YBCO on STO

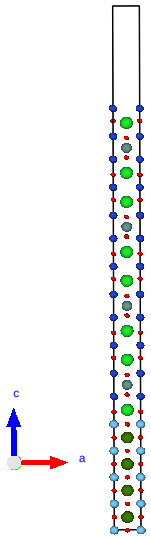

Figure 1: The atoms in the structure.

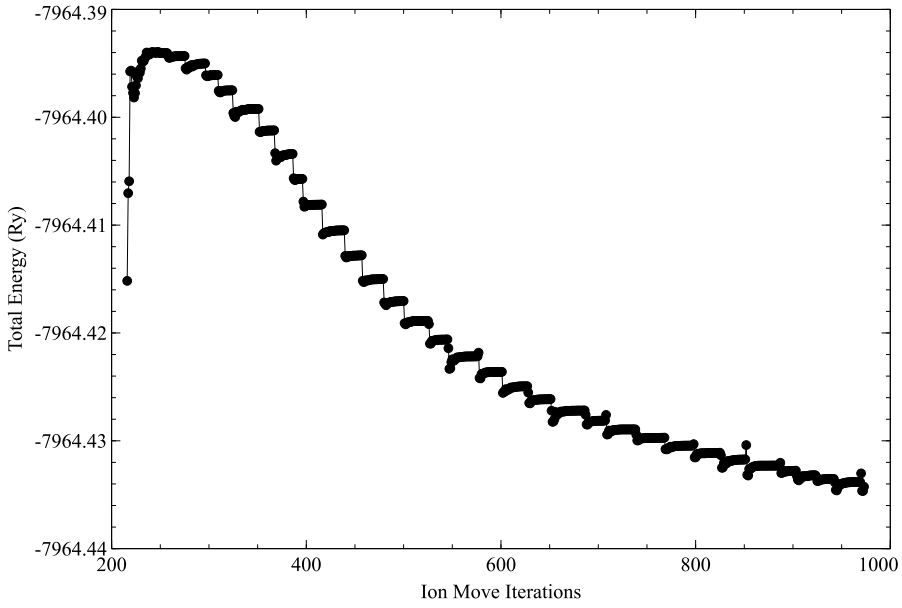

Figure 2: The convergence is shown as the total energy decreases with iterations.

I. THE STRUCTURE

The initial structure before relax is given in Fig. 1

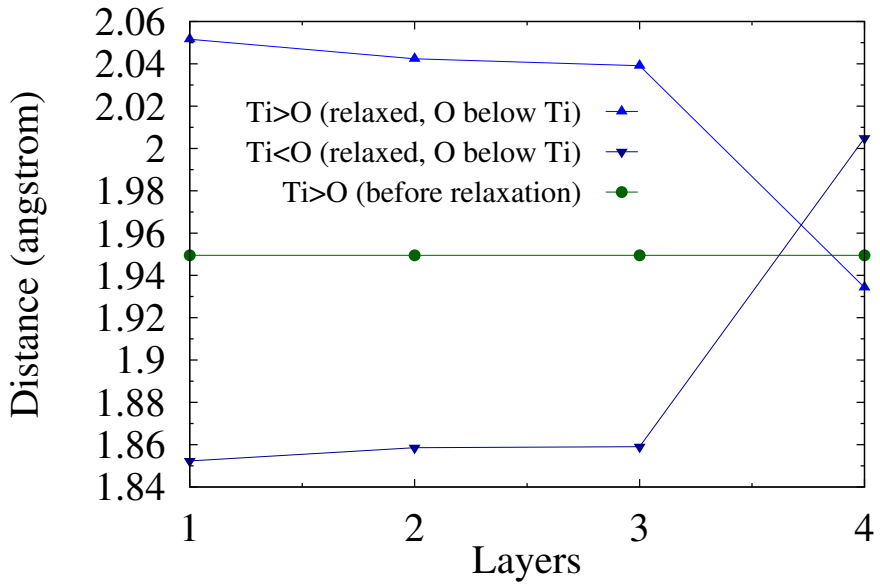

Figure 3: The Ti-O distance, measured in at the x,y positions of $(0.0, 0.0)$. The green line circles are before relaxation. The notation Ti>O means the distance for the Ti above the O atom.

II. THE CONVERGENCE

The result is not totally converged, due to some unknown error (file write error in SSC). I will use the last one to check how the atom positions had shifted.

III. THE CHANGES

The lattice constant along z has changed from 77.1169722464 Åto 77.1169983246 Å(this number is necessary to see how the atoms had moved; note they are quite close).

A. The $SrTiO_3$ layers

Figure 3 shows the O-Ti distance layer by layer. The bottom three layers have almost identical atom shifts – a polarization pointing upward; however the 4th layer (closest to the Ba-O layer) has the opposite behavior, which may be because the Ba-O layer at the interface (or maybe the computation is not entirely converged)?

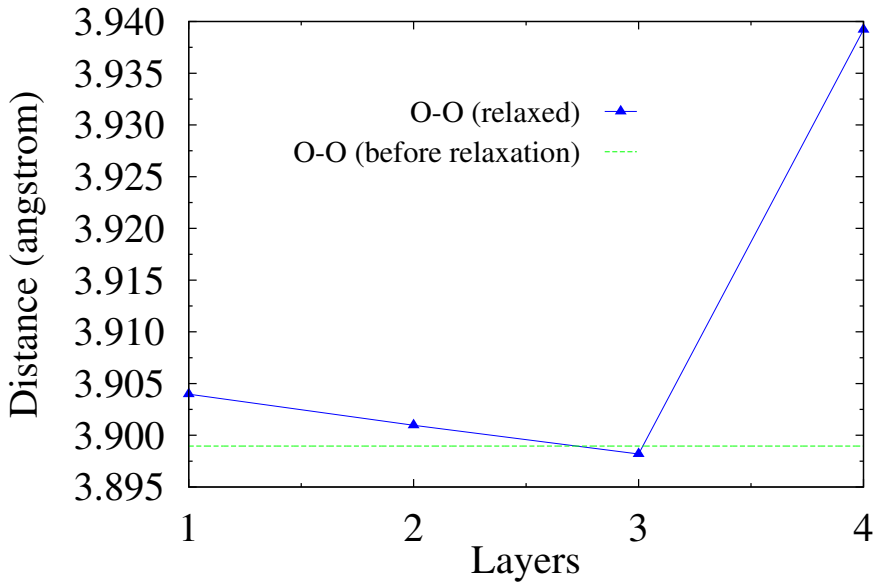

Figure 4: The lattice constant along z as measured from the distance between O atoms.

B. The lattice constant measured in O-O distance

Figure 4 shows the lattice constant variation with respect to layers. The results are obtained by measuring distances between O atoms at x,y positions $(0, 0)$. Interestingly, the lattice constant of the interface layer is about 1% larger than the others.