[Note: This is a reprint of an abstract. Contents of this document should not be quoted or referred to without permission of the author(s).]

Invited talk at the Materials Research Society Fall Meeting, Boston, Massachusetts, November 27-December 1, 2000.

THE ORIGIN OF ELECTRICAL ACTIVITY AT GRAIN BOUNDARIES IN PEROVSKITES AND RELATED MATERIALS

S. J. Pennycook, M. Kim, G. Duscher, N. D. Browning, K. Sohlberg and S. T. Pantelides

Solid State Division
Oak Ridge National Laboratory
Bldg. 3025M, MS-6030
Oak Ridge, Tennessee 37831-6030

"The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. DE-AC05-00OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes."

Prepared by the

SOLID STATE DIVISION
OAK RIDGE NATIONAL LABORATORY
Managed by
UT-BATTELLE, LLC, for the
U.S. DEPARTMENT OF ENERGY
Under Contract DE-AC05-00OR22725

October 2001

THE ORIGIN OF ELECTRICAL ACTIVITY AT GRAIN BOUNDARIES IN PEROVSKITES AND RELATED MATERIALS

S. J. Pennycook, M. Kim, G. Duscher, N. D. Browning, K. Sohlberg and S. T. Pantelides

A combination of atomic-resolution Z-contrast microscopy, electron energy loss spectroscopy and first-principles theory has been used to investigate the origins of electrical activity at grain boundaries in $SrTiO_3$. We show that grain boundaries in $SrTiO_3$ are intrinsically non-stoichiometric. Total-energy calculations reveal that the introduction of nonstoichiometry into the grain boundaries is energetically favorable and results in structures that are consistent with atomic-resolution Z-contrast micrographs. Electron energy-loss spectra provide direct evidence of oxygen deficiency. These results and calculations for model non-stoichiometric grain boundaries provide an explanation of the microscopic origin of the "double-Schottky barriers" that dominate the electrical behavior of polycrystalline perovskites. The same effects also explain the low critical currents that are observed across grain boundaries in the high-temperature superconductors.