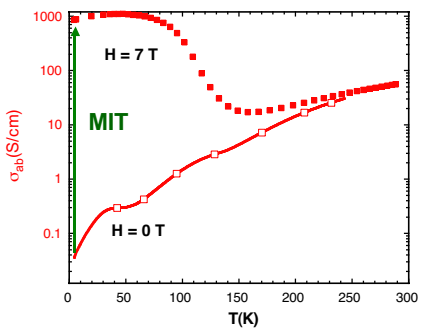
Phenomenological Model of Charge Localization in Layered Manganites

K. E. Gray, Qing'An Li, E. Badica, J. F. Mitchell and Andreas Berger (IBM Almaden)

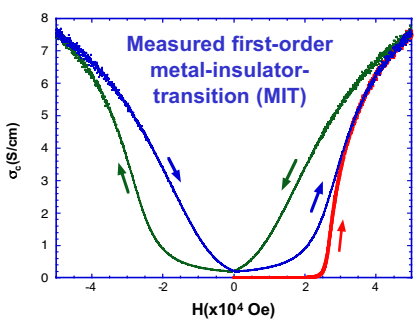
Our motivation is to understand conduction in the colossal magnetoresistive manganites.

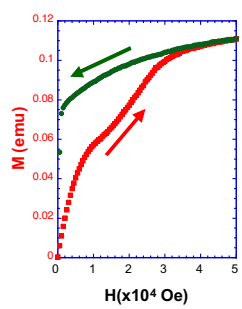
The connection of magnetic order with charge delocalization in manganites has received considerable attention recently, and the need to go beyond double exchange to explain the localized state above T_C starts with Millis, et al [*Phys. Rev. Lett.* 74, 5144 (1995)]

We propose a simple model to explain the ground states of layered manganites, $La_{2-2x}Sr_{1+2x}Mn_2O_7$, in terms of the energy gain due to double exchange, J_{DE}, compared to a new, phenomenological localization parameter, L



The layered manganite for x=0.48 is insulating in zero field but shows metallic conductivity at 7 T. It affords the opportunity to study the metal-insulator transition (MIT) as a function of field at low temperatures





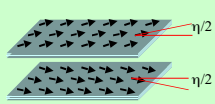
The conductivity, σ, turns on very abruptly at ~3 T with hysteresis-----two signatures of a first-order metal-insulator transition

The magnetization, M, exhibits a high susceptibility even at zero field then begins to saturate before an increase that is associated with the metal-insulator transition in the conductivity

To understand this we have constructed a phenomenological model for the insulating (localized) and metallic (delocalized) states:

$E_{loc}(\eta) = J_{SE}\cos(\eta) - L$

$E_{deloc}(\eta) = J_{SE}\cos(\eta) - J_{DE}\cos(\eta/2)$



by introducing a localization energy (L) with the *intrabilayer* superexchange (SE) and double exchange (DE)

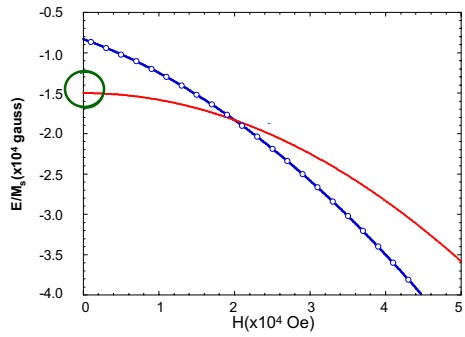
Phenomenological Model

Including magnetic fields adds the Zeeman term

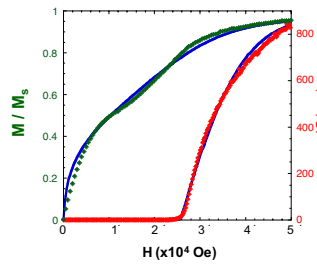
$E_{loc}(\eta) = J_{SE}\cos(\eta) - M_sH\cos(\eta/2) - L$

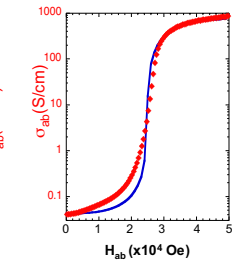
$E_{deloc}(\eta) = J_{SE}\cos(\eta) - (J_{DE}+M_sH)\cos(\eta/2) - J_{DEab}$

and delocalization in each monolayer adds J_{DEab}



The energy of the delocalized state decreases faster with field, so an initially localized state can experience a first-order metal-insulator transition





Using Bruggeman's symmetric effective medium theory, both magnetization and conductivity data are well-fit by this model, in the latter case over many orders-of-magnitude

Implications

The electronically-driven first-order metal-insulator transition has not been predicted for this material

It may help us unravel the complex transitions in these novel, coupled, two order parameter manganites

Future directions

Explore whether the MIT is intrinsically of first-order in the manganites:

Study the zero-field transitions at T_C

Study the colossal magnetoresistance above T_C

Address the scaling of magnetization at T_C in Perovskite manganites *vis-à-vis* a first-order MIT

Qing'An Li, K.E. Gray, A. Berger and J.F. Mitchell, Phys. Rev. B67 184426 (2003)

BES - DOE

This work was supported by the U. S. Department of Energy, Basic Energy Sciences, under contract W-31-109-ENG-38.

MSD - ANL