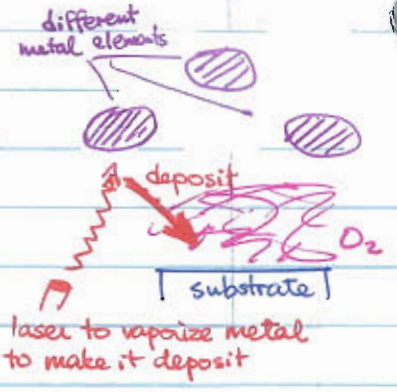
Surfaces & Interfaces (II) [Millis]

- We shall consider explicitly superlattice of perovskite ABO_3
  - ▲ perovskite: { A sits on corner of cubic lattice; B sits on center of cubic lattice; O sits on the faces of cubic lattice }
  - ▲ We shall assume B transition metal, & A = La, Sr, ...
  - ▲ The general superlattice is 001 (along cubic axis)
- Homometallic: "A" changes, "B" stays the same
  e.g. $LaTiO_3 / SrTiO_3$
- Hetrometallic: "B" changes ("A" may of may not change)
  case A: hard wall, e.g.
  case B: different correlated material, e.g. $LaMnO_3 / YBa_2Cu_2O_7$



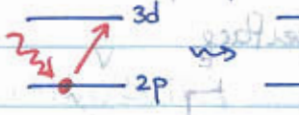
- Fabrication methods (all variation on film)
  - ▲ Oxide epitaxy
  - ▲ MBE
  - ▲ Pulsed Laser Deposition
- Image can be obtain because different atoms have different cross sections.
  - ▲ But reality is often less "clean & clear" than the image suggests.
- Consider

	...	Sr^{2+}	La^{3+}	La^{3+}	La^{3+}	Sr^{2+}	Sr^{2+}	Sr^{2+} ...
	...	Ti	Ti	Ti	Ti	Ti	Ti	Ti ...
naive:		0.5	1	1	0.5	0	0	0

  - ▲ $LaTiO_3$ is Mott insulator, $SrTiO_3$ is band insulator

▲ The charge distribution can be measured by TEM/EELS

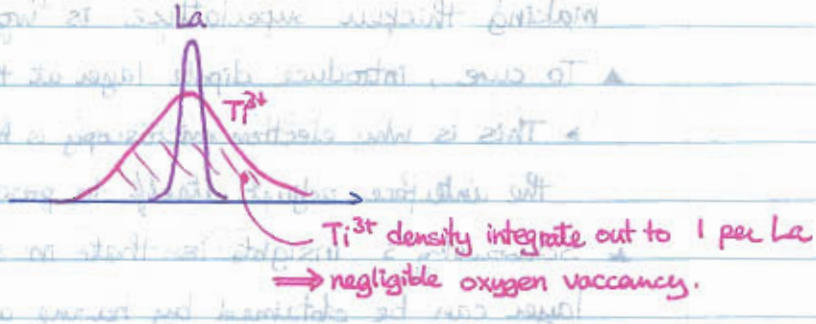
▶ look for inelastic processes, in particular:

Ti: 

probability depends on what's already in d-shell.

▶ The Ti state with (say) +0.5 charge can be decompose into superposition of +0 & +1 charge (not clear why it is just superposition)

▶ Result:



▲ One can also measure longitudinal Hall resistance to find carrier density

▶ Get ~2/3 carrier per La naively. Still close to ~1 as expected.

▲ Now it is also possible to do optical measurement (drude peak)

▲ In above TEM can truely resolve individal layer, while Hall probe/optical measure involve averaging between layers.

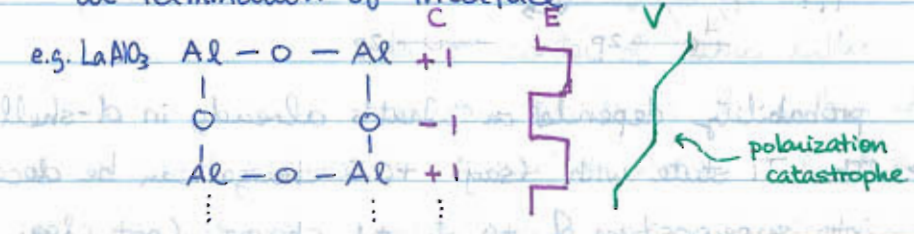
• Magnetization can be seen at interface

• Consider $LaMnO_3/YBa_2Cu_3O_7$:

▲ Orbital occupation can be measured using polarized light.

