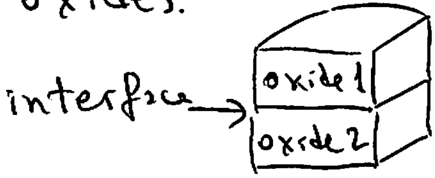
Oxide Interfaces

A goal of nanoscience research is to control materials at the atomic level. An example is the recent large effort focused on interfaces between oxides.



Modern "growth" techniques, called "pulsed laser deposition" and "molecular beam epitaxy" allow the growth of layers of oxides one over the other with atomic accuracy

(See Fig. 4 of Nakagawa et al.) for the case $LaAlO_3/SrTiO_3$

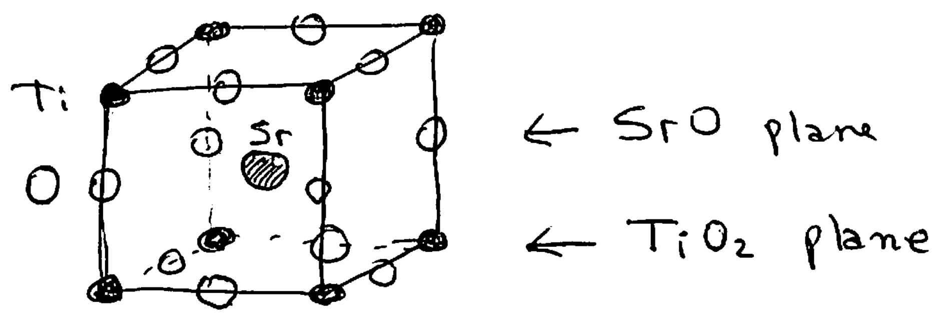
What happens at the interface?
New phases (states of matter) may appear.
For instance $LaAlO_3$ and $SrTiO_3$ are both insulators. Yet, the interface is metallic.

This area of research is vast, but let us focus here on a phenomenon called

"polar catastrophe"

where the simple electrostatic physics we learned plays an important role.

$SrTiO_3$ is in states Sr^{++}, Ti^{++++}, O^{--} so that overall it is neutral. The crystal structure is a "perovskite"



TiO_2 is $Ti^{++++}O^{--}O^{--}$ i.e. <u>neutral</u>

SrO is $Sr^{++}O^{--}$, i.e. also <u>neutral</u>

Consider now $LaAlO_3$. In this case La is La^{+++}, Al is Al^{+++} and O is O^{--}. The crystal structure is the same (perovskite). Thus, we have AlO_2 planes and LaO planes

$A^{+++}O^{--}O^{--}$ is charge (−)

$La^{+++}O^{--}$ is charge (+)

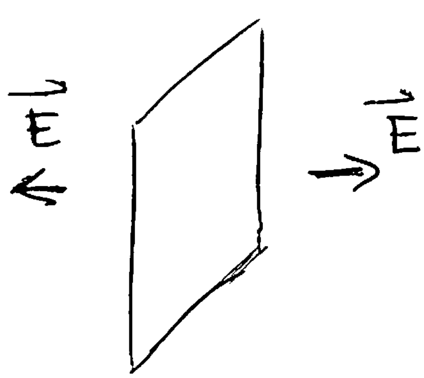
So in the case of $LaAlO_3$ the individual planes have charge.

