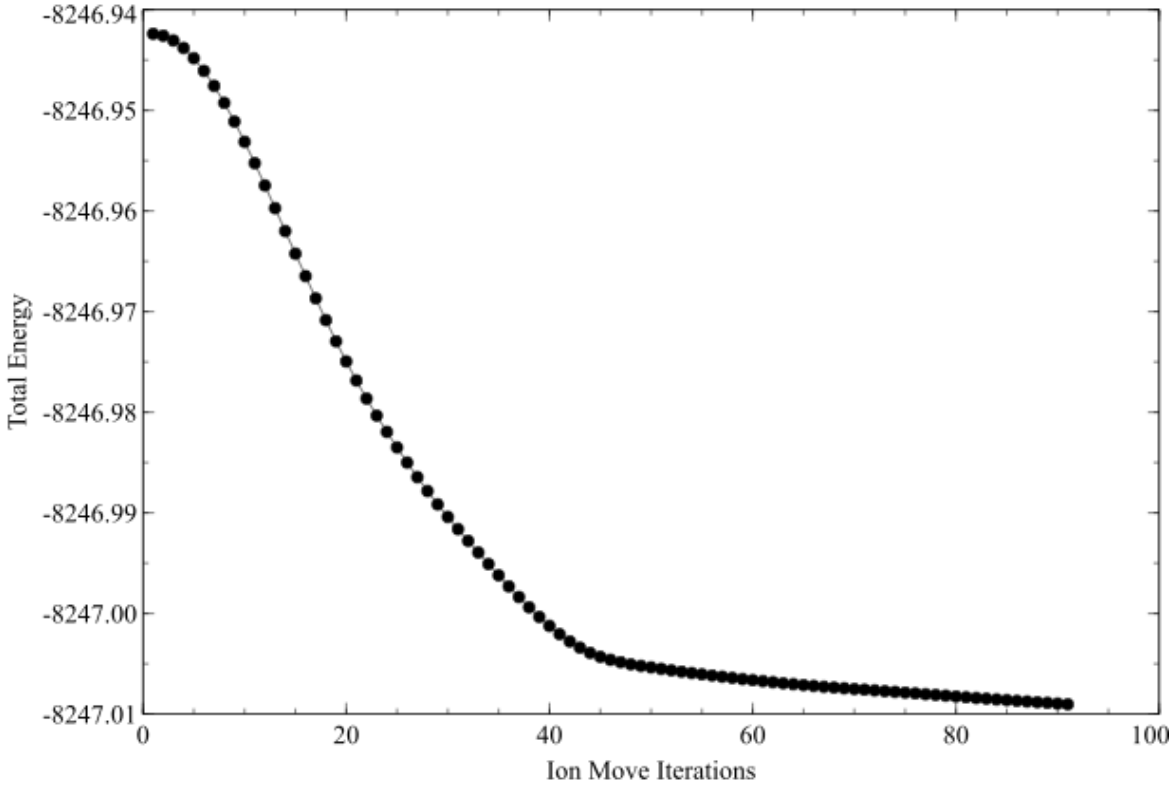
Second results obtained with "Quantum Espresso"

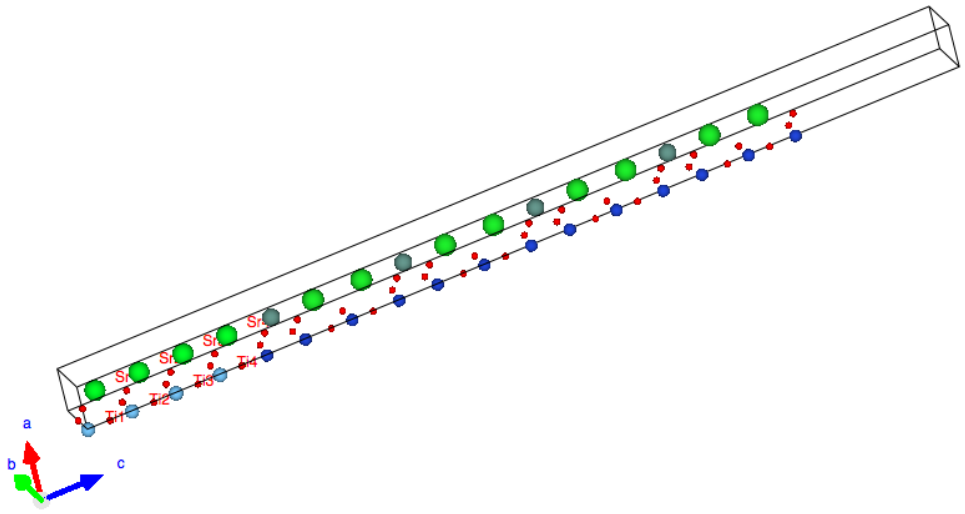
The results are for 4 layers of YBCO and 4 layers of STO, a total of 75 atoms.

YBCO-STO (4+4)

- The system is not completed relaxed, but I believe it is quite close as can be seen from the energy versus relaxation iterations.



- The system is shown in the image. Note the bottom layer is a Ti-O layer.



Atom postions

- Here I list the positions of selected atoms in the SrTiO3 layer before and after relaxation.
  - The Sr atoms:
    The x,y postitions of Sr atoms are (0.5,0.5) and don't change in the relaxation process.
  - The O atoms
    The x,y postitions of the O atoms I am interestend are (0.0,0.0) and don't change in the relaxation process.
  - The Ti atoms
    The x,y postitions of Ti atoms are (0.0,0.0) and don't change in the relaxation process.
- The initial postitions are at their ideal positions, they are here to double check if things work as expected.

