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Twin boundary energy and characterization of charge redistribution near the twin boundaries of cupperate superconductors

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ABSTRACT

Ab-initio calculations under general gradient approximation have been employed for the first time to find out twin boundary energy, γ, in twined YBCO systems. Despite a vast discrepancy in reported experimental values, our results show that the γ value falls in the range of 40–85 mJ/m^2. On the other hand, functional form of γ versus inserted strains shows that the mean value for the twin width lamella would tend to approach zero as the strain goes to zero. We have also investigated the local charge transfer and the modification of the electronic states of the basal and twin planes in YBCO, because the charge redistribution at interfaces can modify transport across the grains considerably and determine the applicability of high-T_c superconductors in the electronic applications. The total density of electronic states at the Fermi level for the twined system is enhanced in comparison with the untwined one. Our results explain the influence of twin boundaries in superconductive properties of YBCO, in experimental situations.

1. Introduction

New materials manifest reversible plasticity properties like: elastic twinning, thermoelastic martensitic transformation, superelasticity, shape memory effect and reversible behavior in ferroelastic domains [1–4]. These materials have low-symmetry crystal structure and frequently exhibit twinning [5]. Twin structures have been observed from the first structural investigations of high T_c superconductors and their influences have already been discussed intensively [1,6–8]. On the other hand, one major problem in high-T_c material technology is their low current carrying capability of the sintered ceramic materials. Their critical currents, J_c, at 77 K and zero magnetic field, is typically between 100 and 1000 A/cm^2 which is at least two orders of magnitude lower than the needs for large scale applications [9–12]. Therefore, it is important to study the limiting factors of the critical current for practical purposes and obviously, anisotropic grains, grain boundaries, phase impurity and oxygen deficiency are among the important factors.

Experimental results intensively show that twin boundaries (TBs) are effective magnetic flux pinning centers at intermediate temperatures, 40–80 K, via blocking the motions of the magnetic vortices; therefore, the TBs behave as conduits or weak links for the vortices [13–16].

In this regard, the main factor for adjusting the TB's separation length (twin lamella width, TW) is TB's energy, γ, whose lower value causes generating finer twin lamellas and vice versa [17]. By the way, the γ parameter is a function of annealing temperature, oxygen partial pressure and also the impurity doped elements [18].

Generally speaking, the γ parameter is an important parameter for engineering of the twin microstructures to improve electrical and magnetic properties of the high T_c systems. Unfortunately, the main difficulty in empirical study of the twinning effects arises from their interference with the other plainer defects and imperfections. On the other hand, comprehensive physical model for the role of twin boundaries in superconductor properties has remained elusive.

In this article we employ density functional theory method to obtain and study the fully relaxed $YBa_2Cu_3O_{6+x}$ ($YBCO_x$) twin boundary. We find out the γ energy and its dependence on the oxygen stoichiometry(x). Effects of twinning on the electronic density of states (DOS) and charge redistribution in the interfaces that would influence superconductivity properties (T_c and J_c values) will be investigated.

1.1. Background

By oxygen adsorption in the $YBCO_x$ samples the resultant local strain fields cause a second order structural phase transition from the higher symmetry paraelastic tetragonal phase (Tet), to the

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lower symmetry ferroelastic orthorhombic phase (Ort). During this Tet/Ort structural phase transition, the resulting internal elastic shear stress fields (originating from changing the lattice parameters) can be released through twinning process along the (1 1 0) and (1 $\bar{1}$ 0) crystallographic planes (twin planes). The estimated expression for the average value of the TWs, can be obtained by balancing the elastic and the TB energies thus leading to the following equation [19–21]:

$$TW = [G\gamma/ES^2]^{1/2} \quad (1)$$

where G is the grain size (or twin colony size), E is the elastic modulus and S is the orthorhombicity ($S = 2(b-a)/(b+a)$) so it is a measure of the induced strain field after oxygen uptake. Moreover it is assumed that each grain is elastically bound to the neighboring grains and also entropy effects expectedly would introduce fluctuations around the above predicted value for the TWs (in the case of thin layer samples the G parameter is replaced by the layer's thickness) [22]. The validity of the above equation has also been confirmed in poly-crystalline samples by various authors [23–26].

An empirical method to determine the γ parameter could be possible by measuring the TW and G values directly via electron microscopy techniques and using the Eq. (1) or more accurately it can be obtained from slope of a linear fitting of the TWs versus the $G^{1/2}$, (the S and E values must be already determined by crystallographic and direct measuring methods).

