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LEED study of TMOs surfaces V.B. NASCIMENTO, R.G. MOORE, The Univ of Tennesse, Knoxville, TN 37996, J. RUNDGREN, Theory of Materials, Phys Dept, Royal Inst of Tech, SE-10691, Stockholm, Sweden, JIANDI ZHANG , LEI CAI, Florida International Univ., Miami, FL 33199, R. JIN, D. G. MANDRUS, E.W. PLUMMER, Oak Ridge National Lab, Oak Ridge, TN 37831 — In contrast with the case of metals and semiconductors, the final theory-experiment agreement obtained for LEED $I-V$ data for TMOs is generally not very satisfactory. One reason is that the calculations of the phase shifts for metal oxides is not a straightforward procedure due to the charge transfer. In this work we address this issue of phase shift generation for TMOs by determining the structure of the (001) surface of $Ca_{1.5}Sr_{0.5}RuO_4$, a prototype layered TMS system. The adoption of an optimized muffin-tin potential approach, as proposed by Rundgren, has enabled reaching an acceptable final theory-experiment agreement. Our results indicate that the determination of an energy dependent inner potential plays a key role in the final agreement. *Work supported jointly by NSF and DOE (DMS) NSF -DMR-0451163, NSF DMR-0346826 and by U.S. DOE under DE-FG02-04ER46125 and DE-AC05-00OR22725.

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