Transformations of faceted grain boundaries in high-T_c superconductors

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A theoretical model is suggested that describes the transformations of faceted low-angle grain boundaries in high-T_c superconductors. Conditions are theoretically revealed at which the formation of split dislocation configurations at facet junctions and central parts of facets of low-angle tilt boundaries is energetically favorable. The results of the suggested model account for experimental data reported in the literature on observation of faceted low-angle tilt boundaries consisting of split dislocation configurations in high-T_c superconductors.

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The effects of grain boundaries on high-T_c superconductivity in cuprates are the subject of intensive fundamental research efforts (see, e.g., Refs. 1–21) motivated by a range of technological applications of polycrystalline high-T_c superconductors. Of special interest from both fundamental and applied viewpoints is the drastic reduction of the critical current density across grain boundaries. Though a systematic understanding of suppression of the transport properties of grain boundaries is still expected, there are no doubts in the crucial influence of grain boundary structures on these properties. This causes interest for experimental identification and theoretical description of grain boundary structures in high-T_c superconductors. Faceted structure[19,20,22–24] [Fig. 1(a)] and split dislocation configurations[17–20] are among the experimentally detected specific structural peculiarities of low-angle grain boundaries, which are expected to strongly affect their transport properties. Recently, a theoretical model[15] has been suggested describing the experimentally observed[17] split dislocation configurations at plane low-angle tilt boundaries in YBaCuO superconductors. These split configurations have been assumed to be identical along a grain boundary plane, as it has been detected in experiments.[17] However, in contrast to the case of plane grain boundaries, the split dislocation configurations belonging to one faceted grain boundary are very different in the case of faceted grain boundaries. Following experimental data,[19,20] central parts of facets contain split dislocation configurations with partial dislocations well distant from each other [Fig. 1(b)], while dislocations in the vicinity of junctions of grain boundary facets either do not split or split into partial dislocations closely distant from each other [Fig. 1(b)]. The main aim of this paper is to propose a theoretical model which describes the experimentally observed[19,20] split dislocation configurations at faceted grain boundaries in high-T_c superconductors.

Let us discuss geometric peculiarities of faceted structures of low-angle boundaries and their effects on the dislocation configurations at grain boundaries with focuses placed on the exemplary case of low-angle boundaries in $YBa_2Cu_3O_{7-\delta}$ superconductors. Dislocations at facet junctions and central parts of grain boundary facets have different arrangements of their neighboring dislocations (Fig. 1). As a result, stress fields of these neighboring dislocations cause different conditions of the formation of split dislocation configurations [Fig. 1(b)] at facet junction and a central part of a facet, which is driven by a release of the elastic energy of the system. Conditions of the formation of split dislocations at the facet center are very similar to those in the case of the plane grain boundary, because of the similarity in neighboring-dislocation arrangement in these cases. In the context of the similarity in question, we will not consider in detail calculation of energetic characteristics of split dislocation configurations at facet centers, which, in fact, is the same as in the previously examined situation[15] with split dislocations at plane grain boundaries. In this paper, we will focus our analysis on split dislocation configurations at facet junctions, where the dislocations are placed in the stress field, being the superposition of the stress fields created by two finite dislocation walls at adjacent (misoriented) boundary facets.

So, let us consider two neighboring facets of the boundary in its initial state, containing N_1 and N_2 perfect lattice dislocations periodically arranged along the first facet with period h_1 and along the second facet with period h_2, respectively. Burgers vectors of the dislocations belonging to the first (second, respectively) facet are denoted as $\mathbf{B}_1$ ($\mathbf{B}_2$, respectively). In order to theoretically characterize the conditions at which the structural transformations of faceted tilt boundaries occur in high-T_c superconductors, we will distinguish the two basic structures of such boundaries, conventional [Fig. 1(a)] and split [Fig. 1(b)] structures. A faceted tilt

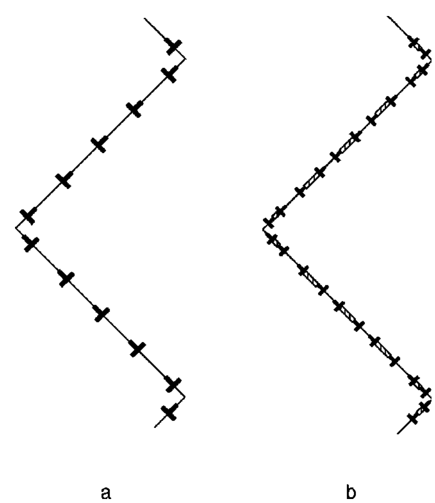

FIG. 1. Structures of faceted tilt boundaries in high-T_c superconductors: (a) conventional and (b) split structures.

