

## Charge Compensated Perovskite Polar Surface: SrTiO<sub>3</sub>(111)-3x3

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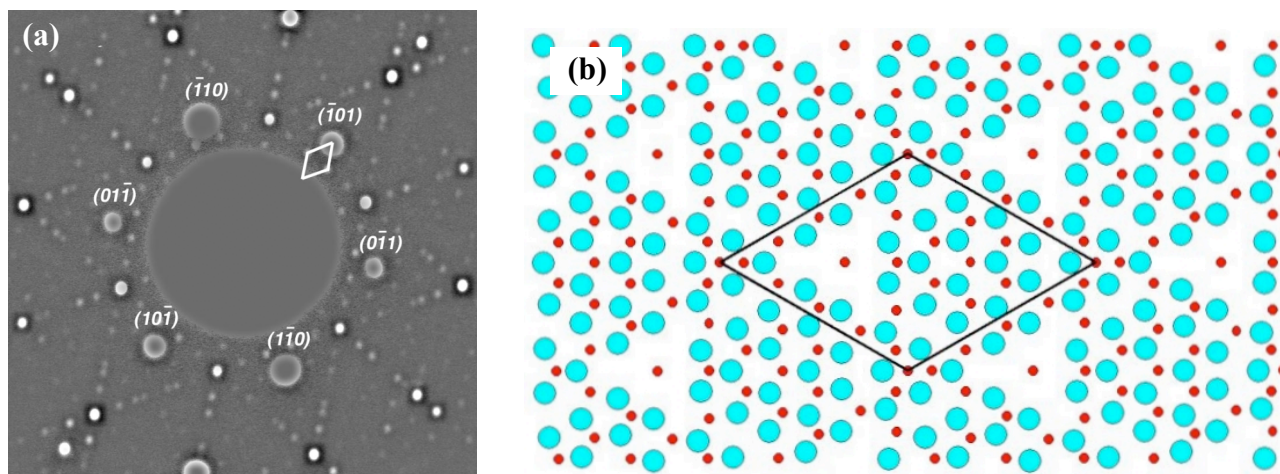
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SrTiO<sub>3</sub> is a prototypical perovskite, representing one of the most widely studied and characterized materials systems. SrTiO<sub>3</sub> has application in photoelectrolysis, heterogeneous catalysis, and as a substrate in the growth of high T<sub>c</sub> superconductors and functional ferroelectrics among others. The (111) surface of this simple mixed metal oxide is polar, meaning that it bears a non-zero charge density within each layer and a non-zero macroscopic dipole moment. By classic electrostatic arguments, this surface has a diverging electrostatic surface energy, is inherently unstable, and therefore should not exist as such [1]. Nevertheless, this surface has been prepared experimentally and here we report the first atomic-level experimental structure solution of a reconstructed SrTiO<sub>3</sub>(111) surface.

