetic, phases, in which case the antiferromagnetic phase effectively destroys the coupling of Cooper electrons in vicinities of grain boundaries.

In this paper we suggest an alternative model of the grain boundary effect on high-Tc superconductivity, based on both the idea on critical stress σ_c and that on disorder in spatial arrangement of grain boundary dislocations in high-T_c superconductors. Actually, high-T_c superconducting materials commonly are synthesized at non-equilibrium conditions at which grain boundary dislocations can form “non-equilibrium” structures (Figs. 1b and 2b) that are different from “equilibrium”, periodic ones (Figs. 1a and 2a). It this situation, grain boundaries in high-T_c superconducting materials, as with boundaries in conventional materials synthesized at non-equilibrium conditions [15,16], create long-range stress fields which drop as $x^{-1/2}$ or $x^{-3/2}$. The main aim of this paper is to calculate the angular dependence of the critical current density, $j_c(\theta)$, in high-T_c superconductors with tilt boundaries containing disorderedly distributed dislocations.

2. MODELS OF LOW- AND HIGH-ANGLE TILT BOUNDARIES IN HIGH-T_C SUPERCONDUCTORS

Stress fields of grain boundaries, in fact, are created by boundary defects (first of all, dislocations) whose parameters are caused by the structural geometry of boundaries. So, low-angle tilt boundaries (with misorientation θ ranging from 0° to $\theta_c \approx 15°$) are effectively represented as walls of lattice dislocations (of the edge type) with Burgers vectors being those of the crystalline lattice [17,18] (Fig.1). For $\theta > \theta_c$, cores of lattice dislocations overlap which compose grain boundaries. As a corollary, high-angle tilt boundaries (with $\theta > \theta_c$) have layer-like cores (characterized by thickness ≈ 1 nm) (Fig.2) with the structure being different from the crystalline structure of adjacent grains. The layer-like cores of high-angle boundaries commonly contain grain boundary dislocations (Fig.2) with Burgers vectors being those of displacement-shift-complete lattices of high-angle boundaries [18]. Moduli of such Burgers vectors commonly are lower than moduli of Burgers vectors of crystal lattice dislocations composing low-angle boundaries.

Grain boundaries at equilibrium conditions form either periodic (Figs.1a and 2a) [17,18] or quasiperiodic [18-20] ensembles that correspond to minimum elastic energy density of such boundaries. Grain boundaries in polycrystalline materials synthesized at highly non-equilibrium conditions are non-equilibrium in the sense that they are characterized by disorder in spatial arrangement of boundary dislocations (see Figs.1b and 2b). In doing so, ensembles of grain boundary dislocations at high-angle boundaries (Fig. 2b), in general, are more disorderedly distributed than lattice dislocations composing low-angle boundaries (Fig. 1b). The aforesaid is related to the fact that dislocations at high-angle boundaries are characterized by small Burgers vectors as compared to those at low-angle boundaries; in this case displacements of dislocations from their equilibrium positions at high-angle boundaries are accompanied by low changes in the elastic energy density as compared to those of dislocations composing low-angle boundaries.

Now let us consider a low-angle tilt boundary of infinite extent, which consists of lattice dislocations periodically spaced in plane *yz* in coordinate system shown in (Fig. 1a). Such dislocations are characterized by ordinates $y_n = nh_0$ and Burgers vectors $\vec{b} = (b,0,0)$ with h_0 and b being in the Frank's relationship [18]: $b = 2h_0\sin(\theta/2)$. Dislocations at "non-equilibrium" tilt boundary (Fig. 1b) are assumed to be displaced by $h_0\,\delta_n(-a < \delta_n < a)$ in a randomly uniform way from their "equilibrium" positions corresponding to the periodic arrangement shown in Fig. 1a. In other words, the probability of finding the *n*th dislocation in an infinitesimal interval $(y,y + dy)$ belonging to the interval $y_n - a \le y \le y_n + a$ is equal to $dy/2a$. In the situation discussed, ordinates of the dislocations composing the "non-equilibrium" tilt boundary (Fig. 1b) are given as:

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

where

$$<\delta_n>= 0,\ <\delta_n^2>= \frac{a^2}{3},\ <\delta_m\delta_n>= 0\,, \tag{2}$$

with <...> being the averaging on the non-equilibrium dislocation ensemble. The dispersion of grain boundary stress is equal to the sum of the dispersions of stresses induced by the boundary dislocations:

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

with $\sigma_{\alpha\beta}^{(n)}$ (on the r.h.s. of formula (3)) being the stress field of the *n*th dislocation, which, following [17], can be written as:

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

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

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

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

Here G denotes the shear modulus, and μ the Poisson ratio.