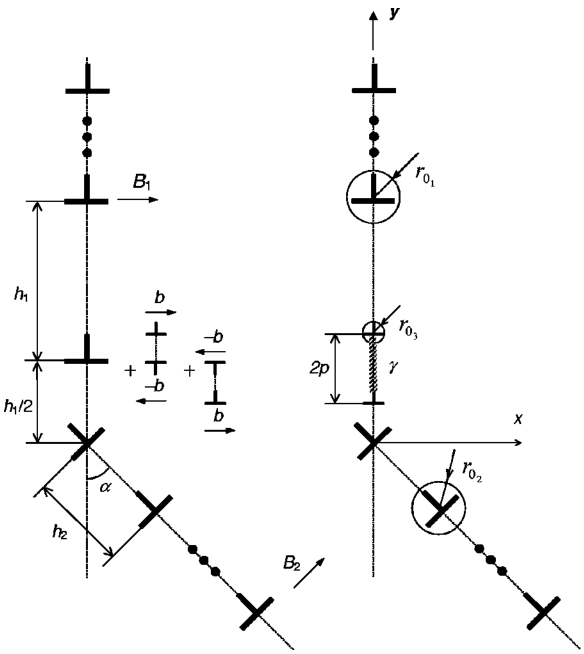

FIG. 2. Low-angle boundary structure 1-2. (a) Two facets of a low-angle boundary consisting of perfect dislocations with one dislocation being replaced by a split dislocation configuration at facet junction. (b) Split dislocation configuration is represented as a perfect dislocation and two dipoles of partial dislocations.

boundary with the conventional structure (before the transformation) represents a consequence of facets of two types, each consisting of periodically spaced perfect lattice dislocations [Fig. 1(a)]. The split structure of a faceted tilt boundary (after the transformation) corresponds to a consequence of facets of two types, each consisting of split dislocation configurations [Fig. 1(b)]. For purposes of this paper dealing with a theoretical description of the structural transformations of faceted tilt boundaries in high-T_c superconductors, we will focus on the situation with an element of the split structure being generated in the preexistent conventional structure at facet junction [Fig. 2(a)]. In other words, we will theoretically examine characteristics of the new dislocation structure: A conventional faceted tilt boundary with one perfect dislocation being replaced by a split dislocation configuration at a facet junction [Fig. 2(a)]. In these circumstances, in order to quantitatively describe the conditions at which the structural transformation in question occur, we will examine the conditions at which the formation of new dislocation structure is energetically favourable.

Following the theory of dislocations in solids,[25] the split dislocation configuration [Fig. 2(a)] can be represented as a perfect dislocation and two dipoles of partial dislocations, as shown in Fig. 2(b). In the framework of this representation, the lower dislocation of the top dipole and the top dislocation of the lower dipole are located at the same position as the perfect dislocation, in which case their combination is equivalent to the absence of any dislocation at the initial position of the perfect dislocation.

With the representation [Fig. 2(b)] taken into account, let us consider the difference in the energy (per unit length of dislocations) between the conventional dislocation structure [Fig. 1(a)] and the new dislocation structure shown in Fig. 2(a). For shortness, hereinafter, the conventional dislocation structure [Fig. 1(a)] and the dislocation structure shown in Fig. 2(a) will be denoted as structure 1 and structure 1–2, respectively. The energy of structure 1 can be written as follows:

$$W_1 = N_1 W_1^{\mathrm{el}} + N_2 W_2^{\mathrm{el}} + W_{\mathrm{int}}^{B_1-B_2} + N_1 W_1^c + N_2 W_2^c, \qquad (1)$$

where W_1^{el} (W_2^{el}, respectively) the elastic energy of a perfect dislocation belonging to the first (second, respectively) facet of structure 1 per its unit length, W_1^c (W_2^c, respectively) the energy of a perfect dislocation core at the first (second, respectively) facet, and $W_{\mathrm{int}}^{B_1\text{-}B_2}$ the energy of interaction between facets.

