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Epitaxial Thin Films of Titanium Oxyhydride

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We recently succeeded to incorporate a large amount of hydrogen into $BaTiO_3$ as an anionic solid solution, $BaTiO_{3-x}H_x$ ($x < 0.6$) [1]. Likewise, $SrTiO_{3-x}H_x$ and $CaTiO_{3-x}H_x$ can also be synthesized [2]. However, only powder samples are available so far, and the transport properties are not well understood in qualitative or quantitative terms. Here, we show the fabrication and transport properties of epitaxial thin films of titanium perovskite oxyhydride $ATiO_{3-x}H_x$ (A = Ba, Sr, Ca). $ATiO_{3-x}H_x$ were prepared by CaH_2 reduction of epitaxial $ATiO_3$ thin films deposited on a $(LaAlO_3)_{0.3}(SrAl_{0.5}Ta_{0.5}O_3)_{0.7}$ (LSAT) substrate [3]. Secondary ion mass spectroscopy detected a substantial amount and uniform distribution of hydride within the film. The amount of hydride depends on the severity of the reaction condition. $SrTiO_3$/LSAT thin film hydridized at 530 °C for 1 day had hydride concentration of 4.0×10^{21} atoms/cm^3 (i.e., $SrTiO_{2.75}H_{0.25}$). The electric resistivity of all the $ATiO_{3-x}H_x$ films exhibited metallic temperature dependence and high conductivity of 10^2 – 10^4 S/cm, revealing that $ATiO_{3-x}H_x$ are intrinsically metallic. Hall measurements for $SrTiO_{2.75}H_{0.25}$ indicate a carrier density of 4.1×10^{21} cm^{-3} at 300 K. This corresponds reasonably well with the H^- amount observed with SIMS, meaning the high carrier activation while oxygen deficiency in $SrTiO_3$ results in relatively low carrier activation. While large amounts of oxygen vacancies readily induce a random potential, H^- with the close ionic radius to O^{2-}, results in significantly less random potential, even at high doping levels. Another advantage of H– incorporation as a dopant is the ability to generate unprecendented amounts of carrier concentrations in oxides, as seen in $SrTiO_{2.75}H_{0.25}$. Incorporation of hydride offers a new way to control carrier levels and realize exotic properties in oxides.

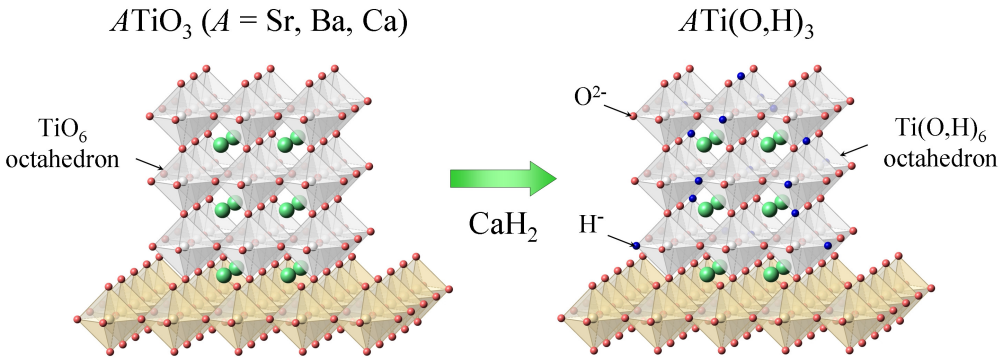

Figure 1. Schematic figure of the hydridization.

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[2] T. Sakaguchi *et al*., Inorganic Chemistry, 51, 11371-11376, (2012)
[3] T. Yajima *et al*., Journal of the American Chemical Society, 134, 8782-8785 (2012)