Then, overall we have

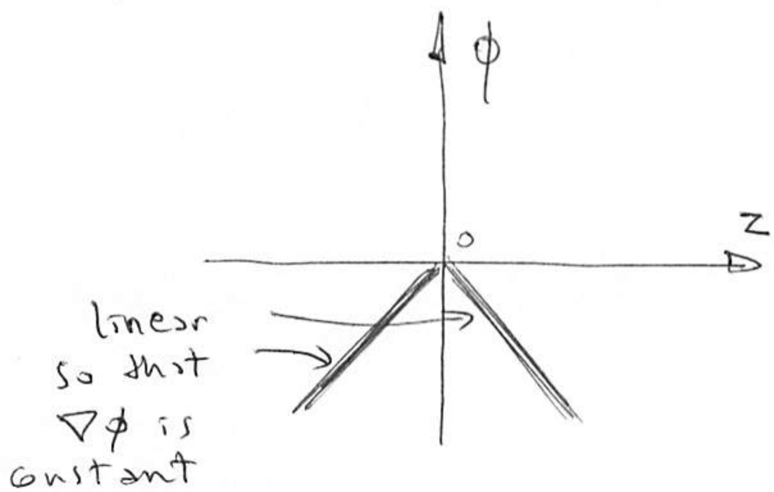
————	AlO_2	$-$
————	LaO	$+$
————	AlO_2	$-$
————	LaO	$+$
————	AlO_2	$-$
————	LaO	$+$
————	TiO_2	0
————	SrO	0
————	TiO_2	0
————	SrO	0

Each individual pair
— AlO_2 $-$
— LaO $+$

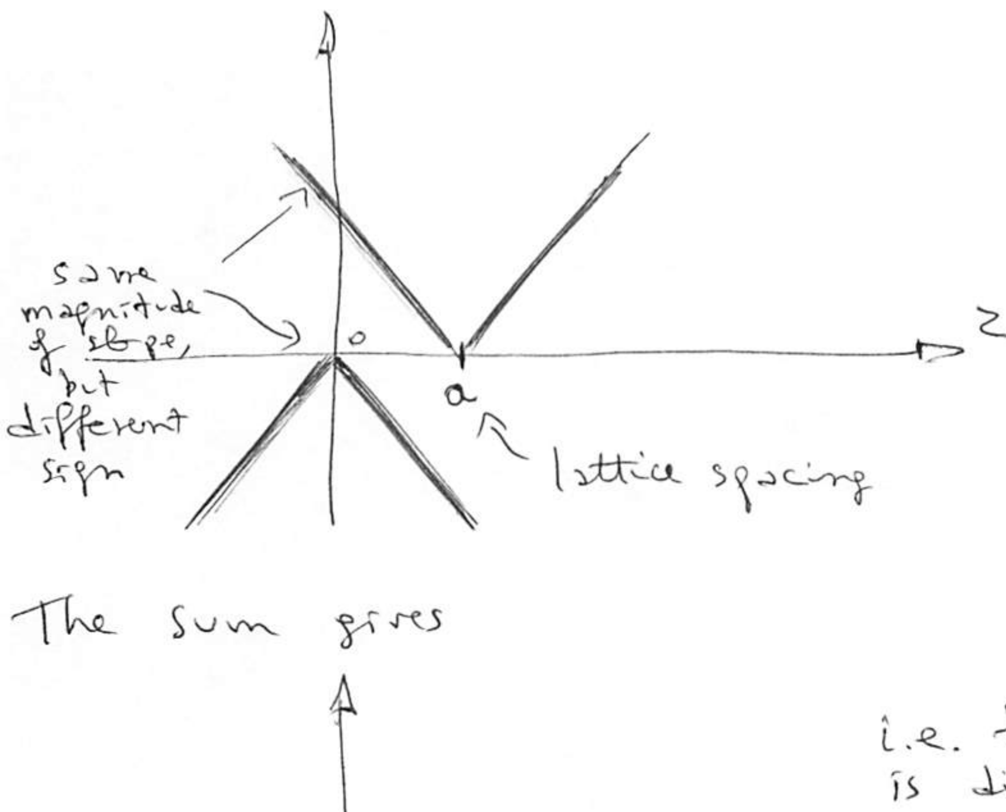
can be considered as one of the <u>dipole layers</u> that we discussed before. What is the potential of such a layer? An individual charged layer that is uniformly charged produces a constant electric field, of opposite sign at opposites sides of the layer



