Electronic properties of structural twin and antiphase boundaries in materials with strong electron-lattice couplings

K. H. AHN, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, T. LOOKMAN, A. SAXENA, A. R. BISHOP, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545 — Using a symmetry-based atomic scale theory of lattice distortions, we show that in functional materials with strong electron lattice coupling, the electronic properties are distinctly modified near elastic textures such as twin boundaries (TBs) and antiphase boundaries (APBs), which can be directly measured by STM. The results also show that the heterogeneities of electron local DOS are not confined within TBs and APBs, but can propagate into domains in the form of Friedel oscillations for TBs and with the wave vector related to short wave length lattice distortions for APBs. The results are discussed in relation with perovskite manganites and other functional electronic materials. Reference: Ahn, Lookman, Saxena, and Bishop, Phys. Rev. B 71, 212102 (2005).

This work is supported by US DOE.