The energy of structure 1-2 is given as

$$W_2 = N_1 W_1^{\mathrm{el}} + N_2 W_2^{\mathrm{el}} + W_{\mathrm{int}}^{B_1-B_2} + (N_1-1) W_1^c + N_2 W_2^c + 2 W_{\mathrm{dip}}^{\mathrm{el}} + 2 W_3^c + W_{\mathrm{int}}^{\mathrm{dip}} + W_{\mathrm{int}}^{\mathrm{dip1\text{-}dis}} + W_{\mathrm{int}}^{\mathrm{dip2\text{-}dis}} + 2(p - r_{0_3})\gamma. \qquad (2)$$

Here $W_{\mathrm{dip}}^{\mathrm{el}}$ denotes the proper energy of a dipole of partial dislocations, W_3^c the energy of a partial dislocation core, $W_{\mathrm{int}}^{\mathrm{dip}}$ the energy of interaction between the dipoles [Fig. 2(b)], $W_{\mathrm{int}}^{\mathrm{dip1\text{-}dis}}$ the energy of interaction between the upper dipole of partial dislocations and the structure 1, $W_{\mathrm{int}}^{\mathrm{dip2\text{-}dis}}$ the energy of interaction of the lower dipole and structure 1, r_{0_3} the radius of a partial dislocation core, and $2p$ and γ are, respectively, the length and the energy of stacking fault formed between the partial dislocations composing the split dislocation configuration [Fig. 2(a)].

From Eqs. (1) and (2) we find that the change in the energy that accompanies transformation of structure 1 into structure 1-2 is as follows:

$$\Delta W_{1-2} = W_2 - W_1 = -W_1^c + 2 W_{\mathrm{dip}}^{\mathrm{el}} + 2 W_3^c + W_{\mathrm{int}}^{\mathrm{dip}} + W_{\mathrm{int}}^{\mathrm{dip1\text{-}dis}} + W_{\mathrm{int}}^{\mathrm{dip2\text{-}dis}} + 2(p - r_{0_3})\gamma. \qquad (3)$$

The equation $\Delta W_{1-2} = 0$ corresponds to the critical conditions at which the structure-1-to-structure-1-2 transformation occurs.

Let us consider terms on the right-hand side of formula (3). The dislocation core energy for a perfect dislocation (W_1^c) and a partial dislocation (W_3^c) are given by known formulas:[25]

$$W_1^c = \frac{G B_1^2}{4\pi(1-\nu)}, \qquad W_3^c = \frac{G b^2}{4\pi(1-\nu)}, \qquad (4)$$

where B_1 and b are Burgers vectors of perfect (from the first facet) and partial dislocations, respectively; G denotes the shear modulus and ν the Poisson ratio. Following Ref. 15 the energies $W_{\mathrm{dip}}^{\mathrm{el}}$ and $W_{\mathrm{int}}^{\mathrm{dip}}$ are as follows:

$$W_{\mathrm{dip}}^{\mathrm{el}} = \frac{G b^2}{2\pi(1-\nu)} \ln\frac{p - r_{0_3}}{r_{0_3}}, \qquad W_{\mathrm{int}}^{\mathrm{dip}} = \frac{G b^2}{2\pi(1-\nu)} \ln\frac{p + r_{0_3}}{2 r_{0_3}}. \qquad (5)$$

Now let us consider the energies $W_{\rm int}^{\rm dip1\text{-}dis}$ and $W_{\rm int}^{\rm dip2\text{-}dis}$. Following the approach in Ref. 26 the energy that characterizes elastic interaction between two defects can be calculated as the work spent to transfer one defect from a free surface of a solid to its current position in the stress field created by another defect. In this context, in our case, the interaction energies $W_{\rm int}^{\rm dip1\text{-}dis}$ and $W_{\rm int}^{\rm dip2\text{-}dis}$ can be written in the general form as follows:

$$W_{\rm int}^{\rm dip1\text{-}dis}=b\int_{h_1/2+r_{0_3}}^{h_1/2+p}[\sigma_{xx}^{(1)}(x=0,y)+\sigma_{xx}^{(2)}(x=0,y)]dy, \tag{6}$$

$$W_{\rm int}^{\rm dip2\text{-}dis}=b\int_{h_1/2-r_{0_3}}^{h_1/2-p}[\sigma_{xx}^{(1)}(x=0,y)+\sigma_{xx}^{(2)}(x=0,y)]dy. \tag{7}$$