Table 2
Calculated γ values under GGA and GGA + U calculation methods and the lattice constants for the twined and untwined super-cells. The experimental values report lattice constants for a twined sample as shown in the last row (for comparison).

YBCO system (calculated method)	γ(mJ/m^2)	a(Å)	b(Å)	c(Å)
Twined (GGA), smallest super-cell	81.64	3.89	3.87	11.63
Twined (GGA + U), smallest super-cell	84.52	3.83	3.93	11.63
Untwined YBCO	–	3.79	3.94	11.68
Twined (GGA), extended super-cell	23.57	3.82	3.9	11.68
Experimental values [42]	–	3.82	3.88	11.68

Mei and Chan [17] have shown the huge discrepancy between various reported γ values (via different experimental and inductive methods) and in Table 1 an updated summery of the issue is presented.

As Table 1 shows the reported values of the γ are spanned from 0.1 to 1000 mJ/m^2; therefore, it is essential to have further investigations along with a solid theoretical method for its determination. Recently Lopez et al. [35] have reported first principle calculations results about band structures and magnetic properties of the $YBCO_x$ samples [34] but up to the best of our knowledge there is

Table 1
Twin boundary energy in YBCO.

γ (mJ/m^2)	Method	Ref.; year
17	Morphology of coherent mixture of cubic and tetragonal phases controlled by elastic strain effect	[21]; 1983
0.1–0.2	Measurement of T in lamellae	[27]; 1990
1000	Dislocation theory	[28]; 1991
2.8	Twin spacing method	[25]; 1991
80	Twin spacing method	[29]; 1991
<40	Coercive stress	[30]; 1992
28.9 (without PtO_2)11.35 (with PtO_2)	Measurement of T in lamellae	[31]; 1996
8.5–2.6	Twin spacing method	[32]; 1996
46.5	T in equilamellar structure	[33]; 2001
60.0	Wedged twin tip shape	
75.7(450 °C) −17.47(680 °C)	Twin tip method	[17]; 2005
20.1–3.7 (from 450 to 680 °C)	Twin spacing method	

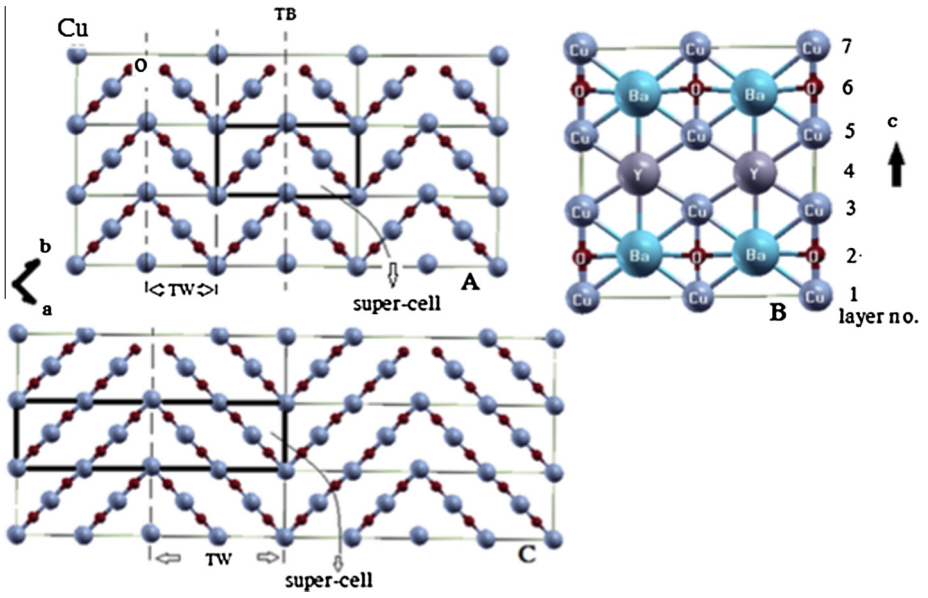

Fig. 1. A-top view of a Cu–O layer with marked (bold boundaries) smallest super-cells for (1 1 0) twin boundaries, B-side view of the super-cell with 7 layers, C-top view of the extended super-cell in the Cu–O plane (super-cells are chosen according to the HREM images).