

## ***In Situ* Studies on the Effect of Oxygen Partial Pressure on Ferroelectric Thin Films**

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From previous studies [1], it is known that the behavior of ferroelectric thin films can depend strongly on oxygen partial pressure ( $pO_2$ ) as well as temperature. This can have significant implications in understanding both ferroelectricity (e.g., switching without domain formation [2]) and the reactivity of oxide surfaces. Others have recently shown that polarization at  $BaTiO_3$  and  $LiNbO_3$  surfaces can affect adsorption behavior [3, 4], suggesting that ferroelectricity may be a potential route for modulating surface catalytic properties.

We use *in situ* synchrotron x-ray scattering to study the  $pO_2$  dependent properties of  $PbTiO_3$  and  $BaTiO_3$  films grown on 0.5 wt% Nb-doped  $SrTiO_3$  (001) substrates. In high  $pO_2$  conditions,  $PbTiO_3$  is in the "up" polarized state; the film forms  $180^\circ$  stripe domains at low  $pO_2$ . A  $c(2 \times 2)$  surface structure is observed under both conditions. Conversely,  $BaTiO_3$  is polarized down regardless of  $pO_2$ ; changes in  $pO_2$  result only in piezoelectric response from the lattice. The  $BaTiO_3$  surface shows a  $(3 \times n)$  surface structure that is also independent of  $pO_2$ . Differences between the  $PbTiO_3$  and  $BaTiO_3$  behavior will be discussed in terms of oxygen surface reactivity. Recent results on the effect of a one-unit-cell capping layer of  $SrTiO_3$  on  $BaTiO_3$  will also be discussed.

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[1] R.-V. Wang, D. D. Fong, F. Jiang, M. J. Highland, P. H. Fuoss, et al., *Phys. Rev. Lett.* 102, 047601 (2009).

[2] M. J. Highland, T. T. Fister, M.-I. Richard, D. D. Fong, P. H. Fuoss, et al., *Phys. Rev. Lett.* 105, 167601 (2010).

[3] D. Li, M. H. Zhao, J. Garra, A. M. Kolpak, A. M. Rappe et al., *Nature Mater.* 7, 473 (2008).

[4] J. Garra, J. M. Vohs, and D. A. Bonnell, *Surf. Sci.* 603, 1106 (2009).