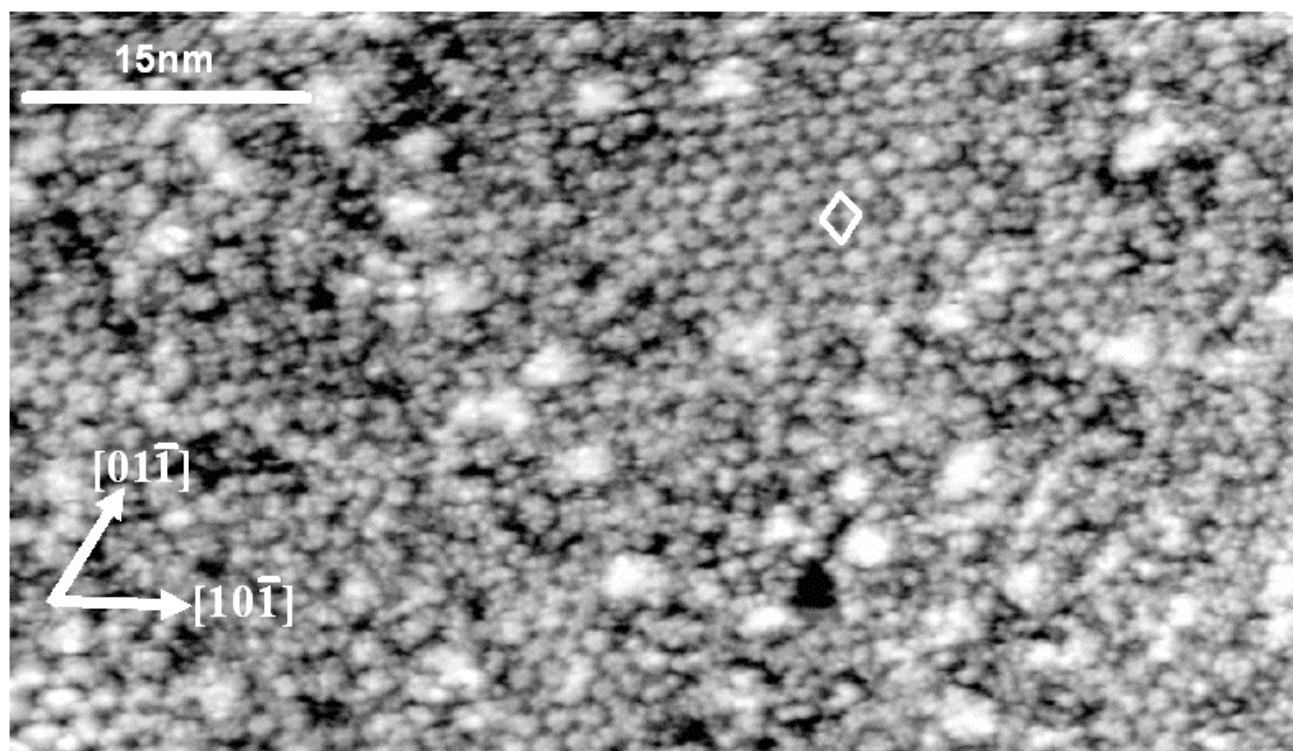
Following Ar<sup>+</sup> ion bombardment and thermal annealing in an oxygen rich environment, a (3x3) equilibrium surface reconstruction has been observed experimentally (Figure 1a) and solved in two dimensions (Figure 1b) by theoretical Direct Methods applied to transmission electron diffraction data [2]. Because of the transmission geometry, this method can only give two dimensional structure information and must be coupled with other techniques in order to get a complete picture of the surface. To that end, we performed Auger electron spectroscopy (AES) and scanning tunneling microscopy (STM) experiments to fill in some of the missing information. The AES data reveals a surface enhancement of Ti relative to the UHV cleaved surface, which is assumed to be stoichiometric. STM imaging (Figure 2) was only possible at sample biases above 1 V, and no negative bias imaging was possible. This indicates that the surface has a substantial bandgap. Combining this information with our 2-d structure from Direct Methods, we are able to say that charge compensation in this polar surface has to come from a change in stoichiometry of a subsurface SrO<sub>3</sub> layer where *all* of the Sr is missing. Given the fact that the surface has a bandgap, this is the only way to compensate the charge given the Ti-O surface stoichiometry determined via Direct Methods. This interpretation is consistent with several recent studies of oxidized SrTiO<sub>3</sub> prepared under similar conditions where the surface selvages were found to be deficient in Sr [3,4,5].

### References

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**Figure 1:** (a)  $\text{SrTiO}_3(111)$ - $3 \times 3$  TEM diffraction pattern (image has been high pass filtered). A  $3 \times 3$  unit cell is denoted. (b) Two-dimensional structure solution from Direct Methods applied to transmission electron diffraction data. Titanium atoms are small red circles, oxygen are large blue circles.



**Figure 2:** STM image showing  $(3 \times 3)$  reconstructed regions, as indicated. The imaging conditions were +1.0 V sample bias, and 0.2 nA tunneling current.