WEEKLY CALENDAR

September 29, 2008

Department Colloquium

"The Structure of Transition Metal Oxide Surfaces, probed by Low Energy Electron Diffraction (LEED)"

3:40 PM, October 2, 2008
109 Nicholson Hall

Von Braun Nascimento
University of Tennessee
Host: Michael Cherry

• Refreshments served at 3:15 PM in 201 Nicholson Hall •

An atomic level knowledge of the structure of the surface is a crucial step for understanding its physical and chemical properties. This is specially true in the case of transition metal oxides (TMOs), whose functionality is a close coupling between structure, charge, and spin. The creation of a surface breaks the translational symmetry, driving a lattice distortion or surface reconstruction, and may lead to lattice distortions. Due to the subtle balance present in the TMOs, those distortions can create new functionality: an Emerging Functionality in Transition-Metal Oxides Driven by Broken Symmetry.

The Low Energy Electron Diffraction (LEED) technique has been between the most reliable experimental techniques for surface structure analysis. The strong interaction of the probing low energy electrons with the surface atoms (multiple scattering) allows a high surface sensitivity (reduced penetration depth), but forces LEED structure determination to be performed in an indirect way, by a comparison between theory and experiment. Due do the ionic character of the chemical species in the oxide, the final theory-experiment for LEED on TMOS has historically not been as good as in the case of simple metallic surfaces, drastically reducing the reliability of the structural analysis. In a recent work, our research group at University of Tennessee has proposed a new effective theoretical approach for LEED on TMOs, based on the optimized muffin-tin approach.[1] This new approach has been successfully applied to several different TMOs systems, leading to very good final theory-experiment agreement.

This presentation will start with a brief introduction to the LEED technique, describing its experimental and theoretical aspects. The theoretical and experimental issues associated with LEED analysis of TMOs will be addressed. The new theoretical approach for LEED on TMOs will be discussed, using the prototype $Ca1.5Sr0.5RuO4(001)$ system as an example.[1] Some interesting results obtained for different oxide systems will be presented: i) $Ca1.9Sr0.1RuO4(001)$, an inherent metal-Mott insulator transition at the surface;[2] ii) $Ca2-xSrMxRuO4(001)$, the broken symmetry giving rise to new "surface phases";[3] iii) $BaTiO3(001)$ thin films, single-domain vertically upward polarized state, questioning about the critical thickness for ferroelectric phase stability in thin films;[4] iv) $La2-2xSr1+2xMn3O7(001)$, an anti-ferromagnetic phase is stabilized at the surface by a Jahn-Teller distortion induced change in orbital occupancy.[5] Some future projects will also be addressed: i) clean and deposited (001) surface of $BaFe2As2$ (parent compound of the new FeAs superconductors); ii) controlled molecular adsorption on TMO surfaces; iii) new codes for LEED-IV.

References:
[1] V. B. Nascimento, et al., Physical Review B 75 (2007), 035408.
[2] R. G. Moore, et al., Science 318 (2007), 615.
[3] R. G. Moore, et. al., Physical Review Letters 100 (2008), 066102.
[4] Junsoo Shin, et al., Physical Review B 77 (2008), 245437.
[5] V. B. Nascimento, et al., Nature Physics (to be submitted).

Welcome To:

Stephanie Crews, a Coordinator with the Department. She is in Room 202-L, 578-6351.

Gretchan Raterman, a Research Associate with Dr. Jonathan Dowling. She is located in Room 425, 578-0946.

Reminder:

There will be a Steering Committee meeting on Tuesday, September 30, 2008 at 3:15 p.m. in Room 109.

Publications:

"Constraint preserving boundary conditions for the Ideal Newtonian MHD equations," M. Cecere, **L. Lehner** and O. Reula, Computer Physics Communications, V 179, pp 545 (2008).