After some algebra based on the calculation scheme [15], from (1)–(7) we have found the averaged (on the ordinate *y*) dispersion, $D\sigma_{\alpha\beta}(x)$, of stress tensor components in vicinity of a non-equilibrium tilt boundary. Following the results of our calculations, the largest dispersion is that of σ_{xx}:

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

For any x, values of $D\sigma_{xy}$ and $D\sigma_{yy}$ are lower by factor 5, while values of $D\sigma_{zz}$ (for μ=0.2; see experimental data [21]) are lower by factor ≈ 4 than those of $D\sigma_{xx}$. Therefore, in context of the idea [7-10] on the crucial effect of the largest stress tensor component on high-T_c superconductivity, here and in the following we will focus on analysis of the dispersion $D\sigma_{xx}$. In doing so, we find the mean value of modulus of σ_{xx} in vicinity of a non-equilibrium tilt boundary of infinite extent to be as follows :

$$<|\sigma_{xx}|>= \sqrt{\frac{D\sigma_{xx}}{\pi}}, \tag{10}$$

because $<\sigma_{xx}> = 0$.

The dispersion of stress tensor components in the case of grain boundaries with partly relaxed dislocation distributions can be calculated by the same methods as with previously examined non-relaxed disordered dislocation ensembles. So, in paper [16] it has been shown that the dispersion in question can be written as $\Delta^2 D\sigma_{xx}$ with Δ $(0 < \Delta < 1)$ being the factor of relaxation. In these circumstances, the mean value of modulus of σ_{xx} depends on the distance, x, from a partly relaxed tilt boundary as follows:

$$\sigma(x) \equiv <|\sigma_{xx}|>= \Delta\sqrt{\frac{D\sigma_{xx}}{\pi}} = \frac{G\Delta}{2\pi(1-\mu)} \times \\ \sqrt{\frac{5\sin(\theta/2)}{2\dfrac{x}{b}\left[1+4\dfrac{x^2}{a^2b^2}\sin^2(\theta/2)\right]}} \tag{11}$$

According to formula (10), $\sigma(x)$ is strongly affected by the two non-dimensional parameters, a and Δ: $\sigma \propto x^{-3/2}$, if $x \ll ab/2\sin(\theta/2)$; and $\sigma \propto x^{-1/2}$, if $x \ll ab/2\sin(\theta/2)$ [15].

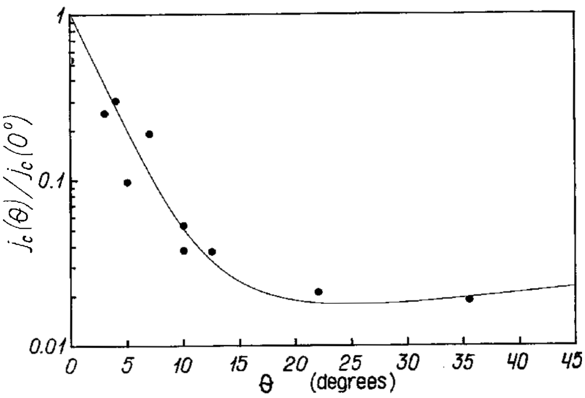

Fig.3. Theoretical (solid curve) and experimental [1] (dots) dependences of the averaged density (j_c) of the superconducting critical current accross "non-equilibrium" tilt boundaries on boundary misorientation (θ).

3. CRITICAL CURRENT DENSITY ACROSS DISORDERED TILT BOUNDARIES

In spirit of models [7-10], let us assume that high-T_c superconductivity disappears in stressed regions in which $\sigma(x) > \sigma_c = \alpha_c G$, where $\alpha_c \ll 1$. Following [8], $\alpha_c \approx 10^{-2}$. In the situation discussed, we find that the non-superconducting phase in vicinity of a tilt boundary with a partly relaxed dislocation distribution lies in the layer: $-x_c < x < x_c$, where x_c is extracted from equation $\sigma(x = x_c) = \alpha_c G$. For definiteness, let us assume that the non-superconducting phase exhibits the normal metal properties. Then, according to the theory of Cooper pairs tunneling [22,23], we find the critical current density across a normal metal layer of thickness $2x_c$ in vicinity of the tilt boundary to be as follows:

$$\frac{j_c(\theta)}{j_c(0°)} = \exp(-2x_c(\theta)/\xi), \qquad (11)$$

where ξ is the electron coherence length in the normal metal phase. Formula (10) and (11) allow one to calculate $x_c(\theta)$ and, therefore, the dependence of the critical current density, j_c, on boundary misorientation.

In the framework of the suggested model, the angular dependence of j_c was calculated as that optimally corresponding to the experimental data [1], in which case parameters, a and Δ, was used as adjusting parameters. In doing so, for characteristic values of $\mu = 0.2$ [21], $\alpha_c = 10^{-2}$ and $\xi/b=5$, we find the optimal correspondence between our theoretical calculations of $j_c(\theta)$ and the experiments [1] (Fig.3) to come into play at $a_{opt} \approx 4.13$ and $\Delta_{opt} = 0.313$. Fig.3 is indicative of a satisfactory agreement between the model under consideration and the experimental data [1].

