

The Grain Boundary Problem in High-Tc Superconductors

S. Graser¹, P. J. Hirschfeld², R. Gutser¹, B. M. Andersen³, J. Mannhart¹, and T. Kopp¹

¹ Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany

² Department of Physics, University of Florida, Gainesville, FL 32611, USA

³ Niels Bohr Institute, University of Copenhagen, Universitetsparken 5 DK-2100 Copenhagen, Denmark

e-mail: thilo.kopp@physik.uni-augsburg.de

The interface properties of high-temperature cuprate superconductors have been of interest for many years, and play an essential role in Josephson junctions, superconducting cables, and microwave electronics. In particular, the maximum critical current achievable in high- T_c wires and tapes is well known to be limited by the presence of grain boundaries,^a regions of mismatch between crystallites with misoriented crystalline axes. In studies of single, artificially fabricated grain boundaries the striking observation has been made that the critical current J_c of a grain boundary junction depends *exponentially* on the misorientation angle.^b Until now microscopic understanding of this apparently universal behavior has been lacking. We present the results of a microscopic evaluation based on a construction of fully three-dimensional $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ grain boundaries by molecular dynamics. With these structures, an effective tight-binding Hamiltonian is calculated for the d -wave superconductor with a grain boundary. The critical current is then shown to follow an exponential suppression with grain boundary angle.^c We identify the buildup of charge inhomogeneities as the dominant mechanism for the suppression of the supercurrent.

^a H. Hilgenkamp and J. Mannhart, *Grain boundaries in high- T_c superconductors*, Rev. Mod. Phys. **74**, 485 (2002).

^b D. Dimos, P. Chaudhari, J. Mannhart, and F. K. LeGoues, *Orientation dependence of grain-boundary critical currents in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ bicrystals*, Phys. Rev. Lett. **61**, 219 (1988).

^c S. Graser, P. J. Hirschfeld, T. Kopp, R. Gutser, B. M. Andersen, and J. Mannhart, *How grain boundaries limit supercurrents in high-temperature superconductors*, Nature Physics, **6**, 609 (2010).