Millis Boulder II

Discussion so far: - surfaces (ill controlled)
QN: How "passivate" a TMO surface
- speculation

Rest of lectures: superlattice. Apparently better controlled system

Ohtomo, Muller Grazul Hwang. Nature 419 378 (2002)
"Oxide epitaxy" = "careful pulsed laser deposition"

Idea

Shoot calibrated "puffs" of ions at substrate, under appropriate oxygen pressure. Monitor result by high class scattering

- Can grow many "materials by design"

So far: mainly studied variants on "ABO_3" perovskite. structure.
- B site: simple cubic lattice. Latt. par $\approx 4\mathring{A}$
- O : in between each pair of B's
- A : body center of B cube

Typically: B site: electronically active
A site: controls carrier conc. on B

Simplest superlattice: change only A

001 Superlattice: pick 1 cubic axis. Alternate A site:

Ohtomo et. al $(SrTiO_3)_m / (LaTiO_3)_n$
Band insulator: Ti d^0 "Mott" insulator: Ti d^1

Advantageous structure, need only keep La/Sr in place.

TEM image: Thinned sample. Avg over ~ 1000 Å

- Interface appears v. flat
  Qn: How much local disorder (Sr/La exch) there

- Qn Charge:

Sr	Sr	La	La	La	Sr	Sr
	Ti	Ti	Ti	Ti	Ti	Ti
	0	.5	1	1	.5	0

~~each~~ if O ~~all~~ stoichiometry good
each La ⇒ 1 e^- ⇒ 3 e^-.
Where sit.? Natural Guess: edge of La region: ≈ .5 e^-

Obvious questions: how wide is edge
how thick must you make central region to get ~
what can you get edge to do?

<u>TEM-EELS</u> : Inelastic spectrum corr. to transitions from Ti L edge to unocc Ti ~~d~~ stat
(?)

~~Ede~~

(⇒) inverse photoemission + excitonic correct (int. bet. core hole ~~m~~ ~~+~~ el. in unocc. state)

Idea: diff Ti valence ⇒ diff. occ Ti d-states
⇒ diff final state energies
(⇒ differences in spectra larger cf electronic hopping true. Will see explicit ex later)

Found (for these lattices): $n\,Ti^{3+} = n\,La$

Also: meas R_{xy}: $2/3\ e^-/La$. Qn: some carrier trapped
? Compensation

Polarization "Catastrophe"

Simple observation (Sawatzky): most TMO planes are polar = charged

ex) 100 $LaTiO_3$. Formal valence $La^{3+} Ti^{3+} O^{2-}$

Planes $\overset{3+}{Ti}\overset{2\times 2-}{O_2} = -1$ $\overset{3+}{La}\overset{2-}{O} = +1$

La
Ti
La
Ti
La
Ti

La ≠ # Ti Net charge ⇒ Very Bad

But even if # La = # Ti - problem

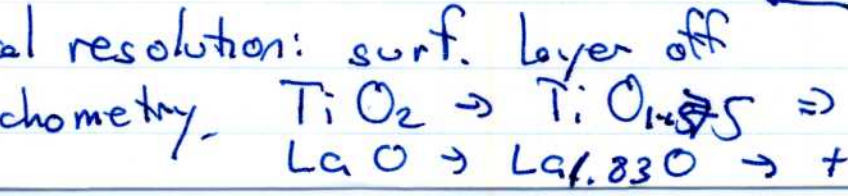
<u>Poisson</u>: $\nabla \cdot E = \frac{4\pi\rho}{\varepsilon}$

2d charged sheet: $\rho = \sigma\,\delta(z - z_n)$

⇒ across sheet $\Delta E = \frac{4\pi\sigma}{\varepsilon}$

E Ti La Ti La Ti L.

