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Atomic arrangement and charge distribution in YBCO tilt grain boundaries J.K. BORDING, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton NY, 11973, J.W. HALLEY, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, Y. ZHU, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton NY, 11973
— It is well known that the critical current, J_c, in high-Tc superconductors is reduced at grain boundaries. Recent high resolution holography experiments show the [100] tilt grain boundaries in $YBa_2Cu_3O_{7-x}$ to have an excess negative charge localized at the boundary dislocation core. Upon doping with Ca, this charge is reduced and the critical current increased. To shed light on this behavior at an atomic scale, we carried out Tight Binding (TB) calculations of these boundaries. Our TB scheme is charge self consistent to allow charge transfer typical for ionic materials. We present the arrangement of atoms and charge in YBCO tilt grain boundaries as determined by a combination of TB calculations, recent high resolution Scanning Transmission Electron Microscopy and Electron Energy Loss Spectroscopy measurements.

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