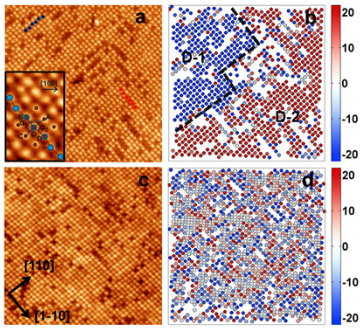
Chemically induced Jahn-Teller ordering on manganite surfaces



Direct visualization of the distortion domains in unoccupied state STM image of LCMO surface (a and b). Such domains are absent in the occupied state image (d and e). Calculation (not shown) of the density of states reveal that the origin of the distortion domains is the formation of the ordered Jahn-Teller distortions on the LCMO surface.

Research performed as staff science at ORNL's Center for Nanophase Materials Sciences and the Materials Sciences and Engineering Division, in collaboration with the University of Nebraska Lincoln and IHI Corporation.

Scientific Achievement

Direct observation of structural domains on manganite surfaces originating from the surface-chemistry-induced stabilization of ordered Jahn-Teller displacements.

Significance and Impact

Measuring the sub 30 pm displacements of atoms from high-symmetry positions in the atomically resolved STM images allows the physical order parameter fields to be visualized in real space on the single atom level.

Research Details

- From atomic resolution STM images, we identify and refine the surface adatom locations and oxygen vacancies.
- Local distortion maps are constructed to demonstrate the domain boundaries.
- Density functional calculations provide insight into the intriguing interplay between the various degrees of freedom now resolved on the atomic level.

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Narrative Highlight Text:
Understanding the emergent physical phenomena at surfaces requires the capability to probe local composition, recognize minute deviations from ideal structures, and explore atomic coupling to electronic properties. We report studies of the chemical and electronic structure and structural distortions of the (001) surface of $La_{5/8}Ca_{3/8}MnO_3$ through direct mapping by high-resolution scanning tunneling microscopy (STM), directly visualizing order parameter fields and associated topological defects. From atomic resolution scanning tunneling microscopy images, we identity and refine the surface adatom locations and oxygen vacancies. From these, local distortion angles are extracted based on the refined coordinates of surface adatoms. In this way, we can obtain surface structure maps that clearly demonstrate the boundary between two domains with different distortion orientations. This behavior is discussed in terms of ordered Jahn-Teller distortions which arise due to the imposed effect of the oxygen adatoms on the surface. Specifically the pattern of oxygen adatoms, i.e. the pattern of *local* oxygen stoichiometry has a strong influence on the electronic structure of the surface. The surface oxygen adatoms impose a checkerboard pattern of crystal field environments, leading to a charge and orbital disproportionation of the surface Mn lattice. Overall, these studies provide an example of order parameter field mapping from high-resolution STM, opening a pathway for probing electronic properties of topological defects and the interaction between order parameter fields and structural defects.

Reference
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