Here $\sigma_{xx}^{(1)}(x,y)$ and $\sigma_{xx}^{(2)}(x,y)$ are the stress components of dislocations belonging to the first and second facets, respectively. Burgers vectors of the dislocations belonging to the first facet are oriented along axis x (Fig. 2). Therefore, $\sigma_{xx}^{(1)}(x,y)$ represents the following sum of stresses of these dislocations:[25]

$$\sigma_{xx}^{(1)}(x,y)=\sum_{n=0}^{N_1-1}\sigma_{xx}^{B_1}(x,y-h_1(n+1/2))=-\frac{GB_1}{2\pi(1-\nu)}\sum_{n=0}^{N_1-1}\frac{[y-h_1(n+1/2)]\{[y-h_1(n+1/2)]^2+3x^2\}}{\{x^2+[y-h_1(n+1/2)]^2\}^2}. \tag{8}$$

Burgers vectors of the dislocations belonging to the second facet (Fig. 2) are not parallel with axis x, in which case it is convenient to write the stress component $\sigma_{xx}^{(2)}(x,y)$ as the sum of stresses created by dislocations with Burgers vectors being projections B_{2x} and B_{2y} of the vector $\mathbf{B}_2$ onto axes x and y, respectively:

$$\sigma_{xx}^{(2)}(x,y)=\sum_{n=0}^{N_2-1}[\sigma_{xx}^{B_{2x}}(x-nh_2\sin\alpha,y+nh_2\cos\alpha)+\sigma_{xx}^{B_{2y}}(x-nh_2\sin\alpha,y+nh_2\cos\alpha)], \tag{9}$$

where

$$\sigma_{xx}^{B_{2x}}(x-nh_2\sin\alpha,y+nh_2\cos\alpha)=\frac{GB_2\cos\alpha}{2\pi(1-\nu)}\frac{[y+nh_2\cos\alpha][(y+nh_2\cos\alpha)^2-3(x-nh_2\sin\alpha)^2]}{[(x-nh_2\sin\alpha)^2+(y+nh_2\cos\alpha)^2]^2}, \tag{10}$$

$$\sigma_{xx}^{B_{2y}}(x-nh_2\sin\alpha,y+nh_2\cos\alpha)=\frac{GB_2\sin\alpha}{2\pi(1-\nu)}\frac{[x-nh_2\sin\alpha][(x-nh_2\sin\alpha)^2-(y+nh_2\cos\alpha)^2]}{[(x-nh_2\sin\alpha)^2+(y+nh_2\cos\alpha)^2]^2}. \tag{11}$$

Now we have formulas (4)–(11), which allow one to calculate all terms of the characteristic energy difference ΔW_{1-2}. With these formulas, we have calculated the dependence of ΔW_{1-2} on p (where $2p$ is the distance between partial dislocations forming a split configuration) in the exemplary case of (100) and (110) facets, for the following characteristic values of parameters: $B_1\approx 3.9$ Å, $B_2\approx 5.5$ Å, $h_1\approx 4.5$ nm, $h_2\approx 6.3$ nm (these values of B_1, B_2, h_1, and h_2 correspond to boundary tilt misorientation $\theta=5°$), $\alpha=45°$, $N_1=N_2=5$, $\gamma=1.1$ J/m^2, $G=113$ GPa, and $\nu=0.3$; see curve 1 in Fig. 3. In Fig. 3 the dependence $\Delta\widetilde{W}_{1-2}$ that characterizes the formation of a split dislocation configuration at the facet center is shown as curve 2. In doing so, $\Delta\widetilde{W}_{1-2}$ is calculated using the approach in Ref. 15, for parameters listed above.