⇒ V

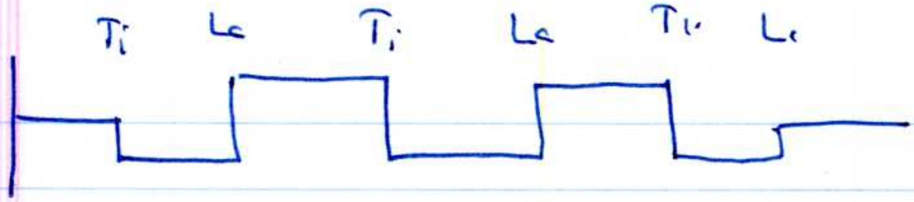


⇒ N Layers, L.c.c

$\Delta V = \frac{N\, 4\pi e^2 \sigma c}{\varepsilon\, z}$

Typical resolution: surf. Layer off stoichometry. $TiO_2 \to TiO_{1.75} \Rightarrow -\frac{1}{2}$

$LaO \to La_{0.83}O \to +\frac{1}{2}$



Principal reason why TMO surfaces are typically <u>bad</u>

Sawatzky realized: can compensate polarization by moving electrons instead

Consider structure: $(LaAlO_3)_n\ (SrTiO_3)_m$

- $LaAlO_3$: wide bandgap insulator (effective barrier to electrons)
- $SrTiO_3$: very small gap to add el to Ti d-states (wider gap to add holes) NON Polar. $Sr^{2+}Ti^{4+}$ $(SrO)(TiO_2)_{neut}$

Materials v. common in technology

Sr Ti Sr Ti La Al La Al ...

.5 Add electron to Ti lay

Sr Ti Sr Ti Sr Al La Al

.5 add hole to Ti or Al layer

⇒ doping by ≈ .5 electron or hole from pol. catast.

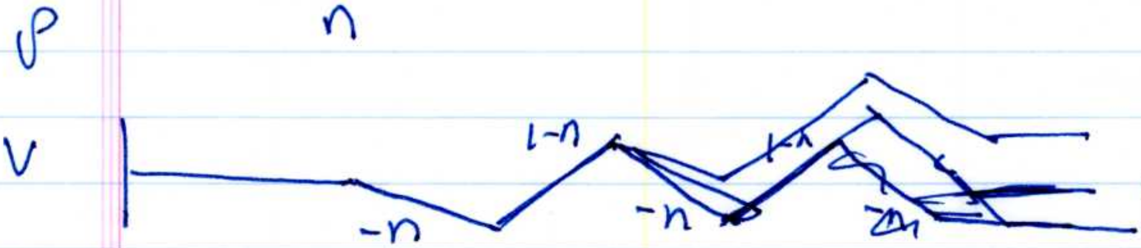
Examine electrostatics in more detail.
Simple model.

Energy to put n electrons on STO in absence of field

$$E = E_\Delta n + \tfrac{1}{2} E_c n^2$$

if have n el., must have surf. charge layer and also have dipole field

Sr Ti La Al La Al n^{sur}



E_p

$$\Delta V = \frac{2\pi e^2}{\varepsilon c}(1-2n)$$

⇒ Dipole. Energy ~ Dipole squared ~ E_D

$$E = E_\Delta n + \tfrac{1}{2} E_c n^2 - N E_p (1-2n) n + \tfrac{1}{2} N^2 E_D (1-2n)^2$$

<u>Minimize</u> : $E_\Delta + E_c n - N E_p - 2N^2 E_D + 4N^2 E_D n + 4 N E_p n$

$$\left(\frac{N E_p + 2N^2 E_D - \Delta}{E_c + 4N E_p + 4N^2 E_D} \right) = n/\text{cell}$$

Characteristics: Threshold. Saturation at ½. Approach rapid if $E_D > E_p$

Examine charge dist. in more detail

Classical appx:

Charge density n_j

$$E = \sum_j \Delta n_j + \frac{1}{2} E_c \sum n_j^2 + 2E_p \sum_{j=0}^{\infty} \sum_{l=j+1}^{\infty} n_j n_l |j-l|$$

- Put all charge in layer 0

$$E = \Delta n + \frac{1}{2} E_c n^2$$

Put δ in layer 1

$$E = \Delta n + \frac{1}{2} E_c \left((n-\delta)^2 + \delta^2\right) + E_p (n-\delta)\delta$$
$$= \Delta n + \frac{1}{2} E_c n^2 - E_c n \delta + E_c \delta^2 + E_p n \delta - E_p \delta^2$$

$\Rightarrow$ only if $E_c > E_p$ does it pay

$$\sum_l l r^l$$

$$r \frac{d}{dr} \sum_l r^l = \frac{r}{(1-r)^2}$$