Thus, the potential is



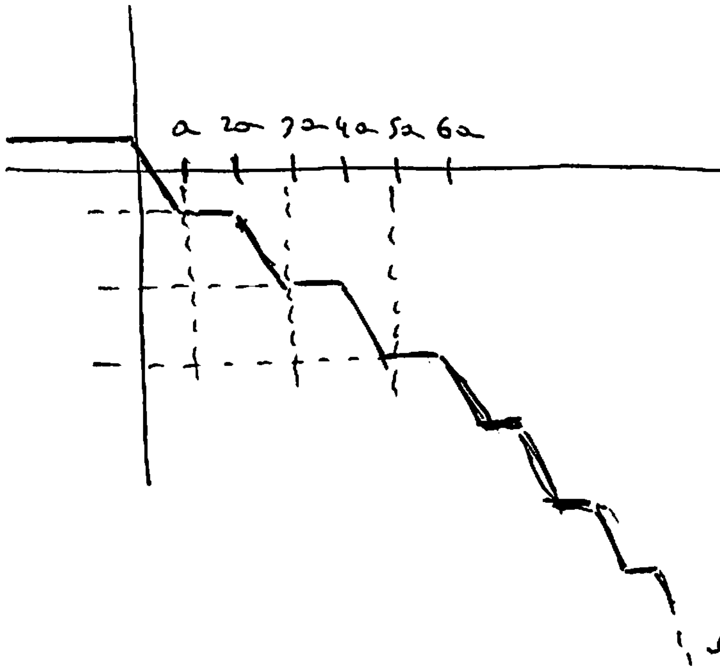
Consider now two layers with opposite charges. The potential will be:



The sum gives

i.e. the potential is discontinuous across the dipole layer

Here is the "punchline". In the $LaAlO_3$ portion of the interface, there are many dipole layers, one over the other. Then, the potential for "many" is:



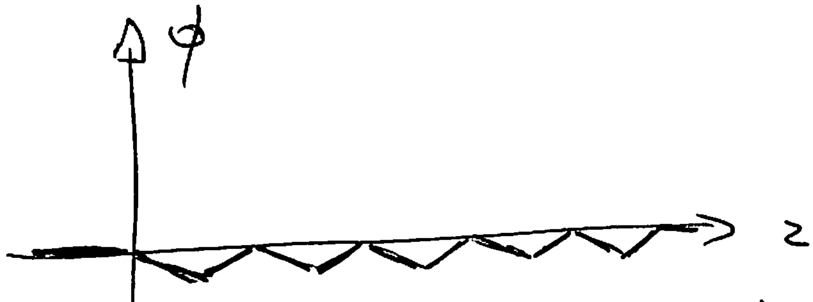
, etc.

As the # of dipole layers grows, the difference is potential grows, creating an <u>unstable</u> situation. "Something" has to happen when this "polar catastrophe" occurs. The way this problem is believed to be cured is by changing the valences. For instance, Ti^{++++} goes into Ti^{+++} at the interface. ↑ or rather $Ti^{3.5+}$
Then, TiO_2 becomes $(TiO_2)^{-1/2}$. At the same time the first layer AlO_2, which is -1, gets an additional $+1/2$ that came from TiO_2, making it $(AlO_2)^{-1/2}$

Then, the profile of charge goes from

-1		$-1/2$
$+1$		$+1$
-1		-1
$+1$	to	$+1$
-1		-1
$+1$		$+1$
-1		-1
$+1$		$+1$
0		$-1/2$
0		0
0		0
$\vdots$		$\vdots$

This charge distribution is <u>symmetric under inversion</u>, thus it cannot make a difference between top and bottom. It can be shown that the potential is now



i.e. <u>no</u> polar catastrophe.

At the TiO_2 layer there is an excess of charge forming a quasi-two dimensional electron gas. Adding an external voltage that is <u>on</u> or <u>off</u>, the metallicity of the interface can be controlled.