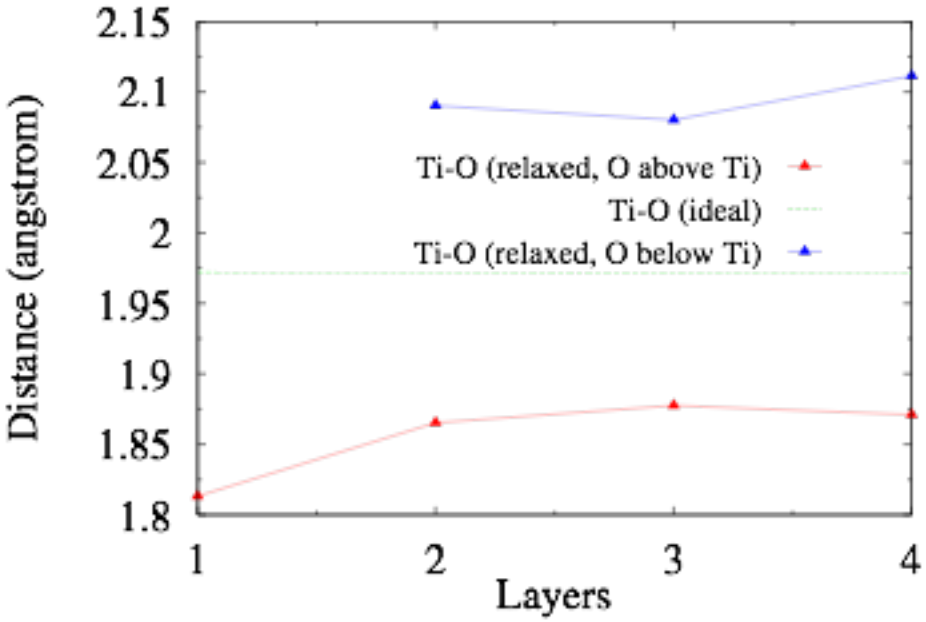
The data

```
#Sr(Init) Ti(Init) O(Init) Sr(Relaxed) Ti(Relaxed) O(Relaxed)
0.025235 0.000000 0.025235 0.024393 0.001220 0.024434
0.075706 0.050471 0.075706 0.075853 0.051195 0.075076
0.126177 0.100942 0.126177 0.126663 0.101707 0.125744
0.176648 0.151413 0.176648 0.177458 0.152774 0.176727
```

- Note the lattice constants (z component) is 78.14397 angstrom before relaxation, and 78.10835 angstrom after.

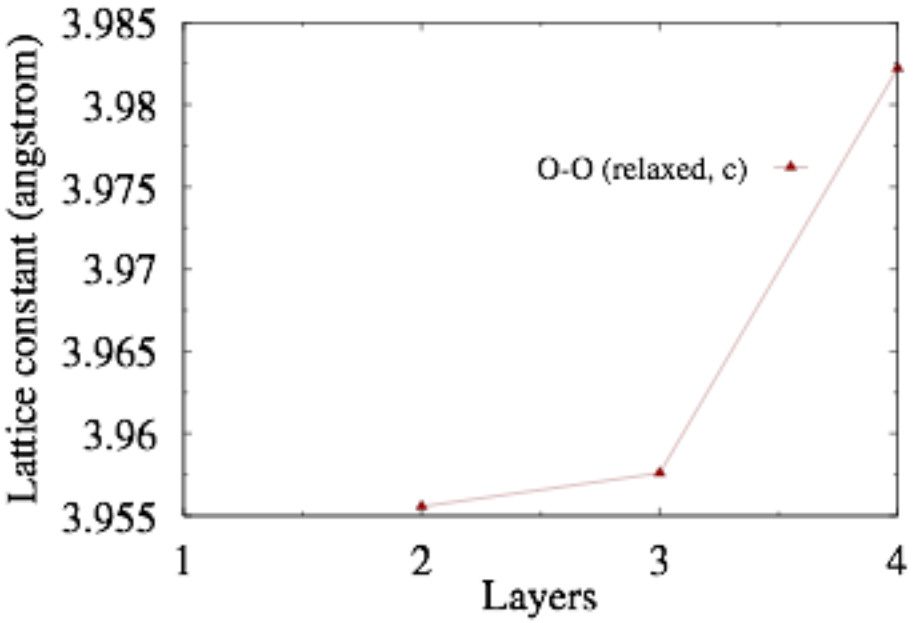
Regarding to changes.

- Since the inital atom postions are set at their ideal positions. So I can compare Ti-O distance (z component) to get an idea of how the structure distorted in the film with respect to its bulk positions.
  Here is the figure showing the Ti-O distance layer by layer from bottom to the interface. The straight line there is the ideal distance in bulk.



This figure clearly shows that Ti atoms had shifted upward with respect to oxygen octahedra, likely producing a polarization upward. However, the results indicate that the polarization persists 4 layers below the interface, which seems not consistent with experiment.

- We can also have an idea about how the lattice constant changes (z component) layer by layer by measing the distances between O atoms. This figure shows the results.



- Note, in this plot, x-index 4 is about the STO layer directly below the YBCO-STO interface, x-index 3 is the 2nd STO below the interface, x-index 2 is the 3rd STO layer below the interface.
- It is worthing noting that the ideal lattice constant of STO is 3.944 angstrom (ab initio values). Therefore this results shows that all the STO lattices are stretched along z and, more importantly, the stretch is larger as the layer get closer to the interface. Hope the result is consistant with experimental.