Analysis of the theoretical dependence $j_c(\theta)$ shows that this dependence is weakly affected by parameters, ξ/b and α_c, because $a_{opt} \approx 0.83\xi/b$, and Δ_{opt} runs parallel with α_c at constant a. When ξ/b grows, value of Δ_{opt} weakly increases. With this taken into conside-ration, we find that "structural transition" from low-angle tilt boundaries (weakly disordered walls of dislocation with large Burgers vectors; see Fig.1b) to high-angle tilt boundaries (containing highly disordered ensembles of dislocations with small Burgers vectors; see Fig.2b) occuring at $\theta \approx \theta_c$ does not result in any jump-like changes of the theoretical dependence $j_c(\theta)$ at $\theta \approx \theta_c$ (see Fig.3).

4. CONCLUSION

In conclusion, in this paper we have developed a theoretical model which describes the tilt boundary effect on high-T_c superconductivity as that related to long-range stresses (which suppress the superconducting order parameter) created by tilt boundaries with disorderdly arranged dislocations. In this context, the disorder of grain boundary dislocation ensembles is caused by highly non-equilibrium conditions of synthesis of polycrystalline high-T_c superconductors. The angular dependence, $j_c(\theta)$, calculated within the framework of the suggested model, is in a satisfactory agreement with the experimental data [1] (see Fig.3).

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REFERENCES

[1] D. Dimos, P. Chaudhari, J. Mannhart and F.K. LeGoues // *Phys. Rev. Lett.* **61** (1988) 219.

[2] D. Dimos, P. Chaudhari and J. Mannhart // *Phys. Rev. B* **41** (1990) 4038.

[3] T. Amrein, M. Seitz, D. Uhe, L. Schultz and K. Urban // *Appl. Phys. Lett.* **63** (1993) 1978.

[4] M. Prester // *Supercond. Sci. Technol.* **11** (1998) 33.

[5] N.D. Browing, E.M. James, K. Kyosuke, I. Arlsan, J.P. Buban, J.A. Zaborac, S.J. Pennycook, Y.Xin and G. Duscher // *Rev. Adv. Mater. Sci.* **1** (2000) 3.

[6] K.E. Bagnall, I.V. Grigirieva and J.W. Steeds // *Supercond. Sci. Technol.* **8** (1995) 605.

[7] D. Agassi, C.S. Pande and R.A. Masumura // *Phys. Rev. B* **52** (1995) 16237.

[8] M.F. Chisholm and S.J. Pennycook // *Nature* **351** (1991) 47.

[9] K. Jagannadham and J. Narayan // *Philos. Mag.* **61** (1990) 129.

[10] A. Gurevich and E.A. Pashitskii // *Phys. Rev. B* **57** (1998) 13878.

[11] H. Hilgenkamp, J. Mannhart and B. Mayer // *Phys. Rev. B* **53** (1996) 14586.

[12] S.E. Babcock and D.C. Larbalestier // *Appl. Phys. Lett.* **55** (1989) 393.

[13] D.M. Kroeger, A. Choudhary, J. Brynestad, R.K. Williams, R.A. Padgett and W. Goghlan // *J. Appl. Phys.* **64** (1988) 331.

[14] A.Yu. Kraevskii and I.A. Ovid'ko // *Phys. Sol. State* **42** (2000).

[15] A.A. Nazarov, A.E. Romanov and B. Baudelet // *Philos. Mag. Lett.* **68** (1993) 303.

[16] A.A. Nazarov, R.Z. Valiev and A.E. Romanov // *Sol. State Phen*. **35/36** (1994) 381.

[17] J.P. Hirth and J. Lothe, *Theory of Dislocations* (N.Y.:McGraw-Hill, 1975).

[18] A.P. Sutton and R.W. Balluffi, *Interfaces in Crystalline Materials* (Oxford, Clarendon Press, 1995).

[19] K.N. Mikaelyan, I.A. Ovid'ko and A.E. Romanov // *Mater. Sci. Eng. A* **259** (1999) 132.

[20] I.A. Ovid'ko // *Mater. Sci. Eng. A* **280** (2000) 355.

[21] M. Cankurtaran, G.A. Saunders, J.R. Willis, A. Al-Kheffaji and D.P. Almond // *Phys. Rev. B* **39** (1989) 2872.

[22] P.G. De Gennes // *Rev. Mod. Phys*. **36** (1964) 225.

[23] A. Barone and G. Paterno, *Physics and Applications of the Josephson Effect* (N.Y., Wiley, 1982).