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Cooperative doping mechanism of YBCO grain boundaries A. FRANCESCHETTI, S.J. PENNYCOOK, S.T. PANTELIDES, Vanderbilt University, Nashville, TN 37235 and Oak Ridge National Laboratory, Oak Ridge, TN 37831
— A major impediment to large-scale applications of high-Tc superconductors has been the low critical crurrent across grain boundaries. Grain-boundary doping, in particular by Ca, was shown to increase the critical current, but an atomic-scale understanding of the underlying mechanism is still lacking. Here we report first-principles, density-functional calculations of Ca-impurity and O-vacancy formation energies in YBCO. Using biaxial strain to mimic the effect of local strain at the grain boundaries, we find that Ca segregates at Cu or Ba sites, depending on the sign and magnitude of the local strain field. In bulk YBCO, Ca^{2+} ions are known to substitute for Y^{3+} ions, thereby providing additional holes. However, the doping mechanism proposed for bulk YBCO does not apply to grain-boundary doping, as Ca substitutes for Cu or Ba atoms. Instead, we propose that Ca doping provide strain relief at the grain boundary, thereby reducing the propensity of O vacancies to segregate, and effectively restoring high hole concentrations.

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