Surface phase diagram of $Ca_{2-x}Sr_xRuO_4$

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Short Abstract

The bulk phase diagram of $Ca_{2-x}Sr_xRuO_4$ contains rich and exotic behavior attributed to numerous, nearly degenerate, structural and magnetic instabilities [1]. For instance, for x <0.2, an antiferromagnetic (AFM) insulating ground state and metal-insulator phase transitions are observed. At the critical concentration x_c ≈ 0.5 it is believed that there is a *quantum critical point* at T=0. Finally, the point x = 2 represents the *p-wave* superconducting phase. We have used LEED, STM, and ELS to measure the surface geometric structure, electron distribution, lattice dynamics and electronic response. This data has been used to prepare a surface phase diagram. Most interesting is the difference in the tilt and rotation or the RuO_6 octahedron at the surface which results in a reconstruction for x=2 creating a non-superconducting surface that is predicted to be magnetically ordered. At x = 0.1 the surface appears to undergo the Mott transition from insulator to metal at a lower temperature than in the bulk creating a unique situation where the surface is metallic and the bulk a Mott-insulator.

Keywords

Phase transitions, structure, lattice dynamics, electronic structure.

Introduction

Understanding the exotic behaviour exhibited by Highly Correlated Electron Systems poses perhaps the deepest intellectual challenge in the physical sciences today [2]. Although correlated electron phenomenon are observed in a wide variety of materials, transition-metal oxides (TMOs) occupy a special position because of the immense richness of the phenomena they display, ranging from ferroelectricity to high-T_C superconductivity to all forms of magnetism to heavy fermion behavior. Many of the spectacular properties of TMOs are believed to result from competing ground states—the balance between phases is very subtle and small perturbations can produce a large response. Breaking the symmetry by the creation of a surface is a controlled way to disturb this coupled system and may lead to the formation of new phases.

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Results and discussion

We have reported the surface structure of Sr_2RuO_4 [3], which is a reconstruction resulting from an in-plane rotation of the RuO_6 octahedron of $8.5^0 \pm 2.5^0$. This alternating clockwise and counter clockwise in-plane rotation results from freezing out a bulk-zone boundary soft phonon. Quantitative LEED *I-V* has been utilized to measure the tilt and rotation of the octhadra as a function of x. The results are shown in Fig. 1. The rotation starts with x = 2 and is basically independent of x. Surprisingly, the tilt begins at a lower value of x than in the bulk and never exceeds the bulk value.

The STM reveals an interesting behaviour with changing x. There is a non-monotonic evolution of the local electronic inhomogeneity on the nanoscale which correlates well with the bulk in-plane resistivity.

Momentum resolved inelastic electron scattering has been utilized to measure the surface phonon dispersion (lattice dynamics) [4] and electronic excitation spectra. In general the surface optical phonon modes are always higher in energy than the corresponding bulk modes, which we attribute to the change in the octahedral aspect ratio at the surface.

For x=0.1 we observe with STM and ELS that the surface insulator to metal transition appears to occur at a lower temperature than in the bulk (155K). This is contour intuitive since one would expect the surface band-width to be smaller than in the bulk and consequently result in a larger U/W at the surface raising the Mott transition temperature at the surface. We also observe only small changes in the surface structure across this transition. In a temperature range between the surface and bulk transition temperatures the surface is a metal on top of a Mott-insulator.

Conclusions

The creation of a surface by cleaving a layered TMO shifts the balance between the competing bulk ground states, producing new and interesting surfaces phases.

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References

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Figures and Tables

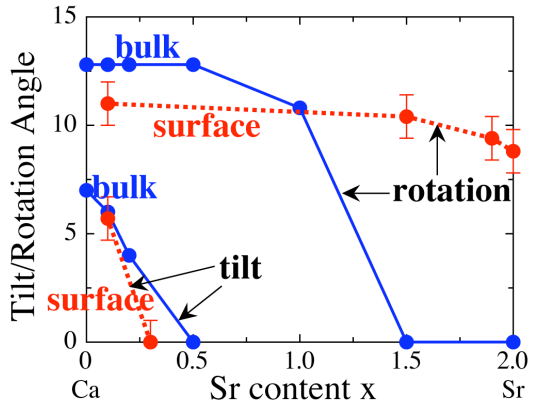

Fig. 1. Tilt and rotation for $Ca_{2-x}Sr_xRuO_4$. The blue lines are for the bulk [1] and the red lines our measurements for the surface structure.