▲ { Bulk: holes found in $|x^2-y^2\rangle$ state
Interface: holes found ALSO in $|3z^2-r^2\rangle$ state.

- Consider electrostatics of these superlattice
  - ▲ Most ABO_3 perovskite are polar ⟹ charges build up at termination of interface



  - ▲ Intuitively, this is why from material science perspective, for thicker polar layer in superlattice, quality of interface reduces.
  - ▲ To cure, introduce dipole layer at the end: C: ½ −1 +1 ... −1 +1 −½
    - ▶ This is why electron microscopy is hard to do in these material, since the interface adjust itself to produce the desired polar charge.
  - ▲ Sawatzky. Insight is that in superlattice, the ±½ charge layer can be obtained by having an 2D e^- gas in the interface (hence interface ⟹ more metallic.
  - ▲ Question: Do we have ion transfer or e^- transfer?
  - ▲ For $SrTiO_3/LaAlO_3$, we have p-type & n-type

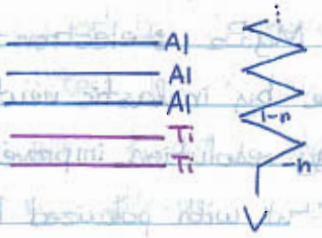
p-type: ... Ti | Sr | Al | La ...
(+½ | +1 | −1)
(−½ | +1 | −1)
n-type: ... Sr | Ti | La | Al ...

  - ▲ For n-type find $-0.6\ e^-$ & ~0.15 O vacancy
    For p-type find $0\ e^-$ & ~0.3 O vacancy
    ⟹ for some reason the material does not want to dope interface with holes.

- Hetrometallic interface is less sharp than homometallic
- For $LaAlO_3/SrTiO_3$, the interface goes superconducting, but mobile carrier ~0.1 per cell.
  - ▲ Similarly, Hall measurement shows fewer mobile carriers

- $SrTiO_3$ is a bulk sc, but can only support few carriers. Matching $\Longrightarrow$ can get interface sc up to 16 layers.

- Consider $LaAlO_3/SrTiO_3$



$\Longrightarrow \Delta V = \underbrace{\frac{2\pi e^2}{\epsilon c}}_{\equiv E_p}(1-2n)N$

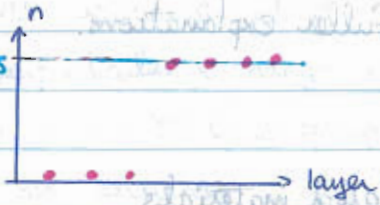
$E_0 = n\Delta + \frac{1}{2}E_{comp}n^2$ ($E_{comp} \sim e^2/\epsilon$)

At the other surface we need { surface charge n ; surface dipole cancel Δn

Combining, $E = \underbrace{n\Delta}_{\text{cost for } e^- \text{ transfer}} + \underbrace{\frac{1}{2}E_{comp}n^2}_{\text{intralayer repulsion}} - \underbrace{NE_p(1-2n)n}_{\text{energy from } \Delta V} + \underbrace{\frac{1}{2}E_D\left[N(1-2n)\right]^2}_{\text{dipolar energy cost at other end of interface}}$

$\Longrightarrow \frac{n}{\text{cell}} = \left(\frac{NE_p + 2N^2E_D - \Delta}{E_{comp} + 4NE_p + 4N^2E_D}\right)$

- In experiment



- Classically, $E = \Delta\sum_j n_j + \frac{1}{2}E_c\sum_j n_j^2 + \frac{2\pi e^2}{\epsilon c}\sum_{j=0}^{\infty}\sum_{\ell=j+1}^{\infty} n_j n_\ell |j-\ell|$

  Putting all n in 0^{th} layer, $E = n\Delta + \frac{1}{2}E_c n^2$

  If we have $n-\delta$ in layer 0, & δ in layer 1

  $\Longrightarrow \Delta E = \delta(E_p - E_c)n + O(\delta^2)$

  Thus only delocalized charge if $E_c > E_p$ [hard!]

  ▲ We've neglected e^- hopping, which will produce the desired charge spreading.