Investigating the Atomic Scale Superconducting Properties of Grain Boundaries in High-\(T_c\) Superconductors

N. D. Browning,¹ J. P. Buban,¹ C. Prouteau,¹,² D. Verebelyi,² D. P. Norton,² D. K. Christen,² S. J. Pennycook,² and P. D. Nellist³

¹University of Illinois at Chicago, 845 West Taylor Street, Chicago, IL 60607-7059
²Solid State Division, Oak Ridge National Laboratory
P.O. Box 2008, Oak Ridge, Tennessee 37831-6030
³Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, United Kingdom

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Investigating the Atomic Scale Superconducting Properties of Grain Boundaries in High-Tc Superconductors

N. D. Browning¹, J. P. Buban¹, C. Prouteau¹², D. Verebelyi², D. P. Norton², D. K. Christen², S. J. Pennycook² and P. D. Nellist³

¹Dept. Physics, University of Illinois at Chicago, 845 W. Taylor St., Chicago, IL 60607-7059. USA.
²Solid State Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6030. USA
³Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE. UK

Over ten years after the discovery of high-Tc superconductors, their widespread application into viable device structures is still limited by the deleterious effect of grain boundaries. One of the main difficulties associated with understanding this effect is that transport measurements are usually performed on the micron scale. However, the critical parameter for superconductivity, the coherence length, is only ~1nm. To understand grain boundaries on a fundamental level it is therefore necessary to investigate the properties on this atomic scale; a scale attainable only by electron microscopy [1,2].

As an example of the observed properties of grain boundaries in YBa₂Cu₃O₇₋ₓ (YBCO), the V(I) curves recorded across a 24° boundary for several magnetic fields are shown in figure 1. To explain these properties, a model where the grain boundary is composed of equally sized and spaced dislocation cores separated by a very small fraction of much stronger links has been developed (figure 1). These strong links may carry either the depairing current, the Jc of the grains or another Josephson current (a depairing current seems unlikely in view of the field dependence of the experimental data). The simulated behavior obtained for this model, where the fraction of strong links is x=0.005 and Jc is the observed Jc(B) of the grains, exhibits qualitatively similar behavior to the experimental data (figure 1). However, the fit is not perfect, suggesting that the strong links are more likely to be regions of grain boundary with a higher Josephson current, rather than links with the Jc(B) of the grains.

Using electron microscopy we can look for the origin of these stronger coupled regions at the grain boundary. Figure 2 shows a Z-contrast image of a similar high-angle [001] tilt grain boundary in YBCO. The image shows that there are some regions where the boundary plane is symmetric, while other regions where it is asymmetric. EELS measurements [1] at such boundaries have shown that the symmetry of the boundary plane plays an important role in determining the properties. Asymmetric high-angle grain boundaries show significant hole depletion whereas symmetric high angle grain boundaries show very little (Figure 3). This effect can be understood using bond valence sum analysis [3]. Figure 4 shows the Cu valence plots across regions of both high angle symmetric and asymmetric boundaries. The asymmetric boundaries show a dramatic drop in the copper valence (charge carrying holes are formed by hybridization of the O 2p and Cu 3d bands), whereas the symmetric regions show areas of dramatic decrease in valence and areas where there is no valence change. The origin of this behavior is that the asymmetric boundaries always show a reconstruction on the Cu sub-lattice while symmetric boundaries show a reconstruction on both the Cu and Y/Ba sub-lattices (figure 2). Regions of the boundary plane where the reconstruction exists on the Y/Ba sub-lattice may be the strong links seen in the transport measurements. Work is continuing to investigate this supposition [4].

References

1. N. D. Browning et al, Physica C 212 (1993), 185
4. We would like to thank J. T. Luck for her help with sample preparation. This research is sponsored
FIG. 1- V(I) curves in several magnetic fields for a high-angle boundary can be modelled by considering the boundary plain to contain a small fraction of strong links. The simulated graph exhibits qualitatively similar behavior for a fraction $x=0.005$, and $J_c$ is the $J_c(B)$ of the grains.

FIG. 2- Z-contrast image of a 30° grain boundary showing an asymmetric segment on the left, containing a distorted unit cell, and a small symmetric segment on the right.

Fig.3- The hole concentration at grain boundaries can be quantified by the oxygen pre-edge. There is a significant difference between high-angle symmetric and asymmetric boundaries.

Fig. 4- Cu valence plot across an asymmetric boundary shows a broad depletion zone, whereas at an ideal grain boundary there is no depletion.