Let us analyze these dependences. Both ΔW_{1-2} and $\Delta\widetilde{W}_{1-2}$ (curves 1 and 2 in Fig. 3, respectively) are negative at any p in the range under consideration. However, the dependence $\Delta\widetilde{W}_{1-2}$ has its minimum at $2p=2p'\approx 6B_1$, whereas the dependence ΔW_{1-2} decreases with decreasing p from $8B_1$ to $B1$, where $B_1=3.9$ Å is close to crystal lattice parameters of YBaCuO cuprate along the a and b axes. In these circumstances, the split dislocation configuration with minimal interspacing between partial dislocations is most energetically favorable at facet junctions. At the same time, the formation of split dislocation configurations with the interspacing $2p=2p'$ (in our case, $2p'\approx 6B_1$) is energetically favorable in the central parts of grain boundary facets. These results obtained in the framework of our model are in agreement with experimental data[19,20] on observation of split dislocation configurations at faceted grain boundaries in YBaCuO superconductors, which are small at facet junctions and extended at central parts of facets.

Thus, in this paper a theoretical model has been suggested describing transformations of boundary dislocation structures at faceted tilt boundaries in high-T_c superconductors. In the framework of the model suggested, boundary dislocations at facet junctions and central parts of boundary facets split into

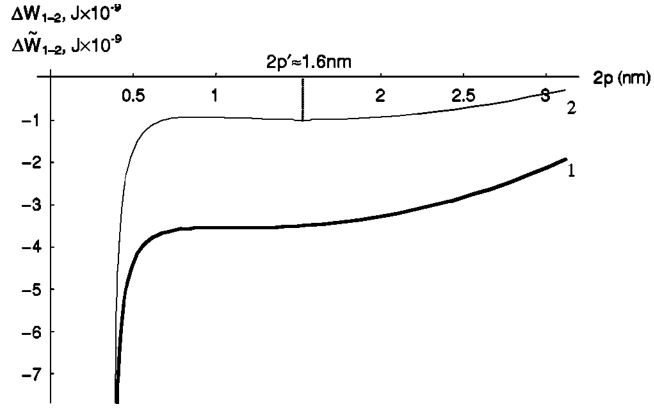

FIG. 3. Dependences of the characteristic energy differences (ΔW_{1-2} and $\Delta \tilde{W}_{1-2}$) on interspacing $2p$ between partial dislocations forming a split dislocation configuration at facet junction (solid curve 1) and central part of a boundary facet (curve 2).

partial dislocations joined by small and extended stacking faults, respectively. The rearrangements of grain boundary dislocations are driven by a release of the elastic energy density of grain boundary dislocation ensemble whose geometry causes different behaviors of dislocations at facet junctions and central parts of facets. In doing so, distribution of grain boundary dislocations varies along the grain boundary [see Fig. 1(b)] and, therefore, is capable of causing spatial variations of its transport properties. These theoretical results are directly supported by experimental data[19,20] on observation of split dislocation configurations at faceted grain boundaries in YBaCuO superconductors and are interesting in interpretation of experimentally observed[27–30] inhomogeneities of the supercurrent along grain boundaries in high-T_c superconductors.

In general, current models[2–13,21] of the grain boundary effect on high-T_c superconductivity are based on the representation of low-angle tilt boundaries as periodic walls of perfect dislocations [Fig. 1(a)]. However, in the light of both experiments[17–20] and theoretical analysis given in this paper, the splitting of dislocations at low-angle tilt boundaries (Fig. 1) should be definitely taken into consideration of the effects of grain boundary strain fields and core structures on high-T_c superconductivity in cuprates. Also, structural variations and the corresponding variations of the transport properties of faceted grain boundaries are worth being taken into account in analysis of percolation processes in polycrystalline high-T_c superconductors.[11,12] More precisely, in the context of experimental data[19,20] and theoretical results of this paper, a faceted grain boundary cannot be treated as a grain boundary network element with its characteristic constant value of critical current density. Such a boundary represents a combination of elements (in particular, facet junctions and central parts of facets) with different structures and, therefore, different transport properties. This view changes the geometry of network of elements conducting the supercurrent, which is very essential in a description[11,12] of percolation processes in polycrystalline high-T_c superconductors. The results of our theoretical analysis can be used also in a description of split dislocation configurations that often exist in semiconductors[31,32] and quasicrystals.[33,34]

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