SURFACE STRUCTURE OF LAYERED PEROVSKITES: A LEED I-V STUDY[1]

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Highly correlated electron materials such as the transition-metal oxides (TMOs) have attracted much attention in the materials community because of the richness and tunability of their novel properties. Specifically, these TMO characteristics are believed to result from an astonishing variety of possible ground states very close together in energy, so that the balance between competing phases is very subtle and small changes can create new phenomena. Creating a surface is a controlled way to disturb this balance and create a new phase. Quantitative low-energy electron diffraction (LEED) I-V has been utilized to measure the surface structure of cleaved layered TMOs. The surface of the unconventional (spin-triplet-coupled) superconductor Sr_2RuO_4 reconstructs into a $(\sqrt{2} \times \sqrt{2})R45^o$ structure by a clockwise and counterclockwise (8.5^o) rotation of the octoctahedra (RuO_6) around the surface normal. The surface is magnetically ordered and non-superconducting.

The bulk of $La_{0.5}Sr_{1.5}MnO_4$ is a charge-ordered antiferromagnetic insulator at low temperatures (<110 K). The charge-ordered state should have created a$\sqrt{2} \times \sqrt{2}$ structure at the cleaved surface of a single crystal. LEED shows only a (1×1) structure with small distortions, as observed in Fig. 1. Cleaving a surface like this at room temperature results in segregation of Sr to the surface, as shown in Fig. 2. The surface plane is $La_{0.15}Sr_{0.85}O$. The segregated surface is still a polar surface (it is not charge neutral) unless there is 7.5% excess oxygen.

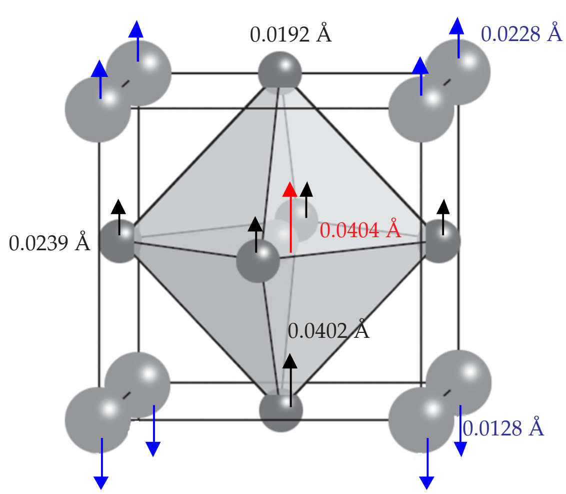

Fig. 1. Best fit structure to the experimental data. The motion of the atoms with respect to the bulk are shown by the arrows.

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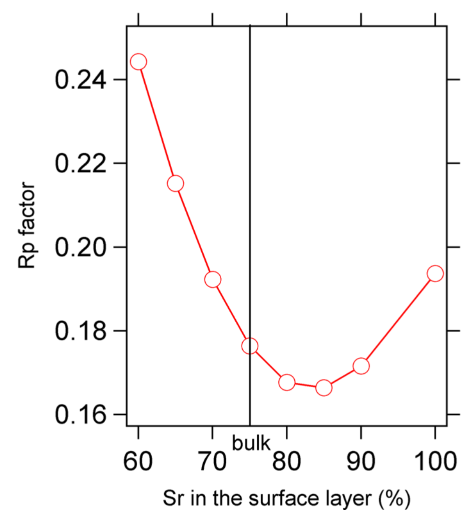

Fig. 2. Best fit to experimental data for the % Sr in the first layer.