Sufaces & Interfaces (I) [Millis]

- The field is still in early stage. Not clear what it will end up with.

- Basic Questions: How do exotic behaviors of strongly correlated systems change in proximity of sufaces/interfaces
  - ▲ Particular important for device engineering, since most devices involve intefaces.

- Transition metal oxides → Examples:
  - ▲ $La_{1-x} Sr_x Cu O_4$ [high-T_c SC]
  - ▲ $La_{1-x} Sr_x Mn O_3$ ["half metal"]
    - ▸ Charge & orbital magnetism
    - ▸ Colossal magnetoresistance.
  - ▲ VO_2 & V_2O_3 [metal–insulator transition]
    - ▸ enhanced TEP.

- All the above has enhanced response functions
  - ▲ Partially filled d-shell
    - ▸ interaction effects: { charging energy $U = E(N+1) + E(N-1) - 2E(N)$; internal energy (e.g. Hund's rule "J") }
  - ▲ Existence of "Ligand field" that split degeneracies
  - ▲ Electron itineracy
  - ▲ Carrier density

- States with very different properties are close in energy
  $\Longrightarrow$ small tuning can change properties of material

- Difference between suface & bulk:
  - ▲ suface has lower coordination (Potthoff/Nolting, PRB-2000)
  - ▲ different interaction, e.g. phonon 3D & 2D

    interaction U screening (Sawatzhy)

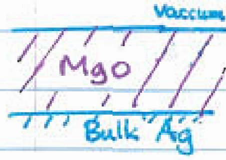
    - ▶ Sawatzhy considered MgO (wide gap insulator)

      $1s^2 2s^2 2p^6$ ← MgO → $1s^2 2s^2 2p^6$

      Put MgO flim on top of metal substrate, vary thickness.

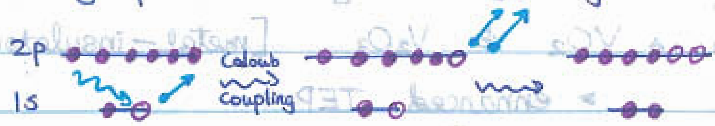
      Measure $E = Mg(2p^4) + Mg(2p^6) - 2\,Mg(2p^5)$

      via X-ray photon spectoscopy



      Found detectable changes in energy (~1 eV)

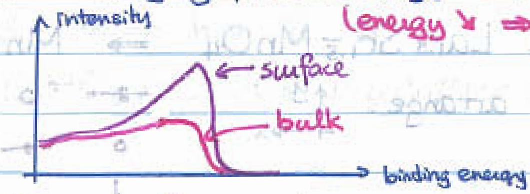
      To measure $Mg(2p^4)$, need to tune X-ray to eject $1s\ e^-$, then consider:



      $$\hbar\omega = KE_1 + KE_2 + (2E_{2p}^5 + U) - E_{1s}$$

    - ▶ Similar experiment can be done on Mn.
    - ▶ Conclusion: U is greatly affected by interface, other interaction (e.g. Hund's rule "J") do not.
    - ▶ Alternatively (generalizing), processes that change charges configuration is affect greater by interface. Processes that does not change total charge but rearrange them has weaker interface effect.
  - ▲ Different Symmetry at surface (typically lower)
  - ▲ Ligand field changes
  - ▲ All these effect suggests that interface is more insulating.

- Example: $SrVO_3$ & $CaVO_3$
  - ▲ Photoemission — varying photon energy ⇒ varying skin sensitivity (energy ↘ ⇒ bulk sensitive ↗)



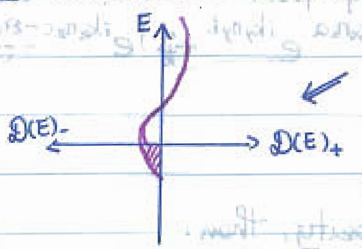
  - ▲ From experiment, interface is less insulating

- Example Ca/Sr-O-Ru Science 318 (2007)
  - ▲ Metal – insulator transition occur at 30K lower at surface
  - ▲ Again, interface is more metallic

- Possible Application: "Spin Valve"

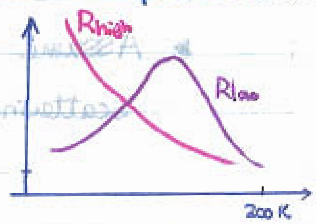
spin parallel ⇒ more current
spin antiparallel ⇒ less current

  - ▲ Consider Mn d^{4-x} $1-x\{$ — e_g ⟹ $\mathcal{H}_{int} \propto -J\vec{S}_c \cdot \vec{\sigma}_{e_g}$
    $S=\frac{3}{2}\{$ ↑↑↑ t_{2g} (cost ~ 0.5 eV per spin)



⟹ conduction band spin polarized.
⟹ (ideally) perfect spin valve ...

  - ▲ But at interface the magnetoresistance dies much faster in T than the Bulk Curie temperature indicates

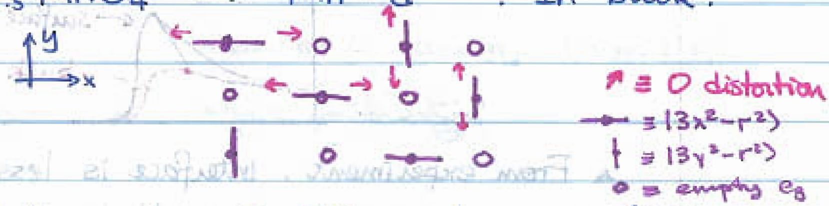


  - ▲ Now recall $e_g = \{ |3z^2-r^2\rangle, |x^2-y^2\rangle \}$

▲ Alternatively use $\{|3x^2-r^2\rangle, |3y^2-r^2\rangle\}$ not truely orthogonal

▲ Take $La_{1.5}Sr_{1.5}MnO_4 \Longrightarrow Mn: d^{3.5}$. In bulk:

Can arrange:



▶ Mn orbital shifts position of O^{2-}, producing a lattice distortion, which produces new Bragg peak, hence can be measured.

▶ Another possible way to measure pattern is to use photon to drive transition between bands. Different band filled implies different transition allowed.

▶ The orbital order produces non-trivial magnetic interaction

▲ What happens to $La_{1.5}Sr_{1.5}MnO_4$ in interface?

▶ Recall in bulk if $\varphi(x,y,z) = \sum_{\{n_i\}} f(x-n_xa, y-n_yb, z-n_zc)$

Then $\varphi_k = \int dxdydz\, e^{ik\cdot r}\varphi(x,y,z)$

But at suface z runs only from 0 to ∞. ← material

i.e. $\varphi(\vec{k}) = \int d^3\vec{r} \sum_{n_z=0}^{\infty} \left(\sum_{n_x,n_y} e^{ik_xn_xa} e^{ik_yn_yb} f_{\vec{k}}\right) e^{ik_zn_zc-\epsilon n_z}$ vacuum ← regularize

$$= \frac{f(\vec{k})}{1-e^{ik_zc}e^{-\epsilon}}$$

▶ If suface has different property, then:

$$\varphi(\vec{k}) = \frac{f(\vec{k})}{1-e^{ik_zc}} + (f^{top} - f)$$

▶ Assume phase incoherence,

scattering intensity $I = \frac{|f|^2}{|\vec{k}-\vec{G}|^2} + |f_{top}|^2$

- Question: Is there surface behavior that is not exhibit in bulks?
  - ▲ Proposal: empirically, symmetry breaking from superlattice picks out f
    $d_{x^2-y^2}$ orbital $\Longrightarrow$ high T_c SC
    Hence take $LaMO_3$ / $LaNiO_3$ superlattice: